Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 05:00 pm GMT

PDB ID	:	2WIN
Title	:	C3 convertase (C3bBb) stabilized by SCIN
Authors	:	Wu, J.; Janssen, B.J.; Gros, P.
Deposited on	:	2009-05-13
Resolution	:	3.90 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 (i) 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 (1)) were used in the production of this report:

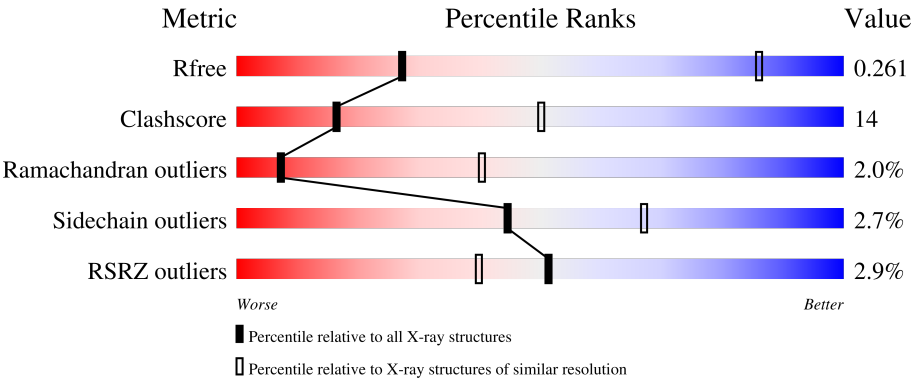
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	645	2% 72% 25%
1	C	645	2% 72% 26%
1	E	645	2% 72% 26%
1	G	645	9% 71% 27%
2	B	915	% 69% 26%

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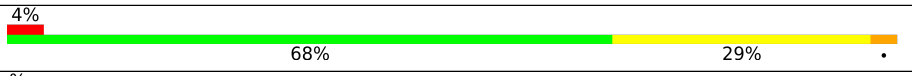
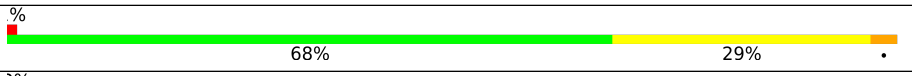
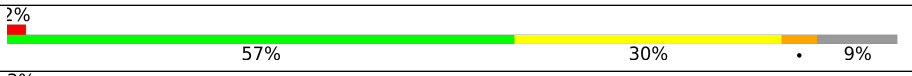
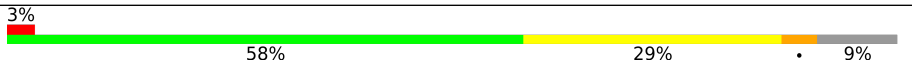
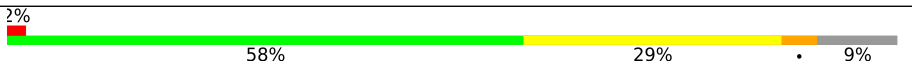
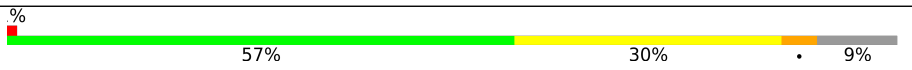
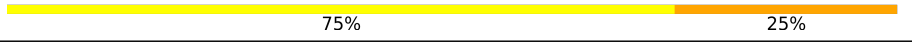
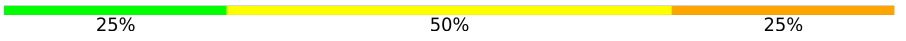
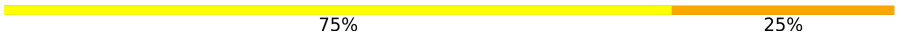
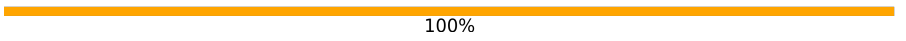
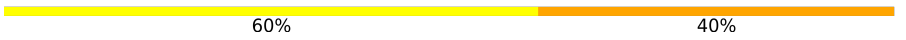
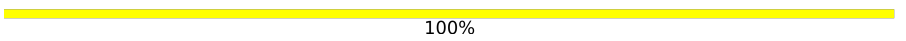
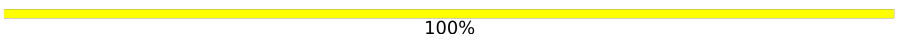
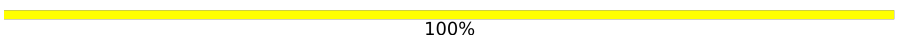
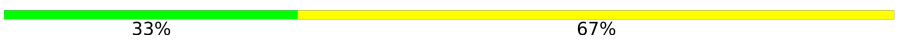
Mol	Chain	Length	Quality of chain
2	D	915	
2	F	915	
2	H	915	
3	I	507	
3	J	507	
3	K	507	
3	L	507	
4	M	92	
4	N	92	
4	P	92	
4	Q	92	
5	O	4	
5	R	4	
5	T	4	
5	U	4	
6	S	5	
6	W	5	
7	V	6	
8	X	4	
9	Y	3	
9	a	3	
10	Z	2	
11	b	5	
12	c	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	Z	1	X	-	-	-
11	NAG	b	1	X	-	-	-
11	MAN	b	3	X	-	-	-
11	MAN	b	4	X	-	-	-
11	MAN	b	5	X	-	-	-
16	NAG	K	1749	X	-	-	-
16	NAG	L	1746	X	-	-	-
5	NAG	O	1	X	-	-	-
6	BMA	W	5	-	-	-	X
7	NAG	V	1	X	-	-	-
8	MAN	X	3	X	-	-	-
8	MAN	X	4	X	-	-	-
9	MAN	Y	3	X	-	-	-
9	MAN	a	3	X	-	-	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 67989 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 COMPLEMENT C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	C	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	E	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	G	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	901	Total	C	N	O	S	0	0	0
			7177	4545	1209	1386	37			
2	D	901	Total	C	N	O	S	0	0	0
			7166	4537	1208	1384	37			
2	F	900	Total	C	N	O	S	0	0	0
			7172	4545	1206	1384	37			
2	H	900	Total	C	N	O	S	2313	0	0
			7175	4547	1209	1382	37			

- Molecule 3 is a protein called COMPLEMENT FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	J	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	K	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	L	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			

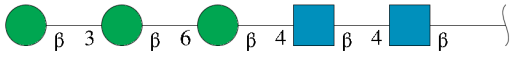
- Molecule 4 is a protein called STAPHYLOCOCