Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:03 PM EDT

PDB ID	:	1JJK
Title	:	Selenomethionine Substitution of Orotidine-5'-monophosphate Decarboxylase from E. coli Causes a Change in Crystal Contacts and Space Group
Authors	:	Poulsen, J.-C.N.; Harris, P.; Jensen, K.F.; Larsen, S.
Deposited on	:	2001-07-06
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

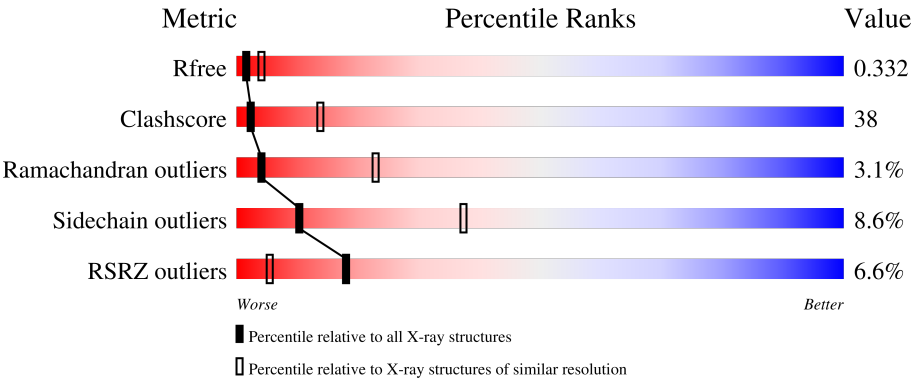
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	245	2% 41% 46% 6% • 6%
1	B	245	2% 40% 48% 6% • 6%
1	C	245	41% 47% 6% • 6%
1	D	245	2% 40% 47% 6% • 6%
1	E	245	3% 41% 47% 6% • 6%

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Mol	Chain	Length	Quality of chain
1	F	245	2% 41% 47% 6% • 6%
1	G	245	2% 40% 47% 6% • 6%
1	H	245	2% 41% 46% 6% • 6%
1	I	245	6% 40% 47% 6% • 6%
1	J	245	9% 40% 47% 6% • 6%
1	K	245	5% 40% 47% 6% • 6%
1	L	245	9% 41% 46% 6% • 6%
1	M	245	7% 40% 47% 6% • 6%
1	N	245	14% 40% 47% 6% • 6%
1	O	245	19% 42% 46% 6% • 6%
1	P	245	12% 40% 48% 6% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 28336 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called OROTIDINE 5'-PHOSPHATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	B	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	C	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	D	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	E	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	F	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	G	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	H	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	I	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	J	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	K	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	L	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	M	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	N	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	O	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			
1	P	231	Total	C	N	O	S	Se	0	0	0
			1749	1104	306	328	3	8			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
A	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
B	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
C	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
D	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	133	MSE	MET	MODIFIED RESIDUE	UNP P08244

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Chain	Residue	Modelled	Actual	Comment	Reference
E	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
E	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
F	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
G	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
H	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
I	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	95	MSE	MET	MODIFIED RESIDUE	UNP P08244

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Chain	Residue	Modelled	Actual	Comment	Reference
J	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
J	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
K	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
L	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
M	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
N	218	MSE	MET	MODIFIED RESIDUE	UNP P08244

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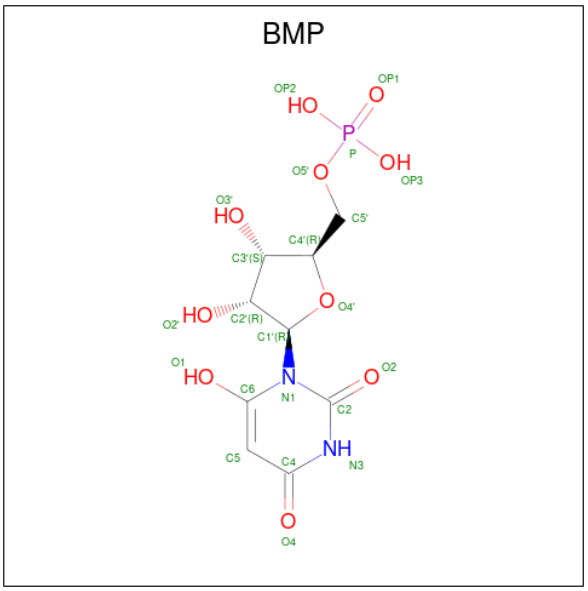
Chain	Residue	Modelled	Actual	Comment	Reference
O	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
O	218	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	1	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	49	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	95	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	106	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	107	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	133	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	143	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	205	MSE	MET	MODIFIED RESIDUE	UNP P08244
P	218	MSE	MET	MODIFIED RESIDUE	UNP P08244

- Molecule 2 is 6-HYDROXYURIDINE-5'-PHOSPHATE (three-letter code: BMP) (formula: $C_9H_{13}N_2O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	B	1	Total	C	N	O	P	0	0
			22	9	2	10	1		

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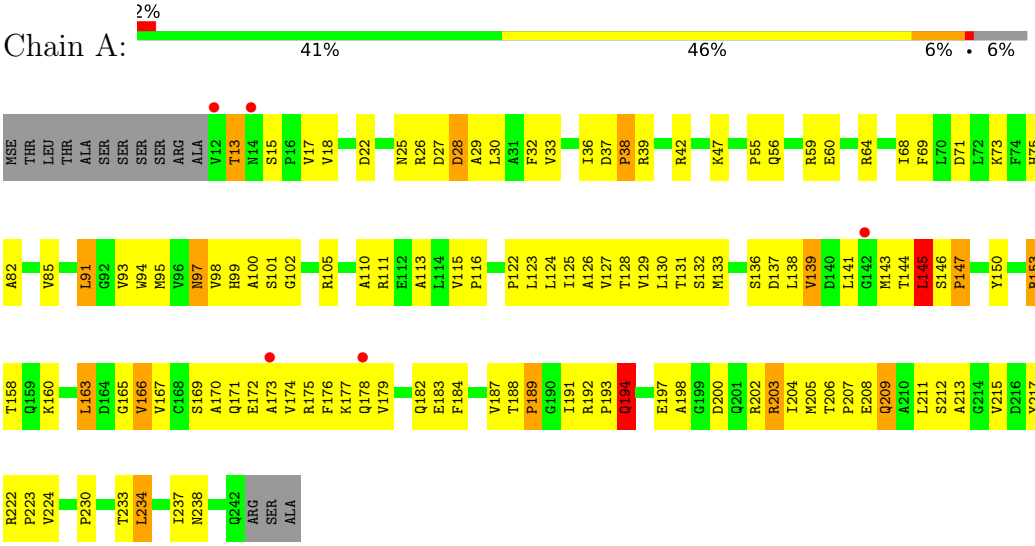
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	D	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	E	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	F	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	G	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	H	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	I	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	J	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	K	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	L	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	M	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	N	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	O	1	Total	C	N	O	P	0	0
			22	9	2	10	1		
2	P	1	Total	C	N	O	P	0	0
			22	9	2	10	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

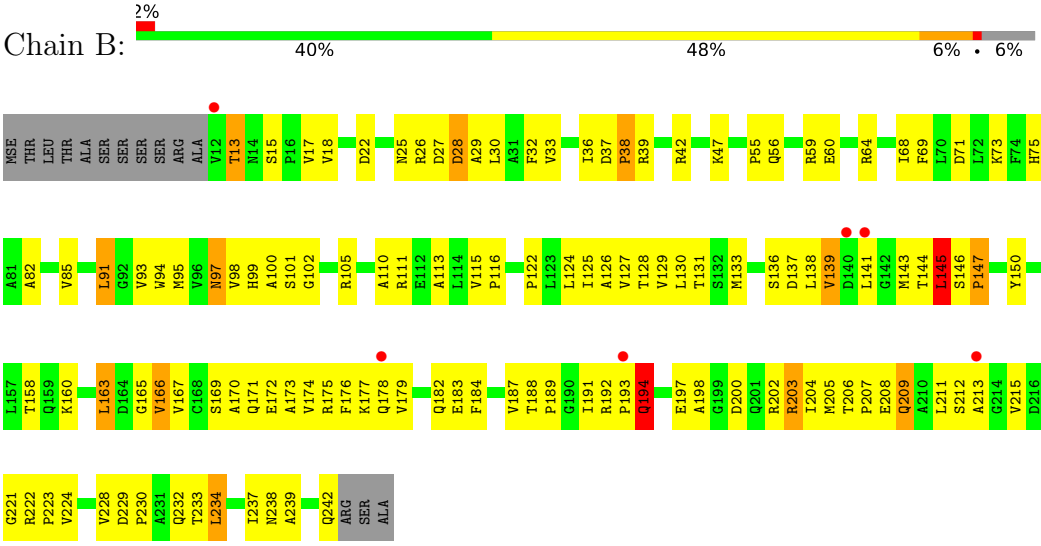
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain A:



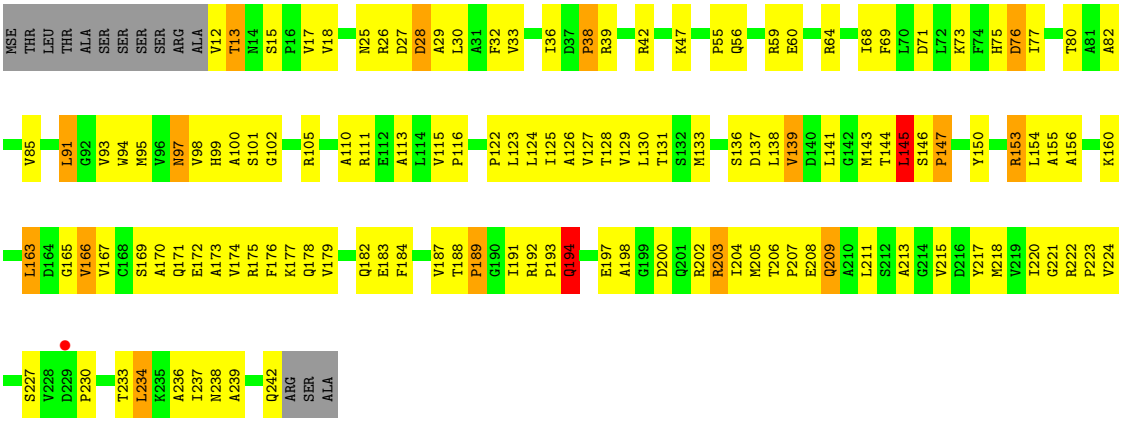
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain B:

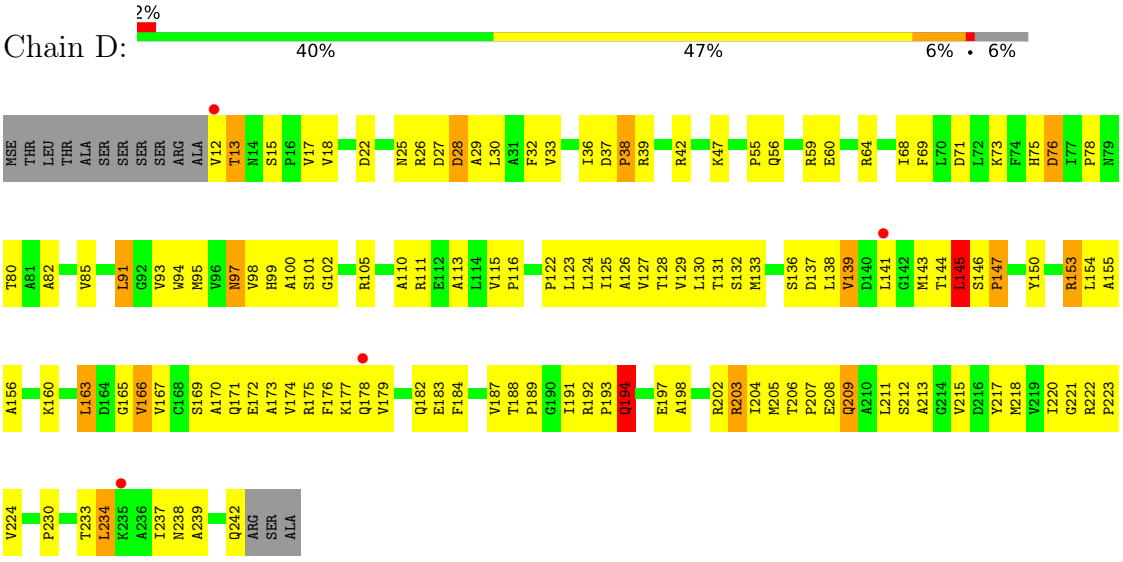


• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

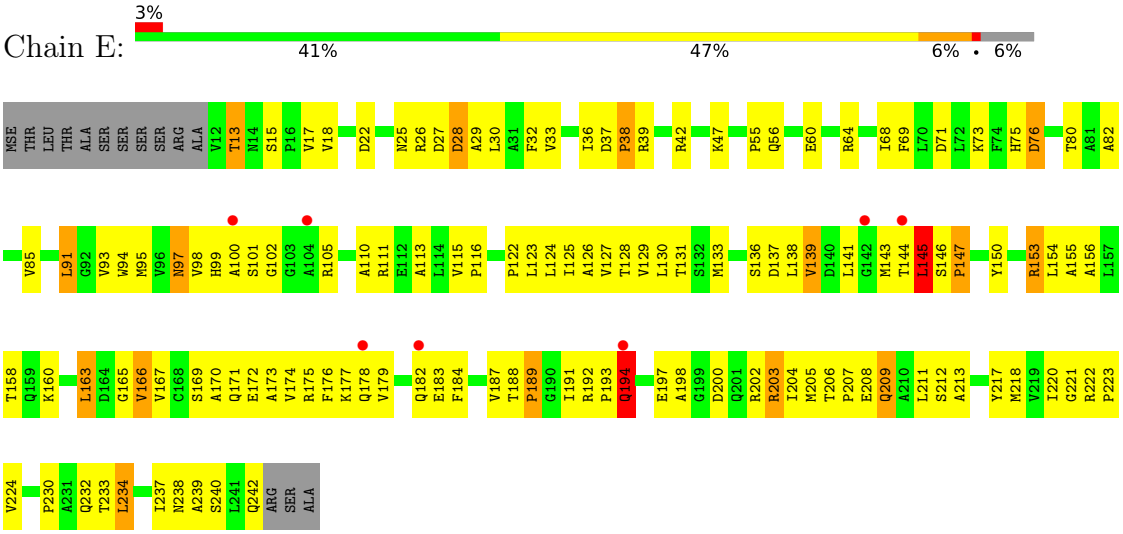
Chain C:



• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

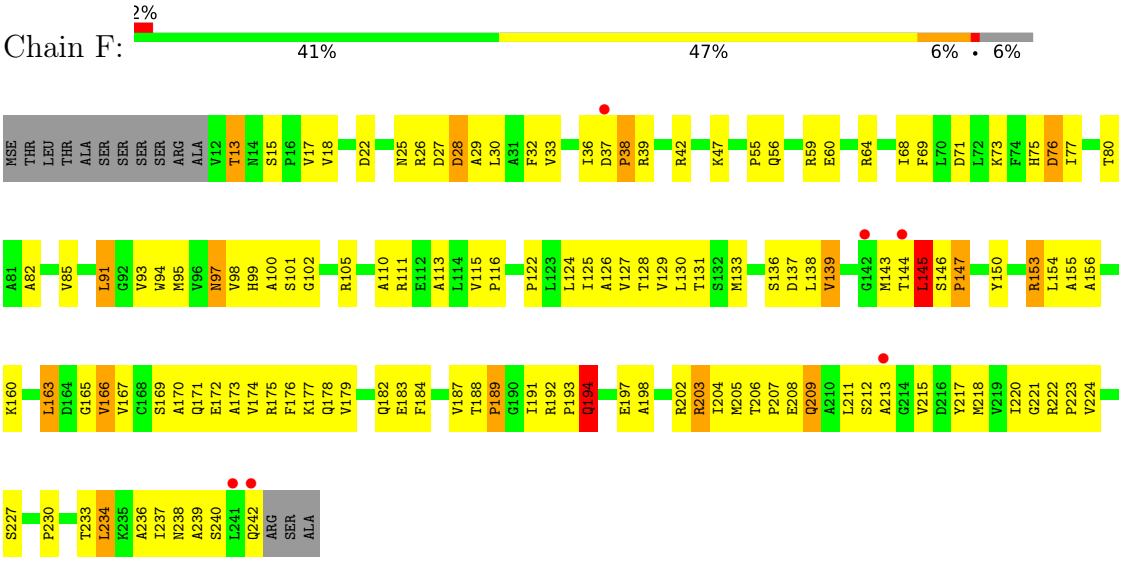


• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE



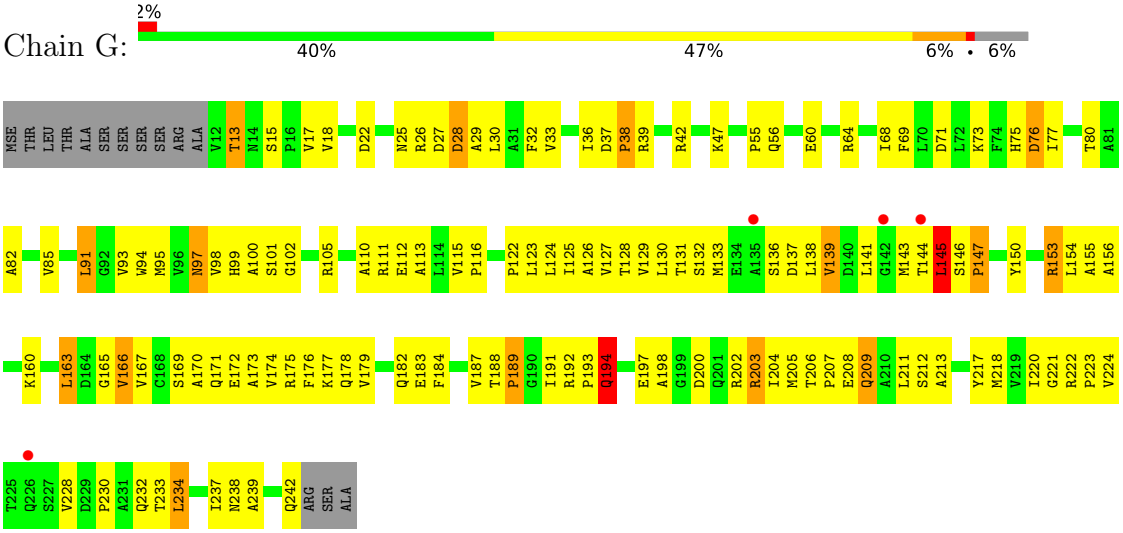
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain F:



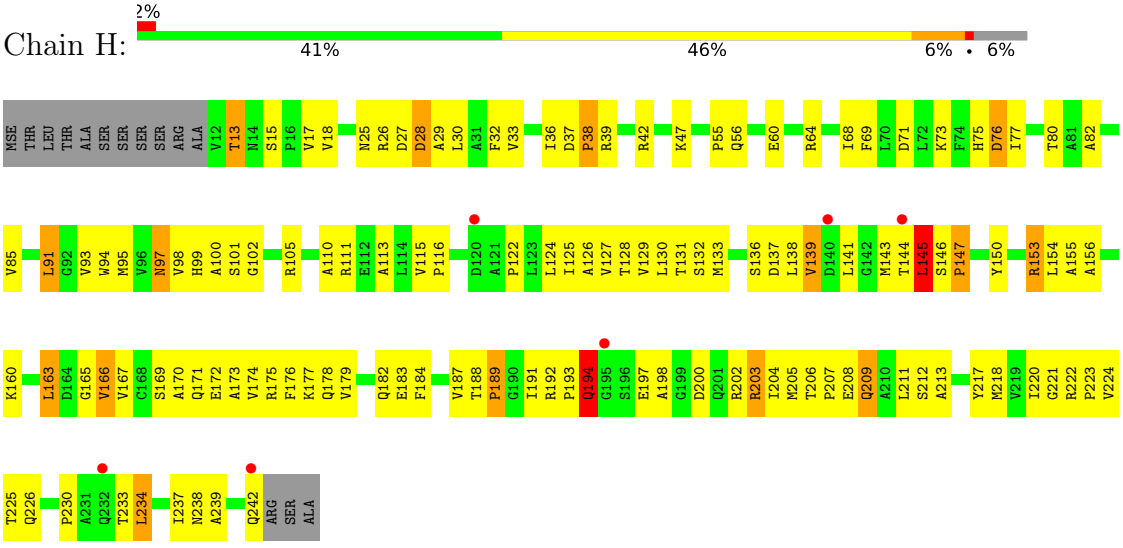
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain G:



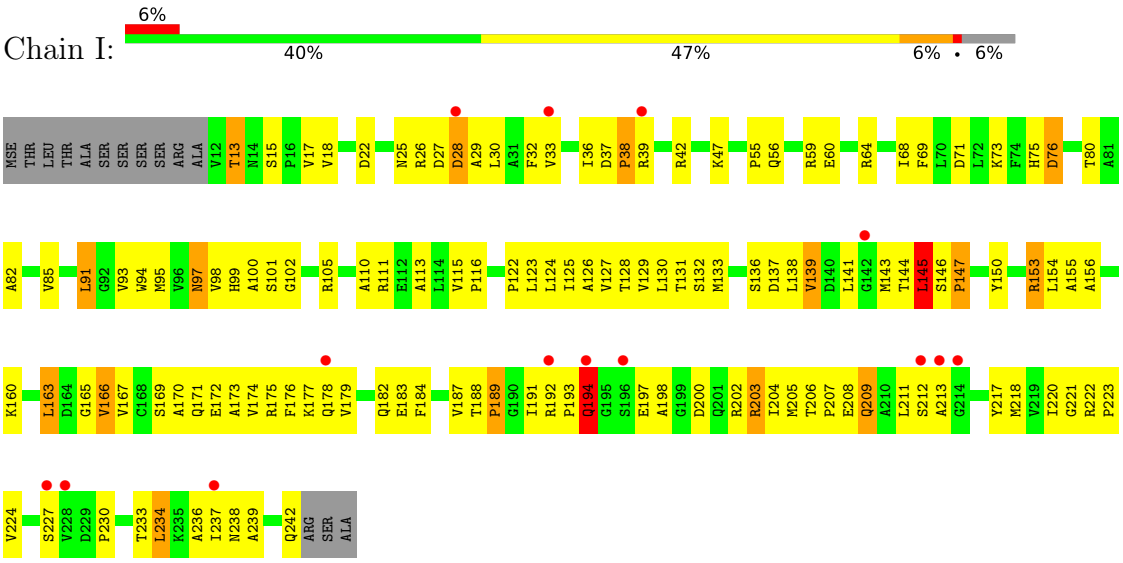
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain H:



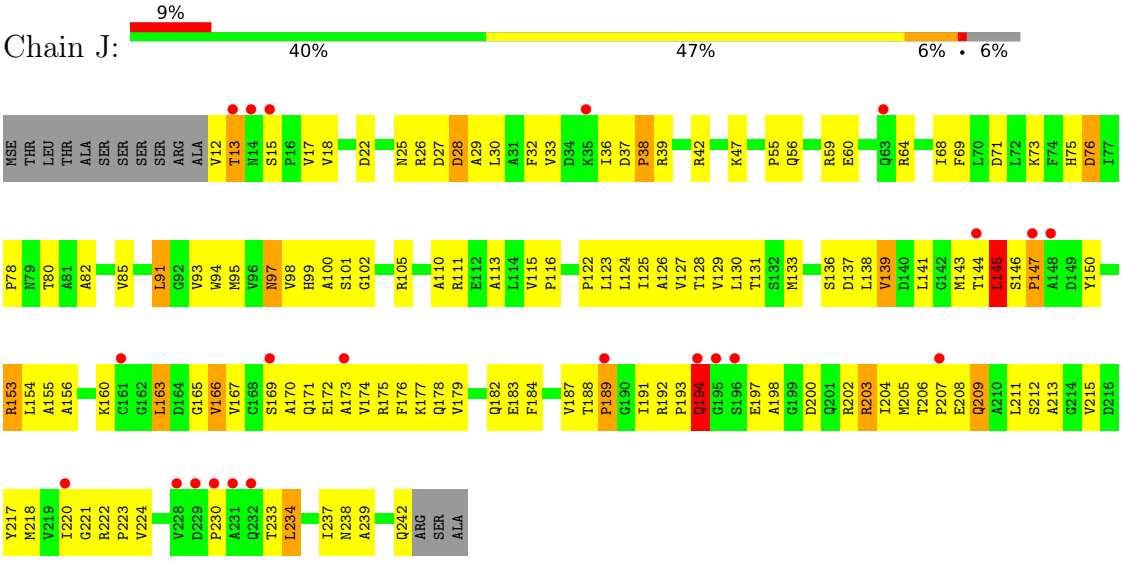
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain I:



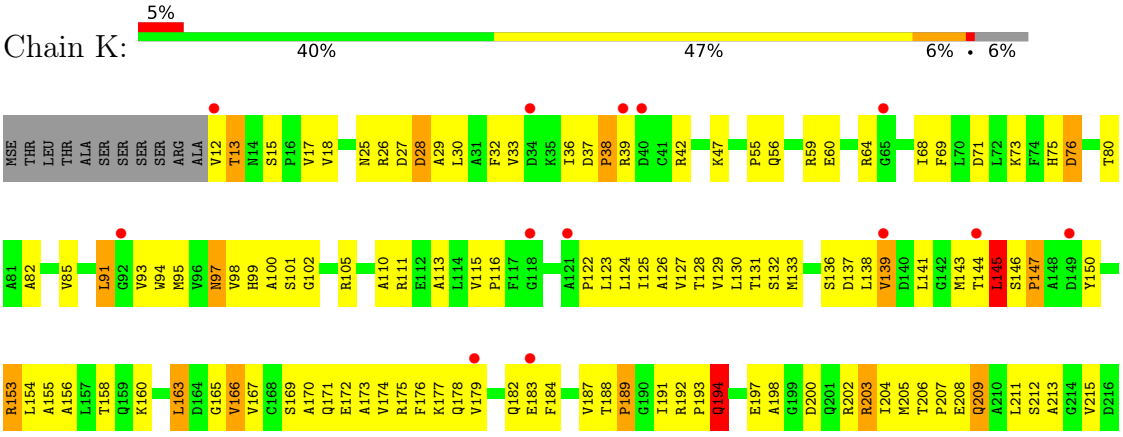
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

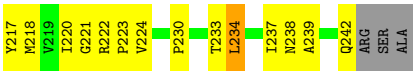
Chain J:



• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

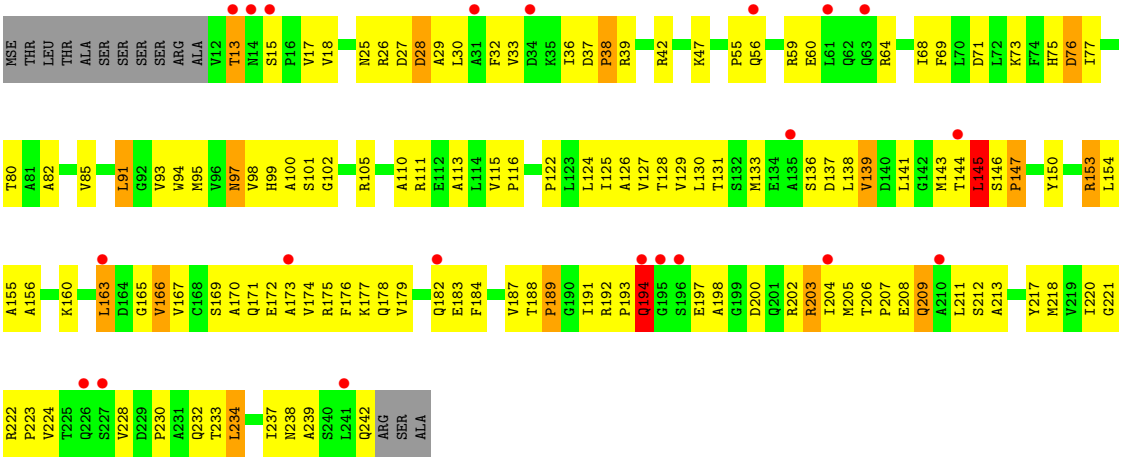
Chain K:





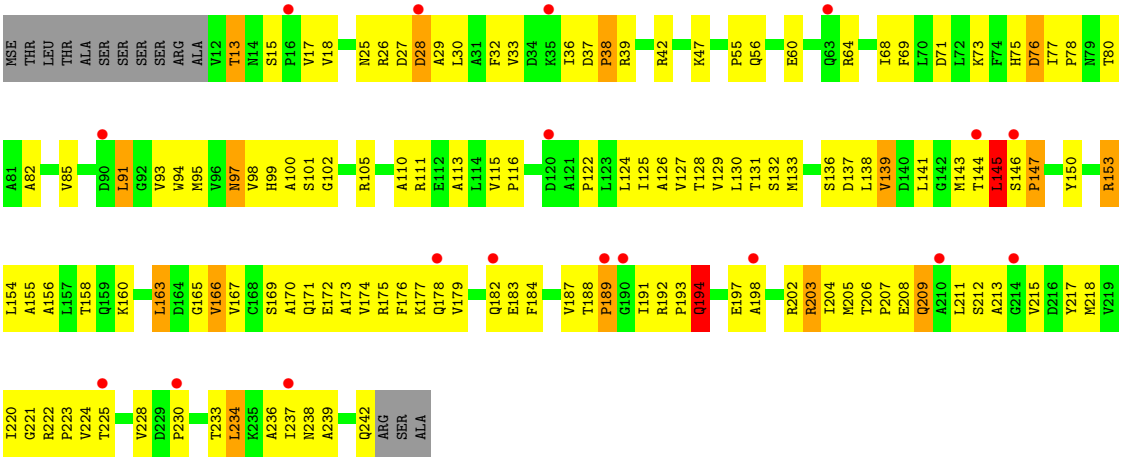
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain L:



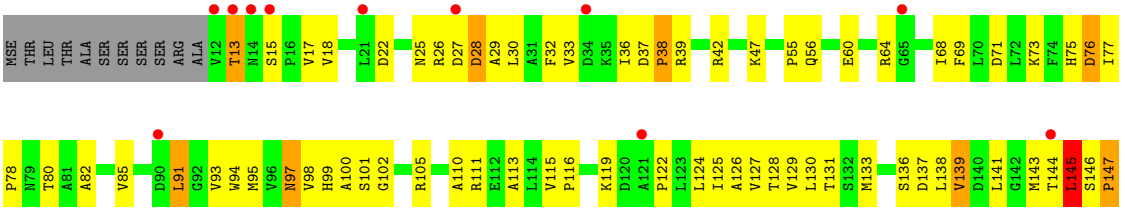
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

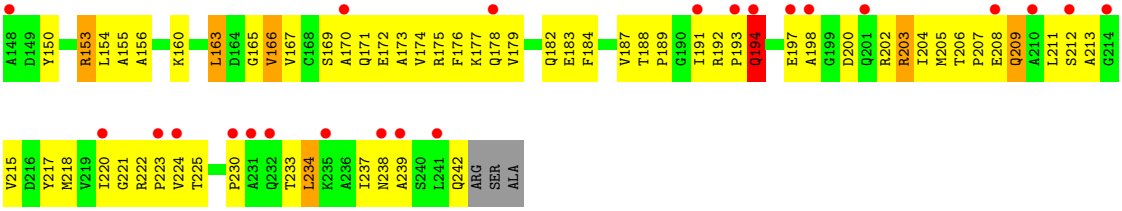
Chain M:



• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

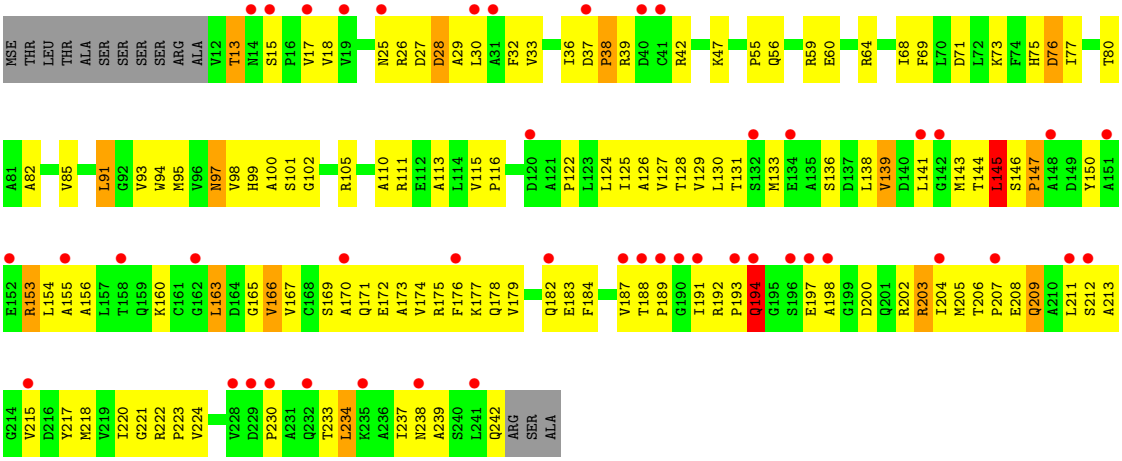
Chain N:





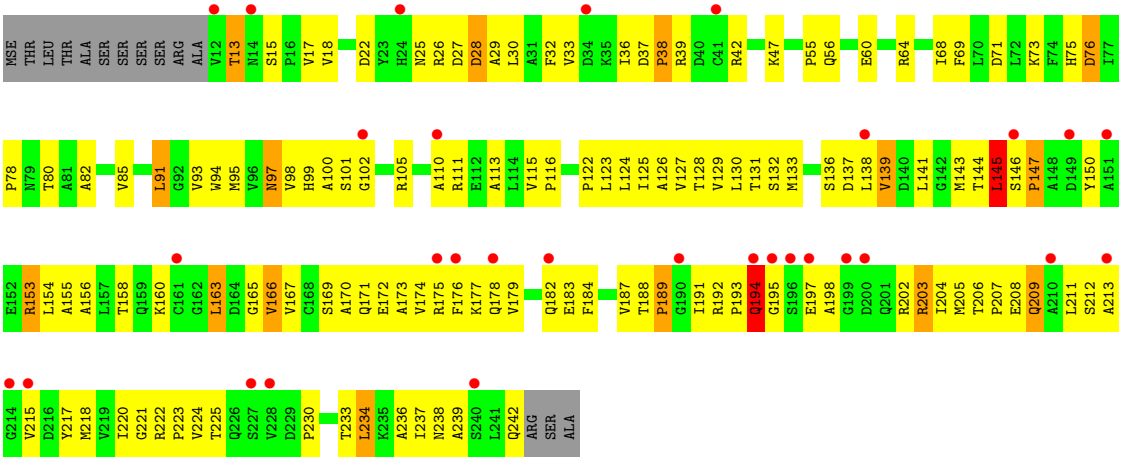
• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain O:



• Molecule 1: OROTIDINE 5'-PHOSPHATE DECARBOXYLASE

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	115.50Å 149.00Å 115.60Å 90.00° 115.30° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.5 (30.00-3.00) 91.2 (29.82-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.41 (at 3.00Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.344 , 0.344 0.338 , 0.332	Depositor DCC
R_{free} test set	3281 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 0.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.376 for l,-k,h	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	28336	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 76.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1146e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/1772	0.67	0/2392
1	B	0.40	0/1772	0.67	0/2392
1	C	0.40	0/1772	0.67	0/2392
1	D	0.40	0/1772	0.67	0/2392
1	E	0.40	0/1772	0.67	0/2392
1	F	0.40	0/1772	0.67	0/2392
1	G	0.40	0/1772	0.67	0/2392
1	H	0.40	0/1772	0.67	0/2392
1	I	0.40	0/1772	0.67	0/2392
1	J	0.40	0/1772	0.67	0/2392
1	K	0.40	0/1772	0.67	0/2392
1	L	0.40	0/1772	0.67	0/2392
1	M	0.40	0/1772	0.67	0/2392
1	N	0.40	0/1772	0.67	0/2392
1	O	0.40	0/1772	0.67	0/2392
1	P	0.40	0/1772	0.67	0/2392
All	All	0.40	0/28352	0.67	0/38272

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1749	0	1758	139	1
1	B	1749	0	1758	162	0
1	C	1749	0	1758	163	0
1	D	1749	0	1758	141	0
1	E	1749	0	1758	138	3
1	F	1749	0	1758	152	0
1	G	1749	0	1758	155	0
1	H	1749	0	1758	135	1
1	I	1749	0	1758	138	2
1	J	1749	0	1758	148	1
1	K	1749	0	1758	145	2
1	L	1749	0	1758	138	2
1	M	1749	0	1758	144	2
1	N	1749	0	1758	143	0
1	O	1749	0	1758	135	1
1	P	1749	0	1758	141	3
2	A	22	0	11	2	0
2	B	22	0	11	2	0
2	C	22	0	11	2	0
2	D	22	0	11	2	0
2	E	22	0	11	3	0
2	F	22	0	11	2	0
2	G	22	0	11	2	0
2	H	22	0	11	2	0
2	I	22	0	11	2	0
2	J	22	0	11	2	0
2	K	22	0	11	2	0
2	L	22	0	11	2	0
2	M	22	0	11	3	0
2	N	22	0	11	4	0
2	O	22	0	11	2	0
2	P	22	0	11	2	0
All	All	28336	0	28304	2177	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (2177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:GLN:HG3	1:J:12:VAL:CG1	1.65	1.26
1:B:232:GLN:NE2	1:C:227:SER:HA	1.53	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:236:ALA:CB	1:G:228:VAL:HG21	1.77	1.13
1:F:236:ALA:CB	1:G:228:VAL:CG2	2.26	1.11
1:F:236:ALA:HB3	1:G:228:VAL:HG21	1.37	1.04
1:O:218:MSE:HE2	1:O:220:ILE:HD11	1.42	1.02
1:K:218:MSE:HE2	1:K:220:ILE:HD11	1.42	1.02
1:I:218:MSE:HE2	1:I:220:ILE:HD11	1.42	1.01
1:C:182:GLN:HG3	1:J:12:VAL:HG11	1.05	1.01
1:P:218:MSE:HE2	1:P:220:ILE:HD11	1.42	1.01
1:G:218:MSE:HE2	1:G:220:ILE:HD11	1.42	1.01
1:H:218:MSE:HE2	1:H:220:ILE:HD11	1.42	1.01
1:N:218:MSE:HE2	1:N:220:ILE:HD11	1.42	1.01
1:A:218:MSE:HE2	1:A:220:ILE:HD11	1.42	1.00
1:E:218:MSE:HE2	1:E:220:ILE:HD11	1.42	1.00
1:F:218:MSE:HE2	1:F:220:ILE:HD11	1.42	1.00
1:M:218:MSE:HE2	1:M:220:ILE:HD11	1.42	0.99
1:D:218:MSE:HE2	1:D:220:ILE:HD11	1.42	0.99
1:C:218:MSE:HE2	1:C:220:ILE:HD11	1.42	0.99
1:B:218:MSE:HE2	1:B:220:ILE:HD11	1.42	0.98
1:F:227:SER:HA	1:G:232:GLN:NE2	1.78	0.98
1:B:228:VAL:CG2	1:C:236:ALA:CB	2.40	0.98
1:D:12:VAL:HG11	1:K:182:GLN:HG3	1.43	0.98
1:C:182:GLN:CG	1:J:12:VAL:HG11	1.93	0.98
1:J:218:MSE:HE2	1:J:220:ILE:HD11	1.42	0.97
1:L:218:MSE:HE2	1:L:220:ILE:HD11	1.42	0.97
1:D:182:GLN:HG3	1:K:12:VAL:HG11	1.45	0.97
1:B:228:VAL:HG21	1:C:236:ALA:HB3	1.46	0.95
1:B:232:GLN:HE21	1:C:227:SER:HA	1.13	0.94
1:C:182:GLN:CG	1:J:12:VAL:CG1	2.46	0.93
1:F:236:ALA:HB1	1:G:228:VAL:CG2	1.98	0.92
1:M:25:ASN:HD22	1:M:28:ASP:HB2	1.35	0.92
1:B:25:ASN:HD22	1:B:28:ASP:HB2	1.35	0.92
1:I:25:ASN:HD22	1:I:28:ASP:HB2	1.35	0.91
1:N:25:ASN:HD22	1:N:28:ASP:HB2	1.35	0.91
1:D:25:ASN:HD22	1:D:28:ASP:HB2	1.35	0.91
1:O:25:ASN:HD22	1:O:28:ASP:HB2	1.35	0.91
1:E:25:ASN:HD22	1:E:28:ASP:HB2	1.35	0.91
1:J:147:PRO:HB3	1:J:203:ARG:HE	1.36	0.91
1:B:147:PRO:HB3	1:B:203:ARG:HE	1.36	0.91
1:A:25:ASN:HD22	1:A:28:ASP:HB2	1.35	0.91
1:G:25:ASN:HD22	1:G:28:ASP:HB2	1.35	0.91
1:J:25:ASN:HD22	1:J:28:ASP:HB2	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:PRO:HB3	1:F:203:ARG:HE	1.36	0.90
1:O:147:PRO:HB3	1:O:203:ARG:HE	1.36	0.90
1:I:147:PRO:HB3	1:I:203:ARG:HE	1.36	0.90
1:K:25:ASN:HD22	1:K:28:ASP:HB2	1.35	0.90
1:H:25:ASN:HD22	1:H:28:ASP:HB2	1.35	0.90
1:D:147:PRO:HB3	1:D:203:ARG:HE	1.36	0.90
1:P:25:ASN:HD22	1:P:28:ASP:HB2	1.35	0.90
1:C:25:ASN:HD22	1:C:28:ASP:HB2	1.35	0.90
1:H:147:PRO:HB3	1:H:203:ARG:HE	1.36	0.90
1:L:147:PRO:HB3	1:L:203:ARG:HE	1.36	0.90
1:F:25:ASN:HD22	1:F:28:ASP:HB2	1.35	0.90
1:P:25:ASN:ND2	1:P:28:ASP:H	1.71	0.89
1:F:25:ASN:ND2	1:F:28:ASP:H	1.71	0.89
1:L:25:ASN:HD22	1:L:28:ASP:HB2	1.35	0.89
1:M:75:HIS:H	1:N:47:LYS:HZ2	1.17	0.89
1:E:25:ASN:ND2	1:E:28:ASP:H	1.71	0.89
1:G:25:ASN:ND2	1:G:28:ASP:H	1.71	0.89
1:N:25:ASN:ND2	1:N:28:ASP:H	1.71	0.89
1:A:25:ASN:ND2	1:A:28:ASP:H	1.71	0.89
1:M:75:HIS:H	1:N:47:LYS:NZ	1.71	0.89
1:C:25:ASN:ND2	1:C:28:ASP:H	1.71	0.89
1:B:25:ASN:ND2	1:B:28:ASP:H	1.71	0.89
1:D:25:ASN:ND2	1:D:28:ASP:H	1.71	0.89
1:H:25:ASN:ND2	1:H:28:ASP:H	1.71	0.88
1:M:147:PRO:HB3	1:M:203:ARG:HE	1.36	0.88
1:A:147:PRO:HB3	1:A:203:ARG:HE	1.36	0.88
1:N:147:PRO:HB3	1:N:203:ARG:HE	1.36	0.88
1:P:147:PRO:HB3	1:P:203:ARG:HE	1.36	0.88
1:K:147:PRO:HB3	1:K:203:ARG:HE	1.36	0.88
1:C:147:PRO:HB3	1:C:203:ARG:HE	1.36	0.88
1:E:147:PRO:HB3	1:E:203:ARG:HE	1.36	0.88
1:K:25:ASN:ND2	1:K:28:ASP:H	1.71	0.88
1:G:147:PRO:HB3	1:G:203:ARG:HE	1.36	0.87
1:L:25:ASN:ND2	1:L:28:ASP:H	1.71	0.87
1:I:25:ASN:ND2	1:I:28:ASP:H	1.71	0.87
1:O:25:ASN:ND2	1:O:28:ASP:H	1.71	0.87
1:J:25:ASN:ND2	1:J:28:ASP:H	1.71	0.87
1:M:25:ASN:ND2	1:M:28:ASP:H	1.71	0.87
1:B:232:GLN:HE21	1:C:227:SER:CA	1.89	0.86
1:B:228:VAL:HG23	1:C:236:ALA:CB	2.06	0.85
1:B:228:VAL:CG2	1:C:236:ALA:HB3	2.05	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:204:ILE:HG22	1:O:205:MSE:N	1.93	0.84
1:D:204:ILE:HG22	1:D:205:MSE:N	1.93	0.84
1:F:204:ILE:HG22	1:F:205:MSE:N	1.93	0.84
1:H:192:ARG:HG3	1:H:204:ILE:HD13	1.60	0.84
1:H:204:ILE:HG22	1:H:205:MSE:N	1.93	0.84
1:N:192:ARG:HG3	1:N:204:ILE:HD13	1.60	0.84
1:N:204:ILE:HG22	1:N:205:MSE:N	1.93	0.84
1:M:192:ARG:HG3	1:M:204:ILE:HD13	1.60	0.84
1:F:192:ARG:HG3	1:F:204:ILE:HD13	1.60	0.83
1:B:204:ILE:HG22	1:B:205:MSE:N	1.93	0.83
1:J:204:ILE:HG22	1:J:205:MSE:N	1.93	0.83
1:G:204:ILE:HG22	1:G:205:MSE:N	1.93	0.83
1:P:204:ILE:HG22	1:P:205:MSE:N	1.93	0.83
1:C:204:ILE:HG22	1:C:205:MSE:N	1.93	0.83
1:E:204:ILE:HG22	1:E:205:MSE:N	1.93	0.83
1:O:192:ARG:HG3	1:O:204:ILE:HD13	1.60	0.83
1:A:204:ILE:HG22	1:A:205:MSE:N	1.93	0.82
1:E:192:ARG:HG3	1:E:204:ILE:HD13	1.60	0.82
1:K:192:ARG:HG3	1:K:204:ILE:HD13	1.60	0.82
1:F:236:ALA:CB	1:G:228:VAL:HG23	2.07	0.82
1:P:192:ARG:HG3	1:P:204:ILE:HD13	1.60	0.82
1:K:204:ILE:HG22	1:K:205:MSE:N	1.93	0.82
1:B:192:ARG:HG3	1:B:204:ILE:HD13	1.60	0.82
1:A:192:ARG:HG3	1:A:204:ILE:HD13	1.60	0.82
1:G:192:ARG:HG3	1:G:204:ILE:HD13	1.60	0.82
1:L:192:ARG:HG3	1:L:204:ILE:HD13	1.60	0.82
1:M:204:ILE:HG22	1:M:205:MSE:N	1.93	0.82
1:E:153:ARG:HH11	1:E:153:ARG:HB2	1.45	0.82
1:G:153:ARG:HB2	1:G:153:ARG:HH11	1.45	0.82
1:C:192:ARG:HG3	1:C:204:ILE:HD13	1.60	0.81
1:D:192:ARG:HG3	1:D:204:ILE:HD13	1.60	0.81
1:I:204:ILE:HG22	1:I:205:MSE:N	1.93	0.81
1:J:192:ARG:HG3	1:J:204:ILE:HD13	1.60	0.81
1:L:204:ILE:HG22	1:L:205:MSE:N	1.93	0.81
1:O:153:ARG:HB2	1:O:153:ARG:HH11	1.45	0.81
1:I:192:ARG:HG3	1:I:204:ILE:HD13	1.60	0.81
1:H:153:ARG:HH11	1:H:153:ARG:HB2	1.45	0.81
1:J:153:ARG:HH11	1:J:153:ARG:HB2	1.45	0.81
1:D:153:ARG:HB2	1:D:153:ARG:HH11	1.45	0.81
1:A:153:ARG:HB2	1:A:153:ARG:HH11	1.45	0.81
1:B:153:ARG:HH11	1:B:153:ARG:HB2	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:ARG:HB2	1:F:153:ARG:HH11	1.45	0.80
1:N:153:ARG:HB2	1:N:153:ARG:HH11	1.45	0.80
1:K:153:ARG:HB2	1:K:153:ARG:HH11	1.45	0.80
1:L:153:ARG:HB2	1:L:153:ARG:HH11	1.45	0.80
1:M:204:ILE:HG22	1:M:205:MSE:H	1.47	0.80
1:A:204:ILE:HG22	1:A:205:MSE:H	1.47	0.80
1:B:204:ILE:HG22	1:B:205:MSE:H	1.47	0.80
1:D:204:ILE:HG22	1:D:205:MSE:H	1.47	0.80
1:C:153:ARG:HB2	1:C:153:ARG:HH11	1.45	0.80
1:I:153:ARG:HB2	1:I:153:ARG:HH11	1.45	0.80
1:I:204:ILE:HG22	1:I:205:MSE:H	1.47	0.79
1:K:204:ILE:HG22	1:K:205:MSE:H	1.47	0.79
1:A:75:HIS:H	1:B:47:LYS:HZ2	1.31	0.79
1:J:204:ILE:HG22	1:J:205:MSE:H	1.47	0.79
1:M:153:ARG:HH11	1:M:153:ARG:HB2	1.45	0.79
1:P:69:PHE:CD2	1:P:95:MSE:HE3	2.18	0.79
1:P:153:ARG:HH11	1:P:153:ARG:HB2	1.45	0.79
1:C:182:GLN:HG3	1:J:12:VAL:HG12	1.65	0.78
1:N:69:PHE:CD2	1:N:95:MSE:HE3	2.18	0.78
1:D:69:PHE:CD2	1:D:95:MSE:HE3	2.18	0.78
1:H:69:PHE:CD2	1:H:95:MSE:HE3	2.19	0.78
1:B:69:PHE:CD2	1:B:95:MSE:HE3	2.18	0.78
1:N:204:ILE:HG22	1:N:205:MSE:H	1.47	0.78
1:G:204:ILE:HG22	1:G:205:MSE:H	1.47	0.78
1:M:69:PHE:CD2	1:M:95:MSE:HE3	2.19	0.78
1:E:204:ILE:HG22	1:E:205:MSE:H	1.47	0.78
1:I:69:PHE:CD2	1:I:95:MSE:HE3	2.18	0.78
1:F:69:PHE:CD2	1:F:95:MSE:HE3	2.18	0.78
1:F:204:ILE:HG22	1:F:205:MSE:H	1.47	0.78
1:G:69:PHE:CD2	1:G:95:MSE:HE3	2.18	0.78
1:H:204:ILE:HG22	1:H:205:MSE:H	1.47	0.78
1:C:204:ILE:HG22	1:C:205:MSE:H	1.47	0.77
1:E:69:PHE:CD2	1:E:95:MSE:HE3	2.19	0.77
1:A:69:PHE:CD2	1:A:95:MSE:HE3	2.18	0.77
1:C:69:PHE:CD2	1:C:95:MSE:HE3	2.18	0.77
1:B:228:VAL:HB	1:C:236:ALA:HB1	1.65	0.77
1:J:69:PHE:CD2	1:J:95:MSE:HE3	2.18	0.77
1:L:204:ILE:HG22	1:L:205:MSE:H	1.47	0.77
1:O:204:ILE:HG22	1:O:205:MSE:H	1.47	0.77
1:K:69:PHE:CD2	1:K:95:MSE:HE3	2.18	0.77
1:O:69:PHE:CD2	1:O:95:MSE:HE3	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:THR:O	1:B:237:ILE:HG13	1.85	0.76
1:J:233:THR:O	1:J:237:ILE:HG13	1.85	0.76
1:L:69:PHE:CD2	1:L:95:MSE:HE3	2.18	0.76
1:P:204:ILE:HG22	1:P:205:MSE:H	1.47	0.76
1:P:233:THR:O	1:P:237:ILE:HG13	1.85	0.76
1:C:47:LYS:NZ	1:D:75:HIS:H	1.83	0.76
1:E:47:LYS:NZ	1:F:75:HIS:H	1.83	0.76
1:H:233:THR:O	1:H:237:ILE:HG13	1.85	0.76
1:K:233:THR:O	1:K:237:ILE:HG13	1.85	0.76
1:F:233:THR:O	1:F:237:ILE:HG13	1.85	0.76
1:N:233:THR:O	1:N:237:ILE:HG13	1.85	0.76
1:M:233:THR:O	1:M:237:ILE:HG13	1.85	0.76
1:A:233:THR:O	1:A:237:ILE:HG13	1.85	0.76
1:I:233:THR:O	1:I:237:ILE:HG13	1.85	0.76
1:G:233:THR:O	1:G:237:ILE:HG13	1.85	0.76
1:F:227:SER:HA	1:G:232:GLN:HE22	1.51	0.76
1:D:233:THR:O	1:D:237:ILE:HG13	1.85	0.76
1:L:124:LEU:HG	1:L:163:LEU:HD13	1.68	0.76
1:D:130:LEU:HB2	1:D:133:MSE:HE2	1.68	0.75
1:B:124:LEU:HG	1:B:163:LEU:HD13	1.68	0.75
1:M:130:LEU:HB2	1:M:133:MSE:HE2	1.68	0.75
1:F:130:LEU:HB2	1:F:133:MSE:HE2	1.68	0.75
1:L:130:LEU:HB2	1:L:133:MSE:HE2	1.68	0.75
1:L:233:THR:O	1:L:237:ILE:HG13	1.85	0.75
1:B:130:LEU:HB2	1:B:133:MSE:HE2	1.68	0.75
1:J:124:LEU:HG	1:J:163:LEU:HD13	1.68	0.75
1:O:124:LEU:HG	1:O:163:LEU:HD13	1.68	0.75
1:P:130:LEU:HB2	1:P:133:MSE:HE2	1.68	0.75
1:D:124:LEU:HG	1:D:163:LEU:HD13	1.68	0.75
1:E:233:THR:O	1:E:237:ILE:HG13	1.85	0.75
1:I:75:HIS:H	1:J:47:LYS:NZ	1.84	0.75
1:H:130:LEU:HB2	1:H:133:MSE:HE2	1.68	0.75
1:O:233:THR:O	1:O:237:ILE:HG13	1.85	0.75
1:C:233:THR:O	1:C:237:ILE:HG13	1.85	0.75
1:G:130:LEU:HB2	1:G:133:MSE:HE2	1.68	0.74
1:I:47:LYS:NZ	1:J:75:HIS:H	1.86	0.74
1:A:124:LEU:HG	1:A:163:LEU:HD13	1.68	0.74
1:K:130:LEU:HB2	1:K:133:MSE:HE2	1.68	0.74
1:G:124:LEU:HG	1:G:163:LEU:HD13	1.68	0.74
1:I:124:LEU:HG	1:I:163:LEU:HD13	1.68	0.74
1:A:130:LEU:HB2	1:A:133:MSE:HE2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:130:LEU:HB2	1:N:133:MSE:HE2	1.68	0.74
1:F:124:LEU:HG	1:F:163:LEU:HD13	1.68	0.74
1:C:124:LEU:HG	1:C:163:LEU:HD13	1.68	0.74
1:I:130:LEU:HB2	1:I:133:MSE:HE2	1.68	0.74
1:O:130:LEU:HB2	1:O:133:MSE:HE2	1.68	0.74
1:E:130:LEU:HB2	1:E:133:MSE:HE2	1.68	0.74
1:J:130:LEU:HB2	1:J:133:MSE:HE2	1.68	0.74
1:M:124:LEU:HG	1:M:163:LEU:HD13	1.68	0.74
1:C:130:LEU:HB2	1:C:133:MSE:HE2	1.68	0.73
1:E:124:LEU:HG	1:E:163:LEU:HD13	1.68	0.73
1:N:124:LEU:HG	1:N:163:LEU:HD13	1.68	0.73
1:K:124:LEU:HG	1:K:163:LEU:HD13	1.68	0.73
1:P:124:LEU:HG	1:P:163:LEU:HD13	1.68	0.73
1:H:124:LEU:HG	1:H:163:LEU:HD13	1.68	0.73
1:M:47:LYS:NZ	1:N:75:HIS:H	1.86	0.73
1:M:137:ASP:OD2	1:N:105:ARG:HD3	1.88	0.73
1:B:232:GLN:HE22	1:C:227:SER:HA	1.53	0.73
1:B:69:PHE:CG	1:B:95:MSE:HE3	2.25	0.72
1:E:47:LYS:HZ2	1:F:75:HIS:H	1.36	0.72
1:K:69:PHE:CG	1:K:95:MSE:HE3	2.25	0.72
1:A:69:PHE:CG	1:A:95:MSE:HE3	2.25	0.72
1:M:69:PHE:CG	1:M:95:MSE:HE3	2.25	0.72
1:P:69:PHE:CG	1:P:95:MSE:HE3	2.25	0.72
1:D:69:PHE:CG	1:D:95:MSE:HE3	2.25	0.72
1:N:69:PHE:CG	1:N:95:MSE:HE3	2.25	0.72
1:O:69:PHE:CG	1:O:95:MSE:HE3	2.25	0.72
1:C:69:PHE:CG	1:C:95:MSE:HE3	2.25	0.72
1:G:69:PHE:CG	1:G:95:MSE:HE3	2.25	0.72
1:E:69:PHE:CG	1:E:95:MSE:HE3	2.25	0.72
1:F:69:PHE:CG	1:F:95:MSE:HE3	2.25	0.72
1:E:75:HIS:H	1:F:47:LYS:NZ	1.87	0.72
1:L:191:ILE:HG21	1:L:218:MSE:HE3	1.72	0.71
1:O:191:ILE:HG21	1:O:218:MSE:HE3	1.72	0.71
1:P:191:ILE:HG21	1:P:218:MSE:HE3	1.72	0.71
1:I:69:PHE:CG	1:I:95:MSE:HE3	2.25	0.71
1:F:236:ALA:HB2	1:G:228:VAL:HG23	1.71	0.71
1:H:69:PHE:CG	1:H:95:MSE:HE3	2.25	0.71
1:L:69:PHE:CG	1:L:95:MSE:HE3	2.25	0.71
1:N:191:ILE:HG21	1:N:218:MSE:HE3	1.72	0.71
1:O:47:LYS:NZ	1:P:75:HIS:H	1.88	0.71
1:K:75:HIS:H	1:L:47:LYS:HZ2	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LYS:HZ2	1:D:75:HIS:H	1.39	0.71
1:F:191:ILE:HG21	1:F:218:MSE:HE3	1.72	0.71
1:J:25:ASN:HD22	1:J:28:ASP:H	1.39	0.71
1:K:191:ILE:HG21	1:K:218:MSE:HE3	1.72	0.71
1:A:75:HIS:H	1:B:47:LYS:NZ	1.89	0.71
1:E:191:ILE:HG21	1:E:218:MSE:HE3	1.72	0.71
1:M:191:ILE:HG21	1:M:218:MSE:HE3	1.72	0.71
1:H:191:ILE:HG21	1:H:218:MSE:HE3	1.72	0.71
1:G:191:ILE:HG21	1:G:218:MSE:HE3	1.72	0.70
1:J:69:PHE:CG	1:J:95:MSE:HE3	2.25	0.70
1:I:25:ASN:HD22	1:I:28:ASP:H	1.39	0.70
1:J:191:ILE:HG21	1:J:218:MSE:HE3	1.72	0.70
1:A:25:ASN:HD22	1:A:28:ASP:H	1.39	0.70
1:M:47:LYS:HZ2	1:N:75:HIS:H	1.36	0.70
1:I:191:ILE:HG21	1:I:218:MSE:HE3	1.72	0.70
1:A:191:ILE:HG21	1:A:218:MSE:HE3	1.72	0.70
1:B:229:ASP:OD1	1:C:227:SER:HB2	1.91	0.70
1:G:75:HIS:H	1:H:47:LYS:NZ	1.90	0.70
1:K:207:PRO:HA	1:K:218:MSE:HE1	1.74	0.70
1:D:191:ILE:HG21	1:D:218:MSE:HE3	1.72	0.70
1:G:25:ASN:HD22	1:G:28:ASP:H	1.39	0.70
1:A:207:PRO:HA	1:A:218:MSE:HE1	1.74	0.70
1:C:207:PRO:HA	1:C:218:MSE:HE1	1.74	0.70
1:F:207:PRO:HA	1:F:218:MSE:HE1	1.74	0.70
1:P:207:PRO:HA	1:P:218:MSE:HE1	1.74	0.69
1:H:207:PRO:HA	1:H:218:MSE:HE1	1.74	0.69
1:I:207:PRO:HA	1:I:218:MSE:HE1	1.74	0.69
1:L:25:ASN:HD22	1:L:28:ASP:H	1.39	0.69
1:N:25:ASN:HD22	1:N:28:ASP:H	1.39	0.69
1:N:207:PRO:HA	1:N:218:MSE:HE1	1.74	0.69
1:P:25:ASN:HD22	1:P:28:ASP:H	1.39	0.69
1:D:25:ASN:HD22	1:D:28:ASP:H	1.39	0.69
1:D:192:ARG:HH22	2:D:304:BMP:P	2.16	0.69
1:F:192:ARG:HH22	2:F:306:BMP:P	2.16	0.69
1:M:192:ARG:HH22	2:M:313:BMP:P	2.15	0.69
1:C:25:ASN:HD22	1:C:28:ASP:H	1.39	0.69
1:G:192:ARG:HH22	2:G:307:BMP:P	2.15	0.69
1:H:192:ARG:HH22	2:H:308:BMP:P	2.16	0.69
1:K:75:HIS:H	1:L:47:LYS:NZ	1.89	0.69
1:C:192:ARG:HH22	2:C:303:BMP:P	2.16	0.69
1:E:25:ASN:HD22	1:E:28:ASP:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:25:ASN:HD22	1:O:28:ASP:H	1.39	0.69
1:B:191:ILE:HG21	1:B:218:MSE:HE3	1.72	0.69
1:B:228:VAL:HG23	1:C:236:ALA:HB2	1.74	0.69
1:C:191:ILE:HG21	1:C:218:MSE:HE3	1.72	0.69
1:K:192:ARG:HH22	2:K:311:BMP:P	2.16	0.69
1:N:192:ARG:HH22	2:N:314:BMP:P	2.16	0.69
1:M:204:ILE:CG2	1:M:205:MSE:H	2.06	0.69
1:O:204:ILE:CG2	1:O:205:MSE:H	2.06	0.69
1:B:25:ASN:HD22	1:B:28:ASP:H	1.39	0.69
1:B:204:ILE:CG2	1:B:205:MSE:H	2.06	0.69
1:D:204:ILE:CG2	1:D:205:MSE:H	2.06	0.69
1:E:192:ARG:HH22	2:E:305:BMP:P	2.15	0.69
1:F:25:ASN:HD22	1:F:28:ASP:H	1.39	0.69
1:G:47:LYS:NZ	1:H:75:HIS:H	1.91	0.69
1:H:25:ASN:HD22	1:H:28:ASP:H	1.39	0.69
1:H:204:ILE:CG2	1:H:205:MSE:H	2.06	0.69
1:K:25:ASN:HD22	1:K:28:ASP:H	1.39	0.69
1:L:192:ARG:HH22	2:L:312:BMP:P	2.16	0.69
1:O:207:PRO:HA	1:O:218:MSE:HE1	1.74	0.69
1:B:228:VAL:CG2	1:C:233:THR:HA	2.23	0.69
1:M:25:ASN:HD22	1:M:28:ASP:H	1.39	0.69
1:J:192:ARG:HH22	2:J:310:BMP:P	2.15	0.69
1:F:204:ILE:CG2	1:F:205:MSE:H	2.06	0.68
1:P:192:ARG:HH22	2:P:316:BMP:P	2.16	0.68
1:I:192:ARG:HH22	2:I:309:BMP:P	2.15	0.68
1:B:192:ARG:HH22	2:B:302:BMP:P	2.16	0.68
1:L:207:PRO:HA	1:L:218:MSE:HE1	1.74	0.68
1:A:204:ILE:CG2	1:A:205:MSE:H	2.06	0.68
1:C:12:VAL:HG11	1:J:182:GLN:HG3	1.75	0.68
1:E:207:PRO:HA	1:E:218:MSE:HE1	1.74	0.68
1:O:192:ARG:HH22	2:O:315:BMP:P	2.15	0.68
1:A:192:ARG:HH22	2:A:301:BMP:P	2.15	0.68
1:A:47:LYS:NZ	1:B:75:HIS:H	1.90	0.68
1:C:182:GLN:CG	1:J:12:VAL:HG12	2.22	0.68
1:C:204:ILE:CG2	1:C:205:MSE:H	2.06	0.68
1:G:207:PRO:HA	1:G:218:MSE:HE1	1.74	0.68
1:K:47:LYS:NZ	1:L:75:HIS:H	1.92	0.68
1:M:207:PRO:HA	1:M:218:MSE:HE1	1.74	0.67
1:E:75:HIS:H	1:F:47:LYS:HZ2	1.43	0.67
1:E:204:ILE:CG2	1:E:205:MSE:H	2.06	0.67
1:I:47:LYS:HZ2	1:J:75:HIS:H	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:207:PRO:HA	1:J:218:MSE:HE1	1.74	0.67
1:D:207:PRO:HA	1:D:218:MSE:HE1	1.74	0.67
1:J:204:ILE:CG2	1:J:205:MSE:H	2.06	0.67
1:K:138:LEU:O	1:K:143:MSE:HB3	1.95	0.67
1:E:138:LEU:O	1:E:143:MSE:HB3	1.95	0.67
1:L:204:ILE:CG2	1:L:205:MSE:H	2.06	0.67
1:N:204:ILE:CG2	1:N:205:MSE:H	2.06	0.67
1:G:138:LEU:O	1:G:143:MSE:HB3	1.95	0.67
1:O:138:LEU:O	1:O:143:MSE:HB3	1.95	0.67
1:P:169:SER:HB3	1:P:172:GLU:OE1	1.95	0.67
1:G:204:ILE:CG2	1:G:205:MSE:H	2.06	0.67
1:N:169:SER:HB3	1:N:172:GLU:OE1	1.95	0.67
1:P:204:ILE:CG2	1:P:205:MSE:H	2.06	0.67
1:A:218:MSE:CE	1:A:220:ILE:HD11	2.23	0.67
1:C:138:LEU:O	1:C:143:MSE:HB3	1.95	0.67
1:G:169:SER:HB3	1:G:172:GLU:OE1	1.95	0.67
1:K:204:ILE:CG2	1:K:205:MSE:H	2.06	0.67
1:B:207:PRO:HA	1:B:218:MSE:HE1	1.74	0.67
1:D:169:SER:HB3	1:D:172:GLU:OE1	1.95	0.67
1:I:204:ILE:CG2	1:I:205:MSE:H	2.06	0.67
1:M:218:MSE:CE	1:M:220:ILE:HD11	2.23	0.67
1:N:138:LEU:O	1:N:143:MSE:HB3	1.95	0.67
1:P:138:LEU:O	1:P:143:MSE:HB3	1.95	0.67
1:A:138:LEU:O	1:A:143:MSE:HB3	1.95	0.66
1:D:138:LEU:O	1:D:143:MSE:HB3	1.95	0.66
1:I:138:LEU:O	1:I:143:MSE:HB3	1.95	0.66
1:B:169:SER:HB3	1:B:172:GLU:OE1	1.95	0.66
1:E:169:SER:HB3	1:E:172:GLU:OE1	1.95	0.66
1:G:75:HIS:H	1:H:47:LYS:HZ2	1.43	0.66
1:L:138:LEU:O	1:L:143:MSE:HB3	1.95	0.66
1:C:75:HIS:H	1:D:47:LYS:NZ	1.93	0.66
1:M:138:LEU:O	1:M:143:MSE:HB3	1.95	0.66
1:I:75:HIS:H	1:J:47:LYS:HZ2	1.43	0.66
1:K:169:SER:HB3	1:K:172:GLU:OE1	1.95	0.66
1:J:138:LEU:O	1:J:143:MSE:HB3	1.95	0.66
1:H:98:VAL:O	1:H:126:ALA:HA	1.96	0.66
1:H:169:SER:HB3	1:H:172:GLU:OE1	1.95	0.66
1:O:169:SER:HB3	1:O:172:GLU:OE1	1.95	0.66
1:G:47:LYS:HZ2	1:H:75:HIS:H	1.42	0.66
1:K:98:VAL:O	1:K:126:ALA:HA	1.96	0.66
1:B:138:LEU:O	1:B:143:MSE:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:206:THR:OG1	1:P:209:GLN:HG2	1.96	0.66
1:C:218:MSE:CE	1:C:220:ILE:HD11	2.23	0.66
1:M:98:VAL:O	1:M:126:ALA:HA	1.96	0.66
1:O:206:THR:OG1	1:O:209:GLN:HG2	1.96	0.66
1:A:206:THR:OG1	1:A:209:GLN:HG2	1.96	0.66
1:C:169:SER:HB3	1:C:172:GLU:OE1	1.95	0.66
1:C:206:THR:OG1	1:C:209:GLN:HG2	1.96	0.66
1:F:98:VAL:O	1:F:126:ALA:HA	1.96	0.66
1:F:138:LEU:O	1:F:143:MSE:HB3	1.95	0.66
1:F:206:THR:OG1	1:F:209:GLN:HG2	1.96	0.66
1:K:206:THR:OG1	1:K:209:GLN:HG2	1.96	0.66
1:F:30:LEU:HD22	1:F:64:ARG:HH21	1.61	0.65
1:H:206:THR:OG1	1:H:209:GLN:HG2	1.96	0.65
1:I:169:SER:HB3	1:I:172:GLU:OE1	1.95	0.65
1:C:30:LEU:HD22	1:C:64:ARG:HH21	1.61	0.65
1:D:204:ILE:CG2	1:D:205:MSE:N	2.60	0.65
1:H:30:LEU:HD22	1:H:64:ARG:HH21	1.61	0.65
1:I:98:VAL:O	1:I:126:ALA:HA	1.96	0.65
1:M:169:SER:HB3	1:M:172:GLU:OE1	1.95	0.65
1:A:169:SER:HB3	1:A:172:GLU:OE1	1.95	0.65
1:B:204:ILE:CG2	1:B:205:MSE:N	2.60	0.65
1:H:138:LEU:O	1:H:143:MSE:HB3	1.95	0.65
1:I:206:THR:OG1	1:I:209:GLN:HG2	1.96	0.65
1:J:30:LEU:HD22	1:J:64:ARG:HH21	1.61	0.65
1:J:169:SER:HB3	1:J:172:GLU:OE1	1.95	0.65
1:F:169:SER:HB3	1:F:172:GLU:OE1	1.95	0.65
1:G:30:LEU:HD22	1:G:64:ARG:HH21	1.61	0.65
1:G:98:VAL:O	1:G:126:ALA:HA	1.96	0.65
1:H:218:MSE:CE	1:H:220:ILE:HD11	2.23	0.65
1:K:218:MSE:CE	1:K:220:ILE:HD11	2.23	0.65
1:N:206:THR:OG1	1:N:209:GLN:HG2	1.96	0.65
1:O:105:ARG:HD3	1:P:137:ASP:OD2	1.97	0.65
1:P:30:LEU:HD22	1:P:64:ARG:HH21	1.61	0.65
1:L:204:ILE:CG2	1:L:205:MSE:N	2.60	0.65
1:A:204:ILE:CG2	1:A:205:MSE:N	2.60	0.65
1:E:98:VAL:O	1:E:126:ALA:HA	1.96	0.65
1:I:218:MSE:CE	1:I:220:ILE:HD11	2.23	0.65
1:L:30:LEU:HD22	1:L:64:ARG:HH21	1.61	0.65
1:P:218:MSE:CE	1:P:220:ILE:HD11	2.23	0.65
1:L:98:VAL:O	1:L:126:ALA:HA	1.96	0.65
1:M:204:ILE:CG2	1:M:205:MSE:N	2.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:204:ILE:CG2	1:O:205:MSE:N	2.60	0.65
1:A:30:LEU:HD22	1:A:64:ARG:HH21	1.61	0.65
1:L:169:SER:HB3	1:L:172:GLU:OE1	1.95	0.65
1:N:98:VAL:O	1:N:126:ALA:HA	1.96	0.65
1:C:204:ILE:CG2	1:C:205:MSE:N	2.60	0.65
1:F:69:PHE:CD1	1:F:95:MSE:HG2	2.33	0.65
1:H:69:PHE:CD1	1:H:95:MSE:HG2	2.32	0.65
1:N:30:LEU:HD22	1:N:64:ARG:HH21	1.61	0.65
1:N:204:ILE:CG2	1:N:205:MSE:N	2.60	0.65
1:D:30:LEU:HD22	1:D:64:ARG:HH21	1.61	0.64
1:E:30:LEU:HD22	1:E:64:ARG:HH21	1.61	0.64
1:H:204:ILE:CG2	1:H:205:MSE:N	2.60	0.64
1:O:218:MSE:CE	1:O:220:ILE:HD11	2.23	0.64
1:P:204:ILE:CG2	1:P:205:MSE:N	2.60	0.64
1:B:206:THR:OG1	1:B:209:GLN:HG2	1.96	0.64
1:G:69:PHE:CD1	1:G:95:MSE:HG2	2.32	0.64
1:N:69:PHE:CD1	1:N:95:MSE:HG2	2.33	0.64
1:B:30:LEU:HD22	1:B:64:ARG:HH21	1.61	0.64
1:C:98:VAL:O	1:C:126:ALA:HA	1.96	0.64
1:E:69:PHE:CD1	1:E:95:MSE:HG2	2.33	0.64
1:G:206:THR:OG1	1:G:209:GLN:HG2	1.96	0.64
1:J:206:THR:OG1	1:J:209:GLN:HG2	1.96	0.64
1:L:69:PHE:CD1	1:L:95:MSE:HG2	2.33	0.64
1:M:206:THR:OG1	1:M:209:GLN:HG2	1.96	0.64
1:O:98:VAL:O	1:O:126:ALA:HA	1.96	0.64
1:A:98:VAL:O	1:A:126:ALA:HA	1.96	0.64
1:E:206:THR:OG1	1:E:209:GLN:HG2	1.96	0.64
1:K:30:LEU:HD22	1:K:64:ARG:HH21	1.61	0.64
1:O:69:PHE:CD1	1:O:95:MSE:HG2	2.33	0.64
1:P:69:PHE:CD1	1:P:95:MSE:HG2	2.33	0.64
1:D:69:PHE:CD1	1:D:95:MSE:HG2	2.32	0.64
1:G:204:ILE:CG2	1:G:205:MSE:N	2.60	0.64
1:J:98:VAL:O	1:J:126:ALA:HA	1.96	0.64
1:B:98:VAL:O	1:B:126:ALA:HA	1.96	0.64
1:I:69:PHE:CD1	1:I:95:MSE:HG2	2.33	0.64
1:A:69:PHE:CD1	1:A:95:MSE:HG2	2.33	0.64
1:D:206:THR:OG1	1:D:209:GLN:HG2	1.96	0.64
1:J:204:ILE:CG2	1:J:205:MSE:N	2.60	0.64
1:K:69:PHE:CD1	1:K:95:MSE:HG2	2.33	0.64
1:B:69:PHE:CD1	1:B:95:MSE:HG2	2.32	0.64
1:D:98:VAL:O	1:D:126:ALA:HA	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:THR:OG1	1:L:209:GLN:HG2	1.96	0.64
1:F:204:ILE:CG2	1:F:205:MSE:N	2.60	0.64
1:J:69:PHE:CD1	1:J:95:MSE:HG2	2.33	0.64
1:M:69:PHE:CD1	1:M:95:MSE:HG2	2.32	0.64
1:O:30:LEU:HD22	1:O:64:ARG:HH21	1.61	0.64
1:P:98:VAL:O	1:P:126:ALA:HA	1.96	0.64
1:G:218:MSE:CE	1:G:220:ILE:HD11	2.23	0.63
1:C:69:PHE:CD1	1:C:95:MSE:HG2	2.33	0.63
1:M:30:LEU:HD22	1:M:64:ARG:HH21	1.61	0.63
1:I:30:LEU:HD22	1:I:64:ARG:HH21	1.61	0.63
1:I:137:ASP:OD2	1:J:105:ARG:HD3	1.99	0.63
1:D:182:GLN:HG3	1:K:12:VAL:CG1	2.25	0.63
1:E:218:MSE:CE	1:E:220:ILE:HD11	2.23	0.63
1:A:47:LYS:HZ2	1:B:75:HIS:H	1.48	0.62
1:A:56:GLN:HA	1:A:56:GLN:NE2	2.15	0.62
1:D:218:MSE:CE	1:D:220:ILE:HD11	2.23	0.62
1:D:59:ARG:HD3	1:H:28:ASP:OD1	2.00	0.62
1:F:227:SER:HA	1:G:232:GLN:HE21	1.60	0.62
1:H:56:GLN:HA	1:H:56:GLN:NE2	2.15	0.62
1:C:56:GLN:HA	1:C:56:GLN:NE2	2.15	0.62
1:F:56:GLN:HA	1:F:56:GLN:NE2	2.15	0.62
1:K:94:TRP:CZ3	1:K:95:MSE:HE2	2.35	0.62
1:P:56:GLN:HA	1:P:56:GLN:NE2	2.15	0.62
1:L:94:TRP:CZ3	1:L:95:MSE:HE2	2.35	0.62
1:E:56:GLN:HA	1:E:56:GLN:NE2	2.15	0.62
1:L:218:MSE:CE	1:L:220:ILE:HD11	2.23	0.62
1:F:94:TRP:CZ3	1:F:95:MSE:HE2	2.35	0.61
1:I:94:TRP:CZ3	1:I:95:MSE:HE2	2.35	0.61
1:N:218:MSE:CE	1:N:220:ILE:HD11	2.23	0.61
1:C:75:HIS:H	1:D:47:LYS:HZ2	1.48	0.61
1:D:71:ASP:OD1	1:D:97:ASN:ND2	2.34	0.61
1:H:94:TRP:CZ3	1:H:95:MSE:HE2	2.35	0.61
1:K:56:GLN:HA	1:K:56:GLN:NE2	2.15	0.61
1:N:56:GLN:HA	1:N:56:GLN:NE2	2.15	0.61
1:C:71:ASP:OD1	1:C:97:ASN:ND2	2.33	0.61
1:G:56:GLN:NE2	1:G:56:GLN:HA	2.15	0.61
1:N:94:TRP:CZ3	1:N:95:MSE:HE2	2.35	0.61
1:B:71:ASP:OD1	1:B:97:ASN:ND2	2.34	0.61
1:F:71:ASP:OD1	1:F:97:ASN:ND2	2.34	0.61
1:I:56:GLN:HA	1:I:56:GLN:NE2	2.15	0.61
1:O:56:GLN:NE2	1:O:56:GLN:HA	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:71:ASP:OD1	1:O:97:ASN:ND2	2.34	0.61
1:A:71:ASP:OD1	1:A:97:ASN:ND2	2.34	0.61
1:E:94:TRP:CZ3	1:E:95:MSE:HE2	2.35	0.61
1:F:236:ALA:HB1	1:G:228:VAL:CB	2.30	0.61
1:O:94:TRP:CZ3	1:O:95:MSE:HE2	2.35	0.61
1:B:56:GLN:NE2	1:B:56:GLN:HA	2.15	0.61
1:C:105:ARG:HD3	1:D:137:ASP:OD2	2.00	0.61
1:K:71:ASP:OD1	1:K:97:ASN:ND2	2.34	0.61
1:M:56:GLN:HA	1:M:56:GLN:NE2	2.15	0.61
1:M:71:ASP:OD1	1:M:97:ASN:ND2	2.34	0.61
1:M:94:TRP:CZ3	1:M:95:MSE:HE2	2.35	0.61
1:G:94:TRP:CZ3	1:G:95:MSE:HE2	2.35	0.61
1:J:94:TRP:CZ3	1:J:95:MSE:HE2	2.35	0.61
1:H:71:ASP:OD1	1:H:97:ASN:ND2	2.34	0.61
1:P:94:TRP:CZ3	1:P:95:MSE:HE2	2.35	0.61
1:B:94:TRP:CZ3	1:B:95:MSE:HE2	2.35	0.61
1:D:94:TRP:CZ3	1:D:95:MSE:HE2	2.35	0.61
1:O:47:LYS:HZ2	1:P:75:HIS:H	1.49	0.61
1:A:94:TRP:CZ3	1:A:95:MSE:HE2	2.35	0.61
1:C:94:TRP:CZ3	1:C:95:MSE:HE2	2.35	0.61
1:D:56:GLN:NE2	1:D:56:GLN:HA	2.15	0.61
1:F:236:ALA:HB1	1:G:228:VAL:HB	1.83	0.60
1:P:71:ASP:OD1	1:P:97:ASN:ND2	2.34	0.60
1:I:71:ASP:OD1	1:I:97:ASN:ND2	2.33	0.60
1:J:56:GLN:NE2	1:J:56:GLN:HA	2.15	0.60
1:L:56:GLN:NE2	1:L:56:GLN:HA	2.15	0.60
1:B:218:MSE:CE	1:B:220:ILE:HD11	2.23	0.60
1:J:218:MSE:CE	1:J:220:ILE:HD11	2.23	0.60
1:L:71:ASP:OD1	1:L:97:ASN:ND2	2.34	0.60
1:N:71:ASP:OD1	1:N:97:ASN:ND2	2.33	0.60
1:E:71:ASP:OD1	1:E:97:ASN:ND2	2.34	0.60
1:G:71:ASP:OD1	1:G:97:ASN:ND2	2.34	0.60
1:H:192:ARG:HB2	1:H:204:ILE:HG21	1.84	0.60
1:J:71:ASP:OD1	1:J:97:ASN:ND2	2.34	0.60
1:A:192:ARG:HB2	1:A:204:ILE:HG21	1.84	0.60
1:M:130:LEU:HD13	1:N:76:ASP:C	2.22	0.60
1:C:192:ARG:HB2	1:C:204:ILE:HG21	1.84	0.60
1:L:192:ARG:HB2	1:L:204:ILE:HG21	1.84	0.60
1:K:47:LYS:HZ3	1:L:75:HIS:H	1.50	0.60
1:P:192:ARG:HB2	1:P:204:ILE:HG21	1.84	0.60
1:J:192:ARG:HB2	1:J:204:ILE:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:ARG:HB2	1:F:204:ILE:HG21	1.84	0.59
1:B:169:SER:HB2	1:B:203:ARG:HH11	1.68	0.59
1:B:228:VAL:HG21	1:C:233:THR:HA	1.83	0.59
1:E:105:ARG:HD3	1:F:137:ASP:OD2	2.01	0.59
1:I:192:ARG:HB2	1:I:204:ILE:HG21	1.84	0.59
1:D:169:SER:HB2	1:D:203:ARG:HH11	1.68	0.59
1:N:169:SER:HB2	1:N:203:ARG:HH11	1.68	0.59
1:N:175:ARG:O	1:N:179:VAL:HG23	2.03	0.59
1:A:169:SER:HB2	1:A:203:ARG:HH11	1.68	0.59
1:F:175:ARG:O	1:F:179:VAL:HG23	2.03	0.59
1:F:218:MSE:CE	1:F:220:ILE:HD11	2.23	0.59
1:F:236:ALA:HB2	1:G:228:VAL:CG2	2.26	0.59
1:G:175:ARG:O	1:G:179:VAL:HG23	2.03	0.59
1:K:204:ILE:CG2	1:K:205:MSE:N	2.60	0.59
1:K:192:ARG:HB2	1:K:204:ILE:HG21	1.84	0.59
1:O:169:SER:HB2	1:O:203:ARG:HH11	1.68	0.59
1:E:175:ARG:O	1:E:179:VAL:HG23	2.03	0.59
1:J:175:ARG:O	1:J:179:VAL:HG23	2.03	0.59
1:A:175:ARG:O	1:A:179:VAL:HG23	2.03	0.59
1:C:169:SER:HB2	1:C:203:ARG:HH11	1.67	0.59
1:C:175:ARG:O	1:C:179:VAL:HG23	2.03	0.59
1:D:192:ARG:HB2	1:D:204:ILE:HG21	1.84	0.59
1:H:175:ARG:O	1:H:179:VAL:HG23	2.03	0.59
1:O:192:ARG:HB2	1:O:204:ILE:HG21	1.84	0.59
1:B:192:ARG:HB2	1:B:204:ILE:HG21	1.84	0.59
1:K:137:ASP:OD2	1:L:105:ARG:HD3	2.03	0.59
1:M:192:ARG:HB2	1:M:204:ILE:HG21	1.84	0.59
1:A:137:ASP:OD2	1:B:105:ARG:HD3	2.03	0.59
1:K:175:ARG:O	1:K:179:VAL:HG23	2.03	0.59
1:L:175:ARG:O	1:L:179:VAL:HG23	2.03	0.58
1:B:228:VAL:CB	1:C:236:ALA:HB1	2.31	0.58
1:I:169:SER:HB2	1:I:203:ARG:HH11	1.68	0.58
1:K:169:SER:HB2	1:K:203:ARG:HH11	1.68	0.58
1:A:234:LEU:HD13	1:A:238:ASN:HD21	1.69	0.58
1:M:169:SER:HB2	1:M:203:ARG:HH11	1.68	0.58
1:P:175:ARG:O	1:P:179:VAL:HG23	2.03	0.58
1:C:234:LEU:HD13	1:C:238:ASN:HD21	1.69	0.58
1:D:234:LEU:HD13	1:D:238:ASN:HD21	1.69	0.58
1:M:175:ARG:O	1:M:179:VAL:HG23	2.03	0.58
1:B:234:LEU:HD13	1:B:238:ASN:HD21	1.69	0.58
1:F:94:TRP:HZ3	1:F:95:MSE:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175:ARG:O	1:I:179:VAL:HG23	2.03	0.58
1:L:94:TRP:HZ3	1:L:95:MSE:HE2	1.68	0.58
1:C:94:TRP:HZ3	1:C:95:MSE:HE2	1.68	0.58
1:C:191:ILE:HG21	1:C:218:MSE:CE	2.34	0.58
1:L:169:SER:HB2	1:L:203:ARG:HH11	1.67	0.58
1:M:132:SER:OG	1:N:78:PRO:HD3	2.04	0.58
1:O:175:ARG:O	1:O:179:VAL:HG23	2.03	0.58
1:A:191:ILE:HG21	1:A:218:MSE:CE	2.34	0.58
1:F:169:SER:HB2	1:F:203:ARG:HH11	1.68	0.58
1:H:94:TRP:HZ3	1:H:95:MSE:HE2	1.68	0.58
1:J:169:SER:HB2	1:J:203:ARG:HH11	1.68	0.58
1:M:170:ALA:HA	1:M:188:THR:HG21	1.86	0.58
1:N:192:ARG:HB2	1:N:204:ILE:HG21	1.84	0.58
1:B:170:ALA:HA	1:B:188:THR:HG21	1.86	0.58
1:E:170:ALA:HA	1:E:188:THR:HG21	1.86	0.58
1:G:192:ARG:HB2	1:G:204:ILE:HG21	1.84	0.58
1:H:169:SER:HB2	1:H:203:ARG:HH11	1.67	0.58
1:I:191:ILE:HG21	1:I:218:MSE:CE	2.34	0.58
1:K:191:ILE:HG21	1:K:218:MSE:CE	2.34	0.58
1:B:175:ARG:O	1:B:179:VAL:HG23	2.03	0.58
1:D:175:ARG:O	1:D:179:VAL:HG23	2.03	0.58
1:N:94:TRP:HZ3	1:N:95:MSE:HE2	1.68	0.58
1:C:177:LYS:HE3	1:C:182:GLN:HA	1.86	0.58
1:G:234:LEU:HD13	1:G:238:ASN:HD21	1.69	0.58
1:I:234:LEU:HD13	1:I:238:ASN:HD21	1.69	0.58
1:J:177:LYS:HE3	1:J:182:GLN:HA	1.86	0.58
1:M:234:LEU:HD13	1:M:238:ASN:HD21	1.69	0.58
1:O:234:LEU:HD13	1:O:238:ASN:HD21	1.69	0.58
1:A:94:TRP:HZ3	1:A:95:MSE:HE2	1.68	0.57
1:D:170:ALA:HA	1:D:188:THR:HG21	1.86	0.57
1:E:234:LEU:HD13	1:E:238:ASN:HD21	1.69	0.57
1:F:234:LEU:HD13	1:F:238:ASN:HD21	1.69	0.57
1:M:94:TRP:HZ3	1:M:95:MSE:HE2	1.68	0.57
1:N:234:LEU:HD13	1:N:238:ASN:HD21	1.69	0.57
1:B:150:TYR:CE1	1:B:154:LEU:HD11	2.40	0.57
1:E:192:ARG:HB2	1:E:204:ILE:HG21	1.84	0.57
1:G:170:ALA:HA	1:G:188:THR:HG21	1.86	0.57
1:D:150:TYR:CE1	1:D:154:LEU:HD11	2.40	0.57
1:E:94:TRP:HZ3	1:E:95:MSE:HE2	1.68	0.57
1:E:177:LYS:HE3	1:E:182:GLN:HA	1.87	0.57
1:G:169:SER:HB2	1:G:203:ARG:HH11	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:TRP:HZ3	1:J:95:MSE:HE2	1.68	0.57
1:J:150:TYR:CE1	1:J:154:LEU:HD11	2.39	0.57
1:J:170:ALA:HA	1:J:188:THR:HG21	1.86	0.57
1:N:150:TYR:CE1	1:N:154:LEU:HD11	2.40	0.57
1:B:191:ILE:HG21	1:B:218:MSE:CE	2.34	0.57
1:C:124:LEU:CG	1:C:163:LEU:HD13	2.35	0.57
1:E:169:SER:HB2	1:E:203:ARG:HH11	1.68	0.57
1:J:234:LEU:HD13	1:J:238:ASN:HD21	1.69	0.57
1:N:124:LEU:CG	1:N:163:LEU:HD13	2.35	0.57
1:O:170:ALA:HA	1:O:188:THR:HG21	1.86	0.57
1:P:169:SER:HB2	1:P:203:ARG:HH11	1.68	0.57
1:P:234:LEU:HD13	1:P:238:ASN:HD21	1.68	0.57
1:A:177:LYS:HE3	1:A:182:GLN:HA	1.86	0.57
1:G:191:ILE:HG21	1:G:218:MSE:CE	2.34	0.57
1:K:94:TRP:HZ3	1:K:95:MSE:HE2	1.68	0.57
1:K:177:LYS:HE3	1:K:182:GLN:HA	1.87	0.57
1:L:124:LEU:CG	1:L:163:LEU:HD13	2.35	0.57
1:L:170:ALA:HA	1:L:188:THR:HG21	1.86	0.57
1:A:170:ALA:HA	1:A:188:THR:HG21	1.86	0.57
1:G:177:LYS:HE3	1:G:182:GLN:HA	1.86	0.57
1:I:94:TRP:HZ3	1:I:95:MSE:HE2	1.68	0.57
1:I:177:LYS:HE3	1:I:182:GLN:HA	1.86	0.57
1:K:150:TYR:CE1	1:K:154:LEU:HD11	2.40	0.57
1:M:150:TYR:CE1	1:M:154:LEU:HD11	2.40	0.57
1:A:138:LEU:HB3	1:A:143:MSE:HG2	1.87	0.57
1:C:194:GLN:HG3	1:C:194:GLN:O	2.05	0.57
1:E:191:ILE:HG21	1:E:218:MSE:CE	2.34	0.57
1:F:124:LEU:CG	1:F:163:LEU:HD13	2.35	0.57
1:G:94:TRP:HZ3	1:G:95:MSE:HE2	1.68	0.57
1:H:234:LEU:HD13	1:H:238:ASN:HD21	1.69	0.57
1:L:177:LYS:HE3	1:L:182:GLN:HA	1.86	0.57
1:N:191:ILE:HG21	1:N:218:MSE:CE	2.34	0.57
1:O:94:TRP:HZ3	1:O:95:MSE:HE2	1.68	0.57
1:O:191:ILE:HG21	1:O:218:MSE:CE	2.34	0.57
1:P:191:ILE:HG21	1:P:218:MSE:CE	2.34	0.57
1:A:124:LEU:CG	1:A:163:LEU:HD13	2.35	0.57
1:A:194:GLN:O	1:A:194:GLN:HG3	2.05	0.57
1:E:150:TYR:CE1	1:E:154:LEU:HD11	2.40	0.57
1:G:138:LEU:HB3	1:G:143:MSE:HG2	1.87	0.57
1:H:194:GLN:HG3	1:H:194:GLN:O	2.05	0.57
1:I:150:TYR:CE1	1:I:154:LEU:HD11	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:170:ALA:HA	1:K:188:THR:HG21	1.86	0.57
1:K:234:LEU:HD13	1:K:238:ASN:HD21	1.69	0.57
1:L:234:LEU:HD13	1:L:238:ASN:HD21	1.69	0.57
1:M:138:LEU:HB3	1:M:143:MSE:HG2	1.87	0.57
1:P:138:LEU:HB3	1:P:143:MSE:HG2	1.87	0.57
1:B:177:LYS:HE3	1:B:182:GLN:HA	1.86	0.57
1:C:138:LEU:HB3	1:C:143:MSE:HG2	1.87	0.57
1:C:150:TYR:CE1	1:C:154:LEU:HD11	2.39	0.57
1:E:138:LEU:HB3	1:E:143:MSE:HG2	1.87	0.57
1:F:150:TYR:CE1	1:F:154:LEU:HD11	2.40	0.57
1:H:191:ILE:HG21	1:H:218:MSE:CE	2.34	0.57
1:M:194:GLN:HG3	1:M:194:GLN:O	2.05	0.57
1:N:138:LEU:HB3	1:N:143:MSE:HG2	1.87	0.57
1:N:177:LYS:HE3	1:N:182:GLN:HA	1.87	0.57
1:F:191:ILE:HG21	1:F:218:MSE:CE	2.34	0.57
1:F:194:GLN:HG3	1:F:194:GLN:O	2.05	0.57
1:H:150:TYR:CE1	1:H:154:LEU:HD11	2.39	0.57
1:M:124:LEU:CG	1:M:163:LEU:HD13	2.35	0.57
1:O:124:LEU:CG	1:O:163:LEU:HD13	2.35	0.57
1:P:194:GLN:HG3	1:P:194:GLN:O	2.05	0.57
1:O:150:TYR:CE1	1:O:154:LEU:HD11	2.40	0.56
1:O:177:LYS:HE3	1:O:182:GLN:HA	1.86	0.56
1:P:150:TYR:CE1	1:P:154:LEU:HD11	2.40	0.56
1:E:137:ASP:OD2	1:F:105:ARG:HD3	2.04	0.56
1:I:194:GLN:O	1:I:194:GLN:HG3	2.05	0.56
1:K:194:GLN:HG3	1:K:194:GLN:O	2.05	0.56
1:M:191:ILE:HG21	1:M:218:MSE:CE	2.34	0.56
1:P:94:TRP:HZ3	1:P:95:MSE:HE2	1.68	0.56
1:B:194:GLN:HG3	1:B:194:GLN:O	2.05	0.56
1:C:170:ALA:HA	1:C:188:THR:HG21	1.86	0.56
1:D:194:GLN:HG3	1:D:194:GLN:O	2.05	0.56
1:I:170:ALA:HA	1:I:188:THR:HG21	1.86	0.56
1:J:191:ILE:HG21	1:J:218:MSE:CE	2.34	0.56
1:K:124:LEU:CG	1:K:163:LEU:HD13	2.35	0.56
1:L:150:TYR:CE1	1:L:154:LEU:HD11	2.40	0.56
1:L:191:ILE:HG21	1:L:218:MSE:CE	2.34	0.56
1:N:170:ALA:HA	1:N:188:THR:HG21	1.86	0.56
1:B:94:TRP:HZ3	1:B:95:MSE:HE2	1.68	0.56
1:G:150:TYR:CE1	1:G:154:LEU:HD11	2.40	0.56
1:K:192:ARG:HD2	1:K:198:ALA:HA	1.88	0.56
1:B:138:LEU:HB3	1:B:143:MSE:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:TRP:HZ3	1:D:95:MSE:HE2	1.68	0.56
1:H:170:ALA:HA	1:H:188:THR:HG21	1.86	0.56
1:I:124:LEU:CG	1:I:163:LEU:HD13	2.35	0.56
1:O:138:LEU:HB3	1:O:143:MSE:HG2	1.87	0.56
1:P:177:LYS:HE3	1:P:182:GLN:HA	1.86	0.56
1:A:150:TYR:CE1	1:A:154:LEU:HD11	2.40	0.56
1:P:124:LEU:CG	1:P:163:LEU:HD13	2.35	0.56
1:D:177:LYS:HE3	1:D:182:GLN:HA	1.86	0.56
1:D:191:ILE:HG21	1:D:218:MSE:CE	2.34	0.56
1:I:138:LEU:HB3	1:I:143:MSE:HG2	1.87	0.56
1:M:177:LYS:HE3	1:M:182:GLN:HA	1.86	0.56
1:D:138:LEU:HB3	1:D:143:MSE:HG2	1.87	0.56
1:I:192:ARG:HD2	1:I:198:ALA:HA	1.88	0.56
1:J:194:GLN:HG3	1:J:194:GLN:O	2.05	0.56
1:K:138:LEU:HB3	1:K:143:MSE:HG2	1.87	0.56
1:C:192:ARG:HD2	1:C:198:ALA:HA	1.88	0.56
1:F:170:ALA:HA	1:F:188:THR:HG21	1.86	0.56
1:G:173:ALA:O	1:G:177:LYS:HB2	2.06	0.56
1:J:138:LEU:HB3	1:J:143:MSE:HG2	1.87	0.56
1:L:194:GLN:HG3	1:L:194:GLN:O	2.05	0.56
1:E:192:ARG:HD2	1:E:198:ALA:HA	1.88	0.56
1:F:177:LYS:HE3	1:F:182:GLN:HA	1.86	0.56
1:G:192:ARG:HD2	1:G:198:ALA:HA	1.88	0.56
1:L:138:LEU:HB3	1:L:143:MSE:HG2	1.87	0.56
1:N:192:ARG:HD2	1:N:198:ALA:HA	1.88	0.56
1:N:194:GLN:HG3	1:N:194:GLN:O	2.05	0.56
1:H:138:LEU:HB3	1:H:143:MSE:HG2	1.87	0.55
1:A:192:ARG:HD2	1:A:198:ALA:HA	1.88	0.55
1:E:194:GLN:HG3	1:E:194:GLN:O	2.05	0.55
1:G:137:ASP:OD2	1:H:105:ARG:HD3	2.05	0.55
1:H:177:LYS:HE3	1:H:182:GLN:HA	1.86	0.55
1:J:124:LEU:CG	1:J:163:LEU:HD13	2.35	0.55
1:M:192:ARG:HD2	1:M:198:ALA:HA	1.88	0.55
1:B:173:ALA:O	1:B:177:LYS:HB2	2.06	0.55
1:E:173:ALA:O	1:E:177:LYS:HB2	2.06	0.55
1:J:192:ARG:HD2	1:J:198:ALA:HA	1.88	0.55
1:M:173:ALA:O	1:M:177:LYS:HB2	2.06	0.55
1:O:194:GLN:HG3	1:O:194:GLN:O	2.05	0.55
1:P:170:ALA:HA	1:P:188:THR:HG21	1.86	0.55
1:P:171:GLN:HG2	1:P:205:MSE:CE	2.37	0.55
1:E:171:GLN:HG2	1:E:205:MSE:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:173:ALA:O	1:N:177:LYS:HB2	2.06	0.55
1:B:124:LEU:CG	1:B:163:LEU:HD13	2.35	0.55
1:F:138:LEU:HB3	1:F:143:MSE:HG2	1.87	0.55
1:G:194:GLN:HG3	1:G:194:GLN:O	2.05	0.55
1:K:171:GLN:HG2	1:K:205:MSE:CE	2.37	0.55
1:L:192:ARG:HD2	1:L:198:ALA:HA	1.88	0.55
1:O:192:ARG:HD2	1:O:198:ALA:HA	1.88	0.55
1:D:173:ALA:O	1:D:177:LYS:HB2	2.06	0.55
1:H:192:ARG:HD2	1:H:198:ALA:HA	1.88	0.55
1:I:171:GLN:HG2	1:I:205:MSE:CE	2.37	0.55
1:A:171:GLN:HG2	1:A:205:MSE:CE	2.37	0.55
1:D:192:ARG:HD2	1:D:198:ALA:HA	1.88	0.55
1:G:171:GLN:HG2	1:G:205:MSE:CE	2.37	0.55
1:I:105:ARG:HD3	1:J:137:ASP:OD2	2.06	0.55
1:N:171:GLN:HG2	1:N:205:MSE:CE	2.37	0.55
1:F:192:ARG:HD2	1:F:198:ALA:HA	1.88	0.55
1:L:173:ALA:O	1:L:177:LYS:HB2	2.06	0.55
1:A:173:ALA:O	1:A:177:LYS:HB2	2.06	0.55
1:C:171:GLN:HG2	1:C:205:MSE:CE	2.37	0.55
1:E:124:LEU:CG	1:E:163:LEU:HD13	2.35	0.55
1:F:227:SER:CB	1:G:232:GLN:HE21	2.19	0.55
1:H:171:GLN:HG2	1:H:205:MSE:CE	2.37	0.55
1:J:173:ALA:O	1:J:177:LYS:HB2	2.06	0.55
1:N:125:ILE:HG23	1:N:165:GLY:C	2.28	0.55
1:A:127:VAL:HA	1:A:167:VAL:HB	1.89	0.54
1:C:173:ALA:O	1:C:177:LYS:HB2	2.06	0.54
1:F:173:ALA:O	1:F:177:LYS:HB2	2.06	0.54
1:J:171:GLN:HG2	1:J:205:MSE:CE	2.37	0.54
1:L:125:ILE:HG23	1:L:165:GLY:C	2.28	0.54
1:O:171:GLN:HG2	1:O:205:MSE:CE	2.37	0.54
1:A:125:ILE:HG23	1:A:165:GLY:C	2.28	0.54
1:B:228:VAL:CG2	1:C:236:ALA:HB1	2.36	0.54
1:L:127:VAL:HA	1:L:167:VAL:HB	1.89	0.54
1:P:125:ILE:HG23	1:P:165:GLY:C	2.28	0.54
1:D:205:MSE:HG3	1:D:209:GLN:CD	2.28	0.54
1:F:171:GLN:HG2	1:F:205:MSE:CE	2.37	0.54
1:I:127:VAL:HA	1:I:167:VAL:HB	1.89	0.54
1:K:127:VAL:HA	1:K:167:VAL:HB	1.89	0.54
1:M:127:VAL:HA	1:M:167:VAL:HB	1.89	0.54
1:M:171:GLN:HG2	1:M:205:MSE:CE	2.37	0.54
1:O:173:ALA:O	1:O:177:LYS:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:127:VAL:HA	1:P:167:VAL:HB	1.89	0.54
1:B:127:VAL:HA	1:B:167:VAL:HB	1.89	0.54
1:B:171:GLN:HG2	1:B:205:MSE:CE	2.37	0.54
1:B:192:ARG:HD2	1:B:198:ALA:HA	1.88	0.54
1:B:205:MSE:HG3	1:B:209:GLN:CD	2.28	0.54
1:C:205:MSE:HG3	1:C:209:GLN:CD	2.28	0.54
1:G:205:MSE:HG3	1:G:209:GLN:CD	2.28	0.54
1:I:173:ALA:O	1:I:177:LYS:HB2	2.06	0.54
1:N:127:VAL:HA	1:N:167:VAL:HB	1.89	0.54
1:A:205:MSE:HG3	1:A:209:GLN:CD	2.28	0.54
1:C:127:VAL:HA	1:C:167:VAL:HB	1.90	0.54
1:D:171:GLN:HG2	1:D:205:MSE:CE	2.37	0.54
1:E:205:MSE:HG3	1:E:209:GLN:CD	2.28	0.54
1:H:173:ALA:O	1:H:177:LYS:HB2	2.06	0.54
1:P:173:ALA:O	1:P:177:LYS:HB2	2.06	0.54
1:P:192:ARG:HD2	1:P:198:ALA:HA	1.88	0.54
1:B:125:ILE:HG23	1:B:165:GLY:C	2.28	0.54
1:D:124:LEU:CG	1:D:163:LEU:HD13	2.35	0.54
1:E:204:ILE:CG2	1:E:205:MSE:N	2.60	0.54
1:F:205:MSE:HG3	1:F:209:GLN:CD	2.28	0.54
1:G:124:LEU:CG	1:G:163:LEU:HD13	2.35	0.54
1:G:125:ILE:HG23	1:G:165:GLY:C	2.28	0.54
1:I:205:MSE:HG3	1:I:209:GLN:CD	2.28	0.54
1:J:125:ILE:HG23	1:J:165:GLY:C	2.28	0.54
1:L:171:GLN:HG2	1:L:205:MSE:CE	2.37	0.54
1:C:125:ILE:HG23	1:C:165:GLY:C	2.28	0.54
1:D:125:ILE:HG23	1:D:165:GLY:C	2.28	0.54
1:D:127:VAL:HA	1:D:167:VAL:HB	1.89	0.54
1:I:207:PRO:CA	1:I:218:MSE:HE1	2.38	0.54
1:J:205:MSE:HG3	1:J:209:GLN:CD	2.28	0.54
1:M:207:PRO:CA	1:M:218:MSE:HE1	2.38	0.54
1:F:125:ILE:HG23	1:F:165:GLY:C	2.28	0.54
1:H:127:VAL:HA	1:H:167:VAL:HB	1.89	0.54
1:J:127:VAL:HA	1:J:167:VAL:HB	1.90	0.54
1:K:205:MSE:HG3	1:K:209:GLN:CD	2.28	0.54
1:N:205:MSE:HG3	1:N:209:GLN:CD	2.28	0.54
1:E:125:ILE:HG23	1:E:165:GLY:C	2.28	0.54
1:H:147:PRO:HB3	1:H:203:ARG:NE	2.17	0.54
1:O:25:ASN:HD22	1:O:28:ASP:CB	2.16	0.54
1:B:232:GLN:HE21	1:C:227:SER:CB	2.20	0.54
1:E:207:PRO:CA	1:E:218:MSE:HE1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:SER:CA	1:G:232:GLN:NE2	2.64	0.54
1:G:127:VAL:HA	1:G:167:VAL:HB	1.89	0.54
1:H:205:MSE:HG3	1:H:209:GLN:CD	2.28	0.54
1:M:125:ILE:HG23	1:M:165:GLY:C	2.28	0.54
1:P:205:MSE:HG3	1:P:209:GLN:CD	2.28	0.54
1:D:12:VAL:HG11	1:K:182:GLN:CG	2.27	0.53
1:H:124:LEU:CG	1:H:163:LEU:HD13	2.35	0.53
1:I:125:ILE:HG23	1:I:165:GLY:C	2.28	0.53
1:I:234:LEU:HD13	1:I:238:ASN:ND2	2.24	0.53
1:P:234:LEU:HD13	1:P:238:ASN:ND2	2.24	0.53
1:C:25:ASN:HD22	1:C:28:ASP:CB	2.16	0.53
1:E:234:LEU:HD13	1:E:238:ASN:ND2	2.24	0.53
1:F:127:VAL:HA	1:F:167:VAL:HB	1.89	0.53
1:G:207:PRO:CA	1:G:218:MSE:HE1	2.38	0.53
1:G:234:LEU:HD13	1:G:238:ASN:ND2	2.24	0.53
1:H:125:ILE:HG23	1:H:165:GLY:C	2.28	0.53
1:K:173:ALA:O	1:K:177:LYS:HB2	2.06	0.53
1:N:234:LEU:HD13	1:N:238:ASN:ND2	2.24	0.53
1:O:127:VAL:HA	1:O:167:VAL:HB	1.89	0.53
1:G:221:GLY:HA3	2:G:307:BMP:OP3	2.09	0.53
1:K:234:LEU:HD13	1:K:238:ASN:ND2	2.24	0.53
1:M:234:LEU:HD13	1:M:238:ASN:ND2	2.24	0.53
1:E:221:GLY:HA3	2:E:305:BMP:OP3	2.09	0.53
1:I:224:VAL:O	1:I:230:PRO:HB3	2.09	0.53
1:M:205:MSE:HG3	1:M:209:GLN:CD	2.28	0.53
1:N:25:ASN:HD22	1:N:28:ASP:CB	2.16	0.53
1:C:207:PRO:CA	1:C:218:MSE:HE1	2.38	0.53
1:C:224:VAL:O	1:C:230:PRO:HB3	2.09	0.53
1:L:205:MSE:HG3	1:L:209:GLN:CD	2.28	0.53
1:O:125:ILE:HG23	1:O:165:GLY:C	2.28	0.53
1:O:205:MSE:HG3	1:O:209:GLN:CD	2.28	0.53
1:P:82:ALA:HB1	1:P:113:ALA:HB2	1.91	0.53
1:A:224:VAL:O	1:A:230:PRO:HB3	2.09	0.53
1:B:207:PRO:CA	1:B:218:MSE:HE1	2.38	0.53
1:D:207:PRO:CA	1:D:218:MSE:HE1	2.38	0.53
1:N:221:GLY:HA3	2:N:314:BMP:OP3	2.09	0.53
1:O:75:HIS:H	1:P:47:LYS:NZ	2.07	0.53
1:P:224:VAL:O	1:P:230:PRO:HB3	2.09	0.53
1:F:234:LEU:HD13	1:F:238:ASN:ND2	2.24	0.53
1:L:221:GLY:HA3	2:L:312:BMP:OP3	2.09	0.53
1:M:224:VAL:O	1:M:230:PRO:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:224:VAL:O	1:N:230:PRO:HB3	2.09	0.53
1:O:234:LEU:HD13	1:O:238:ASN:ND2	2.24	0.53
1:E:127:VAL:HA	1:E:167:VAL:HB	1.89	0.53
1:F:221:GLY:HA3	2:F:306:BMP:OP3	2.09	0.53
1:H:221:GLY:HA3	2:H:308:BMP:OP3	2.09	0.53
1:I:221:GLY:HA3	2:I:309:BMP:OP3	2.09	0.53
1:O:77:ILE:HG22	1:P:132:SER:HB3	1.90	0.53
1:E:82:ALA:HB1	1:E:113:ALA:HB2	1.91	0.53
1:J:207:PRO:CA	1:J:218:MSE:HE1	2.38	0.53
1:J:221:GLY:HA3	2:J:310:BMP:OP3	2.09	0.53
1:K:224:VAL:O	1:K:230:PRO:HB3	2.09	0.53
1:L:73:LYS:H	1:L:97:ASN:HB3	1.74	0.53
1:M:105:ARG:HH22	1:N:200:ASP:HA	1.74	0.53
1:A:105:ARG:HD3	1:B:137:ASP:OD2	2.09	0.53
1:C:221:GLY:HA3	2:C:303:BMP:OP3	2.09	0.53
1:G:82:ALA:HB1	1:G:113:ALA:HB2	1.91	0.53
1:H:234:LEU:HD13	1:H:238:ASN:ND2	2.24	0.53
1:J:73:LYS:H	1:J:97:ASN:HB3	1.74	0.53
1:K:125:ILE:HG23	1:K:165:GLY:C	2.28	0.53
1:K:207:PRO:CA	1:K:218:MSE:HE1	2.38	0.53
1:O:124:LEU:HG	1:O:163:LEU:CD1	2.39	0.53
1:P:207:PRO:CA	1:P:218:MSE:HE1	2.38	0.53
1:A:25:ASN:HD22	1:A:28:ASP:CB	2.16	0.52
1:B:224:VAL:O	1:B:230:PRO:HB3	2.09	0.52
1:D:234:LEU:HD13	1:D:238:ASN:ND2	2.24	0.52
1:G:224:VAL:O	1:G:230:PRO:HB3	2.09	0.52
1:H:82:ALA:HB1	1:H:113:ALA:HB2	1.91	0.52
1:M:221:GLY:HA3	2:M:313:BMP:OP3	2.09	0.52
1:O:221:GLY:HA3	2:O:315:BMP:OP3	2.09	0.52
1:A:207:PRO:CA	1:A:218:MSE:HE1	2.38	0.52
1:B:73:LYS:H	1:B:97:ASN:HB3	1.74	0.52
1:D:82:ALA:HB1	1:D:113:ALA:HB2	1.91	0.52
1:D:221:GLY:HA3	2:D:304:BMP:OP3	2.09	0.52
1:F:73:LYS:H	1:F:97:ASN:HB3	1.74	0.52
1:F:224:VAL:O	1:F:230:PRO:HB3	2.09	0.52
1:A:221:GLY:HA3	2:A:301:BMP:OP3	2.09	0.52
1:I:82:ALA:HB1	1:I:113:ALA:HB2	1.91	0.52
1:M:73:LYS:H	1:M:97:ASN:HB3	1.74	0.52
1:N:124:LEU:HG	1:N:163:LEU:CD1	2.39	0.52
1:A:73:LYS:H	1:A:97:ASN:HB3	1.74	0.52
1:C:183:GLU:OE1	1:C:183:GLU:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:LYS:H	1:D:97:ASN:HB3	1.74	0.52
1:E:25:ASN:HD22	1:E:28:ASP:CB	2.16	0.52
1:F:82:ALA:HB1	1:F:113:ALA:HB2	1.91	0.52
1:H:73:LYS:H	1:H:97:ASN:HB3	1.74	0.52
1:J:82:ALA:HB1	1:J:113:ALA:HB2	1.91	0.52
1:K:73:LYS:H	1:K:97:ASN:HB3	1.74	0.52
1:O:73:LYS:H	1:O:97:ASN:HB3	1.74	0.52
1:B:82:ALA:HB1	1:B:113:ALA:HB2	1.91	0.52
1:H:224:VAL:O	1:H:230:PRO:HB3	2.09	0.52
1:I:183:GLU:OE1	1:I:183:GLU:HA	2.10	0.52
1:K:221:GLY:HA3	2:K:311:BMP:OP3	2.09	0.52
1:L:82:ALA:HB1	1:L:113:ALA:HB2	1.91	0.52
1:L:207:PRO:CA	1:L:218:MSE:HE1	2.38	0.52
1:M:136:SER:O	1:M:139:VAL:HG12	2.10	0.52
1:A:183:GLU:OE1	1:A:183:GLU:HA	2.10	0.52
1:B:221:GLY:HA3	2:B:302:BMP:OP3	2.09	0.52
1:C:73:LYS:H	1:C:97:ASN:HB3	1.74	0.52
1:C:234:LEU:HD13	1:C:238:ASN:ND2	2.24	0.52
1:K:82:ALA:HB1	1:K:113:ALA:HB2	1.91	0.52
1:O:224:VAL:O	1:O:230:PRO:HB3	2.09	0.52
1:P:124:LEU:HG	1:P:163:LEU:CD1	2.39	0.52
1:P:221:GLY:HA3	2:P:316:BMP:OP3	2.09	0.52
1:A:234:LEU:HD13	1:A:238:ASN:ND2	2.24	0.52
1:B:131:THR:HA	1:B:203:ARG:NH1	2.25	0.52
1:B:136:SER:O	1:B:139:VAL:HG12	2.10	0.52
1:B:183:GLU:OE1	1:B:183:GLU:HA	2.10	0.52
1:B:234:LEU:HD13	1:B:238:ASN:ND2	2.24	0.52
1:E:224:VAL:O	1:E:230:PRO:HB3	2.09	0.52
1:G:25:ASN:HD22	1:G:28:ASP:CB	2.16	0.52
1:K:25:ASN:HD22	1:K:28:ASP:CB	2.16	0.52
1:M:128:THR:OG1	1:M:129:VAL:N	2.43	0.52
1:N:73:LYS:H	1:N:97:ASN:HB3	1.74	0.52
1:D:131:THR:HA	1:D:203:ARG:NH1	2.25	0.52
1:D:183:GLU:OE1	1:D:183:GLU:HA	2.10	0.52
1:G:183:GLU:HA	1:G:183:GLU:OE1	2.10	0.52
1:J:136:SER:O	1:J:139:VAL:HG12	2.10	0.52
1:J:224:VAL:O	1:J:230:PRO:HB3	2.09	0.52
1:N:82:ALA:HB1	1:N:113:ALA:HB2	1.91	0.52
1:N:136:SER:O	1:N:139:VAL:HG12	2.10	0.52
1:O:82:ALA:HB1	1:O:113:ALA:HB2	1.91	0.52
1:D:136:SER:O	1:D:139:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:VAL:O	1:D:230:PRO:HB3	2.09	0.52
1:I:136:SER:O	1:I:139:VAL:HG12	2.10	0.52
1:K:147:PRO:HB3	1:K:203:ARG:NE	2.17	0.52
1:M:76:ASP:HB3	1:M:80:THR:HB	1.92	0.52
1:M:183:GLU:OE1	1:M:183:GLU:HA	2.10	0.52
1:N:76:ASP:HB3	1:N:80:THR:HB	1.92	0.52
1:N:183:GLU:OE1	1:N:183:GLU:HA	2.10	0.52
1:D:174:VAL:HG22	1:D:213:ALA:HB1	1.92	0.52
1:E:73:LYS:H	1:E:97:ASN:HB3	1.74	0.52
1:J:76:ASP:HB3	1:J:80:THR:HB	1.92	0.52
1:J:131:THR:HA	1:J:203:ARG:NH1	2.25	0.52
1:J:183:GLU:OE1	1:J:183:GLU:HA	2.10	0.52
1:M:174:VAL:HG22	1:M:213:ALA:HB1	1.92	0.52
1:P:211:LEU:HD12	1:P:211:LEU:O	2.10	0.52
1:A:136:SER:O	1:A:139:VAL:HG12	2.10	0.51
1:C:136:SER:O	1:C:139:VAL:HG12	2.10	0.51
1:H:211:LEU:HD12	1:H:211:LEU:O	2.10	0.51
1:J:124:LEU:HG	1:J:163:LEU:CD1	2.39	0.51
1:J:211:LEU:HD12	1:J:211:LEU:O	2.11	0.51
1:K:183:GLU:OE1	1:K:183:GLU:HA	2.10	0.51
1:L:131:THR:HA	1:L:203:ARG:NH1	2.25	0.51
1:L:136:SER:O	1:L:139:VAL:HG12	2.10	0.51
1:O:147:PRO:HB3	1:O:203:ARG:NE	2.17	0.51
1:O:174:VAL:HG22	1:O:213:ALA:HB1	1.92	0.51
1:P:136:SER:O	1:P:139:VAL:HG12	2.10	0.51
1:C:174:VAL:HG22	1:C:213:ALA:HB1	1.92	0.51
1:E:131:THR:HA	1:E:203:ARG:NH1	2.25	0.51
1:E:183:GLU:OE1	1:E:183:GLU:HA	2.10	0.51
1:G:73:LYS:H	1:G:97:ASN:HB3	1.74	0.51
1:G:174:VAL:HG22	1:G:213:ALA:HB1	1.92	0.51
1:H:131:THR:HA	1:H:203:ARG:NH1	2.25	0.51
1:H:207:PRO:CA	1:H:218:MSE:HE1	2.38	0.51
1:I:131:THR:HA	1:I:203:ARG:NH1	2.25	0.51
1:A:82:ALA:HB1	1:A:113:ALA:HB2	1.91	0.51
1:A:131:THR:HA	1:A:203:ARG:NH1	2.25	0.51
1:E:211:LEU:HD12	1:E:211:LEU:O	2.11	0.51
1:F:207:PRO:CA	1:F:218:MSE:HE1	2.38	0.51
1:F:211:LEU:HD12	1:F:211:LEU:O	2.10	0.51
1:H:174:VAL:HG22	1:H:213:ALA:HB1	1.92	0.51
1:I:25:ASN:HD22	1:I:28:ASP:CB	2.16	0.51
1:J:234:LEU:HD13	1:J:238:ASN:ND2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:174:VAL:HG22	1:K:213:ALA:HB1	1.92	0.51
1:L:183:GLU:OE1	1:L:183:GLU:HA	2.10	0.51
1:L:211:LEU:O	1:L:211:LEU:HD12	2.10	0.51
1:L:224:VAL:O	1:L:230:PRO:HB3	2.09	0.51
1:L:234:LEU:HD13	1:L:238:ASN:ND2	2.24	0.51
1:N:131:THR:HA	1:N:203:ARG:NH1	2.25	0.51
1:O:131:THR:HA	1:O:203:ARG:NH1	2.25	0.51
1:B:174:VAL:HG22	1:B:213:ALA:HB1	1.92	0.51
1:B:228:VAL:HG22	1:C:233:THR:HG23	1.92	0.51
1:H:183:GLU:OE1	1:H:183:GLU:HA	2.10	0.51
1:N:211:LEU:HD12	1:N:211:LEU:O	2.10	0.51
1:O:136:SER:O	1:O:139:VAL:HG12	2.10	0.51
1:O:183:GLU:HA	1:O:183:GLU:OE1	2.10	0.51
1:O:207:PRO:CA	1:O:218:MSE:HE1	2.38	0.51
1:P:73:LYS:H	1:P:97:ASN:HB3	1.74	0.51
1:A:211:LEU:HD12	1:A:211:LEU:O	2.10	0.51
1:B:187:VAL:HG22	1:B:217:TYR:HB2	1.93	0.51
1:N:207:PRO:CA	1:N:218:MSE:HE1	2.38	0.51
1:O:76:ASP:HB3	1:O:80:THR:HB	1.92	0.51
1:A:76:ASP:HB3	1:A:80:THR:HB	1.92	0.51
1:B:128:THR:OG1	1:B:129:VAL:N	2.43	0.51
1:C:82:ALA:HB1	1:C:113:ALA:HB2	1.91	0.51
1:C:131:THR:HA	1:C:203:ARG:NH1	2.25	0.51
1:F:183:GLU:OE1	1:F:183:GLU:HA	2.10	0.51
1:G:131:THR:HA	1:G:203:ARG:NH1	2.25	0.51
1:J:128:THR:OG1	1:J:129:VAL:N	2.43	0.51
1:K:131:THR:HA	1:K:203:ARG:NH1	2.25	0.51
1:O:128:THR:OG1	1:O:129:VAL:N	2.43	0.51
1:D:128:THR:OG1	1:D:129:VAL:N	2.43	0.51
1:D:187:VAL:HG22	1:D:217:TYR:HB2	1.93	0.51
1:F:131:THR:HA	1:F:203:ARG:NH1	2.25	0.51
1:I:73:LYS:H	1:I:97:ASN:HB3	1.74	0.51
1:I:187:VAL:HG22	1:I:217:TYR:HB2	1.93	0.51
1:K:136:SER:O	1:K:139:VAL:HG12	2.10	0.51
1:M:187:VAL:HG22	1:M:217:TYR:HB2	1.93	0.51
1:M:211:LEU:HD12	1:M:211:LEU:O	2.11	0.51
1:P:128:THR:OG1	1:P:129:VAL:N	2.43	0.51
1:B:76:ASP:HB3	1:B:80:THR:HB	1.92	0.51
1:E:136:SER:O	1:E:139:VAL:HG12	2.10	0.51
1:E:174:VAL:HG22	1:E:213:ALA:HB1	1.92	0.51
1:G:136:SER:O	1:G:139:VAL:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:LEU:O	1:G:211:LEU:HD12	2.10	0.51
1:I:174:VAL:HG22	1:I:213:ALA:HB1	1.92	0.51
1:L:76:ASP:HB3	1:L:80:THR:HB	1.92	0.51
1:M:82:ALA:HB1	1:M:113:ALA:HB2	1.91	0.51
1:N:187:VAL:HG22	1:N:217:TYR:HB2	1.93	0.51
1:A:124:LEU:HG	1:A:163:LEU:CD1	2.39	0.51
1:C:137:ASP:OD2	1:D:105:ARG:HD3	2.11	0.51
1:C:211:LEU:HD12	1:C:211:LEU:O	2.10	0.51
1:H:25:ASN:HD22	1:H:28:ASP:CB	2.16	0.51
1:I:76:ASP:HB3	1:I:80:THR:HB	1.92	0.51
1:I:211:LEU:HD12	1:I:211:LEU:O	2.10	0.51
1:K:124:LEU:HG	1:K:163:LEU:CD1	2.39	0.51
1:L:128:THR:OG1	1:L:129:VAL:N	2.43	0.51
1:L:187:VAL:HG22	1:L:217:TYR:HB2	1.93	0.51
1:M:131:THR:HA	1:M:203:ARG:NH1	2.25	0.51
1:N:25:ASN:ND2	1:N:28:ASP:HB2	2.17	0.51
1:P:183:GLU:OE1	1:P:183:GLU:HA	2.10	0.51
1:A:128:THR:OG1	1:A:129:VAL:N	2.43	0.51
1:A:174:VAL:HG22	1:A:213:ALA:HB1	1.92	0.51
1:B:124:LEU:HG	1:B:163:LEU:CD1	2.39	0.51
1:B:211:LEU:HD12	1:B:211:LEU:O	2.11	0.51
1:B:220:ILE:HG21	1:B:224:VAL:HG23	1.93	0.51
1:C:187:VAL:HG22	1:C:217:TYR:HB2	1.93	0.51
1:F:76:ASP:HB3	1:F:80:THR:HB	1.92	0.51
1:F:174:VAL:HG22	1:F:213:ALA:HB1	1.92	0.51
1:F:227:SER:CA	1:G:232:GLN:HE21	2.21	0.51
1:H:136:SER:O	1:H:139:VAL:HG12	2.10	0.51
1:K:187:VAL:HG22	1:K:217:TYR:HB2	1.93	0.51
1:O:211:LEU:O	1:O:211:LEU:HD12	2.10	0.51
1:P:220:ILE:HG21	1:P:224:VAL:HG23	1.93	0.51
1:A:178:GLN:HG3	1:A:179:VAL:N	2.27	0.50
1:B:228:VAL:CB	1:C:236:ALA:CB	2.89	0.50
1:C:124:LEU:HG	1:C:163:LEU:CD1	2.39	0.50
1:C:128:THR:OG1	1:C:129:VAL:N	2.43	0.50
1:D:125:ILE:N	1:D:125:ILE:HD12	2.27	0.50
1:D:220:ILE:HG21	1:D:224:VAL:HG23	1.93	0.50
1:G:105:ARG:HD3	1:H:137:ASP:OD2	2.10	0.50
1:H:76:ASP:HB3	1:H:80:THR:HB	1.92	0.50
1:P:131:THR:HA	1:P:203:ARG:NH1	2.25	0.50
1:A:187:VAL:HG22	1:A:217:TYR:HB2	1.93	0.50
1:D:76:ASP:HB3	1:D:80:THR:HB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:LEU:O	1:D:211:LEU:HD12	2.11	0.50
1:F:136:SER:O	1:F:139:VAL:HG12	2.10	0.50
1:H:178:GLN:HG3	1:H:179:VAL:N	2.27	0.50
1:O:125:ILE:N	1:O:125:ILE:HD12	2.27	0.50
1:B:125:ILE:HD12	1:B:125:ILE:N	2.27	0.50
1:G:76:ASP:HB3	1:G:80:THR:HB	1.92	0.50
1:J:174:VAL:HG22	1:J:213:ALA:HB1	1.92	0.50
1:J:187:VAL:HG22	1:J:217:TYR:HB2	1.93	0.50
1:J:220:ILE:HG21	1:J:224:VAL:HG23	1.93	0.50
1:K:125:ILE:HD12	1:K:125:ILE:N	2.27	0.50
1:L:174:VAL:HG22	1:L:213:ALA:HB1	1.92	0.50
1:C:131:THR:HA	1:C:203:ARG:HH12	1.77	0.50
1:K:178:GLN:HG3	1:K:179:VAL:N	2.27	0.50
1:K:220:ILE:HG21	1:K:224:VAL:HG23	1.93	0.50
1:M:25:ASN:HD22	1:M:28:ASP:CB	2.16	0.50
1:P:174:VAL:HG22	1:P:213:ALA:HB1	1.92	0.50
1:C:76:ASP:HB3	1:C:80:THR:HB	1.92	0.50
1:C:178:GLN:HG3	1:C:179:VAL:N	2.27	0.50
1:E:220:ILE:HG21	1:E:224:VAL:HG23	1.93	0.50
1:F:178:GLN:HG3	1:F:179:VAL:N	2.27	0.50
1:I:220:ILE:HG21	1:I:224:VAL:HG23	1.93	0.50
1:L:125:ILE:N	1:L:125:ILE:HD12	2.27	0.50
1:N:125:ILE:HD12	1:N:125:ILE:N	2.27	0.50
1:O:178:GLN:HG3	1:O:179:VAL:N	2.27	0.50
1:P:187:VAL:HG22	1:P:217:TYR:HB2	1.93	0.50
1:E:76:ASP:HB3	1:E:80:THR:HB	1.92	0.50
1:H:187:VAL:HG22	1:H:217:TYR:HB2	1.93	0.50
1:I:125:ILE:N	1:I:125:ILE:HD12	2.27	0.50
1:K:76:ASP:HB3	1:K:80:THR:HB	1.92	0.50
1:K:128:THR:OG1	1:K:129:VAL:N	2.43	0.50
1:M:220:ILE:HG21	1:M:224:VAL:HG23	1.93	0.50
1:N:174:VAL:HG22	1:N:213:ALA:HB1	1.92	0.50
1:N:178:GLN:HG3	1:N:179:VAL:N	2.27	0.50
1:P:76:ASP:HB3	1:P:80:THR:HB	1.92	0.50
1:P:178:GLN:HG3	1:P:179:VAL:N	2.27	0.50
1:A:131:THR:HA	1:A:203:ARG:HH12	1.77	0.50
1:D:124:LEU:HG	1:D:163:LEU:CD1	2.39	0.50
1:F:25:ASN:HD22	1:F:28:ASP:CB	2.16	0.50
1:G:125:ILE:N	1:G:125:ILE:HD12	2.27	0.50
1:G:220:ILE:HG21	1:G:224:VAL:HG23	1.93	0.50
1:L:178:GLN:HG3	1:L:179:VAL:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:125:ILE:HD12	1:M:125:ILE:N	2.27	0.50
1:N:128:THR:OG1	1:N:129:VAL:N	2.43	0.50
1:J:178:GLN:HG3	1:J:179:VAL:N	2.27	0.50
1:K:105:ARG:HD3	1:L:137:ASP:OD2	2.11	0.50
1:O:131:THR:HA	1:O:203:ARG:HH12	1.77	0.50
1:P:192:ARG:O	1:P:206:THR:HG22	2.12	0.50
1:A:125:ILE:N	1:A:125:ILE:HD12	2.27	0.50
1:C:125:ILE:HD12	1:C:125:ILE:N	2.27	0.50
1:G:187:VAL:HG22	1:G:217:TYR:HB2	1.93	0.50
1:I:128:THR:OG1	1:I:129:VAL:N	2.43	0.50
1:L:124:LEU:HG	1:L:163:LEU:CD1	2.39	0.50
1:L:131:THR:HA	1:L:203:ARG:HH12	1.77	0.50
1:P:25:ASN:HD22	1:P:28:ASP:CB	2.16	0.50
1:A:220:ILE:HG21	1:A:224:VAL:HG23	1.93	0.49
1:B:131:THR:HA	1:B:203:ARG:HH12	1.77	0.49
1:E:125:ILE:HD12	1:E:125:ILE:N	2.27	0.49
1:E:187:VAL:HG22	1:E:217:TYR:HB2	1.93	0.49
1:K:211:LEU:HD12	1:K:211:LEU:O	2.10	0.49
1:L:25:ASN:ND2	1:L:28:ASP:HB2	2.17	0.49
1:L:220:ILE:HG21	1:L:224:VAL:HG23	1.93	0.49
1:M:192:ARG:O	1:M:206:THR:HG22	2.12	0.49
1:N:220:ILE:HG21	1:N:224:VAL:HG23	1.93	0.49
1:O:220:ILE:HG21	1:O:224:VAL:HG23	1.93	0.49
1:A:192:ARG:O	1:A:206:THR:HG22	2.12	0.49
1:C:192:ARG:O	1:C:206:THR:HG22	2.12	0.49
1:G:128:THR:OG1	1:G:129:VAL:N	2.43	0.49
1:H:124:LEU:HG	1:H:163:LEU:CD1	2.39	0.49
1:J:192:ARG:O	1:J:206:THR:HG22	2.12	0.49
1:L:192:ARG:O	1:L:206:THR:HG22	2.12	0.49
1:O:192:ARG:O	1:O:206:THR:HG22	2.12	0.49
1:B:192:ARG:O	1:B:206:THR:HG22	2.12	0.49
1:F:187:VAL:HG22	1:F:217:TYR:HB2	1.93	0.49
1:C:25:ASN:ND2	1:C:28:ASP:HB2	2.17	0.49
1:E:128:THR:OG1	1:E:129:VAL:N	2.43	0.49
1:F:124:LEU:HG	1:F:163:LEU:CD1	2.39	0.49
1:M:178:GLN:HG3	1:M:179:VAL:N	2.27	0.49
1:M:202:ARG:O	1:M:204:ILE:N	2.46	0.49
1:P:202:ARG:O	1:P:204:ILE:N	2.46	0.49
1:D:131:THR:HA	1:D:203:ARG:HH12	1.77	0.49
1:G:192:ARG:O	1:G:206:THR:HG22	2.12	0.49
1:I:178:GLN:HG3	1:I:179:VAL:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:125:ILE:HD12	1:J:125:ILE:N	2.27	0.49
1:O:187:VAL:HG22	1:O:217:TYR:HB2	1.93	0.49
1:O:202:ARG:O	1:O:204:ILE:N	2.46	0.49
1:P:125:ILE:HD12	1:P:125:ILE:N	2.27	0.49
1:D:178:GLN:HG3	1:D:179:VAL:N	2.27	0.49
1:F:125:ILE:HD12	1:F:125:ILE:N	2.27	0.49
1:F:192:ARG:O	1:F:206:THR:HG22	2.12	0.49
1:K:131:THR:HA	1:K:203:ARG:HH12	1.77	0.49
1:N:131:THR:HA	1:N:203:ARG:HH12	1.77	0.49
1:N:192:ARG:O	1:N:206:THR:HG22	2.12	0.49
1:B:178:GLN:HG3	1:B:179:VAL:N	2.27	0.49
1:C:220:ILE:HG21	1:C:224:VAL:HG23	1.93	0.49
1:E:192:ARG:O	1:E:206:THR:HG22	2.12	0.49
1:F:220:ILE:HG21	1:F:224:VAL:HG23	1.93	0.49
1:H:220:ILE:HG21	1:H:224:VAL:HG23	1.93	0.49
1:K:202:ARG:O	1:K:204:ILE:N	2.46	0.49
1:L:202:ARG:O	1:L:204:ILE:N	2.46	0.49
1:J:32:PHE:CE2	1:J:36:ILE:HD13	2.48	0.49
1:J:202:ARG:O	1:J:204:ILE:N	2.46	0.49
1:O:32:PHE:CE2	1:O:36:ILE:HD13	2.48	0.49
1:D:192:ARG:O	1:D:206:THR:HG22	2.12	0.49
1:G:202:ARG:O	1:G:204:ILE:N	2.46	0.49
1:H:125:ILE:HD12	1:H:125:ILE:N	2.27	0.49
1:I:25:ASN:ND2	1:I:28:ASP:HB2	2.17	0.49
1:I:131:THR:HA	1:I:203:ARG:HH12	1.77	0.49
1:K:32:PHE:CE2	1:K:36:ILE:HD13	2.48	0.49
1:L:32:PHE:CE2	1:L:36:ILE:HD13	2.48	0.49
1:M:131:THR:HA	1:M:203:ARG:HH12	1.77	0.49
1:O:25:ASN:ND2	1:O:28:ASP:HB2	2.17	0.49
1:P:131:THR:HA	1:P:203:ARG:HH12	1.77	0.49
1:A:32:PHE:CE2	1:A:36:ILE:HD13	2.48	0.49
1:C:32:PHE:CE2	1:C:36:ILE:HD13	2.48	0.49
1:C:206:THR:H	1:C:209:GLN:HG3	1.78	0.49
1:H:32:PHE:CE2	1:H:36:ILE:HD13	2.48	0.49
1:I:147:PRO:HB3	1:I:203:ARG:NE	2.17	0.49
1:L:193:PRO:O	1:L:194:GLN:O	2.31	0.49
1:N:202:ARG:O	1:N:204:ILE:N	2.46	0.49
1:B:32:PHE:CE2	1:B:36:ILE:HD13	2.48	0.48
1:E:32:PHE:CE2	1:E:36:ILE:HD13	2.48	0.48
1:G:178:GLN:HG3	1:G:179:VAL:N	2.27	0.48
1:H:193:PRO:O	1:H:194:GLN:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:PHE:CE2	1:I:36:ILE:HD13	2.48	0.48
1:A:206:THR:H	1:A:209:GLN:HG3	1.79	0.48
1:D:32:PHE:CE2	1:D:36:ILE:HD13	2.48	0.48
1:F:32:PHE:CE2	1:F:36:ILE:HD13	2.48	0.48
1:G:32:PHE:CE2	1:G:36:ILE:HD13	2.48	0.48
1:I:192:ARG:O	1:I:206:THR:HG22	2.12	0.48
1:J:193:PRO:O	1:J:194:GLN:O	2.31	0.48
1:G:124:LEU:HG	1:G:163:LEU:CD1	2.39	0.48
1:H:128:THR:OG1	1:H:129:VAL:N	2.43	0.48
1:H:192:ARG:O	1:H:206:THR:HG22	2.12	0.48
1:H:202:ARG:O	1:H:204:ILE:N	2.46	0.48
1:J:131:THR:HA	1:J:203:ARG:HH12	1.77	0.48
1:K:25:ASN:ND2	1:K:28:ASP:HB2	2.17	0.48
1:K:192:ARG:O	1:K:206:THR:HG22	2.12	0.48
1:N:193:PRO:O	1:N:194:GLN:O	2.31	0.48
1:F:131:THR:HA	1:F:203:ARG:HH12	1.77	0.48
1:F:193:PRO:O	1:F:194:GLN:O	2.31	0.48
1:I:124:LEU:HG	1:I:163:LEU:CD1	2.39	0.48
1:L:206:THR:H	1:L:209:GLN:HG3	1.78	0.48
1:M:206:THR:H	1:M:209:GLN:HG3	1.79	0.48
1:O:200:ASP:HA	1:P:105:ARG:HH22	1.79	0.48
1:F:202:ARG:O	1:F:204:ILE:N	2.46	0.48
1:F:227:SER:HB2	1:G:232:GLN:HE21	1.76	0.48
1:G:115:VAL:N	1:G:116:PRO:CD	2.77	0.48
1:G:206:THR:H	1:G:209:GLN:HG3	1.78	0.48
1:I:202:ARG:O	1:I:204:ILE:N	2.46	0.48
1:L:115:VAL:N	1:L:116:PRO:CD	2.77	0.48
1:M:32:PHE:CE2	1:M:36:ILE:HD13	2.48	0.48
1:M:193:PRO:O	1:M:194:GLN:O	2.31	0.48
2:M:313:BMP:O2	1:N:77:ILE:HD13	2.14	0.48
1:N:115:VAL:N	1:N:116:PRO:CD	2.77	0.48
1:B:115:VAL:N	1:B:116:PRO:CD	2.77	0.48
1:E:115:VAL:N	1:E:116:PRO:CD	2.77	0.48
1:M:115:VAL:N	1:M:116:PRO:CD	2.77	0.48
1:P:193:PRO:O	1:P:194:GLN:O	2.31	0.48
1:P:206:THR:H	1:P:209:GLN:HG3	1.78	0.48
1:E:178:GLN:HG3	1:E:179:VAL:N	2.27	0.48
1:F:202:ARG:O	1:F:204:ILE:HG13	2.14	0.48
1:A:202:ARG:O	1:A:204:ILE:N	2.46	0.48
1:C:200:ASP:HA	1:D:105:ARG:HH22	1.78	0.48
1:E:131:THR:HA	1:E:203:ARG:HH12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:THR:H	1:E:209:GLN:HG3	1.78	0.48
1:G:193:PRO:O	1:G:194:GLN:O	2.31	0.48
1:H:202:ARG:O	1:H:204:ILE:HG13	2.14	0.48
1:K:115:VAL:N	1:K:116:PRO:CD	2.77	0.48
1:M:13:THR:CG2	1:M:38:PRO:O	2.62	0.48
1:N:32:PHE:CE2	1:N:36:ILE:HD13	2.48	0.48
1:A:13:THR:CG2	1:A:38:PRO:O	2.62	0.48
1:A:193:PRO:O	1:A:194:GLN:O	2.31	0.48
1:C:115:VAL:N	1:C:116:PRO:CD	2.77	0.48
1:C:202:ARG:O	1:C:204:ILE:N	2.46	0.48
1:D:115:VAL:N	1:D:116:PRO:CD	2.77	0.48
1:I:13:THR:CG2	1:I:38:PRO:O	2.62	0.48
1:I:115:VAL:N	1:I:116:PRO:CD	2.77	0.48
1:I:206:THR:H	1:I:209:GLN:HG3	1.79	0.48
1:K:193:PRO:O	1:K:194:GLN:O	2.31	0.48
1:O:193:PRO:O	1:O:194:GLN:O	2.31	0.48
1:O:207:PRO:CB	1:O:218:MSE:HE1	2.44	0.48
1:P:32:PHE:CE2	1:P:36:ILE:HD13	2.48	0.48
1:D:207:PRO:CB	1:D:218:MSE:HE1	2.44	0.48
1:E:124:LEU:HG	1:E:163:LEU:CD1	2.39	0.48
1:E:202:ARG:O	1:E:204:ILE:HG13	2.14	0.48
1:F:207:PRO:CB	1:F:218:MSE:HE1	2.44	0.48
1:J:206:THR:H	1:J:209:GLN:HG3	1.78	0.48
1:M:202:ARG:O	1:M:204:ILE:HG13	2.14	0.48
1:N:206:THR:H	1:N:209:GLN:HG3	1.78	0.48
1:B:207:PRO:CB	1:B:218:MSE:HE1	2.44	0.47
1:H:115:VAL:N	1:H:116:PRO:CD	2.77	0.47
1:H:131:THR:HA	1:H:203:ARG:HH12	1.77	0.47
1:I:202:ARG:O	1:I:204:ILE:HG13	2.14	0.47
1:J:115:VAL:N	1:J:116:PRO:CD	2.77	0.47
1:K:13:THR:CG2	1:K:38:PRO:O	2.62	0.47
1:K:202:ARG:O	1:K:204:ILE:HG13	2.14	0.47
1:L:125:ILE:HG23	1:L:166:VAL:N	2.29	0.47
1:M:75:HIS:N	1:N:47:LYS:NZ	2.52	0.47
1:M:125:ILE:HG23	1:M:166:VAL:N	2.29	0.47
1:N:125:ILE:HG23	1:N:166:VAL:N	2.29	0.47
1:P:13:THR:CG2	1:P:38:PRO:O	2.62	0.47
1:P:125:ILE:HG23	1:P:166:VAL:N	2.29	0.47
1:P:202:ARG:O	1:P:204:ILE:HG13	2.14	0.47
1:B:193:PRO:O	1:B:194:GLN:O	2.31	0.47
1:B:202:ARG:O	1:B:204:ILE:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ARG:O	1:E:204:ILE:N	2.46	0.47
1:I:193:PRO:O	1:I:194:GLN:O	2.31	0.47
1:L:30:LEU:HA	1:L:30:LEU:HD23	1.73	0.47
1:M:207:PRO:CB	1:M:218:MSE:HE1	2.44	0.47
1:N:202:ARG:O	1:N:204:ILE:HG13	2.14	0.47
1:O:25:ASN:HB3	1:O:28:ASP:HB2	1.97	0.47
1:O:202:ARG:O	1:O:204:ILE:HG13	2.14	0.47
1:P:115:VAL:N	1:P:116:PRO:CD	2.77	0.47
1:D:202:ARG:O	1:D:204:ILE:N	2.46	0.47
1:E:13:THR:CG2	1:E:38:PRO:O	2.62	0.47
1:E:193:PRO:O	1:E:194:GLN:O	2.31	0.47
1:G:131:THR:HA	1:G:203:ARG:HH12	1.77	0.47
1:G:202:ARG:O	1:G:204:ILE:HG13	2.14	0.47
1:H:207:PRO:CB	1:H:218:MSE:HE1	2.44	0.47
1:I:207:PRO:CB	1:I:218:MSE:HE1	2.44	0.47
1:J:13:THR:CG2	1:J:38:PRO:O	2.62	0.47
1:K:206:THR:H	1:K:209:GLN:HG3	1.78	0.47
1:N:13:THR:CG2	1:N:38:PRO:O	2.62	0.47
1:N:207:PRO:CB	1:N:218:MSE:HE1	2.44	0.47
1:A:25:ASN:ND2	1:A:28:ASP:HB2	2.17	0.47
1:A:115:VAL:N	1:A:116:PRO:CD	2.77	0.47
1:B:27:ASP:CG	1:N:119:LYS:HB2	2.35	0.47
1:C:13:THR:CG2	1:C:38:PRO:O	2.62	0.47
1:H:125:ILE:HG23	1:H:166:VAL:N	2.29	0.47
1:J:125:ILE:HG23	1:J:166:VAL:N	2.29	0.47
1:J:147:PRO:HB3	1:J:203:ARG:NE	2.17	0.47
1:K:207:PRO:CB	1:K:218:MSE:HE1	2.44	0.47
1:L:115:VAL:HB	1:L:116:PRO:HD3	1.97	0.47
1:L:207:PRO:CB	1:L:218:MSE:HE1	2.44	0.47
1:O:125:ILE:HG23	1:O:166:VAL:N	2.29	0.47
1:A:125:ILE:HG23	1:A:166:VAL:N	2.29	0.47
1:A:207:PRO:CB	1:A:218:MSE:HE1	2.44	0.47
1:F:115:VAL:N	1:F:116:PRO:CD	2.77	0.47
1:F:125:ILE:HG23	1:F:166:VAL:N	2.29	0.47
1:M:147:PRO:HB3	1:M:203:ARG:NE	2.17	0.47
1:B:13:THR:CG2	1:B:38:PRO:O	2.62	0.47
1:D:13:THR:CG2	1:D:38:PRO:O	2.62	0.47
1:G:13:THR:CG2	1:G:38:PRO:O	2.62	0.47
1:K:125:ILE:HG23	1:K:166:VAL:N	2.29	0.47
1:L:13:THR:CG2	1:L:38:PRO:O	2.62	0.47
1:M:141:LEU:O	1:M:143:MSE:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:25:ASN:HB3	1:N:28:ASP:HB2	1.96	0.47
1:O:115:VAL:N	1:O:116:PRO:CD	2.77	0.47
1:B:85:VAL:HG21	1:B:110:ALA:HB1	1.97	0.47
1:B:206:THR:H	1:B:209:GLN:HG3	1.78	0.47
1:C:25:ASN:HB3	1:C:28:ASP:HB2	1.97	0.47
1:C:147:PRO:HB3	1:C:203:ARG:NE	2.17	0.47
1:C:193:PRO:O	1:C:194:GLN:O	2.31	0.47
1:C:207:PRO:CB	1:C:218:MSE:HE1	2.44	0.47
1:D:206:THR:H	1:D:209:GLN:HG3	1.78	0.47
1:E:125:ILE:HG23	1:E:166:VAL:N	2.29	0.47
1:E:188:THR:HA	1:E:189:PRO:HD3	1.75	0.47
1:G:188:THR:HA	1:G:189:PRO:HD3	1.75	0.47
1:H:141:LEU:O	1:H:143:MSE:N	2.45	0.47
1:J:115:VAL:HB	1:J:116:PRO:HD3	1.97	0.47
1:L:202:ARG:O	1:L:204:ILE:HG13	2.14	0.47
1:M:124:LEU:HG	1:M:163:LEU:CD1	2.39	0.47
1:O:206:THR:H	1:O:209:GLN:HG3	1.78	0.47
1:P:207:PRO:CB	1:P:218:MSE:HE1	2.44	0.47
1:B:27:ASP:OD2	1:N:119:LYS:HB2	2.14	0.47
1:D:85:VAL:HG21	1:D:110:ALA:HB1	1.97	0.47
1:F:13:THR:CG2	1:F:38:PRO:O	2.62	0.47
1:G:125:ILE:HG23	1:G:166:VAL:N	2.29	0.47
1:H:115:VAL:HB	1:H:116:PRO:HD3	1.97	0.47
1:J:207:PRO:CB	1:J:218:MSE:HE1	2.44	0.47
1:K:85:VAL:HG21	1:K:110:ALA:HB1	1.97	0.47
1:L:141:LEU:O	1:L:143:MSE:N	2.45	0.47
1:M:25:ASN:HB3	1:M:28:ASP:HB2	1.96	0.47
1:M:85:VAL:HG21	1:M:110:ALA:HB1	1.97	0.47
1:A:15:SER:C	1:A:17:VAL:H	2.18	0.47
1:D:115:VAL:HB	1:D:116:PRO:HD3	1.97	0.47
1:D:193:PRO:O	1:D:194:GLN:O	2.31	0.47
1:F:206:THR:H	1:F:209:GLN:HG3	1.79	0.47
1:G:15:SER:C	1:G:17:VAL:H	2.18	0.47
1:H:13:THR:CG2	1:H:38:PRO:O	2.62	0.47
1:I:125:ILE:HG23	1:I:166:VAL:N	2.29	0.47
1:I:204:ILE:CG2	1:I:205:MSE:N	2.60	0.47
1:O:13:THR:CG2	1:O:38:PRO:O	2.62	0.47
1:A:25:ASN:HB3	1:A:28:ASP:HB2	1.97	0.47
1:B:125:ILE:HG23	1:B:166:VAL:N	2.29	0.47
1:C:15:SER:C	1:C:17:VAL:H	2.18	0.47
1:C:125:ILE:HG23	1:C:166:VAL:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:SER:C	1:D:17:VAL:H	2.18	0.47
1:O:76:ASP:C	1:P:130:LEU:HD13	2.36	0.47
1:B:15:SER:C	1:B:17:VAL:H	2.18	0.46
1:B:115:VAL:HB	1:B:116:PRO:HD3	1.97	0.46
1:B:202:ARG:O	1:B:204:ILE:HG13	2.14	0.46
1:C:115:VAL:HB	1:C:116:PRO:HD3	1.97	0.46
1:C:188:THR:HA	1:C:189:PRO:HD3	1.75	0.46
1:D:202:ARG:O	1:D:204:ILE:HG13	2.14	0.46
1:F:85:VAL:HG21	1:F:110:ALA:HB1	1.97	0.46
1:F:115:VAL:HB	1:F:116:PRO:HD3	1.97	0.46
1:I:25:ASN:HB3	1:I:28:ASP:HB2	1.97	0.46
1:I:85:VAL:HG21	1:I:110:ALA:HB1	1.97	0.46
1:J:25:ASN:HB3	1:J:28:ASP:HB2	1.97	0.46
1:M:105:ARG:HD3	1:N:137:ASP:OD2	2.14	0.46
1:M:115:VAL:HB	1:M:116:PRO:HD3	1.97	0.46
1:P:85:VAL:HG21	1:P:110:ALA:HB1	1.97	0.46
1:B:25:ASN:HB3	1:B:28:ASP:HB2	1.97	0.46
1:C:202:ARG:O	1:C:204:ILE:HG13	2.14	0.46
1:E:25:ASN:HB3	1:E:28:ASP:HB2	1.97	0.46
1:E:207:PRO:CB	1:E:218:MSE:HE1	2.44	0.46
1:F:179:VAL:O	1:F:179:VAL:HG12	2.15	0.46
1:I:73:LYS:HB3	1:I:99:HIS:CD2	2.51	0.46
1:O:15:SER:C	1:O:17:VAL:H	2.18	0.46
1:O:73:LYS:HB3	1:O:99:HIS:CD2	2.51	0.46
1:P:179:VAL:HG12	1:P:179:VAL:O	2.15	0.46
1:C:73:LYS:HB3	1:C:99:HIS:CD2	2.51	0.46
1:D:25:ASN:HB3	1:D:28:ASP:HB2	1.97	0.46
1:G:207:PRO:CB	1:G:218:MSE:HE1	2.44	0.46
1:H:85:VAL:HG21	1:H:110:ALA:HB1	1.97	0.46
1:H:179:VAL:HG12	1:H:179:VAL:O	2.16	0.46
1:I:15:SER:C	1:I:17:VAL:H	2.18	0.46
1:K:25:ASN:HB3	1:K:28:ASP:HB2	1.97	0.46
1:K:73:LYS:HB3	1:K:99:HIS:CD2	2.51	0.46
1:O:85:VAL:HG21	1:O:110:ALA:HB1	1.97	0.46
1:P:25:ASN:HB3	1:P:28:ASP:HB2	1.97	0.46
1:A:147:PRO:HB3	1:A:203:ARG:NE	2.17	0.46
1:C:141:LEU:O	1:C:143:MSE:N	2.45	0.46
1:D:125:ILE:HG23	1:D:166:VAL:N	2.29	0.46
1:E:15:SER:C	1:E:17:VAL:H	2.18	0.46
1:H:206:THR:H	1:H:209:GLN:HG3	1.78	0.46
1:I:75:HIS:H	1:J:47:LYS:HZ3	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:85:VAL:HG21	1:J:110:ALA:HB1	1.97	0.46
1:J:179:VAL:O	1:J:179:VAL:HG12	2.16	0.46
1:P:15:SER:C	1:P:17:VAL:H	2.18	0.46
1:B:73:LYS:HB3	1:B:99:HIS:CD2	2.51	0.46
1:E:30:LEU:HD23	1:E:30:LEU:HA	1.73	0.46
1:K:115:VAL:HB	1:K:116:PRO:HD3	1.97	0.46
1:N:115:VAL:HB	1:N:116:PRO:HD3	1.97	0.46
1:A:73:LYS:HB3	1:A:99:HIS:CD2	2.51	0.46
1:A:85:VAL:HG21	1:A:110:ALA:HB1	1.97	0.46
1:A:115:VAL:HB	1:A:116:PRO:HD3	1.97	0.46
1:C:179:VAL:O	1:C:179:VAL:HG12	2.16	0.46
1:D:73:LYS:HB3	1:D:99:HIS:CD2	2.51	0.46
1:F:25:ASN:HB3	1:F:28:ASP:HB2	1.96	0.46
1:I:115:VAL:HB	1:I:116:PRO:HD3	1.97	0.46
1:J:73:LYS:HB3	1:J:99:HIS:CD2	2.51	0.46
1:J:202:ARG:O	1:J:204:ILE:HG13	2.14	0.46
1:L:85:VAL:HG21	1:L:110:ALA:HB1	1.97	0.46
1:A:179:VAL:O	1:A:179:VAL:HG12	2.16	0.46
1:A:202:ARG:O	1:A:204:ILE:HG13	2.14	0.46
1:B:150:TYR:CZ	1:B:154:LEU:HD11	2.51	0.46
1:D:150:TYR:CZ	1:D:154:LEU:HD11	2.51	0.46
1:E:150:TYR:CZ	1:E:154:LEU:HD11	2.51	0.46
1:G:85:VAL:HG21	1:G:110:ALA:HB1	1.97	0.46
1:G:150:TYR:CZ	1:G:154:LEU:HD11	2.51	0.46
1:J:150:TYR:CZ	1:J:154:LEU:HD11	2.51	0.46
1:L:25:ASN:HB3	1:L:28:ASP:HB2	1.97	0.46
1:N:73:LYS:HB3	1:N:99:HIS:CD2	2.51	0.46
1:O:115:VAL:HB	1:O:116:PRO:HD3	1.97	0.46
1:H:25:ASN:HB3	1:H:28:ASP:HB2	1.97	0.46
1:L:150:TYR:CZ	1:L:154:LEU:HD11	2.51	0.46
1:M:25:ASN:ND2	1:M:28:ASP:HB2	2.17	0.46
1:O:176:PHE:C	1:O:178:GLN:N	2.69	0.46
1:P:115:VAL:HB	1:P:116:PRO:HD3	1.97	0.46
1:H:15:SER:C	1:H:17:VAL:H	2.18	0.46
1:M:78:PRO:HD2	1:N:200:ASP:OD2	2.16	0.46
1:O:179:VAL:O	1:O:179:VAL:HG12	2.16	0.46
1:A:141:LEU:O	1:A:143:MSE:N	2.45	0.46
1:E:179:VAL:O	1:E:179:VAL:HG12	2.16	0.46
1:G:25:ASN:HB3	1:G:28:ASP:HB2	1.97	0.46
1:K:150:TYR:CZ	1:K:154:LEU:HD11	2.51	0.46
1:L:93:VAL:O	1:L:122:PRO:HB3	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:93:VAL:O	1:M:122:PRO:HB3	2.16	0.46
1:P:73:LYS:HB3	1:P:99:HIS:CD2	2.51	0.46
1:P:163:LEU:N	1:P:163:LEU:HD23	2.31	0.46
1:A:150:TYR:CZ	1:A:154:LEU:HD11	2.51	0.45
1:E:73:LYS:HB3	1:E:99:HIS:CD2	2.51	0.45
1:E:85:VAL:HG21	1:E:110:ALA:HB1	1.97	0.45
1:E:115:VAL:HB	1:E:116:PRO:HD3	1.97	0.45
1:I:166:VAL:HG13	1:I:167:VAL:N	2.32	0.45
1:I:179:VAL:O	1:I:179:VAL:HG12	2.16	0.45
1:M:150:TYR:CZ	1:M:154:LEU:HD11	2.51	0.45
1:B:163:LEU:N	1:B:163:LEU:HD23	2.31	0.45
1:C:192:ARG:HD2	1:C:197:GLU:O	2.17	0.45
1:D:26:ARG:NH1	1:D:60:GLU:OE2	2.49	0.45
1:L:15:SER:C	1:L:17:VAL:H	2.18	0.45
1:O:141:LEU:O	1:O:143:MSE:N	2.45	0.45
1:P:25:ASN:ND2	1:P:28:ASP:HB2	2.17	0.45
1:P:166:VAL:HG13	1:P:167:VAL:N	2.32	0.45
1:B:93:VAL:O	1:B:122:PRO:HB3	2.16	0.45
1:C:163:LEU:HD23	1:C:163:LEU:N	2.31	0.45
1:F:192:ARG:HD2	1:F:197:GLU:O	2.17	0.45
1:G:115:VAL:HB	1:G:116:PRO:HD3	1.97	0.45
1:H:150:TYR:CZ	1:H:154:LEU:HD11	2.51	0.45
1:K:179:VAL:O	1:K:179:VAL:HG12	2.16	0.45
1:L:179:VAL:O	1:L:179:VAL:HG12	2.16	0.45
1:N:150:TYR:CZ	1:N:154:LEU:HD11	2.51	0.45
1:N:163:LEU:N	1:N:163:LEU:HD23	2.32	0.45
1:O:166:VAL:HG13	1:O:167:VAL:N	2.32	0.45
1:A:166:VAL:HG13	1:A:167:VAL:N	2.32	0.45
1:D:93:VAL:O	1:D:122:PRO:HB3	2.16	0.45
1:D:163:LEU:N	1:D:163:LEU:HD23	2.31	0.45
1:E:163:LEU:N	1:E:163:LEU:HD23	2.31	0.45
1:F:93:VAL:O	1:F:122:PRO:HB3	2.16	0.45
1:F:150:TYR:CZ	1:F:154:LEU:HD11	2.51	0.45
1:G:30:LEU:HA	1:G:30:LEU:HD23	1.73	0.45
1:G:144:THR:O	1:G:145:LEU:O	2.35	0.45
1:G:179:VAL:O	1:G:179:VAL:HG12	2.16	0.45
1:J:93:VAL:O	1:J:122:PRO:HB3	2.16	0.45
1:K:130:LEU:H	1:K:133:MSE:CE	2.30	0.45
1:L:73:LYS:HB3	1:L:99:HIS:CD2	2.51	0.45
1:L:192:ARG:HD2	1:L:197:GLU:O	2.17	0.45
1:M:15:SER:C	1:M:17:VAL:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:188:THR:HA	1:M:189:PRO:HD3	1.75	0.45
1:N:85:VAL:HG21	1:N:110:ALA:HB1	1.97	0.45
1:N:93:VAL:O	1:N:122:PRO:HB3	2.16	0.45
1:O:163:LEU:N	1:O:163:LEU:HD23	2.31	0.45
1:P:141:LEU:O	1:P:143:MSE:N	2.45	0.45
1:P:150:TYR:CZ	1:P:154:LEU:HD11	2.51	0.45
1:P:192:ARG:HD2	1:P:197:GLU:O	2.17	0.45
1:A:163:LEU:N	1:A:163:LEU:HD23	2.31	0.45
1:A:192:ARG:HD2	1:A:197:GLU:O	2.17	0.45
1:B:26:ARG:NH1	1:B:60:GLU:OE2	2.49	0.45
1:B:144:THR:O	1:B:145:LEU:O	2.35	0.45
1:C:85:VAL:HG21	1:C:110:ALA:HB1	1.97	0.45
1:E:26:ARG:NH1	1:E:60:GLU:OE2	2.49	0.45
1:E:141:LEU:O	1:E:143:MSE:N	2.45	0.45
1:E:144:THR:O	1:E:145:LEU:O	2.35	0.45
1:F:15:SER:C	1:F:17:VAL:H	2.18	0.45
1:H:192:ARG:HD2	1:H:197:GLU:O	2.17	0.45
1:I:150:TYR:CZ	1:I:154:LEU:HD11	2.51	0.45
1:I:192:ARG:HD2	1:I:197:GLU:O	2.17	0.45
1:J:166:VAL:HG13	1:J:167:VAL:N	2.31	0.45
1:M:163:LEU:N	1:M:163:LEU:HD23	2.31	0.45
1:M:176:PHE:C	1:M:178:GLN:N	2.69	0.45
1:M:179:VAL:O	1:M:179:VAL:HG12	2.16	0.45
1:N:166:VAL:HG13	1:N:167:VAL:N	2.31	0.45
1:A:144:THR:O	1:A:145:LEU:O	2.35	0.45
1:B:166:VAL:HG13	1:B:167:VAL:N	2.32	0.45
1:C:77:ILE:HG22	1:D:132:SER:HB3	1.98	0.45
1:C:150:TYR:CZ	1:C:154:LEU:HD11	2.51	0.45
1:E:93:VAL:O	1:E:122:PRO:HB3	2.16	0.45
1:G:26:ARG:NH1	1:G:60:GLU:OE2	2.49	0.45
1:G:163:LEU:N	1:G:163:LEU:HD23	2.31	0.45
1:I:130:LEU:HD13	1:J:76:ASP:C	2.36	0.45
1:I:163:LEU:N	1:I:163:LEU:HD23	2.31	0.45
1:J:111:ARG:HG2	1:J:111:ARG:HH11	1.82	0.45
1:J:176:PHE:C	1:J:178:GLN:N	2.69	0.45
1:J:192:ARG:HD2	1:J:197:GLU:O	2.17	0.45
1:K:93:VAL:O	1:K:122:PRO:HB3	2.16	0.45
1:K:144:THR:O	1:K:145:LEU:O	2.35	0.45
1:M:192:ARG:HD2	1:M:197:GLU:O	2.17	0.45
1:O:192:ARG:HD2	1:O:197:GLU:O	2.17	0.45
1:C:130:LEU:H	1:C:133:MSE:CE	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:LEU:O	1:D:143:MSE:N	2.45	0.45
1:E:224:VAL:O	1:E:230:PRO:CB	2.65	0.45
1:F:73:LYS:HB3	1:F:99:HIS:CD2	2.51	0.45
1:F:111:ARG:HG2	1:F:111:ARG:HH11	1.82	0.45
1:G:93:VAL:O	1:G:122:PRO:HB3	2.16	0.45
1:G:224:VAL:O	1:G:230:PRO:CB	2.65	0.45
1:H:93:VAL:O	1:H:122:PRO:HB3	2.16	0.45
1:I:111:ARG:HH11	1:I:111:ARG:HG2	1.82	0.45
1:I:144:THR:O	1:I:145:LEU:O	2.35	0.45
1:I:206:THR:HG23	1:I:209:GLN:OE1	2.17	0.45
1:K:163:LEU:HD23	1:K:163:LEU:N	2.32	0.45
1:L:111:ARG:HG2	1:L:111:ARG:HH11	1.82	0.45
1:L:224:VAL:O	1:L:230:PRO:CB	2.65	0.45
1:M:137:ASP:OD2	1:N:105:ARG:CD	2.61	0.45
1:O:224:VAL:O	1:O:230:PRO:CB	2.65	0.45
1:P:26:ARG:NH1	1:P:60:GLU:OE2	2.49	0.45
1:A:111:ARG:HG2	1:A:111:ARG:HH11	1.82	0.45
1:B:147:PRO:HB3	1:B:203:ARG:NE	2.17	0.45
1:C:206:THR:HG23	1:C:209:GLN:OE1	2.17	0.45
1:C:224:VAL:O	1:C:230:PRO:CB	2.65	0.45
1:D:144:THR:O	1:D:145:LEU:O	2.35	0.45
1:D:179:VAL:O	1:D:179:VAL:HG12	2.15	0.45
1:G:73:LYS:HB3	1:G:99:HIS:CD2	2.51	0.45
1:I:130:LEU:H	1:I:133:MSE:CE	2.30	0.45
1:I:224:VAL:O	1:I:230:PRO:CB	2.65	0.45
1:J:15:SER:C	1:J:17:VAL:H	2.18	0.45
1:J:163:LEU:N	1:J:163:LEU:HD23	2.31	0.45
1:K:15:SER:C	1:K:17:VAL:H	2.18	0.45
1:K:141:LEU:O	1:K:143:MSE:N	2.45	0.45
1:L:26:ARG:NH1	1:L:60:GLU:OE2	2.49	0.45
1:L:163:LEU:N	1:L:163:LEU:HD23	2.31	0.45
1:M:73:LYS:HB3	1:M:99:HIS:CD2	2.51	0.45
1:N:192:ARG:HD2	1:N:197:GLU:O	2.17	0.45
1:N:224:VAL:O	1:N:230:PRO:CB	2.65	0.45
1:O:150:TYR:CZ	1:O:154:LEU:HD11	2.51	0.45
1:P:147:PRO:HB3	1:P:203:ARG:NE	2.17	0.45
1:A:93:VAL:O	1:A:122:PRO:HB3	2.16	0.45
1:A:130:LEU:H	1:A:133:MSE:CE	2.30	0.45
1:F:166:VAL:HG13	1:F:167:VAL:N	2.32	0.45
1:H:73:LYS:HB3	1:H:99:HIS:CD2	2.51	0.45
1:N:15:SER:C	1:N:17:VAL:H	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:111:ARG:HG2	1:O:111:ARG:HH11	1.82	0.45
1:P:130:LEU:H	1:P:133:MSE:CE	2.30	0.45
1:P:176:PHE:C	1:P:178:GLN:N	2.69	0.45
1:P:224:VAL:O	1:P:230:PRO:CB	2.65	0.45
1:A:206:THR:HG23	1:A:209:GLN:OE1	2.17	0.45
1:B:224:VAL:O	1:B:230:PRO:CB	2.65	0.45
1:C:76:ASP:C	1:D:130:LEU:HD13	2.37	0.45
1:C:111:ARG:HG2	1:C:111:ARG:HH11	1.82	0.45
1:C:144:THR:O	1:C:145:LEU:O	2.35	0.45
1:D:224:VAL:O	1:D:230:PRO:CB	2.65	0.45
1:H:25:ASN:ND2	1:H:28:ASP:HB2	2.17	0.45
1:J:26:ARG:NH1	1:J:60:GLU:OE2	2.49	0.45
1:J:188:THR:HA	1:J:189:PRO:HD3	1.75	0.45
1:K:111:ARG:HG2	1:K:111:ARG:HH11	1.82	0.45
1:L:176:PHE:C	1:L:178:GLN:N	2.69	0.45
1:M:77:ILE:CD1	2:N:314:BMP:H2'	2.47	0.45
1:M:206:THR:HG23	1:M:209:GLN:OE1	2.17	0.45
1:N:130:LEU:H	1:N:133:MSE:CE	2.30	0.45
1:O:93:VAL:O	1:O:122:PRO:HB3	2.16	0.45
1:P:144:THR:O	1:P:145:LEU:O	2.35	0.45
1:B:141:LEU:O	1:B:143:MSE:N	2.45	0.44
1:B:179:VAL:O	1:B:179:VAL:HG12	2.15	0.44
1:B:206:THR:HG23	1:B:209:GLN:OE1	2.17	0.44
1:C:166:VAL:HG13	1:C:167:VAL:N	2.32	0.44
1:D:147:PRO:HB3	1:D:203:ARG:NE	2.17	0.44
1:H:176:PHE:C	1:H:178:GLN:N	2.69	0.44
1:C:12:VAL:CG1	1:J:182:GLN:HG3	2.45	0.44
1:C:93:VAL:O	1:C:122:PRO:HB3	2.16	0.44
1:D:192:ARG:HD2	1:D:197:GLU:O	2.17	0.44
1:F:130:LEU:H	1:F:133:MSE:CE	2.30	0.44
1:H:163:LEU:HD23	1:H:163:LEU:N	2.31	0.44
1:I:132:SER:OG	1:J:78:PRO:HD3	2.17	0.44
1:J:130:LEU:H	1:J:133:MSE:CE	2.30	0.44
1:K:166:VAL:HG13	1:K:167:VAL:N	2.32	0.44
1:M:55:PRO:CB	1:M:91:LEU:HD11	2.48	0.44
1:M:166:VAL:HG13	1:M:167:VAL:N	2.32	0.44
1:P:93:VAL:O	1:P:122:PRO:HB3	2.16	0.44
1:B:176:PHE:C	1:B:178:GLN:N	2.69	0.44
1:D:111:ARG:HG2	1:D:111:ARG:HH11	1.82	0.44
1:D:130:LEU:H	1:D:133:MSE:CE	2.30	0.44
1:F:163:LEU:N	1:F:163:LEU:HD23	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:PRO:CB	1:H:91:LEU:HD11	2.48	0.44
1:I:30:LEU:HD23	1:I:30:LEU:HA	1.73	0.44
1:K:192:ARG:HD2	1:K:197:GLU:O	2.17	0.44
1:K:206:THR:HG23	1:K:209:GLN:OE1	2.17	0.44
1:L:130:LEU:H	1:L:133:MSE:CE	2.30	0.44
1:A:224:VAL:O	1:A:230:PRO:CB	2.65	0.44
1:D:55:PRO:CB	1:D:91:LEU:HD11	2.48	0.44
1:D:176:PHE:C	1:D:178:GLN:N	2.69	0.44
1:D:206:THR:HG23	1:D:209:GLN:OE1	2.17	0.44
1:F:145:LEU:H	1:F:145:LEU:CD2	2.31	0.44
1:F:206:THR:HG23	1:F:209:GLN:OE1	2.17	0.44
1:G:141:LEU:O	1:G:143:MSE:N	2.45	0.44
1:H:130:LEU:H	1:H:133:MSE:CE	2.30	0.44
1:H:144:THR:O	1:H:145:LEU:O	2.35	0.44
1:H:145:LEU:H	1:H:145:LEU:CD2	2.31	0.44
1:H:166:VAL:HG13	1:H:167:VAL:N	2.32	0.44
1:I:145:LEU:H	1:I:145:LEU:CD2	2.31	0.44
1:K:176:PHE:C	1:K:178:GLN:N	2.69	0.44
1:K:224:VAL:O	1:K:230:PRO:CB	2.65	0.44
1:L:166:VAL:HG13	1:L:167:VAL:N	2.32	0.44
1:M:30:LEU:HD23	1:M:30:LEU:HA	1.73	0.44
1:M:224:VAL:O	1:M:230:PRO:CB	2.65	0.44
1:N:144:THR:O	1:N:145:LEU:O	2.35	0.44
1:N:179:VAL:O	1:N:179:VAL:HG12	2.16	0.44
1:O:47:LYS:HZ3	1:P:75:HIS:H	1.61	0.44
1:B:55:PRO:CB	1:B:91:LEU:HD11	2.48	0.44
1:B:111:ARG:HG2	1:B:111:ARG:HH11	1.82	0.44
1:D:166:VAL:HG13	1:D:167:VAL:N	2.32	0.44
1:F:144:THR:O	1:F:145:LEU:O	2.35	0.44
1:G:176:PHE:C	1:G:178:GLN:N	2.69	0.44
1:I:55:PRO:CB	1:I:91:LEU:HD11	2.48	0.44
1:I:93:VAL:O	1:I:122:PRO:HB3	2.16	0.44
1:I:176:PHE:C	1:I:178:GLN:N	2.69	0.44
1:J:145:LEU:CD2	1:J:145:LEU:H	2.31	0.44
1:J:224:VAL:O	1:J:230:PRO:CB	2.65	0.44
1:K:26:ARG:NH1	1:K:60:GLU:OE2	2.49	0.44
1:K:55:PRO:CB	1:K:91:LEU:HD11	2.48	0.44
1:N:176:PHE:C	1:N:178:GLN:N	2.69	0.44
1:O:206:THR:HG23	1:O:209:GLN:OE1	2.17	0.44
1:P:206:THR:HG23	1:P:209:GLN:OE1	2.17	0.44
1:A:145:LEU:H	1:A:145:LEU:CD2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLN:HG2	1:A:205:MSE:HE3	2.00	0.44
1:C:145:LEU:H	1:C:145:LEU:CD2	2.31	0.44
1:C:171:GLN:HG2	1:C:205:MSE:HE3	2.00	0.44
1:E:130:LEU:H	1:E:133:MSE:CE	2.30	0.44
1:F:55:PRO:CB	1:F:91:LEU:HD11	2.48	0.44
1:F:176:PHE:C	1:F:178:GLN:N	2.69	0.44
1:H:111:ARG:HG2	1:H:111:ARG:HH11	1.82	0.44
1:J:55:PRO:CB	1:J:91:LEU:HD11	2.47	0.44
1:L:145:LEU:H	1:L:145:LEU:CD2	2.31	0.44
1:L:147:PRO:HB3	1:L:203:ARG:NE	2.17	0.44
1:O:153:ARG:HH11	1:O:153:ARG:CB	2.25	0.44
1:O:171:GLN:HG2	1:O:205:MSE:HE3	2.00	0.44
1:A:26:ARG:NH1	1:A:60:GLU:OE2	2.49	0.44
1:B:130:LEU:H	1:B:133:MSE:CE	2.30	0.44
1:D:146:SER:O	1:D:147:PRO:C	2.56	0.44
1:E:192:ARG:HD2	1:E:197:GLU:O	2.17	0.44
1:F:128:THR:OG1	1:F:129:VAL:N	2.43	0.44
1:F:222:ARG:O	1:F:223:PRO:C	2.56	0.44
1:I:141:LEU:O	1:I:143:MSE:N	2.45	0.44
1:I:222:ARG:O	1:I:223:PRO:C	2.56	0.44
1:J:25:ASN:HD22	1:J:28:ASP:CB	2.16	0.44
1:L:144:THR:O	1:L:145:LEU:O	2.35	0.44
1:M:144:THR:O	1:M:145:LEU:O	2.35	0.44
1:M:146:SER:O	1:M:147:PRO:C	2.56	0.44
1:N:145:LEU:H	1:N:145:LEU:CD2	2.31	0.44
1:N:147:PRO:HB3	1:N:203:ARG:NE	2.17	0.44
1:O:130:LEU:H	1:O:133:MSE:CE	2.30	0.44
1:O:144:THR:O	1:O:145:LEU:O	2.35	0.44
1:E:176:PHE:C	1:E:178:GLN:N	2.69	0.44
1:G:130:LEU:H	1:G:133:MSE:CE	2.30	0.44
1:G:192:ARG:HD2	1:G:197:GLU:O	2.17	0.44
1:G:200:ASP:HA	1:H:105:ARG:HH22	1.83	0.44
1:M:130:LEU:H	1:M:133:MSE:CE	2.30	0.44
1:N:171:GLN:HG2	1:N:205:MSE:HE3	2.00	0.44
1:A:222:ARG:O	1:A:223:PRO:C	2.56	0.44
1:B:25:ASN:HD22	1:B:28:ASP:CB	2.16	0.44
1:B:55:PRO:HB3	1:B:91:LEU:HD11	2.00	0.44
1:C:55:PRO:CB	1:C:91:LEU:HD11	2.48	0.44
1:C:176:PHE:C	1:C:178:GLN:N	2.69	0.44
1:D:55:PRO:HB3	1:D:91:LEU:HD11	2.00	0.44
1:G:145:LEU:CD2	1:G:145:LEU:H	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:THR:O	1:J:145:LEU:O	2.35	0.44
1:K:222:ARG:O	1:K:223:PRO:C	2.56	0.44
1:L:55:PRO:CB	1:L:91:LEU:HD11	2.48	0.44
1:N:55:PRO:HB3	1:N:91:LEU:HD11	2.00	0.44
1:N:111:ARG:HG2	1:N:111:ARG:HH11	1.82	0.44
1:O:55:PRO:CB	1:O:91:LEU:HD11	2.48	0.44
1:A:55:PRO:HB3	1:A:91:LEU:HD11	2.00	0.43
1:A:169:SER:HB2	1:A:203:ARG:NH1	2.33	0.43
1:B:192:ARG:HD2	1:B:197:GLU:O	2.17	0.43
1:C:222:ARG:O	1:C:223:PRO:C	2.56	0.43
1:E:111:ARG:HG2	1:E:111:ARG:HH11	1.82	0.43
1:E:145:LEU:H	1:E:145:LEU:CD2	2.31	0.43
1:E:200:ASP:HA	1:F:105:ARG:HH22	1.83	0.43
1:F:171:GLN:HG2	1:F:205:MSE:HE3	2.00	0.43
1:H:206:THR:HG23	1:H:209:GLN:OE1	2.17	0.43
1:L:206:THR:HG23	1:L:209:GLN:OE1	2.17	0.43
1:M:76:ASP:OD1	1:N:73:LYS:NZ	2.51	0.43
1:N:55:PRO:CB	1:N:91:LEU:HD11	2.48	0.43
1:O:55:PRO:HB3	1:O:91:LEU:HD11	2.00	0.43
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.73	0.43
1:C:169:SER:HB2	1:C:203:ARG:NH1	2.33	0.43
1:E:76:ASP:C	1:F:130:LEU:HD13	2.39	0.43
1:G:171:GLN:HG2	1:G:205:MSE:HE3	2.00	0.43
1:H:222:ARG:O	1:H:223:PRO:C	2.56	0.43
1:M:111:ARG:HG2	1:M:111:ARG:HH11	1.82	0.43
1:M:145:LEU:H	1:M:145:LEU:CD2	2.31	0.43
1:P:222:ARG:O	1:P:223:PRO:C	2.56	0.43
1:C:55:PRO:HB3	1:C:91:LEU:HD11	2.00	0.43
1:E:55:PRO:HB3	1:E:91:LEU:HD11	2.00	0.43
1:E:206:THR:HG23	1:E:209:GLN:OE1	2.17	0.43
1:F:224:VAL:O	1:F:230:PRO:CB	2.65	0.43
1:G:55:PRO:HB3	1:G:91:LEU:HD11	2.00	0.43
1:G:111:ARG:HG2	1:G:111:ARG:HH11	1.82	0.43
1:G:206:THR:HG23	1:G:209:GLN:OE1	2.17	0.43
1:H:224:VAL:O	1:H:230:PRO:CB	2.65	0.43
1:I:171:GLN:HG2	1:I:205:MSE:HE3	2.00	0.43
1:J:146:SER:O	1:J:147:PRO:C	2.56	0.43
1:M:222:ARG:O	1:M:223:PRO:C	2.56	0.43
1:N:206:THR:HG23	1:N:209:GLN:OE1	2.17	0.43
1:P:55:PRO:CB	1:P:91:LEU:HD11	2.48	0.43
1:P:171:GLN:HG2	1:P:205:MSE:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PRO:CB	1:A:91:LEU:HD11	2.48	0.43
1:E:169:SER:HB2	1:E:203:ARG:NH1	2.33	0.43
1:H:171:GLN:HG2	1:H:205:MSE:HE3	2.00	0.43
1:J:56:GLN:HA	1:J:56:GLN:HE21	1.84	0.43
1:J:206:THR:HG23	1:J:209:GLN:OE1	2.17	0.43
1:M:55:PRO:HB3	1:M:91:LEU:HD11	2.00	0.43
1:O:222:ARG:O	1:O:223:PRO:C	2.56	0.43
1:P:55:PRO:HB3	1:P:91:LEU:HD11	2.00	0.43
1:P:111:ARG:HG2	1:P:111:ARG:HH11	1.82	0.43
1:A:176:PHE:C	1:A:178:GLN:N	2.69	0.43
1:C:26:ARG:NH1	1:C:60:GLU:OE2	2.49	0.43
1:E:55:PRO:CB	1:E:91:LEU:HD11	2.48	0.43
1:F:26:ARG:NH1	1:F:60:GLU:OE2	2.49	0.43
1:G:55:PRO:CB	1:G:91:LEU:HD11	2.48	0.43
1:H:26:ARG:NH1	1:H:60:GLU:OE2	2.49	0.43
1:I:26:ARG:NH1	1:I:60:GLU:OE2	2.49	0.43
1:K:55:PRO:HB3	1:K:91:LEU:HD11	2.00	0.43
1:K:145:LEU:H	1:K:145:LEU:CD2	2.31	0.43
1:M:171:GLN:HG2	1:M:205:MSE:HE3	2.00	0.43
1:B:171:GLN:HG2	1:B:205:MSE:HE3	2.00	0.43
1:G:166:VAL:HG13	1:G:167:VAL:N	2.32	0.43
1:L:188:THR:HA	1:L:189:PRO:HD3	1.75	0.43
1:M:169:SER:HB2	1:M:203:ARG:NH1	2.33	0.43
1:N:141:LEU:O	1:N:143:MSE:N	2.45	0.43
1:N:146:SER:O	1:N:147:PRO:C	2.56	0.43
1:O:26:ARG:NH1	1:O:60:GLU:OE2	2.49	0.43
1:O:145:LEU:CD2	1:O:145:LEU:H	2.31	0.43
1:P:169:SER:HB2	1:P:203:ARG:NH1	2.33	0.43
1:B:145:LEU:H	1:B:145:LEU:CD2	2.31	0.43
1:D:169:SER:HB2	1:D:203:ARG:NH1	2.33	0.43
1:E:166:VAL:HG13	1:E:167:VAL:N	2.32	0.43
1:F:147:PRO:HB3	1:F:203:ARG:NE	2.17	0.43
1:J:171:GLN:HG2	1:J:205:MSE:HE3	2.00	0.43
1:L:25:ASN:HD22	1:L:28:ASP:CB	2.16	0.43
1:M:26:ARG:NH1	1:M:60:GLU:OE2	2.49	0.43
1:O:169:SER:HB2	1:O:203:ARG:NH1	2.33	0.43
1:O:200:ASP:OD2	1:P:78:PRO:HD2	2.18	0.43
1:A:156:ALA:O	1:A:160:LYS:HG3	2.19	0.43
1:L:153:ARG:HH11	1:L:153:ARG:CB	2.25	0.43
1:N:26:ARG:NH1	1:N:60:GLU:OE2	2.49	0.43
1:P:145:LEU:H	1:P:145:LEU:CD2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ALA:O	1:B:160:LYS:HG3	2.19	0.43
1:B:169:SER:HB2	1:B:203:ARG:NH1	2.33	0.43
1:F:55:PRO:HB3	1:F:91:LEU:HD11	2.01	0.43
1:F:202:ARG:HA	1:F:202:ARG:HD3	1.89	0.43
1:G:146:SER:O	1:G:147:PRO:C	2.56	0.43
1:G:156:ALA:O	1:G:160:LYS:HG3	2.19	0.43
1:N:222:ARG:O	1:N:223:PRO:C	2.56	0.43
1:O:75:HIS:H	1:P:47:LYS:HZ2	1.66	0.43
1:C:146:SER:O	1:C:147:PRO:C	2.56	0.43
1:C:156:ALA:O	1:C:160:LYS:HG3	2.19	0.43
1:E:156:ALA:O	1:E:160:LYS:HG3	2.19	0.43
1:E:171:GLN:HG2	1:E:205:MSE:HE3	2.00	0.43
1:H:56:GLN:HA	1:H:56:GLN:HE21	1.84	0.43
1:N:30:LEU:HA	1:N:30:LEU:HD23	1.73	0.43
1:F:25:ASN:ND2	1:F:28:ASP:HB2	2.17	0.42
1:G:25:ASN:HD22	1:G:28:ASP:N	2.13	0.42
1:H:55:PRO:HB3	1:H:91:LEU:HD11	2.00	0.42
1:K:29:ALA:O	1:K:33:VAL:HG23	2.19	0.42
1:L:56:GLN:HA	1:L:56:GLN:HE21	1.84	0.42
1:N:156:ALA:O	1:N:160:LYS:HG3	2.19	0.42
1:D:155:ALA:HA	1:D:166:VAL:HG21	2.02	0.42
1:E:146:SER:O	1:E:147:PRO:C	2.56	0.42
1:F:29:ALA:O	1:F:33:VAL:HG23	2.20	0.42
1:G:206:THR:H	1:G:209:GLN:CG	2.33	0.42
1:I:55:PRO:HB3	1:I:91:LEU:HD11	2.00	0.42
1:J:55:PRO:HB3	1:J:91:LEU:HD11	2.00	0.42
1:L:156:ALA:O	1:L:160:LYS:HG3	2.19	0.42
1:M:100:ALA:C	1:M:102:GLY:H	2.23	0.42
1:N:56:GLN:HA	1:N:56:GLN:HE21	1.84	0.42
1:A:29:ALA:O	1:A:33:VAL:HG23	2.19	0.42
1:B:29:ALA:O	1:B:33:VAL:HG23	2.20	0.42
1:B:155:ALA:HA	1:B:166:VAL:HG21	2.02	0.42
1:D:30:LEU:HD23	1:D:30:LEU:HA	1.73	0.42
1:D:145:LEU:H	1:D:145:LEU:CD2	2.31	0.42
1:E:147:PRO:HB3	1:E:203:ARG:NE	2.17	0.42
1:E:155:ALA:HA	1:E:166:VAL:HG21	2.02	0.42
1:E:206:THR:H	1:E:209:GLN:CG	2.33	0.42
1:F:100:ALA:C	1:F:102:GLY:H	2.23	0.42
1:G:112:GLU:CD	1:K:160:LYS:NZ	2.73	0.42
1:H:29:ALA:O	1:H:33:VAL:HG23	2.19	0.42
1:H:100:ALA:C	1:H:102:GLY:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:THR:H	1:H:209:GLN:CG	2.33	0.42
1:J:156:ALA:O	1:J:160:LYS:HG3	2.19	0.42
1:K:146:SER:O	1:K:147:PRO:C	2.56	0.42
1:K:155:ALA:HA	1:K:166:VAL:HG21	2.02	0.42
1:K:171:GLN:HG2	1:K:205:MSE:HE3	2.00	0.42
1:K:202:ARG:HA	1:K:202:ARG:HD3	1.89	0.42
1:L:222:ARG:O	1:L:223:PRO:C	2.56	0.42
1:O:56:GLN:HA	1:O:56:GLN:HE21	1.84	0.42
1:O:146:SER:O	1:O:147:PRO:C	2.57	0.42
1:O:174:VAL:O	1:O:178:GLN:HB3	2.20	0.42
1:A:130:LEU:HD13	1:B:76:ASP:C	2.40	0.42
1:B:25:ASN:ND2	1:B:28:ASP:HB2	2.17	0.42
1:B:206:THR:H	1:B:209:GLN:CG	2.33	0.42
1:D:25:ASN:HD22	1:D:28:ASP:CB	2.16	0.42
1:D:156:ALA:O	1:D:160:LYS:HG3	2.19	0.42
1:D:171:GLN:HG2	1:D:205:MSE:HE3	2.00	0.42
1:F:206:THR:H	1:F:209:GLN:CG	2.33	0.42
1:I:188:THR:HA	1:I:189:PRO:HD3	1.75	0.42
1:K:156:ALA:O	1:K:160:LYS:HG3	2.19	0.42
1:L:55:PRO:HB3	1:L:91:LEU:HD11	2.00	0.42
1:L:206:THR:H	1:L:209:GLN:CG	2.33	0.42
1:M:156:ALA:O	1:M:160:LYS:HG3	2.19	0.42
1:N:155:ALA:HA	1:N:166:VAL:HG21	2.01	0.42
1:O:77:ILE:CG2	1:P:132:SER:HB3	2.49	0.42
1:A:68:ILE:O	1:A:94:TRP:HB3	2.20	0.42
1:B:228:VAL:HB	1:C:236:ALA:CB	2.42	0.42
1:C:29:ALA:O	1:C:33:VAL:HG23	2.19	0.42
1:C:68:ILE:O	1:C:94:TRP:HB3	2.20	0.42
1:D:18:VAL:HA	1:D:42:ARG:O	2.20	0.42
1:D:29:ALA:O	1:D:33:VAL:HG23	2.19	0.42
1:D:206:THR:H	1:D:209:GLN:CG	2.33	0.42
1:E:68:ILE:O	1:E:94:TRP:HB3	2.20	0.42
1:G:18:VAL:HA	1:G:42:ARG:O	2.20	0.42
1:G:68:ILE:O	1:G:94:TRP:HB3	2.20	0.42
1:G:155:ALA:HA	1:G:166:VAL:HG21	2.02	0.42
1:H:68:ILE:O	1:H:94:TRP:HB3	2.20	0.42
1:H:202:ARG:HA	1:H:202:ARG:HD3	1.89	0.42
1:I:29:ALA:O	1:I:33:VAL:HG23	2.19	0.42
1:J:29:ALA:O	1:J:33:VAL:HG23	2.19	0.42
1:K:68:ILE:O	1:K:94:TRP:HB3	2.20	0.42
1:L:174:VAL:O	1:L:178:GLN:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:25:ASN:HD22	1:P:28:ASP:N	2.13	0.42
1:P:155:ALA:HA	1:P:166:VAL:HG21	2.02	0.42
1:A:174:VAL:O	1:A:178:GLN:HB3	2.20	0.42
1:B:222:ARG:O	1:B:223:PRO:C	2.56	0.42
1:C:18:VAL:HA	1:C:42:ARG:O	2.20	0.42
1:C:25:ASN:HD21	1:C:27:ASP:HB2	1.85	0.42
1:E:18:VAL:HA	1:E:42:ARG:O	2.20	0.42
1:E:174:VAL:O	1:E:178:GLN:HB3	2.19	0.42
1:F:68:ILE:O	1:F:94:TRP:HB3	2.20	0.42
1:I:169:SER:HB2	1:I:203:ARG:NH1	2.33	0.42
1:K:18:VAL:HA	1:K:42:ARG:O	2.20	0.42
1:L:146:SER:O	1:L:147:PRO:C	2.56	0.42
1:M:25:ASN:HD21	1:M:27:ASP:HB2	1.85	0.42
1:M:29:ALA:O	1:M:33:VAL:HG23	2.20	0.42
1:M:68:ILE:O	1:M:94:TRP:HB3	2.20	0.42
1:O:18:VAL:HA	1:O:42:ARG:O	2.20	0.42
1:O:25:ASN:HD21	1:O:27:ASP:HB2	1.85	0.42
1:O:156:ALA:O	1:O:160:LYS:HG3	2.19	0.42
1:P:100:ALA:C	1:P:102:GLY:H	2.23	0.42
1:D:222:ARG:O	1:D:223:PRO:C	2.56	0.42
1:F:146:SER:O	1:F:147:PRO:C	2.56	0.42
1:F:156:ALA:O	1:F:160:LYS:HG3	2.19	0.42
1:J:174:VAL:O	1:J:178:GLN:HB3	2.20	0.42
1:J:222:ARG:O	1:J:223:PRO:C	2.56	0.42
1:L:18:VAL:HA	1:L:42:ARG:O	2.20	0.42
1:M:155:ALA:HA	1:M:166:VAL:HG21	2.02	0.42
1:M:206:THR:H	1:M:209:GLN:CG	2.33	0.42
1:O:206:THR:H	1:O:209:GLN:CG	2.33	0.42
1:P:29:ALA:O	1:P:33:VAL:HG23	2.19	0.42
1:P:30:LEU:HD23	1:P:30:LEU:HA	1.73	0.42
1:A:25:ASN:HD21	1:A:27:ASP:HB2	1.85	0.42
1:C:174:VAL:O	1:C:178:GLN:HB3	2.19	0.42
1:F:56:GLN:HA	1:F:56:GLN:HE21	1.84	0.42
1:G:25:ASN:HD21	1:G:27:ASP:HB2	1.85	0.42
1:G:77:ILE:HG22	1:H:132:SER:HB3	2.02	0.42
1:G:100:ALA:C	1:G:102:GLY:H	2.23	0.42
1:G:147:PRO:HB3	1:G:203:ARG:NE	2.17	0.42
1:I:100:ALA:C	1:I:102:GLY:H	2.23	0.42
1:L:155:ALA:HA	1:L:166:VAL:HG21	2.02	0.42
1:L:171:GLN:HG2	1:L:205:MSE:HE3	2.00	0.42
1:A:146:SER:O	1:A:147:PRO:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASN:HD21	1:B:27:ASP:HB2	1.85	0.42
1:D:100:ALA:C	1:D:102:GLY:H	2.23	0.42
1:D:174:VAL:O	1:D:178:GLN:HB3	2.20	0.42
1:E:25:ASN:HD22	1:E:28:ASP:N	2.13	0.42
1:E:25:ASN:HD21	1:E:27:ASP:HB2	1.85	0.42
1:H:156:ALA:O	1:H:160:LYS:HG3	2.19	0.42
1:I:18:VAL:HA	1:I:42:ARG:O	2.20	0.42
1:I:25:ASN:HD21	1:I:27:ASP:HB2	1.85	0.42
1:J:18:VAL:HA	1:J:42:ARG:O	2.20	0.42
1:J:141:LEU:O	1:J:143:MSE:N	2.45	0.42
1:J:155:ALA:HA	1:J:166:VAL:HG21	2.01	0.42
1:J:206:THR:H	1:J:209:GLN:CG	2.33	0.42
1:K:25:ASN:HD21	1:K:27:ASP:HB2	1.85	0.42
1:K:188:THR:HA	1:K:189:PRO:HD3	1.75	0.42
1:K:206:THR:H	1:K:209:GLN:CG	2.33	0.42
1:L:169:SER:HB2	1:L:203:ARG:NH1	2.33	0.42
1:O:29:ALA:O	1:O:33:VAL:HG23	2.19	0.42
1:A:18:VAL:HA	1:A:42:ARG:O	2.20	0.42
1:B:18:VAL:HA	1:B:42:ARG:O	2.20	0.42
1:B:174:VAL:O	1:B:178:GLN:HB3	2.20	0.42
1:C:182:GLN:HG2	1:J:12:VAL:HG12	2.00	0.42
1:E:56:GLN:HA	1:E:56:GLN:HE21	1.84	0.42
1:I:37:ASP:CG	1:I:38:PRO:HD2	2.41	0.42
1:I:156:ALA:O	1:I:160:LYS:HG3	2.19	0.42
1:J:169:SER:HB2	1:J:203:ARG:NH1	2.33	0.42
1:J:205:MSE:HG3	1:J:209:GLN:CG	2.50	0.42
1:L:29:ALA:O	1:L:33:VAL:HG23	2.19	0.42
1:L:37:ASP:CG	1:L:38:PRO:HD2	2.41	0.42
1:A:145:LEU:CD2	1:A:145:LEU:N	2.83	0.41
1:A:206:THR:H	1:A:209:GLN:CG	2.33	0.41
1:E:100:ALA:C	1:E:102:GLY:H	2.23	0.41
1:E:153:ARG:HH11	1:E:153:ARG:CB	2.25	0.41
1:F:145:LEU:CD2	1:F:145:LEU:N	2.83	0.41
1:F:174:VAL:O	1:F:178:GLN:HB3	2.20	0.41
1:G:29:ALA:O	1:G:33:VAL:HG23	2.20	0.41
1:G:174:VAL:O	1:G:178:GLN:HB3	2.20	0.41
1:H:37:ASP:CG	1:H:38:PRO:HD2	2.41	0.41
1:H:146:SER:O	1:H:147:PRO:C	2.56	0.41
1:I:146:SER:O	1:I:147:PRO:C	2.56	0.41
1:I:155:ALA:HA	1:I:166:VAL:HG21	2.02	0.41
1:J:25:ASN:HD21	1:J:27:ASP:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:56:GLN:HA	1:K:56:GLN:HE21	1.84	0.41
1:K:105:ARG:HH22	1:L:200:ASP:HA	1.84	0.41
1:L:68:ILE:O	1:L:94:TRP:HB3	2.20	0.41
1:N:18:VAL:HA	1:N:42:ARG:O	2.20	0.41
1:P:18:VAL:HA	1:P:42:ARG:O	2.20	0.41
1:P:25:ASN:HD21	1:P:27:ASP:HB2	1.85	0.41
1:P:156:ALA:O	1:P:160:LYS:HG3	2.19	0.41
1:A:25:ASN:HD22	1:A:28:ASP:N	2.13	0.41
1:B:100:ALA:C	1:B:102:GLY:H	2.23	0.41
1:C:145:LEU:CD2	1:C:145:LEU:N	2.83	0.41
1:F:18:VAL:HA	1:F:42:ARG:O	2.20	0.41
1:F:155:ALA:HA	1:F:166:VAL:HG21	2.01	0.41
1:G:145:LEU:CD2	1:G:145:LEU:N	2.83	0.41
1:I:68:ILE:O	1:I:94:TRP:HB3	2.20	0.41
1:J:37:ASP:CG	1:J:38:PRO:HD2	2.40	0.41
1:L:25:ASN:HD21	1:L:27:ASP:HB2	1.85	0.41
1:N:206:THR:H	1:N:209:GLN:CG	2.33	0.41
1:O:100:ALA:C	1:O:102:GLY:H	2.23	0.41
1:O:145:LEU:CD2	1:O:145:LEU:N	2.84	0.41
1:P:37:ASP:CG	1:P:38:PRO:HD2	2.41	0.41
1:P:68:ILE:O	1:P:94:TRP:HB3	2.20	0.41
1:B:25:ASN:HD22	1:B:28:ASP:N	2.13	0.41
1:B:205:MSE:HG3	1:B:209:GLN:CG	2.50	0.41
1:E:130:LEU:HD13	1:F:76:ASP:C	2.41	0.41
1:E:145:LEU:CD2	1:E:145:LEU:N	2.83	0.41
1:E:222:ARG:O	1:E:223:PRO:C	2.56	0.41
1:F:188:THR:HA	1:F:189:PRO:HD3	1.75	0.41
1:G:105:ARG:HH22	1:H:200:ASP:HA	1.85	0.41
1:I:206:THR:H	1:I:209:GLN:CG	2.33	0.41
1:K:30:LEU:HA	1:K:30:LEU:HD23	1.73	0.41
1:K:37:ASP:CG	1:K:38:PRO:HD2	2.41	0.41
1:K:169:SER:HB2	1:K:203:ARG:NH1	2.34	0.41
1:M:37:ASP:CG	1:M:38:PRO:HD2	2.41	0.41
1:M:205:MSE:HG3	1:M:209:GLN:CG	2.50	0.41
1:N:37:ASP:CG	1:N:38:PRO:HD2	2.41	0.41
1:N:169:SER:HB2	1:N:203:ARG:NH1	2.33	0.41
1:O:37:ASP:CG	1:O:38:PRO:HD2	2.41	0.41
1:O:68:ILE:O	1:O:94:TRP:HB3	2.20	0.41
1:P:174:VAL:O	1:P:178:GLN:HB3	2.20	0.41
1:P:206:THR:H	1:P:209:GLN:CG	2.33	0.41
1:A:105:ARG:HH22	1:B:200:ASP:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:MSE:HG3	1:A:209:GLN:CG	2.50	0.41
1:B:68:ILE:O	1:B:94:TRP:HB3	2.20	0.41
1:C:155:ALA:HA	1:C:166:VAL:HG21	2.02	0.41
1:C:206:THR:H	1:C:209:GLN:CG	2.33	0.41
1:D:25:ASN:HD22	1:D:28:ASP:N	2.13	0.41
1:D:205:MSE:HG3	1:D:209:GLN:CG	2.50	0.41
1:F:37:ASP:CG	1:F:38:PRO:HD2	2.41	0.41
1:F:153:ARG:HH11	1:F:153:ARG:CB	2.25	0.41
1:F:209:GLN:O	1:F:212:SER:HB2	2.21	0.41
1:H:145:LEU:CD2	1:H:145:LEU:N	2.83	0.41
1:H:209:GLN:O	1:H:212:SER:HB2	2.21	0.41
1:I:145:LEU:CD2	1:I:145:LEU:N	2.84	0.41
1:I:200:ASP:HA	1:J:105:ARG:HH22	1.85	0.41
1:J:30:LEU:HD23	1:J:30:LEU:HA	1.73	0.41
1:K:174:VAL:O	1:K:178:GLN:HB3	2.20	0.41
1:K:209:GLN:O	1:K:212:SER:HB2	2.20	0.41
1:L:145:LEU:CD2	1:L:145:LEU:N	2.83	0.41
1:L:205:MSE:HG3	1:L:209:GLN:CG	2.50	0.41
1:M:18:VAL:HA	1:M:42:ARG:O	2.20	0.41
1:N:29:ALA:O	1:N:33:VAL:HG23	2.19	0.41
1:N:205:MSE:HG3	1:N:209:GLN:CG	2.50	0.41
1:A:100:ALA:C	1:A:102:GLY:H	2.23	0.41
1:B:30:LEU:HD23	1:B:30:LEU:HA	1.73	0.41
1:C:25:ASN:HD22	1:C:28:ASP:N	2.13	0.41
1:D:56:GLN:HA	1:D:56:GLN:HE21	1.84	0.41
1:F:25:ASN:HD21	1:F:27:ASP:HB2	1.85	0.41
1:H:25:ASN:HD21	1:H:27:ASP:HB2	1.85	0.41
1:H:174:VAL:O	1:H:178:GLN:HB3	2.20	0.41
1:I:174:VAL:O	1:I:178:GLN:HB3	2.20	0.41
1:I:205:MSE:HG3	1:I:209:GLN:CG	2.50	0.41
1:M:174:VAL:O	1:M:178:GLN:HB3	2.20	0.41
1:N:145:LEU:CD2	1:N:145:LEU:N	2.83	0.41
1:O:69:PHE:CE2	1:O:95:MSE:HE3	2.55	0.41
1:B:145:LEU:CD2	1:B:145:LEU:N	2.84	0.41
1:D:25:ASN:HD21	1:D:27:ASP:HB2	1.85	0.41
1:D:37:ASP:CG	1:D:38:PRO:HD2	2.41	0.41
1:D:68:ILE:O	1:D:94:TRP:HB3	2.20	0.41
1:G:56:GLN:HA	1:G:56:GLN:HE21	1.84	0.41
1:G:130:LEU:HD13	1:H:76:ASP:C	2.41	0.41
1:G:222:ARG:O	1:G:223:PRO:C	2.56	0.41
1:H:155:ALA:HA	1:H:166:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:130:LEU:HD13	1:L:76:ASP:C	2.40	0.41
1:L:209:GLN:O	1:L:212:SER:HB2	2.20	0.41
1:P:123:LEU:HB3	1:P:125:ILE:HD11	2.03	0.41
1:B:56:GLN:HA	1:B:56:GLN:HE21	1.84	0.41
1:C:205:MSE:HG3	1:C:209:GLN:CG	2.50	0.41
1:D:209:GLN:O	1:D:212:SER:HB2	2.21	0.41
1:E:29:ALA:O	1:E:33:VAL:HG23	2.20	0.41
1:E:69:PHE:CE2	1:E:95:MSE:HE3	2.55	0.41
1:G:37:ASP:CG	1:G:38:PRO:HD2	2.41	0.41
1:I:202:ARG:HA	1:I:202:ARG:HD3	1.89	0.41
1:N:25:ASN:HD21	1:N:27:ASP:HB2	1.85	0.41
1:N:209:GLN:O	1:N:212:SER:HB2	2.20	0.41
1:P:145:LEU:CD2	1:P:145:LEU:N	2.84	0.41
1:P:205:MSE:HG3	1:P:209:GLN:CG	2.50	0.41
1:A:132:SER:HB3	1:B:77:ILE:HG22	2.03	0.41
1:A:188:THR:HA	1:A:189:PRO:HD3	1.75	0.41
1:B:37:ASP:CG	1:B:38:PRO:HD2	2.41	0.41
1:B:209:GLN:O	1:B:212:SER:HB2	2.21	0.41
1:E:37:ASP:CG	1:E:38:PRO:HD2	2.41	0.41
1:F:239:ALA:HA	1:F:242:GLN:NE2	2.36	0.41
1:J:69:PHE:CE2	1:J:95:MSE:HE3	2.55	0.41
1:J:209:GLN:O	1:J:212:SER:HB2	2.21	0.41
1:K:100:ALA:C	1:K:102:GLY:H	2.23	0.41
1:K:205:MSE:HG3	1:K:209:GLN:CG	2.50	0.41
1:L:56:GLN:NE2	1:L:59:ARG:HH11	2.19	0.41
1:L:239:ALA:HA	1:L:242:GLN:NE2	2.36	0.41
1:M:132:SER:HB3	1:N:77:ILE:HG22	2.03	0.41
1:M:209:GLN:O	1:M:212:SER:HB2	2.21	0.41
1:N:22:ASP:N	1:N:22:ASP:OD1	2.54	0.41
1:N:100:ALA:C	1:N:102:GLY:H	2.23	0.41
1:O:209:GLN:O	1:O:212:SER:HB2	2.21	0.41
1:A:155:ALA:HA	1:A:166:VAL:HG21	2.02	0.41
1:B:22:ASP:N	1:B:22:ASP:OD1	2.54	0.41
1:B:153:ARG:HH11	1:B:153:ARG:CB	2.25	0.41
1:B:239:ALA:HA	1:B:242:GLN:NE2	2.36	0.41
1:C:123:LEU:HB3	1:C:125:ILE:HD11	2.03	0.41
1:E:123:LEU:HB3	1:E:125:ILE:HD11	2.03	0.41
1:E:239:ALA:HA	1:E:242:GLN:HE21	1.86	0.41
1:G:69:PHE:CE2	1:G:95:MSE:HE3	2.55	0.41
1:H:18:VAL:HA	1:H:42:ARG:O	2.20	0.41
1:H:174:VAL:HG22	1:H:213:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:205:MSE:HG3	1:H:209:GLN:CG	2.50	0.41
1:I:56:GLN:NE2	1:I:59:ARG:HH11	2.19	0.41
1:I:209:GLN:O	1:I:212:SER:HB2	2.21	0.41
1:J:68:ILE:O	1:J:94:TRP:HB3	2.20	0.41
1:J:100:ALA:C	1:J:102:GLY:H	2.23	0.41
1:J:174:VAL:HG22	1:J:213:ALA:CB	2.51	0.41
1:K:145:LEU:CD2	1:K:145:LEU:N	2.84	0.41
1:L:25:ASN:HD22	1:L:28:ASP:N	2.13	0.41
1:L:141:LEU:C	1:L:143:MSE:H	2.24	0.41
1:M:158:THR:HG21	1:M:166:VAL:HG23	2.03	0.41
1:M:174:VAL:HG22	1:M:213:ALA:CB	2.51	0.41
1:M:239:ALA:HA	1:M:242:GLN:NE2	2.36	0.41
1:N:68:ILE:O	1:N:94:TRP:HB3	2.20	0.41
1:N:239:ALA:HA	1:N:242:GLN:NE2	2.36	0.41
1:N:239:ALA:HA	1:N:242:GLN:HE21	1.86	0.41
1:O:205:MSE:HG3	1:O:209:GLN:CG	2.50	0.41
1:O:239:ALA:HA	1:O:242:GLN:NE2	2.36	0.41
1:P:188:THR:HA	1:P:189:PRO:HD3	1.75	0.41
1:P:239:ALA:HA	1:P:242:GLN:NE2	2.36	0.41
1:A:200:ASP:HA	1:B:105:ARG:HH22	1.85	0.41
2:E:305:BMP:H2'	1:F:77:ILE:CD1	2.52	0.41
1:F:174:VAL:HG22	1:F:213:ALA:CB	2.51	0.41
1:F:205:MSE:HG3	1:F:209:GLN:CG	2.50	0.41
1:G:169:SER:HB2	1:G:203:ARG:NH1	2.33	0.41
1:H:188:THR:HA	1:H:189:PRO:HD3	1.75	0.41
1:H:239:ALA:HA	1:H:242:GLN:NE2	2.36	0.41
1:I:123:LEU:HB3	1:I:125:ILE:HD11	2.03	0.41
1:I:239:ALA:HA	1:I:242:GLN:NE2	2.36	0.41
1:J:145:LEU:CD2	1:J:145:LEU:N	2.83	0.41
1:K:158:THR:HG21	1:K:166:VAL:HG23	2.03	0.41
1:L:100:ALA:C	1:L:102:GLY:H	2.23	0.41
1:L:174:VAL:HG22	1:L:213:ALA:CB	2.51	0.41
1:M:77:ILE:HD13	2:N:314:BMP:H2'	2.03	0.41
1:M:145:LEU:CD2	1:M:145:LEU:N	2.84	0.41
1:N:174:VAL:O	1:N:178:GLN:HB3	2.20	0.41
1:N:222:ARG:HA	1:N:225:THR:OG1	2.21	0.41
1:P:146:SER:O	1:P:147:PRO:C	2.56	0.41
1:P:153:ARG:HH11	1:P:153:ARG:CB	2.25	0.41
1:A:56:GLN:NE2	1:A:59:ARG:HH11	2.19	0.40
1:A:174:VAL:HG22	1:A:213:ALA:CB	2.51	0.40
1:B:228:VAL:CG2	1:C:233:THR:HG23	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ALA:C	1:C:102:GLY:H	2.23	0.40
1:D:239:ALA:HA	1:D:242:GLN:NE2	2.36	0.40
1:E:205:MSE:HG3	1:E:209:GLN:CG	2.50	0.40
1:F:22:ASP:N	1:F:22:ASP:OD1	2.54	0.40
1:G:132:SER:HB3	1:H:77:ILE:HG22	2.02	0.40
1:G:239:ALA:HA	1:G:242:GLN:HE21	1.86	0.40
1:I:56:GLN:HA	1:I:56:GLN:HE21	1.84	0.40
1:K:200:ASP:HA	1:L:105:ARG:HH22	1.86	0.40
1:L:192:ARG:HH21	1:L:223:PRO:CD	2.35	0.40
1:M:25:ASN:HD22	1:M:28:ASP:N	2.13	0.40
1:M:69:PHE:CE2	1:M:95:MSE:HE3	2.55	0.40
1:P:158:THR:HG21	1:P:166:VAL:HG23	2.03	0.40
1:A:22:ASP:N	1:A:22:ASP:OD1	2.54	0.40
1:A:192:ARG:HH21	1:A:223:PRO:CD	2.35	0.40
1:C:56:GLN:NE2	1:C:59:ARG:HH11	2.19	0.40
1:D:64:ARG:HH11	1:D:64:ARG:HG2	1.87	0.40
1:E:240:SER:H	1:E:240:SER:HG	1.66	0.40
1:I:64:ARG:HG2	1:I:64:ARG:HH11	1.86	0.40
1:K:173:ALA:CB	1:K:215:VAL:HG12	2.52	0.40
1:N:173:ALA:CB	1:N:215:VAL:HG12	2.52	0.40
1:N:174:VAL:HG22	1:N:213:ALA:CB	2.51	0.40
1:P:22:ASP:OD1	1:P:22:ASP:N	2.54	0.40
1:A:37:ASP:CG	1:A:38:PRO:HD2	2.41	0.40
1:A:173:ALA:CB	1:A:215:VAL:HG12	2.52	0.40
1:B:146:SER:O	1:B:147:PRO:C	2.56	0.40
1:B:158:THR:HG21	1:B:166:VAL:HG23	2.03	0.40
1:B:173:ALA:CB	1:B:215:VAL:HG12	2.52	0.40
1:B:174:VAL:HG22	1:B:213:ALA:CB	2.51	0.40
1:D:123:LEU:HB3	1:D:125:ILE:HD11	2.03	0.40
1:D:145:LEU:CD2	1:D:145:LEU:N	2.84	0.40
1:D:173:ALA:CB	1:D:215:VAL:HG12	2.52	0.40
1:E:158:THR:HG21	1:E:166:VAL:HG23	2.03	0.40
1:E:209:GLN:O	1:E:212:SER:HB2	2.21	0.40
1:F:56:GLN:NE2	1:F:59:ARG:HH11	2.19	0.40
1:G:22:ASP:OD1	1:G:22:ASP:N	2.54	0.40
1:G:123:LEU:HB3	1:G:125:ILE:HD11	2.03	0.40
1:G:209:GLN:O	1:G:212:SER:HB2	2.21	0.40
1:G:239:ALA:HA	1:G:242:GLN:NE2	2.36	0.40
1:I:105:ARG:HH22	1:J:200:ASP:HA	1.86	0.40
1:J:22:ASP:N	1:J:22:ASP:OD1	2.54	0.40
1:J:239:ALA:HA	1:J:242:GLN:HE21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:123:LEU:HB3	1:K:125:ILE:HD11	2.03	0.40
1:K:174:VAL:HG22	1:K:213:ALA:CB	2.51	0.40
1:K:239:ALA:HA	1:K:242:GLN:NE2	2.36	0.40
1:O:56:GLN:NE2	1:O:59:ARG:HH11	2.19	0.40
1:P:209:GLN:O	1:P:212:SER:HB2	2.21	0.40
1:A:47:LYS:HZ3	1:B:75:HIS:H	1.69	0.40
1:A:123:LEU:HB3	1:A:125:ILE:HD11	2.03	0.40
1:B:56:GLN:NE2	1:B:59:ARG:HH11	2.19	0.40
1:B:64:ARG:HH11	1:B:64:ARG:HG2	1.87	0.40
1:C:173:ALA:CB	1:C:215:VAL:HG12	2.52	0.40
1:C:174:VAL:HG22	1:C:213:ALA:CB	2.51	0.40
1:C:192:ARG:HH21	1:C:223:PRO:CD	2.35	0.40
1:C:239:ALA:HA	1:C:242:GLN:NE2	2.36	0.40
1:D:69:PHE:CE2	1:D:95:MSE:HE3	2.55	0.40
1:E:174:VAL:HG22	1:E:213:ALA:CB	2.51	0.40
1:F:173:ALA:CB	1:F:215:VAL:HG12	2.52	0.40
1:G:153:ARG:HH11	1:G:153:ARG:CB	2.25	0.40
1:I:22:ASP:N	1:I:22:ASP:OD1	2.54	0.40
1:J:56:GLN:NE2	1:J:59:ARG:HH11	2.19	0.40
1:J:173:ALA:CB	1:J:215:VAL:HG12	2.52	0.40
1:J:192:ARG:HH21	1:J:223:PRO:CD	2.35	0.40
1:K:132:SER:HB3	1:L:77:ILE:HG22	2.02	0.40
1:K:192:ARG:HH21	1:K:223:PRO:CD	2.34	0.40
1:K:239:ALA:HA	1:K:242:GLN:HE21	1.86	0.40
1:M:64:ARG:HG2	1:M:64:ARG:HH11	1.86	0.40
1:M:173:ALA:CB	1:M:215:VAL:HG12	2.52	0.40
1:M:222:ARG:HA	1:M:225:THR:OG1	2.21	0.40
1:O:155:ALA:HA	1:O:166:VAL:HG21	2.02	0.40
1:O:173:ALA:CB	1:O:215:VAL:HG12	2.52	0.40
1:A:158:THR:HG21	1:A:166:VAL:HG23	2.03	0.40
1:A:209:GLN:O	1:A:212:SER:HB2	2.21	0.40
1:C:200:ASP:OD2	1:D:78:PRO:HD2	2.21	0.40
1:D:22:ASP:OD1	1:D:22:ASP:N	2.54	0.40
1:E:22:ASP:OD1	1:E:22:ASP:N	2.54	0.40
1:F:240:SER:H	1:F:240:SER:HG	1.66	0.40
1:G:64:ARG:HG2	1:G:64:ARG:HH11	1.86	0.40
1:H:222:ARG:HA	1:H:225:THR:OG1	2.22	0.40
1:J:123:LEU:HB3	1:J:125:ILE:HD11	2.03	0.40
1:K:56:GLN:NE2	1:K:59:ARG:HH11	2.19	0.40
1:P:173:ALA:CB	1:P:215:VAL:HG12	2.52	0.40
1:P:174:VAL:HG22	1:P:213:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:192:ARG:HH21	1:P:223:PRO:CD	2.35	0.40
1:P:222:ARG:HA	1:P:225:THR:OG1	2.22	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:OE1	1:O:242:GLN:OE1[2_545]	1.39	0.81
1:E:242:GLN:OE1	1:K:178:GLN:OE1[1_454]	1.53	0.67
1:M:228:VAL:CG2	1:P:236:ALA:CB[1_455]	1.84	0.36
1:J:56:GLN:NE2	1:P:27:ASP:CB[2_646]	2.01	0.19
1:M:236:ALA:CB	1:P:195:GLY:O[1_455]	2.07	0.13
1:I:227:SER:CA	1:L:232:GLN:NE2[1_556]	2.10	0.10
1:E:242:GLN:OE1	1:K:178:GLN:CD[1_454]	2.14	0.06
1:I:236:ALA:CB	1:L:228:VAL:CG2[1_556]	2.16	0.04
1:E:232:GLN:NE2	1:H:226:GLN:O[1_454]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4	23
1	B	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4	23
1	C	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4	23
1	D	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4	23
1	E	229/245 (94%)	185 (81%)	37 (16%)	7 (3%)	4	23
1	F	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4	23
1	G	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4	23
1	H	229/245 (94%)	183 (80%)	39 (17%)	7 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4 23
1	J	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4 23
1	K	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4 23
1	L	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4 23
1	M	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4 23
1	N	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4 23
1	O	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4 23
1	P	229/245 (94%)	184 (80%)	38 (17%)	7 (3%)	4 23
All	All	3664/3920 (94%)	2944 (80%)	608 (17%)	112 (3%)	4 23

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	LEU
1	A	194	GLN
1	B	145	LEU
1	B	194	GLN
1	C	145	LEU
1	C	194	GLN
1	D	145	LEU
1	D	194	GLN
1	E	145	LEU
1	E	194	GLN
1	F	145	LEU
1	F	194	GLN
1	G	145	LEU
1	G	194	GLN
1	H	145	LEU
1	H	194	GLN
1	I	145	LEU
1	I	194	GLN
1	J	145	LEU
1	J	194	GLN
1	K	145	LEU
1	K	194	GLN
1	L	145	LEU
1	L	194	GLN
1	M	145	LEU
1	M	194	GLN

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Mol	Chain	Res	Type
1	N	145	LEU
1	N	194	GLN
1	O	145	LEU
1	O	194	GLN
1	P	145	LEU
1	P	194	GLN
1	A	147	PRO
1	B	147	PRO
1	C	147	PRO
1	D	147	PRO
1	E	147	PRO
1	F	147	PRO
1	G	147	PRO
1	H	147	PRO
1	I	147	PRO
1	J	147	PRO
1	K	147	PRO
1	L	147	PRO
1	M	147	PRO
1	N	147	PRO
1	O	147	PRO
1	P	147	PRO
1	A	208	GLU
1	B	208	GLU
1	C	208	GLU
1	D	208	GLU
1	E	208	GLU
1	F	208	GLU
1	G	208	GLU
1	H	208	GLU
1	I	208	GLU
1	J	208	GLU
1	K	208	GLU
1	L	208	GLU
1	M	208	GLU
1	N	208	GLU
1	O	208	GLU
1	P	208	GLU
1	A	203	ARG
1	B	203	ARG
1	C	203	ARG
1	D	203	ARG

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Mol	Chain	Res	Type
1	E	203	ARG
1	F	203	ARG
1	G	203	ARG
1	H	203	ARG
1	I	203	ARG
1	J	203	ARG
1	K	203	ARG
1	L	203	ARG
1	M	203	ARG
1	N	203	ARG
1	O	203	ARG
1	P	203	ARG
1	A	189	PRO
1	B	189	PRO
1	C	189	PRO
1	D	189	PRO
1	E	189	PRO
1	F	189	PRO
1	G	189	PRO
1	H	189	PRO
1	I	189	PRO
1	J	189	PRO
1	K	189	PRO
1	L	189	PRO
1	M	189	PRO
1	N	189	PRO
1	O	189	PRO
1	P	189	PRO
1	A	38	PRO
1	B	38	PRO
1	C	38	PRO
1	D	38	PRO
1	E	38	PRO
1	F	38	PRO
1	G	38	PRO
1	H	38	PRO
1	I	38	PRO
1	J	38	PRO
1	K	38	PRO
1	L	38	PRO
1	M	38	PRO
1	N	38	PRO

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Mol	Chain	Res	Type
1	O	38	PRO
1	P	38	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	B	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	C	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	D	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	E	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	F	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	G	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	H	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	I	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	J	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	K	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	L	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	M	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	N	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	O	185/187 (99%)	169 (91%)	16 (9%)	10	37
1	P	185/187 (99%)	169 (91%)	16 (9%)	10	37
All	All	2960/2992 (99%)	2704 (91%)	256 (9%)	10	37

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	28	ASP

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Mol	Chain	Res	Type
1	A	39	ARG
1	A	76	ASP
1	A	91	LEU
1	A	97	ASN
1	A	101	SER
1	A	139	VAL
1	A	145	LEU
1	A	153	ARG
1	A	163	LEU
1	A	166	VAL
1	A	184	PHE
1	A	194	GLN
1	A	209	GLN
1	A	234	LEU
1	B	13	THR
1	B	28	ASP
1	B	39	ARG
1	B	76	ASP
1	B	91	LEU
1	B	97	ASN
1	B	101	SER
1	B	139	VAL
1	B	145	LEU
1	B	153	ARG
1	B	163	LEU
1	B	166	VAL
1	B	184	PHE
1	B	194	GLN
1	B	209	GLN
1	B	234	LEU
1	C	13	THR
1	C	28	ASP
1	C	39	ARG
1	C	76	ASP
1	C	91	LEU
1	C	97	ASN
1	C	101	SER
1	C	139	VAL
1	C	145	LEU
1	C	153	ARG
1	C	163	LEU
1	C	166	VAL

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Mol	Chain	Res	Type
1	C	184	PHE
1	C	194	GLN
1	C	209	GLN
1	C	234	LEU
1	D	13	THR
1	D	28	ASP
1	D	39	ARG
1	D	76	ASP
1	D	91	LEU
1	D	97	ASN
1	D	101	SER
1	D	139	VAL
1	D	145	LEU
1	D	153	ARG
1	D	163	LEU
1	D	166	VAL
1	D	184	PHE
1	D	194	GLN
1	D	209	GLN
1	D	234	LEU
1	E	13	THR
1	E	28	ASP
1	E	39	ARG
1	E	76	ASP
1	E	91	LEU
1	E	97	ASN
1	E	101	SER
1	E	139	VAL
1	E	145	LEU
1	E	153	ARG
1	E	163	LEU
1	E	166	VAL
1	E	184	PHE
1	E	194	GLN
1	E	209	GLN
1	E	234	LEU
1	F	13	THR
1	F	28	ASP
1	F	39	ARG
1	F	76	ASP
1	F	91	LEU
1	F	97	ASN

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Mol	Chain	Res	Type
1	F	101	SER
1	F	139	VAL
1	F	145	LEU
1	F	153	ARG
1	F	163	LEU
1	F	166	VAL
1	F	184	PHE
1	F	194	GLN
1	F	209	GLN
1	F	234	LEU
1	G	13	THR
1	G	28	ASP
1	G	39	ARG
1	G	76	ASP
1	G	91	LEU
1	G	97	ASN
1	G	101	SER
1	G	139	VAL
1	G	145	LEU
1	G	153	ARG
1	G	163	LEU
1	G	166	VAL
1	G	184	PHE
1	G	194	GLN
1	G	209	GLN
1	G	234	LEU
1	H	13	THR
1	H	28	ASP
1	H	39	ARG
1	H	76	ASP
1	H	91	LEU
1	H	97	ASN
1	H	101	SER
1	H	139	VAL
1	H	145	LEU
1	H	153	ARG
1	H	163	LEU
1	H	166	VAL
1	H	184	PHE
1	H	194	GLN
1	H	209	GLN
1	H	234	LEU

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Mol	Chain	Res	Type
1	I	13	THR
1	I	28	ASP
1	I	39	ARG
1	I	76	ASP
1	I	91	LEU
1	I	97	ASN
1	I	101	SER
1	I	139	VAL
1	I	145	LEU
1	I	153	ARG
1	I	163	LEU
1	I	166	VAL
1	I	184	PHE
1	I	194	GLN
1	I	209	GLN
1	I	234	LEU
1	J	13	THR
1	J	28	ASP
1	J	39	ARG
1	J	76	ASP
1	J	91	LEU
1	J	97	ASN
1	J	101	SER
1	J	139	VAL
1	J	145	LEU
1	J	153	ARG
1	J	163	LEU
1	J	166	VAL
1	J	184	PHE
1	J	194	GLN
1	J	209	GLN
1	J	234	LEU
1	K	13	THR
1	K	28	ASP
1	K	39	ARG
1	K	76	ASP
1	K	91	LEU
1	K	97	ASN
1	K	101	SER
1	K	139	VAL
1	K	145	LEU
1	K	153	ARG

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Mol	Chain	Res	Type
1	K	163	LEU
1	K	166	VAL
1	K	184	PHE
1	K	194	GLN
1	K	209	GLN
1	K	234	LEU
1	L	13	THR
1	L	28	ASP
1	L	39	ARG
1	L	76	ASP
1	L	91	LEU
1	L	97	ASN
1	L	101	SER
1	L	139	VAL
1	L	145	LEU
1	L	153	ARG
1	L	163	LEU
1	L	166	VAL
1	L	184	PHE
1	L	194	GLN
1	L	209	GLN
1	L	234	LEU
1	M	13	THR
1	M	28	ASP
1	M	39	ARG
1	M	76	ASP
1	M	91	LEU
1	M	97	ASN
1	M	101	SER
1	M	139	VAL
1	M	145	LEU
1	M	153	ARG
1	M	163	LEU
1	M	166	VAL
1	M	184	PHE
1	M	194	GLN
1	M	209	GLN
1	M	234	LEU
1	N	13	THR
1	N	28	ASP
1	N	39	ARG
1	N	76	ASP

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Mol	Chain	Res	Type
1	N	91	LEU
1	N	97	ASN
1	N	101	SER
1	N	139	VAL
1	N	145	LEU
1	N	153	ARG
1	N	163	LEU
1	N	166	VAL
1	N	184	PHE
1	N	194	GLN
1	N	209	GLN
1	N	234	LEU
1	O	13	THR
1	O	28	ASP
1	O	39	ARG
1	O	76	ASP
1	O	91	LEU
1	O	97	ASN
1	O	101	SER
1	O	139	VAL
1	O	145	LEU
1	O	153	ARG
1	O	163	LEU
1	O	166	VAL
1	O	184	PHE
1	O	194	GLN
1	O	209	GLN
1	O	234	LEU
1	P	13	THR
1	P	28	ASP
1	P	39	ARG
1	P	76	ASP
1	P	91	LEU
1	P	97	ASN
1	P	101	SER
1	P	139	VAL
1	P	145	LEU
1	P	153	ARG
1	P	163	LEU
1	P	166	VAL
1	P	184	PHE
1	P	194	GLN

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Mol	Chain	Res	Type
1	P	209	GLN
1	P	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	56	GLN
1	A	62	GLN
1	A	83	HIS
1	A	159	GLN
1	A	171	GLN
1	A	194	GLN
1	A	226	GLN
1	A	238	ASN
1	A	242	GLN
1	B	25	ASN
1	B	56	GLN
1	B	62	GLN
1	B	83	HIS
1	B	159	GLN
1	B	171	GLN
1	B	194	GLN
1	B	226	GLN
1	B	232	GLN
1	B	238	ASN
1	B	242	GLN
1	C	25	ASN
1	C	56	GLN
1	C	62	GLN
1	C	83	HIS
1	C	159	GLN
1	C	171	GLN
1	C	194	GLN
1	C	226	GLN
1	C	238	ASN
1	C	242	GLN
1	D	25	ASN
1	D	56	GLN
1	D	62	GLN
1	D	83	HIS
1	D	159	GLN

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Mol	Chain	Res	Type
1	D	171	GLN
1	D	194	GLN
1	D	226	GLN
1	D	238	ASN
1	D	242	GLN
1	E	25	ASN
1	E	56	GLN
1	E	62	GLN
1	E	83	HIS
1	E	159	GLN
1	E	171	GLN
1	E	194	GLN
1	E	226	GLN
1	E	238	ASN
1	E	242	GLN
1	F	25	ASN
1	F	56	GLN
1	F	62	GLN
1	F	83	HIS
1	F	159	GLN
1	F	171	GLN
1	F	194	GLN
1	F	226	GLN
1	F	238	ASN
1	F	242	GLN
1	G	25	ASN
1	G	56	GLN
1	G	62	GLN
1	G	83	HIS
1	G	159	GLN
1	G	171	GLN
1	G	194	GLN
1	G	226	GLN
1	G	232	GLN
1	G	238	ASN
1	G	242	GLN
1	H	25	ASN
1	H	56	GLN
1	H	62	GLN
1	H	83	HIS
1	H	159	GLN
1	H	171	GLN

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Mol	Chain	Res	Type
1	H	194	GLN
1	H	226	GLN
1	H	238	ASN
1	H	242	GLN
1	I	25	ASN
1	I	56	GLN
1	I	62	GLN
1	I	83	HIS
1	I	159	GLN
1	I	171	GLN
1	I	194	GLN
1	I	226	GLN
1	I	238	ASN
1	I	242	GLN
1	J	25	ASN
1	J	56	GLN
1	J	62	GLN
1	J	83	HIS
1	J	159	GLN
1	J	171	GLN
1	J	194	GLN
1	J	226	GLN
1	J	238	ASN
1	J	242	GLN
1	K	25	ASN
1	K	56	GLN
1	K	62	GLN
1	K	83	HIS
1	K	159	GLN
1	K	171	GLN
1	K	194	GLN
1	K	226	GLN
1	K	238	ASN
1	K	242	GLN
1	L	25	ASN
1	L	56	GLN
1	L	62	GLN
1	L	83	HIS
1	L	159	GLN
1	L	171	GLN
1	L	194	GLN
1	L	226	GLN

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Mol	Chain	Res	Type
1	L	238	ASN
1	L	242	GLN
1	M	25	ASN
1	M	56	GLN
1	M	62	GLN
1	M	83	HIS
1	M	159	GLN
1	M	171	GLN
1	M	194	GLN
1	M	226	GLN
1	M	238	ASN
1	M	242	GLN
1	N	25	ASN
1	N	56	GLN
1	N	62	GLN
1	N	83	HIS
1	N	159	GLN
1	N	171	GLN
1	N	194	GLN
1	N	226	GLN
1	N	238	ASN
1	N	242	GLN
1	O	25	ASN
1	O	56	GLN
1	O	62	GLN
1	O	83	HIS
1	O	159	GLN
1	O	171	GLN
1	O	194	GLN
1	O	226	GLN
1	O	238	ASN
1	O	242	GLN
1	P	25	ASN
1	P	56	GLN
1	P	62	GLN
1	P	83	HIS
1	P	159	GLN
1	P	171	GLN
1	P	194	GLN
1	P	226	GLN
1	P	238	ASN
1	P	242	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BMP	M	313	-	22,23,23	2.15	5 (22%)	33,35,35	1.70	8 (24%)
2	BMP	G	307	-	22,23,23	2.16	5 (22%)	33,35,35	1.70	8 (24%)
2	BMP	N	314	-	22,23,23	2.16	5 (22%)	33,35,35	1.70	8 (24%)
2	BMP	I	309	-	22,23,23	2.16	5 (22%)	33,35,35	1.71	8 (24%)
2	BMP	F	306	-	22,23,23	2.16	5 (22%)	33,35,35	1.70	8 (24%)
2	BMP	H	308	-	22,23,23	2.16	5 (22%)	33,35,35	1.70	8 (24%)
2	BMP	E	305	-	22,23,23	2.17	5 (22%)	33,35,35	1.70	8 (24%)
2	BMP	J	310	-	22,23,23	2.17	5 (22%)	33,35,35	1.70	9 (27%)
2	BMP	O	315	-	22,23,23	2.17	5 (22%)	33,35,35	1.70	9 (27%)
2	BMP	B	302	-	22,23,23	2.17	5 (22%)	33,35,35	1.70	8 (24%)
2	BMP	A	301	-	22,23,23	2.16	5 (22%)	33,35,35	1.70	8 (24%)
2	BMP	P	316	-	22,23,23	2.16	5 (22%)	33,35,35	1.70	8 (24%)
2	BMP	C	303	-	22,23,23	2.16	5 (22%)	33,35,35	1.70	8 (24%)
2	BMP	L	312	-	22,23,23	2.16	5 (22%)	33,35,35	1.70	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMP	K	311	-	22,23,23	2.16	5 (22%)	33,35,35	1.69	8 (24%)
2	BMP	D	304	-	22,23,23	2.16	5 (22%)	33,35,35	1.70	8 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMP	M	313	-	-	0/10/26/26	0/2/2/2
2	BMP	G	307	-	-	0/10/26/26	0/2/2/2
2	BMP	N	314	-	-	0/10/26/26	0/2/2/2
2	BMP	I	309	-	-	0/10/26/26	0/2/2/2
2	BMP	F	306	-	-	0/10/26/26	0/2/2/2
2	BMP	H	308	-	-	0/10/26/26	0/2/2/2
2	BMP	E	305	-	-	0/10/26/26	0/2/2/2
2	BMP	J	310	-	-	0/10/26/26	0/2/2/2
2	BMP	O	315	-	-	0/10/26/26	0/2/2/2
2	BMP	B	302	-	-	0/10/26/26	0/2/2/2
2	BMP	A	301	-	-	0/10/26/26	0/2/2/2
2	BMP	P	316	-	-	0/10/26/26	0/2/2/2
2	BMP	C	303	-	-	0/10/26/26	0/2/2/2
2	BMP	L	312	-	-	0/10/26/26	0/2/2/2
2	BMP	K	311	-	-	0/10/26/26	0/2/2/2
2	BMP	D	304	-	-	0/10/26/26	0/2/2/2

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	314	BMP	O2-C2	5.84	1.33	1.23
2	J	310	BMP	O2-C2	5.83	1.33	1.23
2	P	316	BMP	O2-C2	5.82	1.33	1.23
2	O	315	BMP	O2-C2	5.82	1.33	1.23
2	E	305	BMP	O2-C2	5.81	1.33	1.23
2	B	302	BMP	O2-C2	5.81	1.33	1.23
2	D	304	BMP	O2-C2	5.80	1.33	1.23
2	A	301	BMP	O2-C2	5.80	1.33	1.23
2	H	308	BMP	O2-C2	5.80	1.33	1.23
2	G	307	BMP	O2-C2	5.80	1.33	1.23
2	K	311	BMP	O2-C2	5.79	1.33	1.23
2	M	313	BMP	O2-C2	5.78	1.33	1.23
2	L	312	BMP	O2-C2	5.77	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	303	BMP	O2-C2	5.77	1.33	1.23
2	I	309	BMP	O2-C2	5.77	1.33	1.23
2	F	306	BMP	O2-C2	5.76	1.33	1.23
2	O	315	BMP	C1'-N1	4.98	1.55	1.46
2	C	303	BMP	C1'-N1	4.97	1.55	1.46
2	B	302	BMP	C1'-N1	4.96	1.55	1.46
2	J	310	BMP	C1'-N1	4.96	1.55	1.46
2	H	308	BMP	C1'-N1	4.95	1.55	1.46
2	E	305	BMP	C1'-N1	4.94	1.55	1.46
2	K	311	BMP	C1'-N1	4.94	1.54	1.46
2	A	301	BMP	C1'-N1	4.93	1.54	1.46
2	L	312	BMP	C1'-N1	4.92	1.54	1.46
2	I	309	BMP	C1'-N1	4.92	1.54	1.46
2	P	316	BMP	C1'-N1	4.91	1.54	1.46
2	D	304	BMP	C1'-N1	4.90	1.54	1.46
2	M	313	BMP	C1'-N1	4.89	1.54	1.46
2	F	306	BMP	C1'-N1	4.88	1.54	1.46
2	G	307	BMP	C1'-N1	4.87	1.54	1.46
2	N	314	BMP	C1'-N1	4.86	1.54	1.46
2	O	315	BMP	O4'-C4'	4.73	1.55	1.45
2	F	306	BMP	O4'-C4'	4.73	1.55	1.45
2	I	309	BMP	O4'-C4'	4.72	1.55	1.45
2	A	301	BMP	O4'-C4'	4.71	1.55	1.45
2	K	311	BMP	O4'-C4'	4.71	1.55	1.45
2	H	308	BMP	O4'-C4'	4.71	1.55	1.45
2	G	307	BMP	O4'-C4'	4.71	1.55	1.45
2	D	304	BMP	O4'-C4'	4.70	1.55	1.45
2	C	303	BMP	O4'-C4'	4.69	1.55	1.45
2	N	314	BMP	O4'-C4'	4.69	1.55	1.45
2	B	302	BMP	O4'-C4'	4.69	1.55	1.45
2	E	305	BMP	O4'-C4'	4.69	1.55	1.45
2	M	313	BMP	O4'-C4'	4.69	1.55	1.45
2	J	310	BMP	O4'-C4'	4.69	1.55	1.45
2	L	312	BMP	O4'-C4'	4.68	1.55	1.45
2	P	316	BMP	O4'-C4'	4.67	1.55	1.45
2	B	302	BMP	O2'-C2'	-2.46	1.37	1.43
2	E	305	BMP	O2'-C2'	-2.46	1.37	1.43
2	I	309	BMP	O2'-C2'	-2.45	1.37	1.43
2	P	316	BMP	O2'-C2'	-2.45	1.37	1.43
2	D	304	BMP	O2'-C2'	-2.45	1.37	1.43
2	L	312	BMP	O2'-C2'	-2.44	1.37	1.43
2	G	307	BMP	O2'-C2'	-2.44	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	310	BMP	O2'-C2'	-2.44	1.37	1.43
2	A	301	BMP	O2'-C2'	-2.44	1.37	1.43
2	K	311	BMP	O2'-C2'	-2.43	1.37	1.43
2	O	315	BMP	O2'-C2'	-2.43	1.37	1.43
2	N	314	BMP	O2'-C2'	-2.43	1.37	1.43
2	F	306	BMP	O2'-C2'	-2.42	1.37	1.43
2	M	313	BMP	O2'-C2'	-2.42	1.37	1.43
2	C	303	BMP	O2'-C2'	-2.41	1.37	1.43
2	H	308	BMP	O2'-C2'	-2.40	1.37	1.43
2	F	306	BMP	O3'-C3'	2.25	1.48	1.43
2	K	311	BMP	O3'-C3'	2.25	1.48	1.43
2	B	302	BMP	O3'-C3'	2.24	1.48	1.43
2	G	307	BMP	O3'-C3'	2.24	1.48	1.43
2	L	312	BMP	O3'-C3'	2.24	1.48	1.43
2	I	309	BMP	O3'-C3'	2.24	1.48	1.43
2	A	301	BMP	O3'-C3'	2.23	1.48	1.43
2	H	308	BMP	O3'-C3'	2.23	1.48	1.43
2	M	313	BMP	O3'-C3'	2.23	1.48	1.43
2	O	315	BMP	O3'-C3'	2.23	1.48	1.43
2	J	310	BMP	O3'-C3'	2.22	1.48	1.43
2	N	314	BMP	O3'-C3'	2.22	1.48	1.43
2	D	304	BMP	O3'-C3'	2.21	1.48	1.43
2	P	316	BMP	O3'-C3'	2.21	1.48	1.43
2	E	305	BMP	O3'-C3'	2.21	1.48	1.43
2	C	303	BMP	O3'-C3'	2.20	1.48	1.43

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	304	BMP	O1-C6-C5	-4.00	116.72	125.53
2	H	308	BMP	O1-C6-C5	-4.00	116.73	125.53
2	N	314	BMP	O1-C6-C5	-4.00	116.73	125.53
2	O	315	BMP	O1-C6-C5	-3.99	116.73	125.53
2	B	302	BMP	O1-C6-C5	-3.99	116.74	125.53
2	M	313	BMP	O1-C6-C5	-3.99	116.74	125.53
2	E	305	BMP	O1-C6-C5	-3.99	116.74	125.53
2	A	301	BMP	O1-C6-C5	-3.99	116.75	125.53
2	I	309	BMP	O1-C6-C5	-3.99	116.75	125.53
2	L	312	BMP	O1-C6-C5	-3.98	116.76	125.53
2	P	316	BMP	O1-C6-C5	-3.98	116.76	125.53
2	G	307	BMP	O1-C6-C5	-3.98	116.77	125.53
2	K	311	BMP	O1-C6-C5	-3.98	116.77	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	303	BMP	O1-C6-C5	-3.98	116.77	125.53
2	F	306	BMP	O1-C6-C5	-3.98	116.77	125.53
2	J	310	BMP	O1-C6-C5	-3.97	116.78	125.53
2	C	303	BMP	C4-N3-C2	-3.81	121.56	126.58
2	I	309	BMP	C4-N3-C2	-3.79	121.58	126.58
2	P	316	BMP	C4-N3-C2	-3.79	121.58	126.58
2	J	310	BMP	C4-N3-C2	-3.79	121.58	126.58
2	B	302	BMP	C4-N3-C2	-3.78	121.59	126.58
2	D	304	BMP	C4-N3-C2	-3.78	121.59	126.58
2	O	315	BMP	C4-N3-C2	-3.78	121.59	126.58
2	A	301	BMP	C4-N3-C2	-3.78	121.60	126.58
2	L	312	BMP	C4-N3-C2	-3.78	121.60	126.58
2	F	306	BMP	C4-N3-C2	-3.78	121.60	126.58
2	N	314	BMP	C4-N3-C2	-3.77	121.60	126.58
2	M	313	BMP	C4-N3-C2	-3.77	121.60	126.58
2	G	307	BMP	C4-N3-C2	-3.77	121.61	126.58
2	E	305	BMP	C4-N3-C2	-3.76	121.62	126.58
2	K	311	BMP	C4-N3-C2	-3.75	121.64	126.58
2	H	308	BMP	C4-N3-C2	-3.73	121.66	126.58
2	C	303	BMP	C5-C4-N3	3.06	118.84	115.14
2	J	310	BMP	C5-C4-N3	3.03	118.80	115.14
2	I	309	BMP	C5-C4-N3	3.03	118.80	115.14
2	F	306	BMP	C5-C4-N3	3.03	118.79	115.14
2	E	305	BMP	C5-C4-N3	3.02	118.79	115.14
2	G	307	BMP	C5-C4-N3	3.02	118.79	115.14
2	B	302	BMP	C5-C4-N3	3.01	118.78	115.14
2	A	301	BMP	C5-C4-N3	3.00	118.77	115.14
2	M	313	BMP	C5-C4-N3	3.00	118.77	115.14
2	D	304	BMP	C5-C4-N3	3.00	118.76	115.14
2	P	316	BMP	C5-C4-N3	3.00	118.76	115.14
2	N	314	BMP	C5-C4-N3	3.00	118.76	115.14
2	O	315	BMP	C5-C4-N3	2.99	118.75	115.14
2	L	312	BMP	C5-C4-N3	2.98	118.74	115.14
2	H	308	BMP	C5-C4-N3	2.98	118.73	115.14
2	K	311	BMP	C5-C4-N3	2.96	118.72	115.14
2	C	303	BMP	O5'-C5'-C4'	2.73	118.39	108.99
2	B	302	BMP	O5'-C5'-C4'	2.73	118.38	108.99
2	G	307	BMP	O5'-C5'-C4'	2.73	118.38	108.99
2	E	305	BMP	O5'-C5'-C4'	2.72	118.36	108.99
2	D	304	BMP	O5'-C5'-C4'	2.72	118.36	108.99
2	F	306	BMP	O5'-C5'-C4'	2.72	118.35	108.99
2	M	313	BMP	O5'-C5'-C4'	2.72	118.35	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	BMP	O5'-C5'-C4'	2.72	118.35	108.99
2	H	308	BMP	O5'-C5'-C4'	2.72	118.34	108.99
2	I	309	BMP	O5'-C5'-C4'	2.72	118.34	108.99
2	O	315	BMP	O5'-C5'-C4'	2.72	118.34	108.99
2	J	310	BMP	O5'-C5'-C4'	2.72	118.34	108.99
2	L	312	BMP	O5'-C5'-C4'	2.71	118.32	108.99
2	P	316	BMP	O5'-C5'-C4'	2.71	118.32	108.99
2	N	314	BMP	O5'-C5'-C4'	2.71	118.31	108.99
2	I	309	BMP	O4-C4-C5	-2.71	121.68	125.47
2	K	311	BMP	O5'-C5'-C4'	2.70	118.30	108.99
2	G	307	BMP	O4-C4-C5	-2.70	121.69	125.47
2	E	305	BMP	O4-C4-C5	-2.70	121.69	125.47
2	B	302	BMP	O4-C4-C5	-2.70	121.69	125.47
2	L	312	BMP	O4-C4-C5	-2.70	121.69	125.47
2	M	313	BMP	O4-C4-C5	-2.69	121.69	125.47
2	H	308	BMP	O4-C4-C5	-2.69	121.69	125.47
2	F	306	BMP	O4-C4-C5	-2.69	121.70	125.47
2	D	304	BMP	O4-C4-C5	-2.68	121.70	125.47
2	A	301	BMP	O4-C4-C5	-2.68	121.71	125.47
2	C	303	BMP	O4-C4-C5	-2.68	121.71	125.47
2	J	310	BMP	O4-C4-C5	-2.68	121.72	125.47
2	N	314	BMP	O4-C4-C5	-2.66	121.73	125.47
2	P	316	BMP	O4-C4-C5	-2.66	121.74	125.47
2	K	311	BMP	O4-C4-C5	-2.65	121.76	125.47
2	O	315	BMP	O4-C4-C5	-2.64	121.76	125.47
2	N	314	BMP	C5-C6-N1	2.36	124.23	119.06
2	M	313	BMP	C5-C6-N1	2.35	124.20	119.06
2	H	308	BMP	C5-C6-N1	2.34	124.19	119.06
2	P	316	BMP	C5-C6-N1	2.34	124.19	119.06
2	G	307	BMP	C5-C6-N1	2.34	124.18	119.06
2	F	306	BMP	C5-C6-N1	2.33	124.16	119.06
2	D	304	BMP	C5-C6-N1	2.33	124.16	119.06
2	A	301	BMP	C5-C6-N1	2.33	124.16	119.06
2	B	302	BMP	C5-C6-N1	2.33	124.16	119.06
2	J	310	BMP	C5-C6-N1	2.33	124.15	119.06
2	E	305	BMP	C5-C6-N1	2.32	124.15	119.06
2	L	312	BMP	C5-C6-N1	2.32	124.13	119.06
2	O	315	BMP	C5-C6-N1	2.31	124.12	119.06
2	C	303	BMP	C5-C6-N1	2.31	124.12	119.06
2	I	309	BMP	C5-C6-N1	2.31	124.11	119.06
2	K	311	BMP	C5-C6-N1	2.30	124.10	119.06
2	O	315	BMP	O1-C6-N1	2.27	119.15	114.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	309	BMP	O1-C6-N1	2.26	119.13	114.74
2	K	311	BMP	O1-C6-N1	2.26	119.13	114.74
2	D	304	BMP	O1-C6-N1	2.25	119.12	114.74
2	C	303	BMP	O1-C6-N1	2.25	119.11	114.74
2	B	302	BMP	O1-C6-N1	2.25	119.11	114.74
2	E	305	BMP	O1-C6-N1	2.25	119.11	114.74
2	L	312	BMP	O1-C6-N1	2.25	119.11	114.74
2	A	301	BMP	O1-C6-N1	2.24	119.09	114.74
2	H	308	BMP	O1-C6-N1	2.24	119.08	114.74
2	J	310	BMP	O1-C6-N1	2.23	119.06	114.74
2	F	306	BMP	O1-C6-N1	2.23	119.06	114.74
2	M	313	BMP	O1-C6-N1	2.22	119.05	114.74
2	G	307	BMP	O1-C6-N1	2.22	119.05	114.74
2	P	316	BMP	O1-C6-N1	2.22	119.05	114.74
2	N	314	BMP	O1-C6-N1	2.22	119.04	114.74
2	O	315	BMP	C5'-C4'-C3'	2.14	123.20	115.18
2	L	312	BMP	C5'-C4'-C3'	2.13	123.17	115.18
2	D	304	BMP	C5'-C4'-C3'	2.13	123.17	115.18
2	E	305	BMP	C5'-C4'-C3'	2.13	123.16	115.18
2	A	301	BMP	C5'-C4'-C3'	2.13	123.16	115.18
2	H	308	BMP	C5'-C4'-C3'	2.13	123.16	115.18
2	P	316	BMP	C5'-C4'-C3'	2.13	123.16	115.18
2	N	314	BMP	C5'-C4'-C3'	2.13	123.16	115.18
2	F	306	BMP	C5'-C4'-C3'	2.13	123.15	115.18
2	K	311	BMP	C5'-C4'-C3'	2.13	123.15	115.18
2	C	303	BMP	C5'-C4'-C3'	2.13	123.15	115.18
2	J	310	BMP	C5'-C4'-C3'	2.13	123.15	115.18
2	G	307	BMP	C5'-C4'-C3'	2.12	123.14	115.18
2	I	309	BMP	C5'-C4'-C3'	2.12	123.13	115.18
2	M	313	BMP	C5'-C4'-C3'	2.12	123.13	115.18
2	B	302	BMP	C5'-C4'-C3'	2.12	123.12	115.18
2	J	310	BMP	C4'-O4'-C1'	-2.00	105.05	109.47
2	O	315	BMP	C4'-O4'-C1'	-2.00	105.06	109.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	313	BMP	3	0

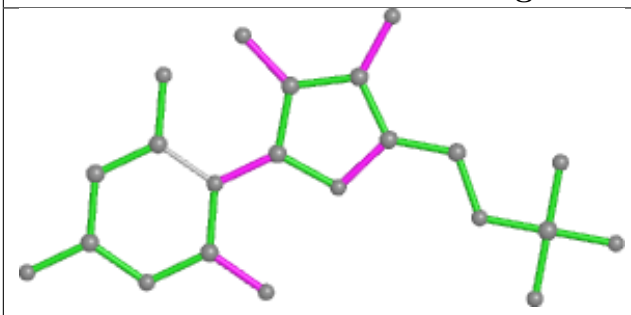
Continued on next page...

Continued from previous page...

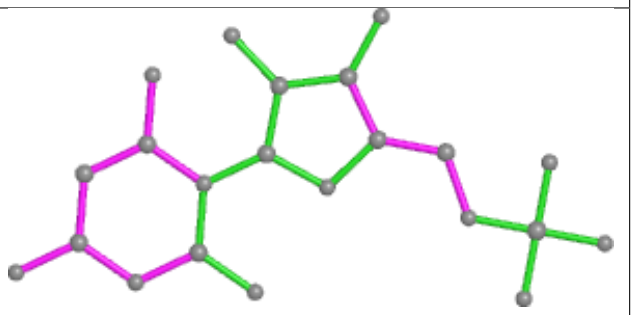
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	307	BMP	2	0
2	N	314	BMP	4	0
2	I	309	BMP	2	0
2	F	306	BMP	2	0
2	H	308	BMP	2	0
2	E	305	BMP	3	0
2	J	310	BMP	2	0
2	O	315	BMP	2	0
2	B	302	BMP	2	0
2	A	301	BMP	2	0
2	P	316	BMP	2	0
2	C	303	BMP	2	0
2	L	312	BMP	2	0
2	K	311	BMP	2	0
2	D	304	BMP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

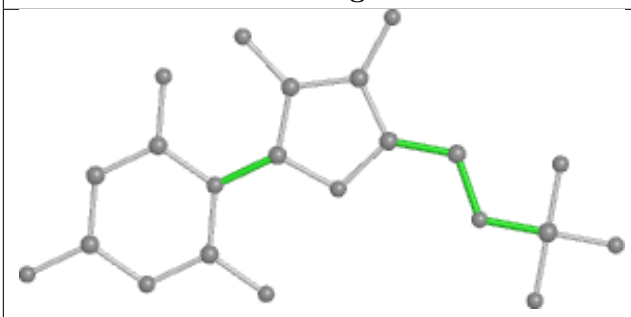
Ligand BMP M 313



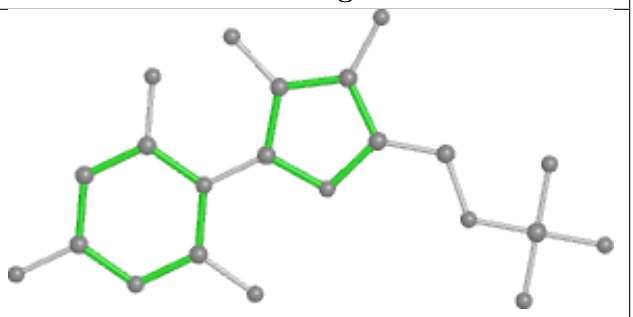
Bond lengths



Bond angles

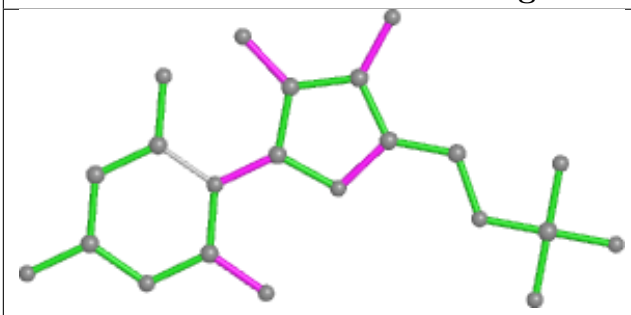


Torsions

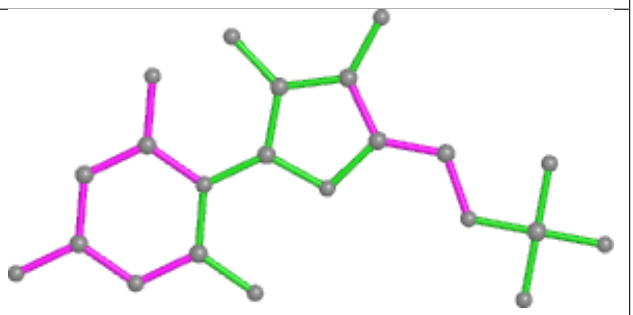


Rings

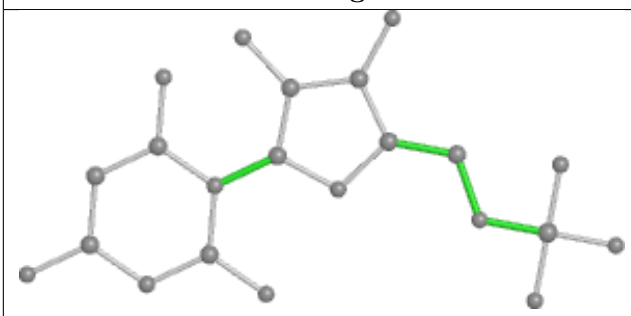
Ligand BMP G 307



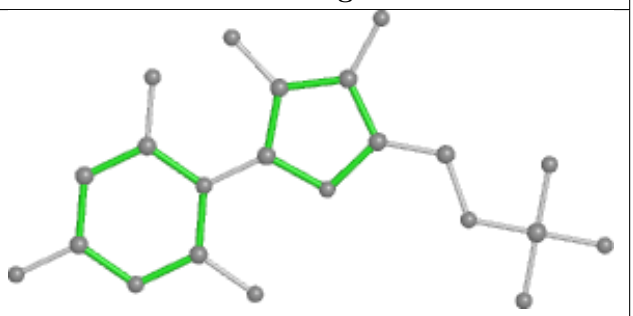
Bond lengths



Bond angles

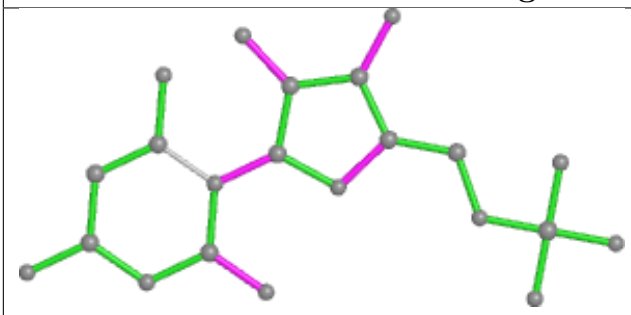


Torsions

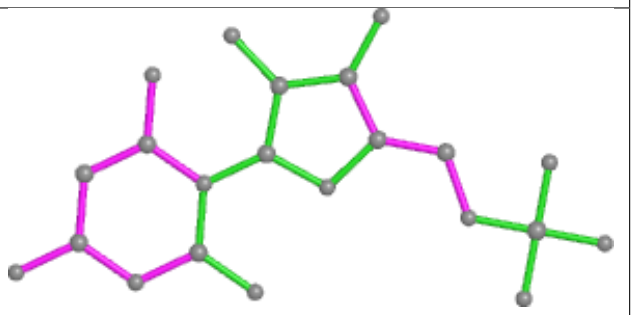


Rings

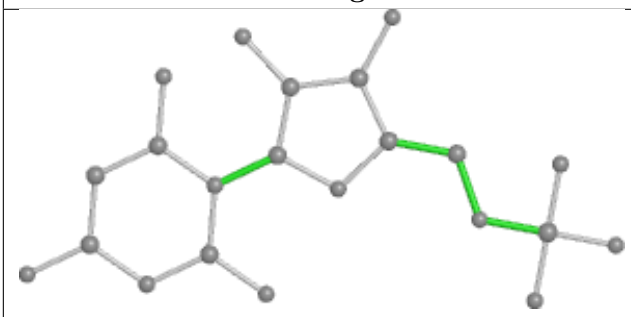
Ligand BMP N 314



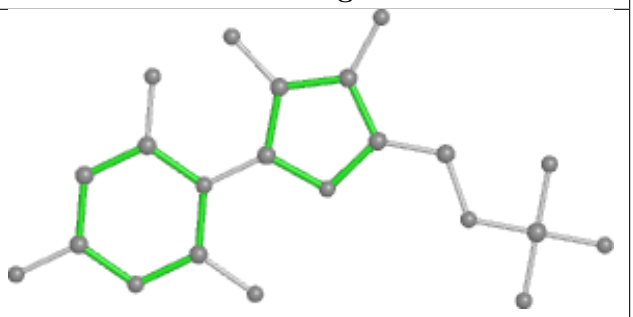
Bond lengths



Bond angles

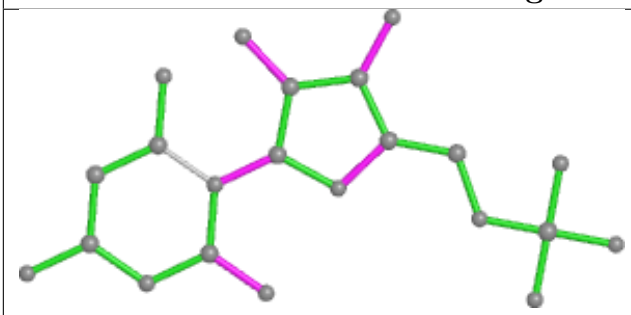


Torsions

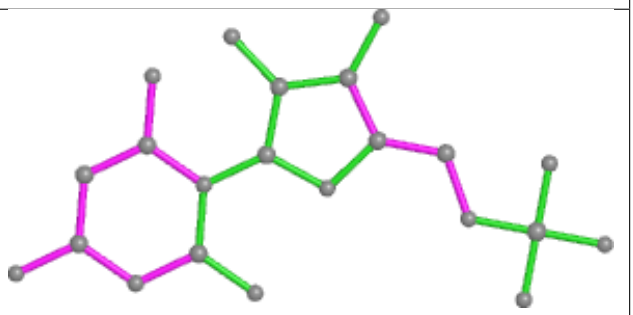


Rings

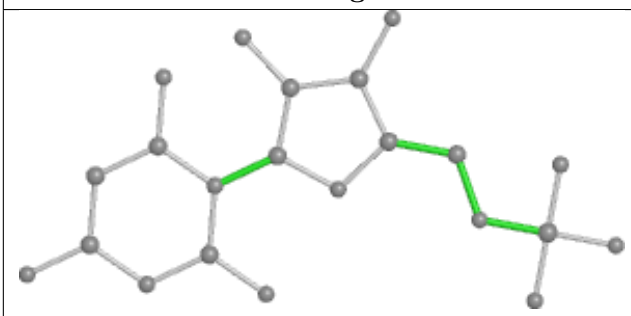
Ligand BMP I 309



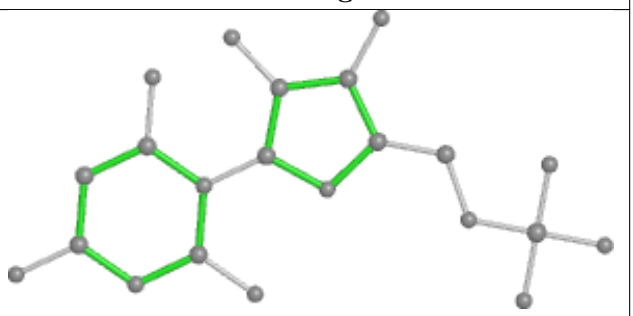
Bond lengths



Bond angles

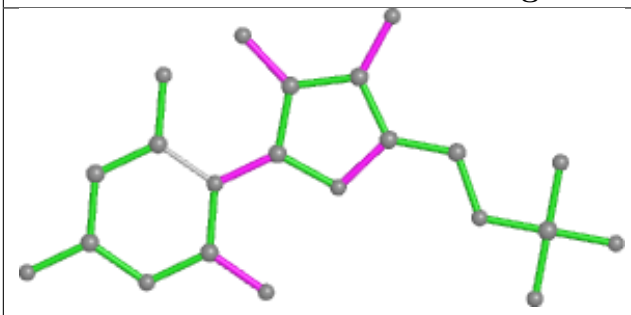


Torsions

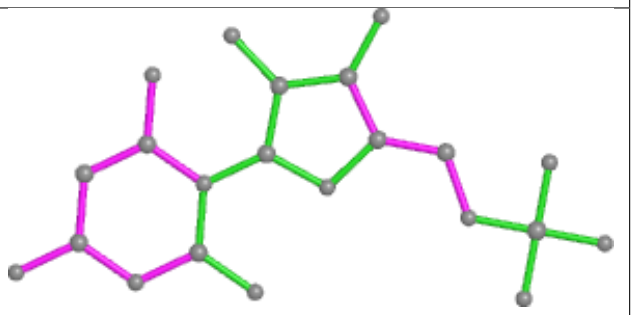


Rings

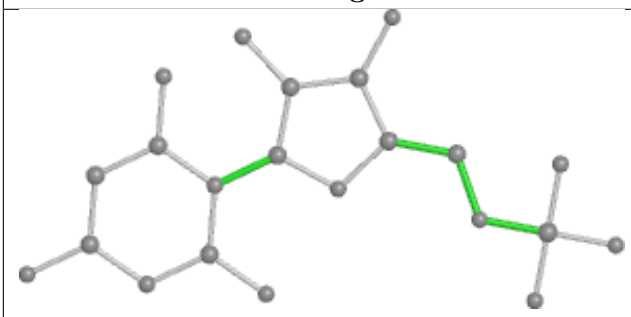
Ligand BMP F 306



Bond lengths



Bond angles



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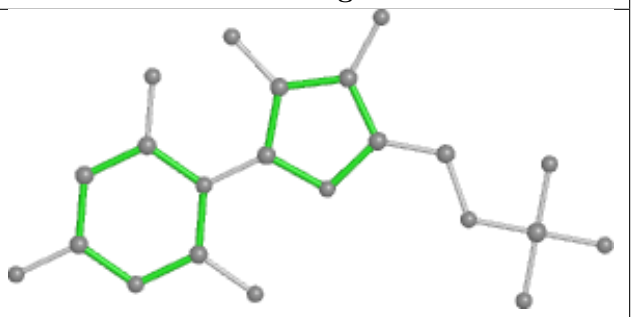
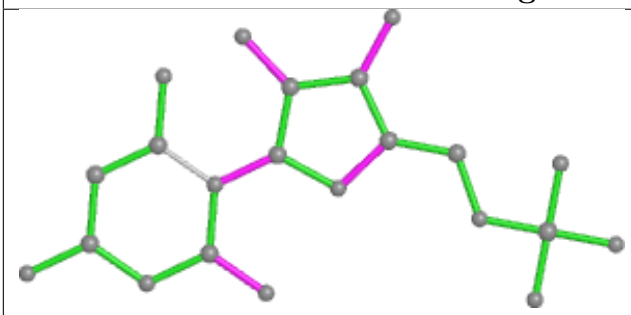


Rings

Ligand BMP H 308



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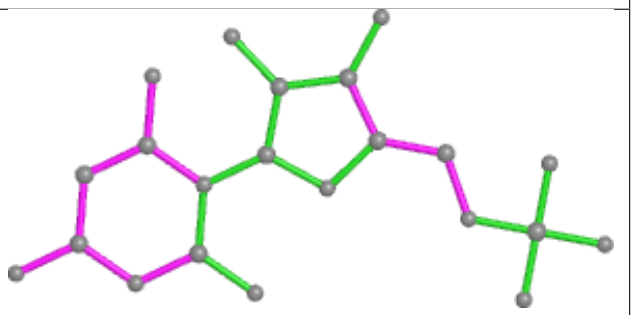
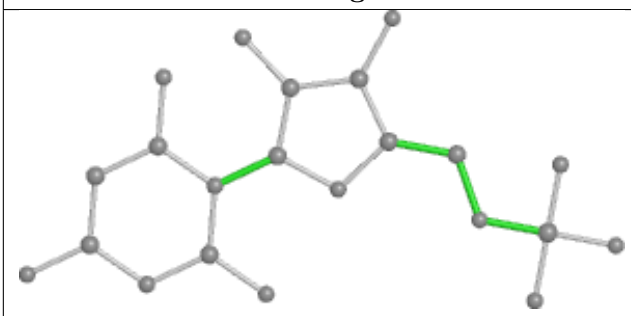
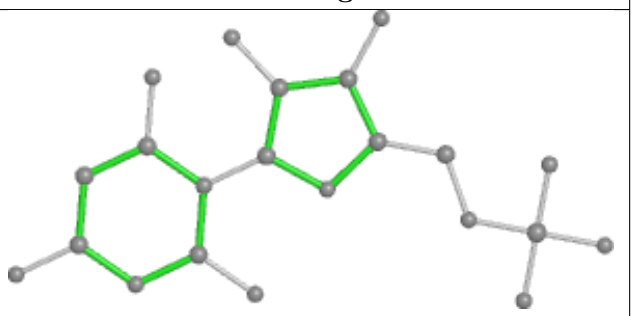


Bond angles

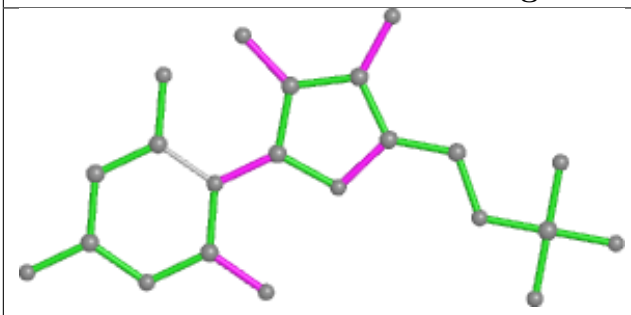


Torsions



Rings

Ligand BMP E 305



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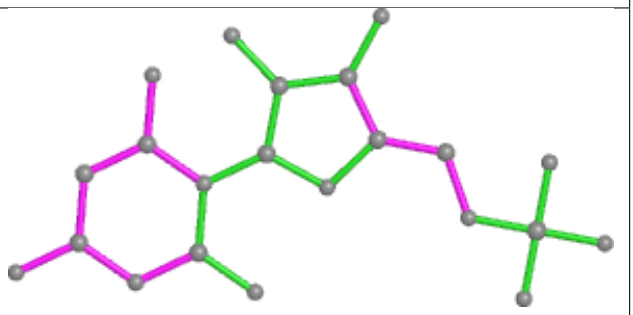

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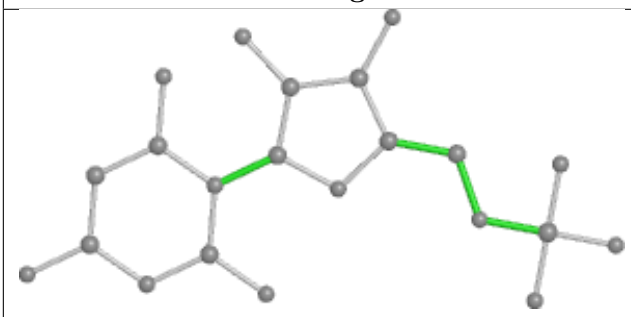

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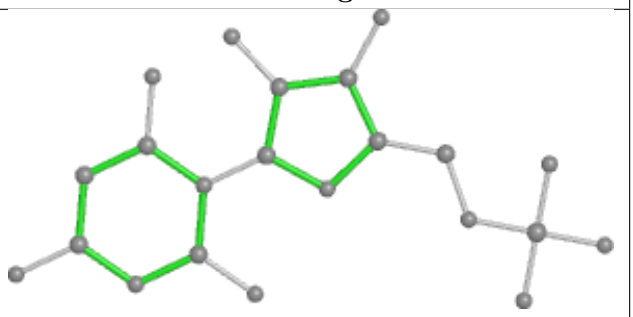
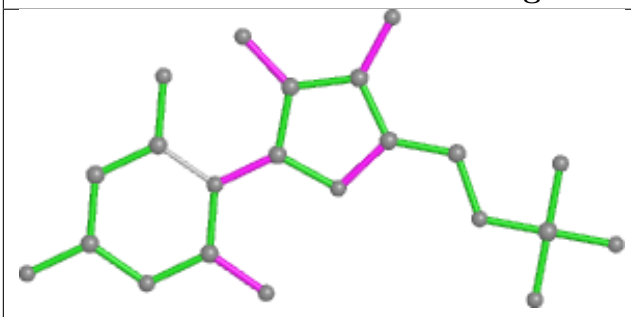


Rings

Ligand BMP J 310



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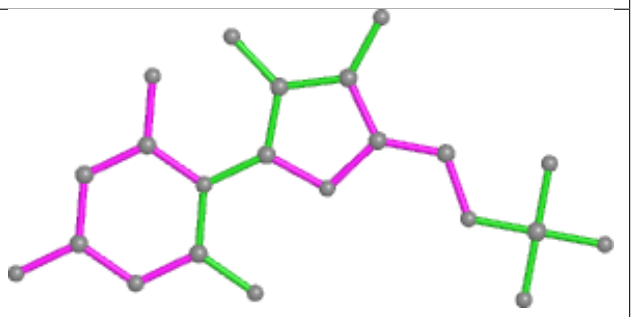
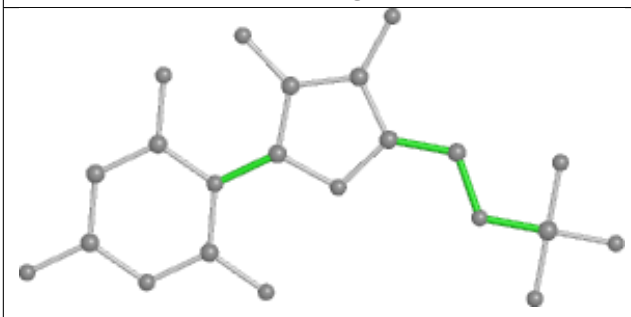
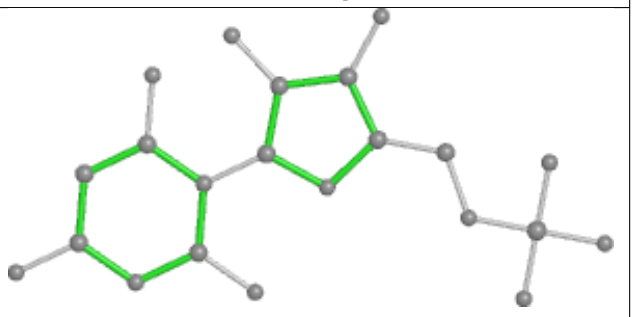


Bond angles

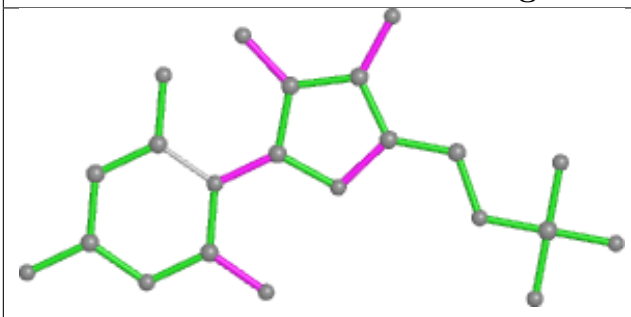


Torsions

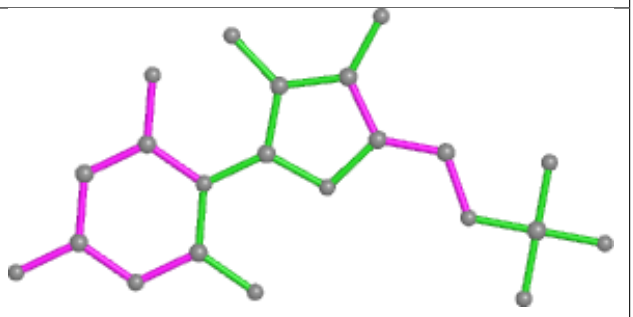


Rings

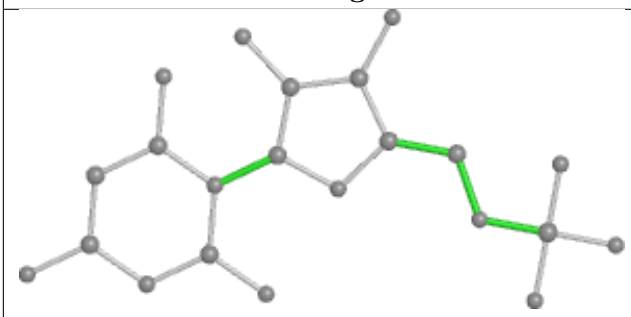
Ligand BMP O 315



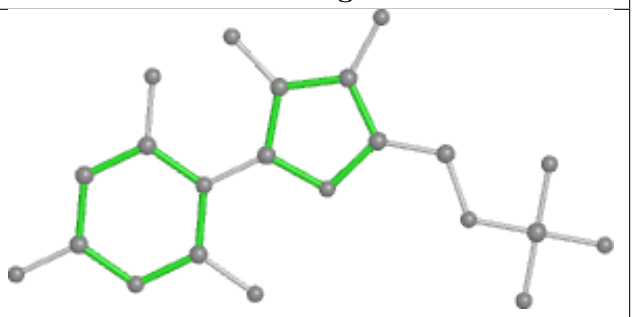
Bond lengths



Bond angles

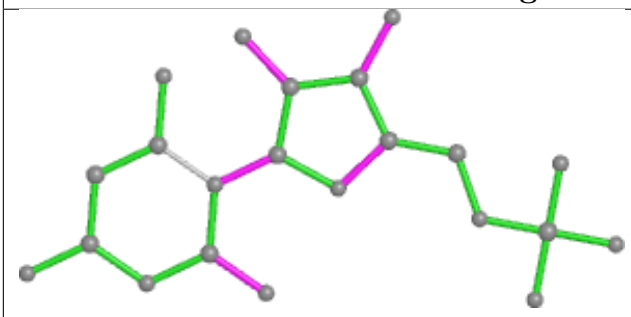


Torsions



Rings

Ligand BMP B 302



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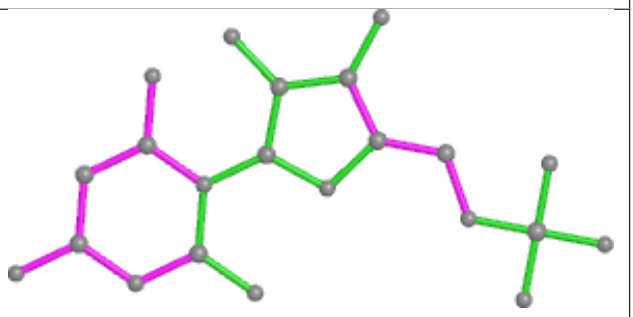
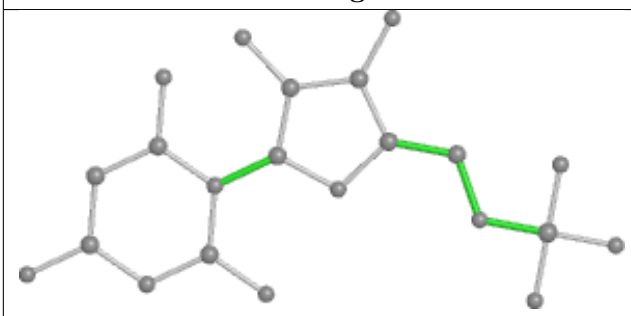


Bond angles



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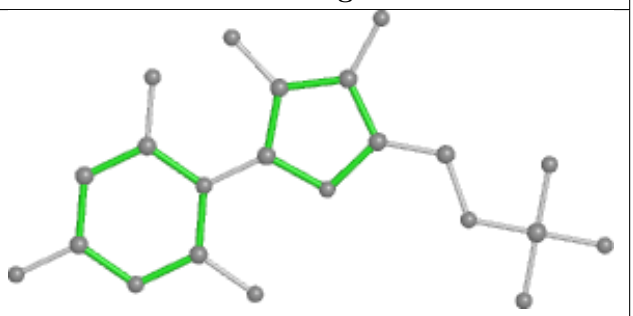
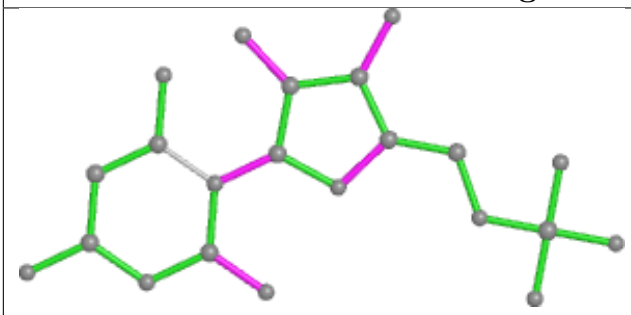
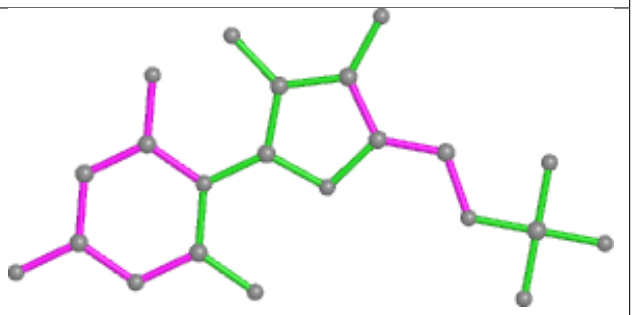


Rings

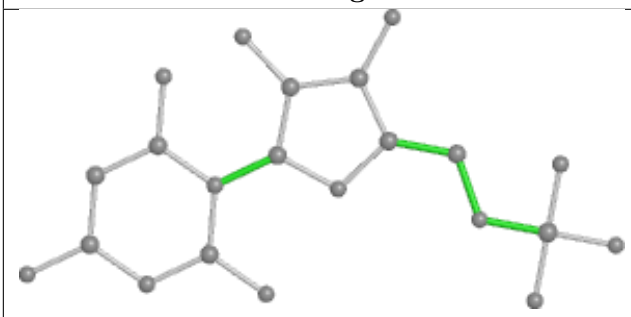
Ligand BMP A 301



Bond lengths



Bond angles



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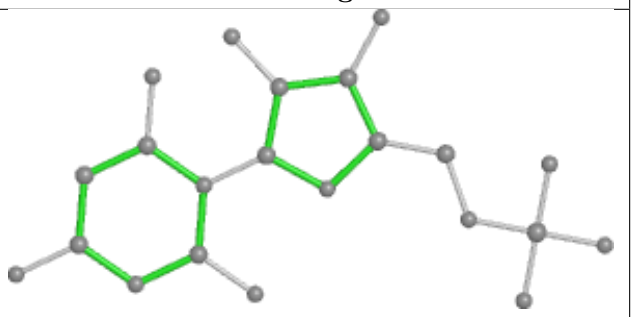
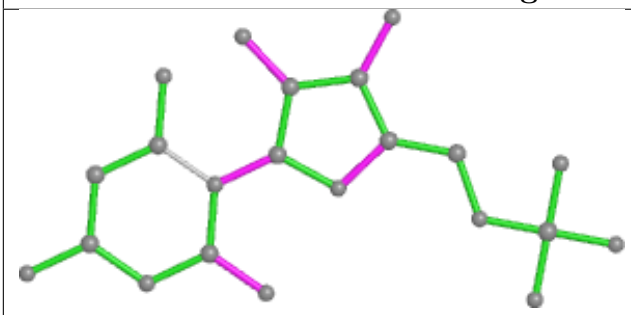
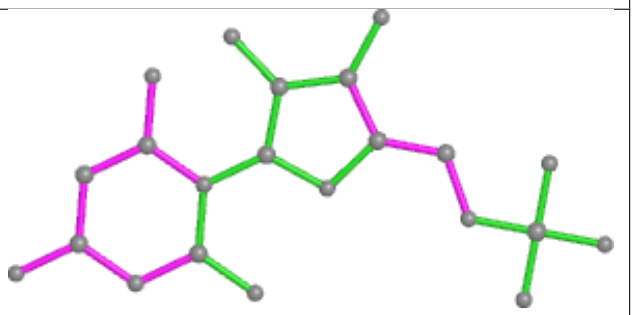


Rings

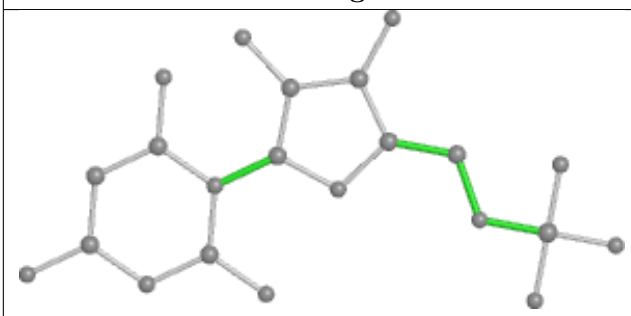
Ligand BMP P 316



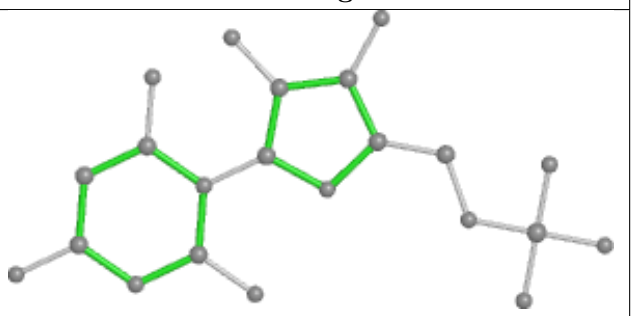
Bond lengths



Bond angles

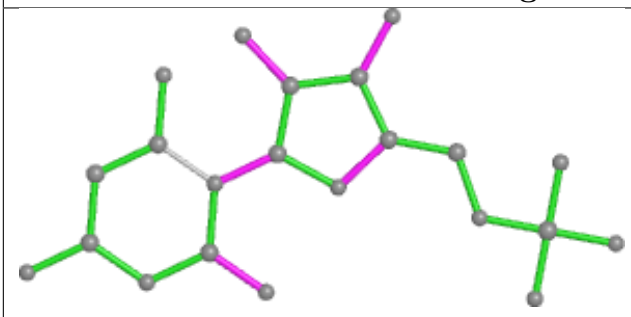


Torsions

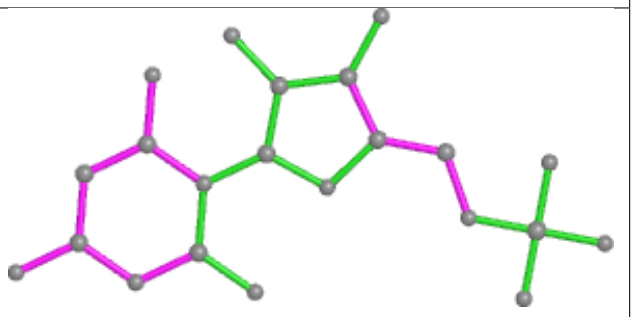


Rings

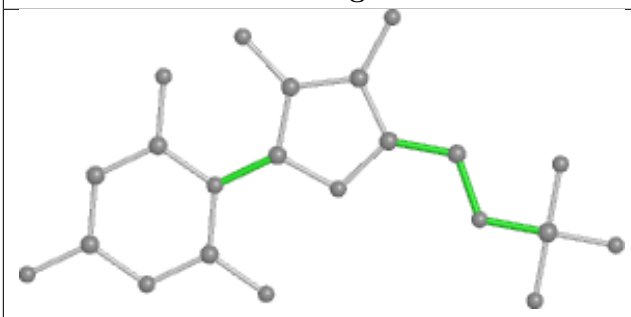
Ligand BMP C 303



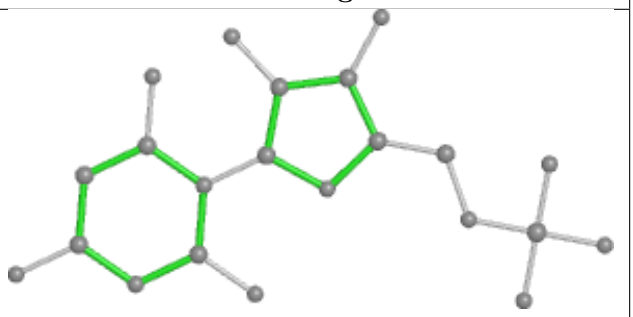
Bond lengths



Bond angles

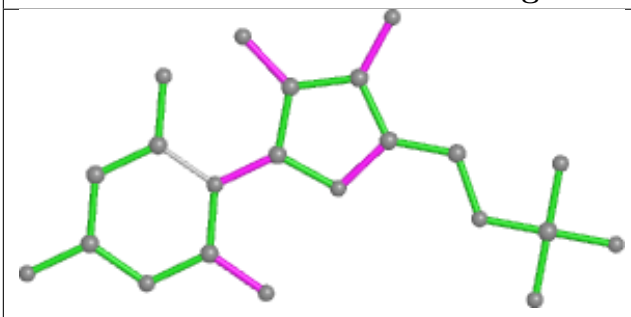


Torsions

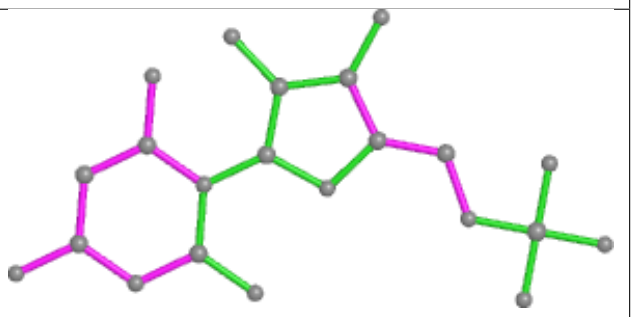


Rings

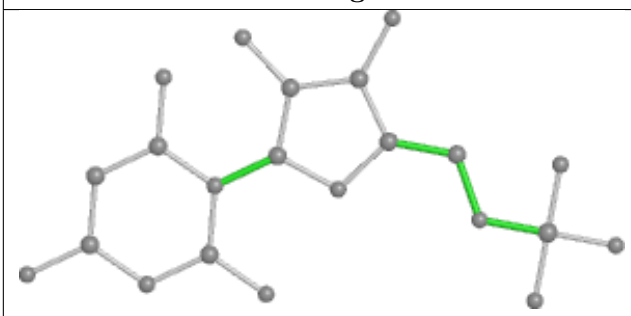
Ligand BMP L 312



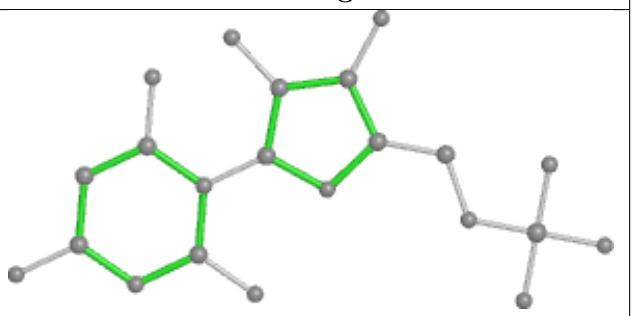
Bond lengths



Bond angles

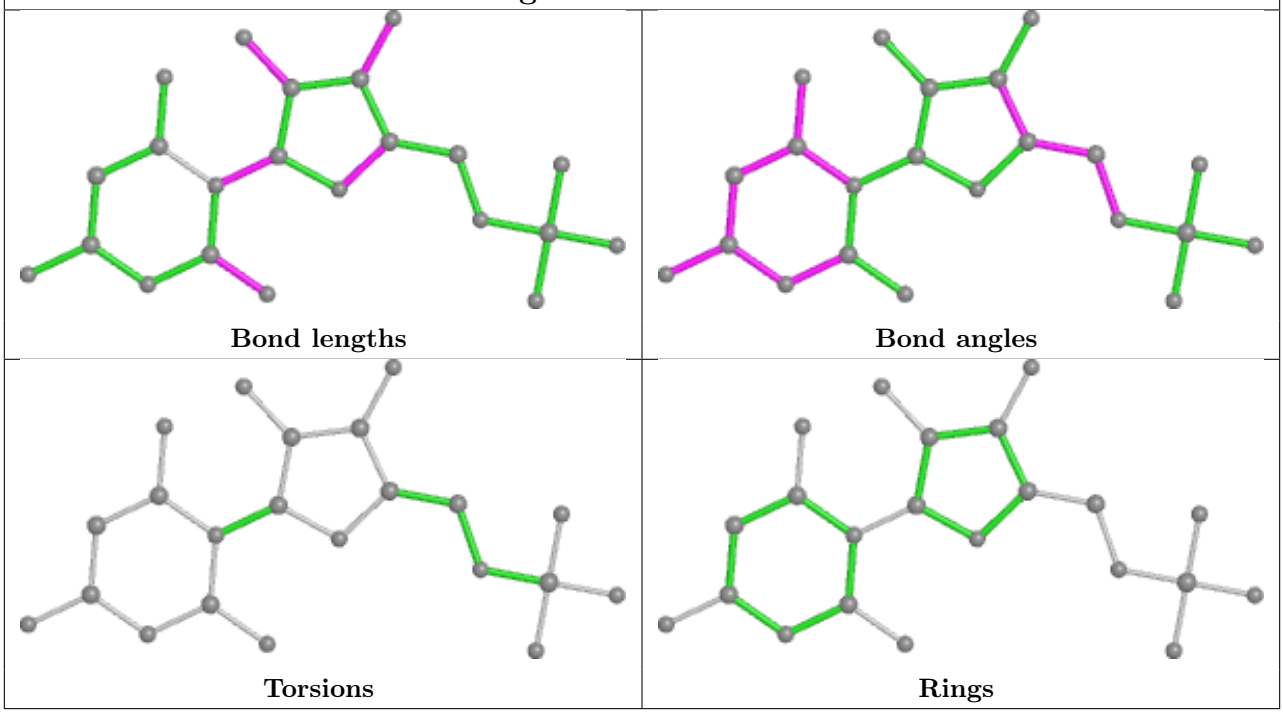


Torsions

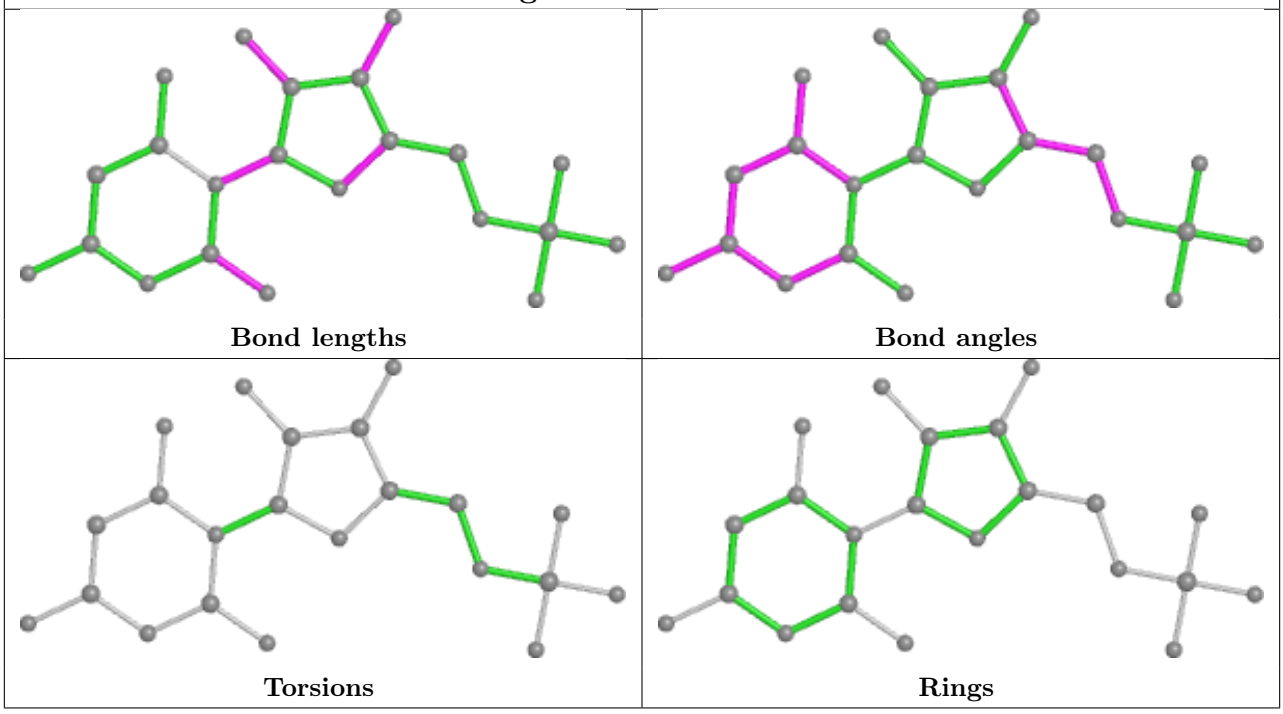


Rings

Ligand BMP K 311



Ligand BMP D 304



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	223/245 (91%)	0.32	5 (2%) 62 33	1, 23, 44, 59	0
1	B	223/245 (91%)	0.34	6 (2%) 54 26	1, 23, 44, 59	0
1	C	223/245 (91%)	0.19	1 (0%) 92 79	1, 23, 44, 59	0
1	D	223/245 (91%)	0.26	4 (1%) 68 40	1, 23, 44, 59	0
1	E	223/245 (91%)	0.40	7 (3%) 49 21	1, 23, 44, 59	0
1	F	223/245 (91%)	0.52	6 (2%) 54 26	1, 23, 44, 59	0
1	G	223/245 (91%)	0.33	4 (1%) 68 40	1, 23, 44, 59	0
1	H	223/245 (91%)	0.26	6 (2%) 54 26	1, 23, 44, 59	0
1	I	223/245 (91%)	0.44	14 (6%) 20 6	1, 23, 44, 59	0
1	J	223/245 (91%)	0.63	22 (9%) 7 2	1, 23, 44, 59	0
1	K	223/245 (91%)	0.79	13 (5%) 23 7	1, 23, 44, 59	0
1	L	223/245 (91%)	0.76	21 (9%) 8 3	1, 23, 44, 59	0
1	M	223/245 (91%)	0.85	18 (8%) 12 3	1, 23, 44, 59	0
1	N	223/245 (91%)	0.95	34 (15%) 2 1	1, 23, 44, 59	0
1	O	223/245 (91%)	1.19	46 (20%) 1 0	1, 23, 44, 59	0
1	P	223/245 (91%)	0.92	30 (13%) 3 1	1, 23, 44, 59	0
All	All	3568/3920 (91%)	0.57	237 (6%) 18 5	1, 23, 45, 59	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	14	ASN	5.8
1	O	197	GLU	5.1
1	O	191	ILE	5.1
1	K	121	ALA	4.7
1	O	148	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	N	238	ASN	4.5
1	B	140	ASP	4.3
1	P	196	SER	4.2
1	J	147	PRO	4.1
1	N	34	ASP	4.1
1	O	193	PRO	4.1
1	O	229	ASP	4.0
1	P	194	GLN	4.0
1	B	12	VAL	3.9
1	N	193	PRO	3.9
1	O	19	VAL	3.9
1	K	12	VAL	3.9
1	P	228	VAL	3.9
1	I	178	GLN	3.8
1	F	144	THR	3.7
1	N	212	SER	3.7
1	P	200	ASP	3.7
1	L	63	GLN	3.7
1	E	194	GLN	3.7
1	J	169	SER	3.6
1	O	142	GLY	3.6
1	J	229	ASP	3.6
1	L	210	ALA	3.6
1	F	142	GLY	3.6
1	P	214	GLY	3.6
1	O	232	GLN	3.6
1	P	12	VAL	3.5
1	M	214	GLY	3.5
1	O	211	LEU	3.5
1	P	151	ALA	3.5
1	N	239	ALA	3.5
1	O	228	VAL	3.5
1	N	214	GLY	3.5
1	N	235	LYS	3.4
1	I	142	GLY	3.4
1	L	195	GLY	3.4
1	L	144	THR	3.4
1	I	213	ALA	3.4
1	J	232	GLN	3.4
1	O	196	SER	3.3
1	G	144	THR	3.3
1	N	170	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	N	197	GLU	3.3
1	N	191	ILE	3.3
1	O	190	GLY	3.3
1	M	178	GLN	3.2
1	L	196	SER	3.2
1	O	151	ALA	3.2
1	L	14	ASN	3.2
1	N	232	GLN	3.2
1	K	39	ARG	3.1
1	O	14	ASN	3.1
1	O	188	THR	3.1
1	J	231	ALA	3.1
1	D	12	VAL	3.1
1	O	212	SER	3.1
1	P	190	GLY	3.1
1	O	15	SER	3.1
1	F	213	ALA	3.1
1	A	142	GLY	3.1
1	O	189	PRO	3.0
1	J	196	SER	3.0
1	P	199	GLY	3.0
1	I	228	VAL	3.0
1	N	224	VAL	3.0
1	L	194	GLN	3.0
1	N	241	LEU	3.0
1	M	230	PRO	3.0
1	P	197	GLU	3.0
1	O	17	VAL	3.0
1	O	132	SER	2.9
1	K	144	THR	2.9
1	N	15	SER	2.9
1	A	173	ALA	2.9
1	J	207	PRO	2.9
1	J	228	VAL	2.9
1	G	135	ALA	2.9
1	J	173	ALA	2.9
1	N	198	ALA	2.9
1	M	189	PRO	2.9
1	N	223	PRO	2.9
1	B	178	GLN	2.9
1	M	28	ASP	2.8
1	N	13	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	226	GLN	2.8
1	O	238	ASN	2.8
1	O	176	PHE	2.8
1	O	182	GLN	2.8
1	O	241	LEU	2.8
1	O	207	PRO	2.8
1	O	198	ALA	2.8
1	P	195	GLY	2.8
1	J	161	CYS	2.8
1	O	40	ASP	2.8
1	O	230	PRO	2.8
1	N	231	ALA	2.7
1	O	170	ALA	2.7
1	L	241	LEU	2.7
1	L	135	ALA	2.7
1	O	41	CYS	2.7
1	O	37	ASP	2.7
1	M	16	PRO	2.7
1	K	139	VAL	2.7
1	N	144	THR	2.7
1	P	110	ALA	2.7
1	N	220	ILE	2.6
1	N	208	GLU	2.6
1	O	155	ALA	2.6
1	P	215	VAL	2.6
1	D	178	GLN	2.6
1	B	141	LEU	2.6
1	J	144	THR	2.6
1	P	213	ALA	2.6
1	I	194	GLN	2.6
1	E	100	ALA	2.6
1	L	31	ALA	2.6
1	F	242	GLN	2.6
1	J	15	SER	2.6
1	K	179	VAL	2.6
1	N	121	ALA	2.6
1	O	194	GLN	2.6
1	J	194	GLN	2.5
1	O	215	VAL	2.5
1	L	173	ALA	2.5
1	P	146	SER	2.5
1	O	31	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	230	PRO	2.5
1	B	213	ALA	2.5
1	O	162	GLY	2.5
1	I	214	GLY	2.5
1	J	14	ASN	2.5
1	N	65	GLY	2.5
1	G	142	GLY	2.5
1	E	144	THR	2.5
1	K	118	GLY	2.5
1	J	220	ILE	2.5
1	I	227	SER	2.4
1	J	148	ALA	2.4
1	M	35	LYS	2.4
1	H	140	ASP	2.4
1	M	120	ASP	2.4
1	O	134	GLU	2.4
1	O	158	THR	2.4
1	N	148	ALA	2.4
1	A	178	GLN	2.4
1	P	182	GLN	2.4
1	I	196	SER	2.4
1	K	92	GLY	2.4
1	L	13	THR	2.4
1	M	237	ILE	2.4
1	O	141	LEU	2.4
1	L	182	GLN	2.4
1	P	14	ASN	2.4
1	O	187	VAL	2.3
1	P	227	SER	2.3
1	H	232	GLN	2.3
1	P	102	GLY	2.3
1	N	90	ASP	2.3
1	J	189	PRO	2.3
1	J	35	LYS	2.3
1	L	163	LEU	2.3
1	L	204	ILE	2.3
1	P	240	SER	2.3
1	O	25	ASN	2.3
1	P	210	ALA	2.3
1	O	152	GLU	2.3
1	D	141	LEU	2.3
1	P	175	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	176	PHE	2.3
1	M	210	ALA	2.3
1	H	120	ASP	2.3
1	L	34	ASP	2.3
1	E	182	GLN	2.3
1	G	226	GLN	2.3
1	H	242	GLN	2.3
1	A	14	ASN	2.3
1	N	21	LEU	2.3
1	O	120	ASP	2.2
1	I	237	ILE	2.2
1	K	183	GLU	2.2
1	N	194	GLN	2.2
1	O	235	LYS	2.2
1	K	65	GLY	2.2
1	M	63	GLN	2.2
1	H	144	THR	2.2
1	M	190	GLY	2.2
1	M	225	THR	2.2
1	L	61	LEU	2.2
1	O	204	ILE	2.2
1	I	33	VAL	2.2
1	L	227	SER	2.2
1	M	198	ALA	2.2
1	I	212	SER	2.2
1	P	138	LEU	2.2
1	P	34	ASP	2.2
1	A	12	VAL	2.2
1	I	192	ARG	2.2
1	K	34	ASP	2.2
1	F	241	LEU	2.1
1	B	193	PRO	2.1
1	N	27	ASP	2.1
1	E	104	ALA	2.1
1	P	178	GLN	2.1
1	J	230	PRO	2.1
1	M	90	ASP	2.1
1	P	149	ASP	2.1
1	I	39	ARG	2.1
1	P	24	HIS	2.1
1	M	146	SER	2.1
1	E	178	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	201	GLN	2.1
1	J	195	GLY	2.1
1	H	195	GLY	2.1
1	M	182	GLN	2.1
1	E	142	GLY	2.1
1	I	28	ASP	2.1
1	N	210	ALA	2.1
1	C	229	ASP	2.1
1	O	30	LEU	2.1
1	P	41	CYS	2.1
1	D	235	LYS	2.1
1	M	144	THR	2.1
1	N	12	VAL	2.1
1	L	15	SER	2.1
1	J	13	THR	2.0
1	J	63	GLN	2.0
1	K	149	ASP	2.0
1	K	40	ASP	2.0
1	P	161	CYS	2.0
1	L	56	GLN	2.0
1	N	178	GLN	2.0
1	F	37	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMP	O	315	22/22	0.73	0.31	6,8,12,13	0

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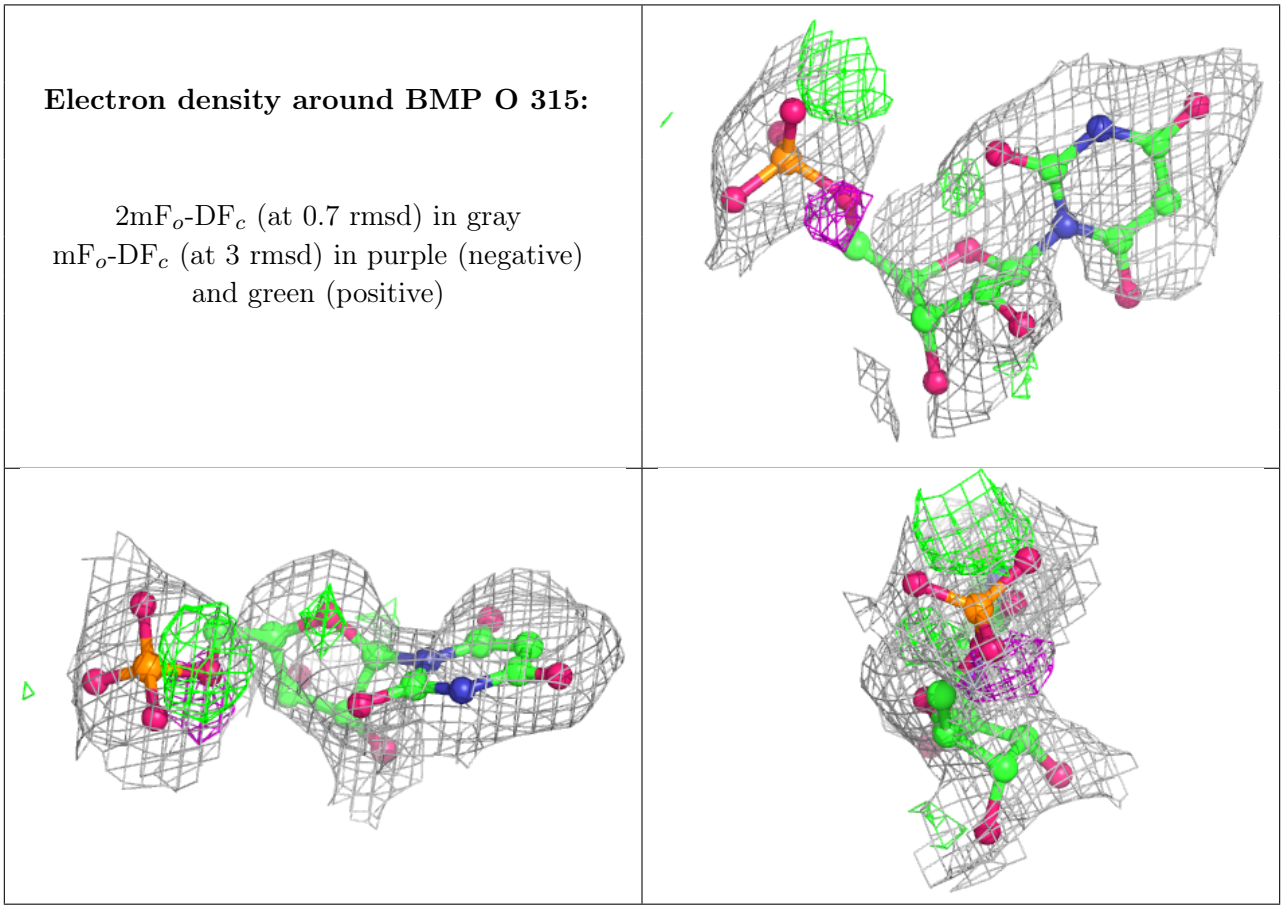
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMP	M	313	22/22	0.76	0.29	6,8,12,13	0
2	BMP	N	314	22/22	0.80	0.28	6,8,12,13	0
2	BMP	L	312	22/22	0.84	0.22	6,8,12,13	0
2	BMP	E	305	22/22	0.84	0.25	6,8,12,13	0
2	BMP	B	302	22/22	0.85	0.23	6,8,12,13	0
2	BMP	F	306	22/22	0.85	0.20	6,8,12,13	0
2	BMP	G	307	22/22	0.87	0.23	6,8,12,13	0
2	BMP	A	301	22/22	0.88	0.21	6,8,12,13	0
2	BMP	J	310	22/22	0.88	0.21	6,8,12,13	0
2	BMP	P	316	22/22	0.88	0.20	6,8,12,13	0
2	BMP	K	311	22/22	0.90	0.17	6,8,12,13	0
2	BMP	I	309	22/22	0.90	0.20	6,8,12,13	0
2	BMP	D	304	22/22	0.91	0.18	6,8,12,13	0
2	BMP	C	303	22/22	0.91	0.17	6,8,12,13	0
2	BMP	H	308	22/22	0.93	0.15	6,8,12,13	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

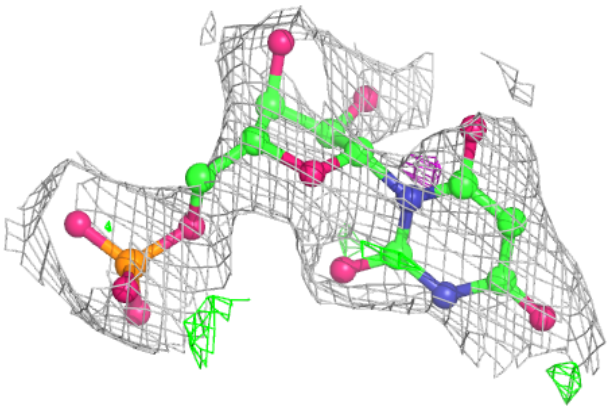
Electron density around BMP O 315:

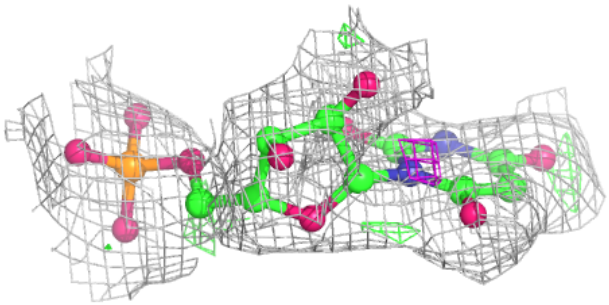
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BMP M 313:

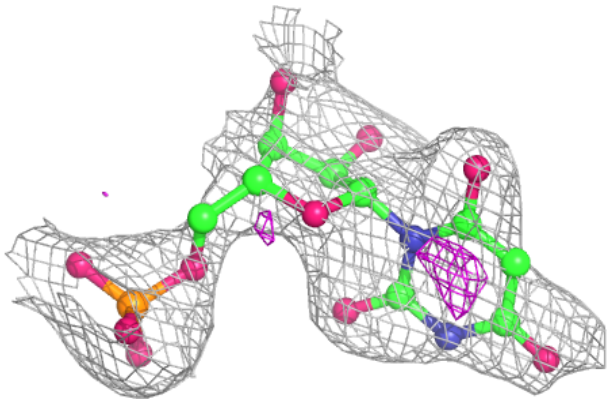
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

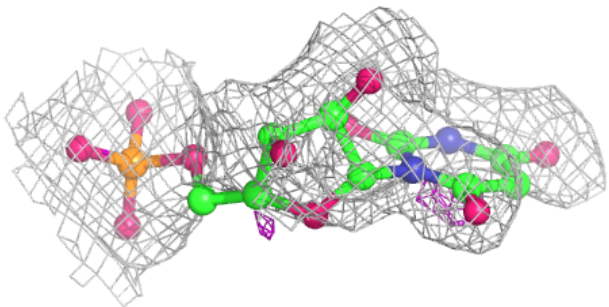


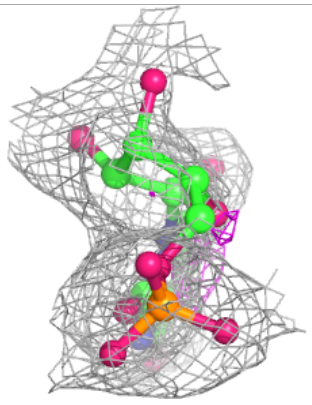


Electron density around BMP N 314:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

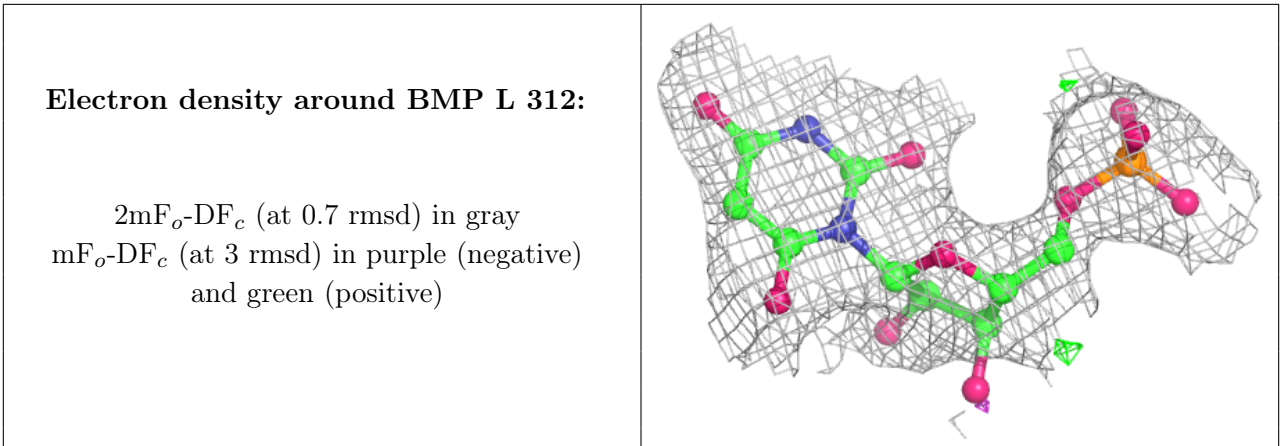






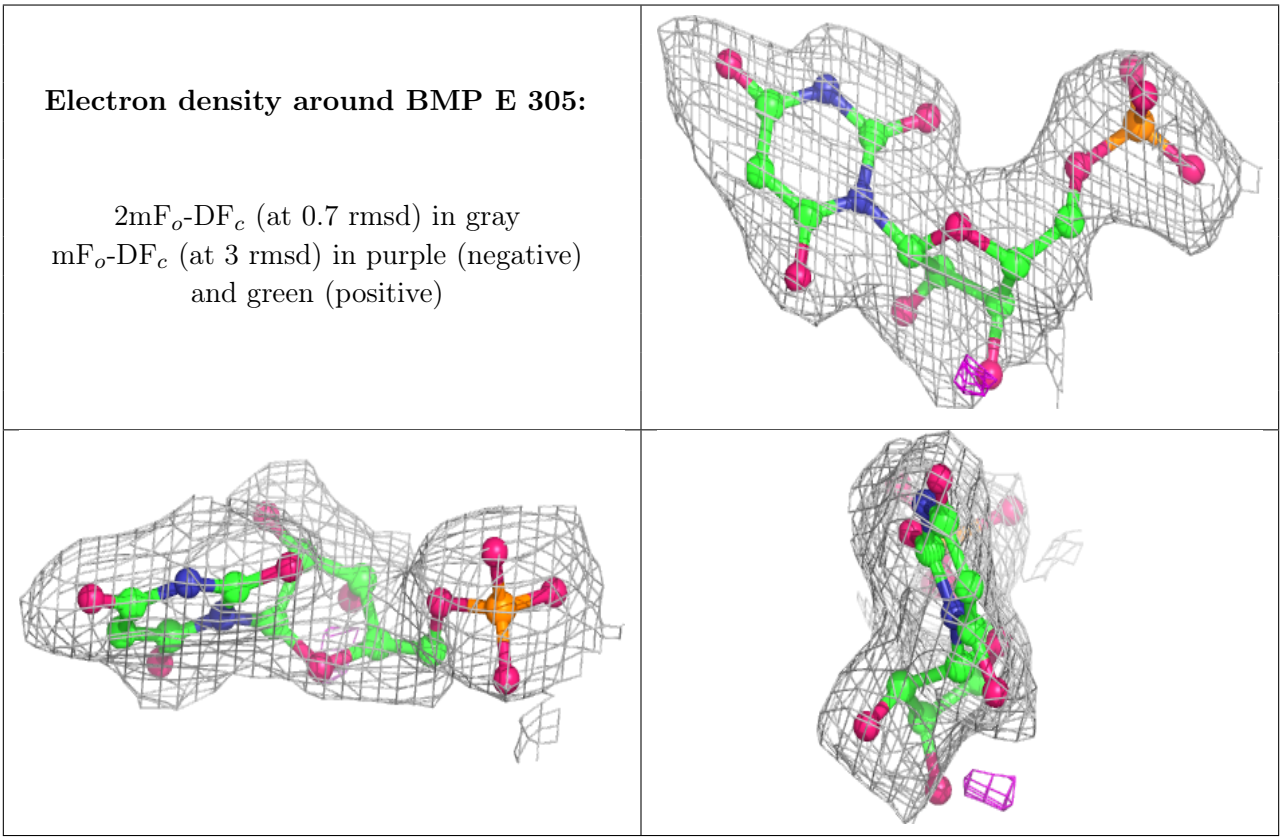
Electron density around BMP L 312:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



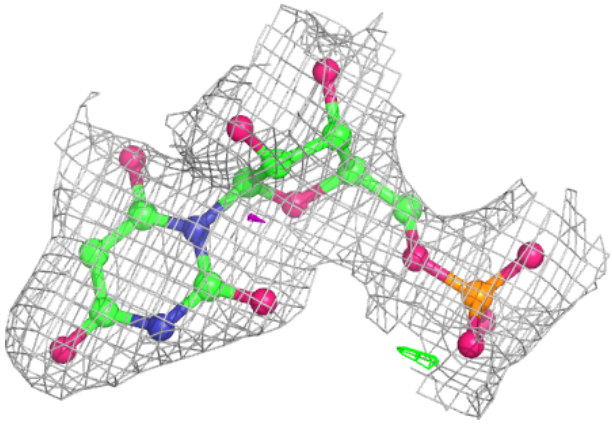
Electron density around BMP E 305:

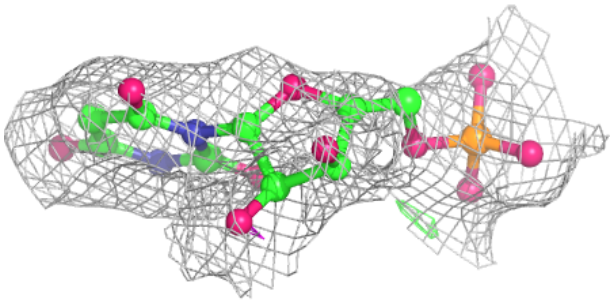
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

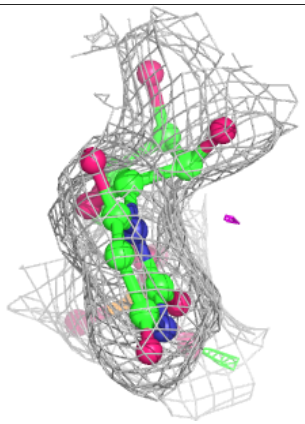


Electron density around BMP B 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

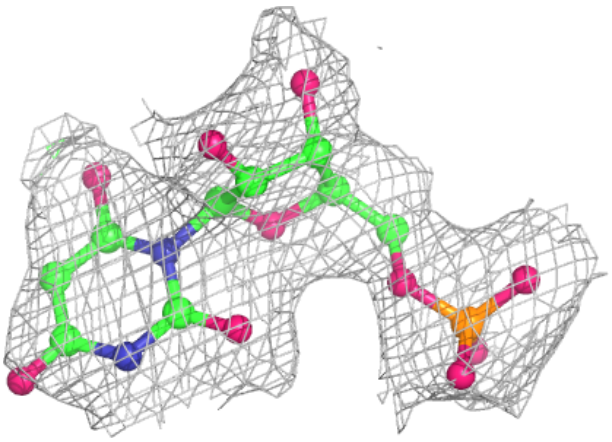


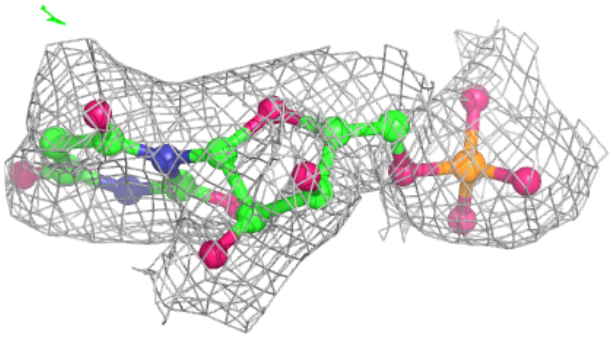


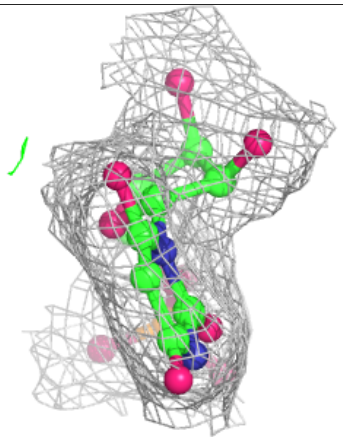


Electron density around BMP F 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

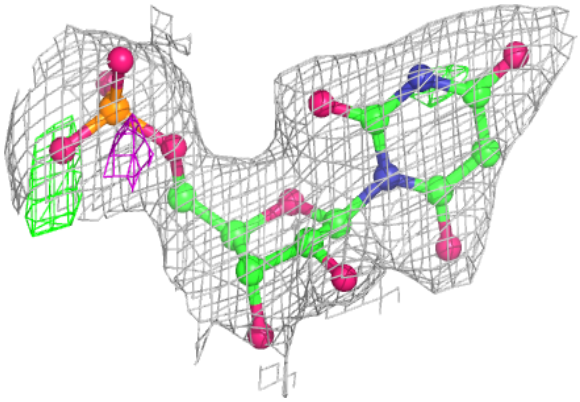


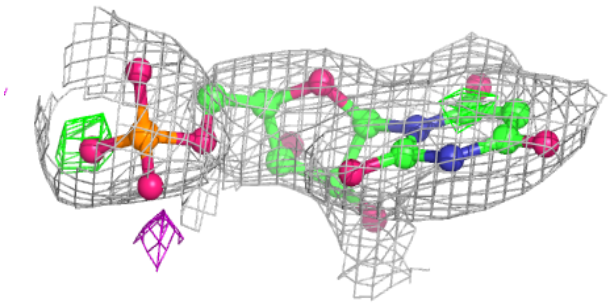


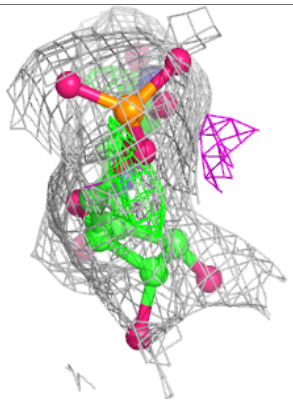


Electron density around BMP G 307:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

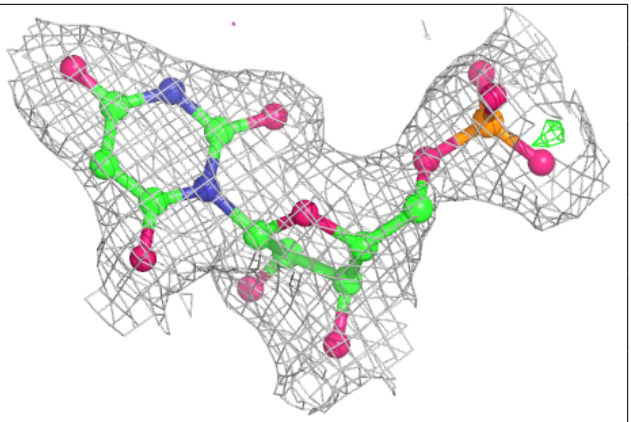


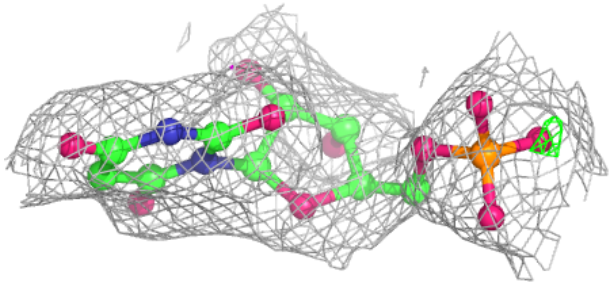


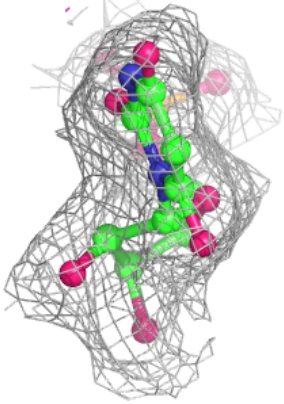


Electron density around BMP A 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

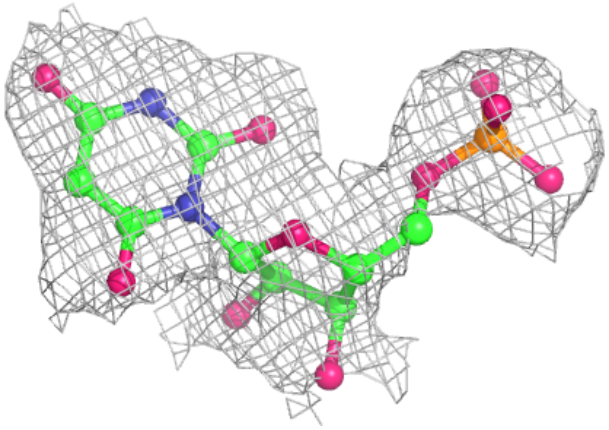


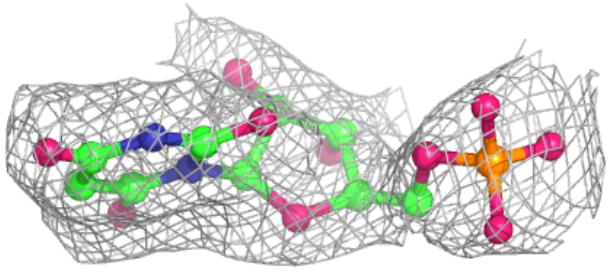


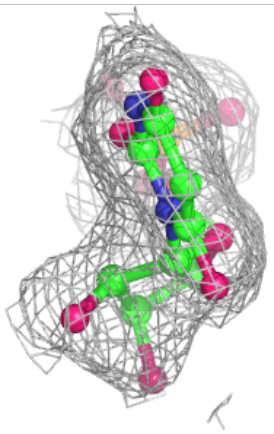


Electron density around BMP J 310:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

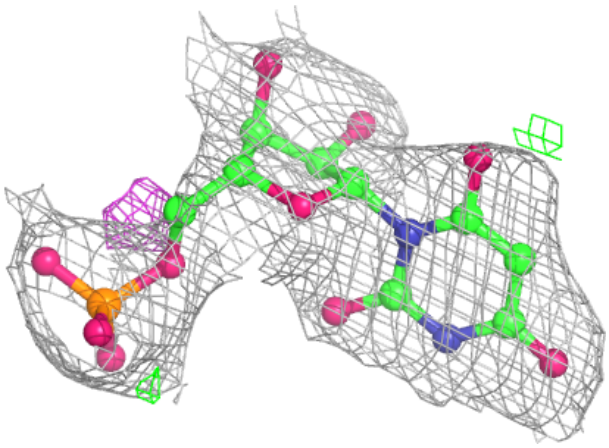


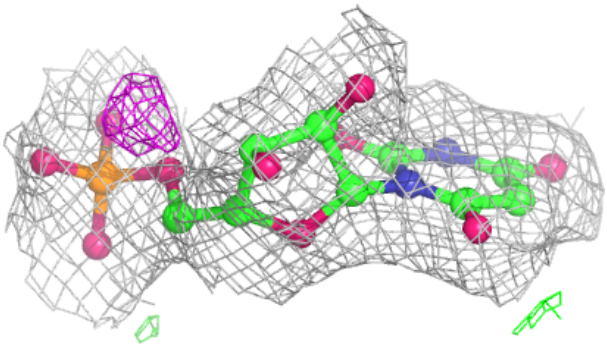


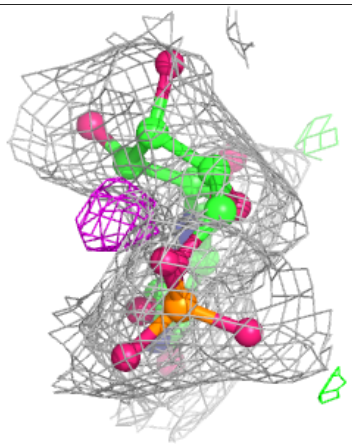


Electron density around BMP P 316:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

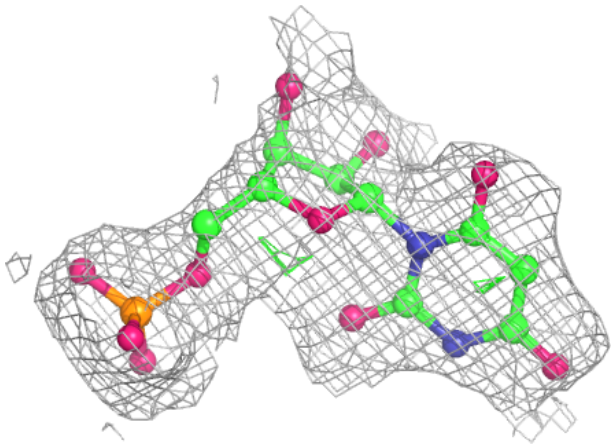


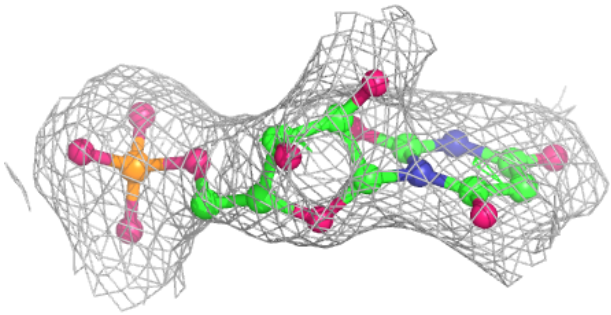


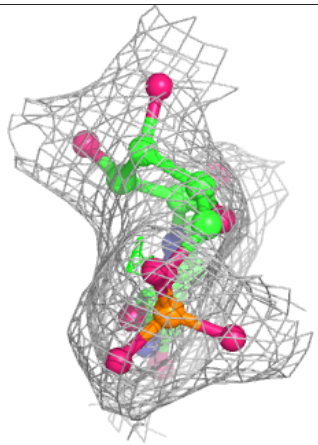


Electron density around BMP K 311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

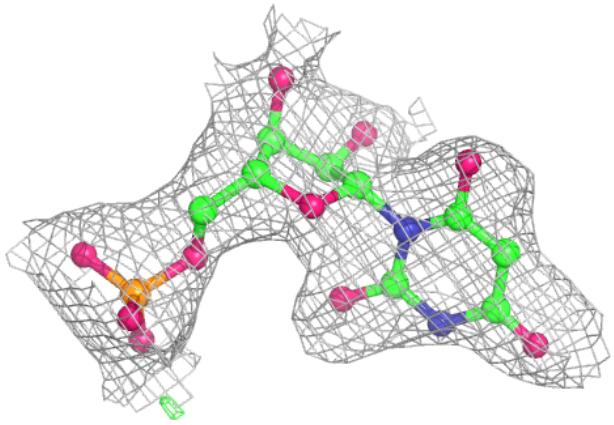


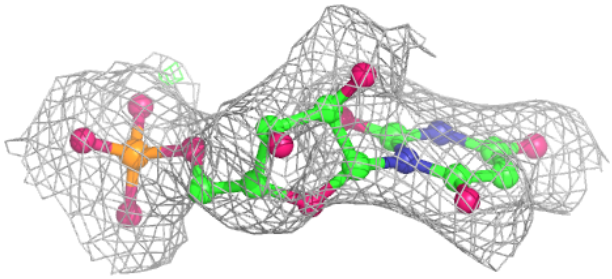


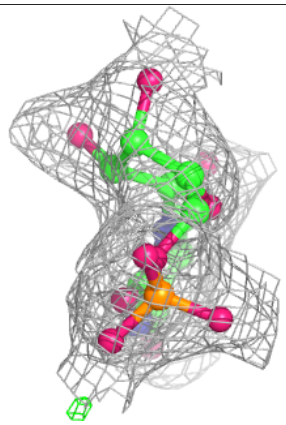


Electron density around BMP I 309:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

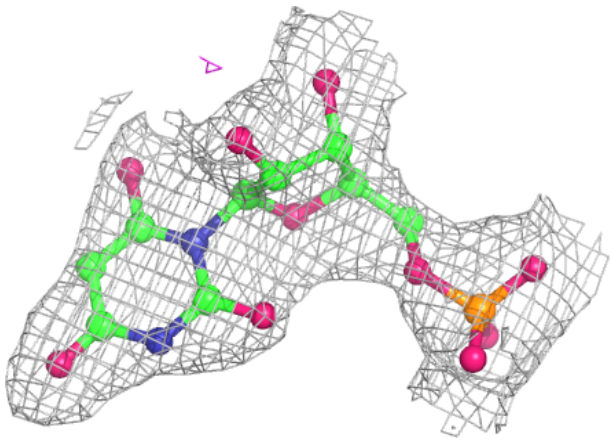


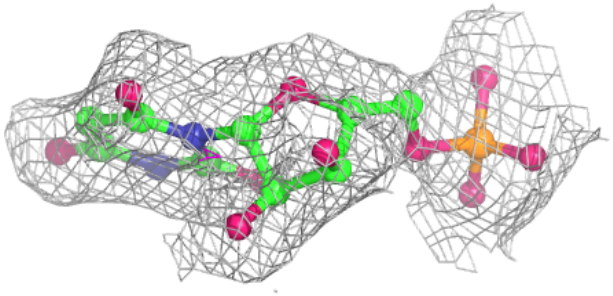


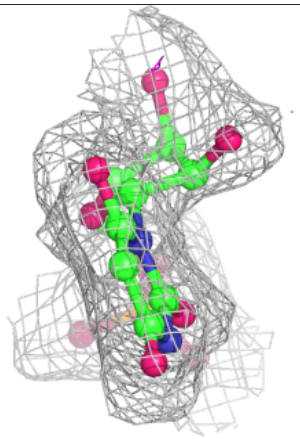


Electron density around BMP D 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

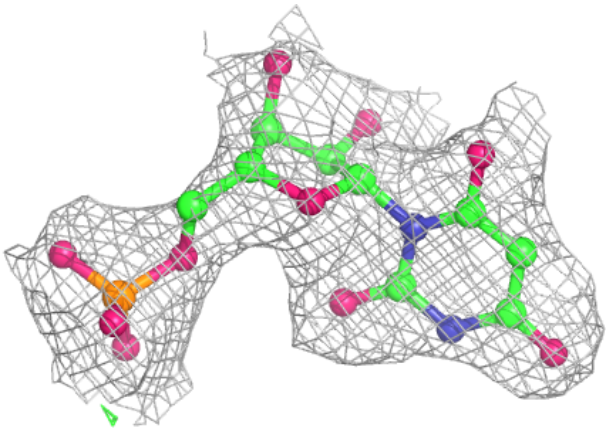


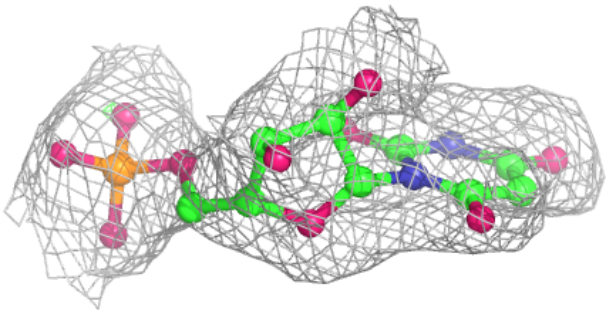


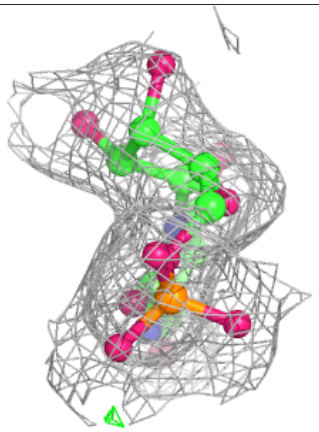


Electron density around BMP C 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

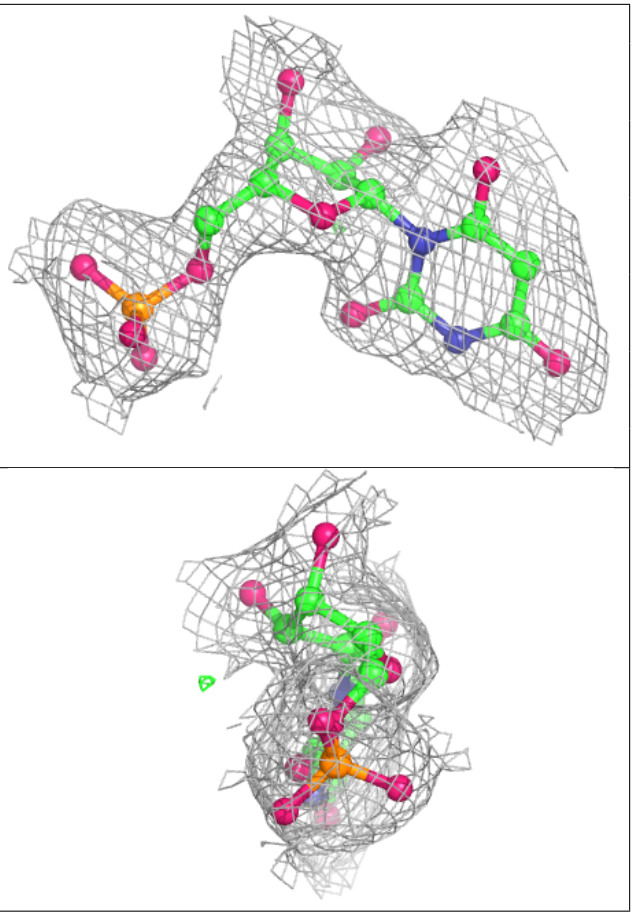






Electron density around BMP H 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.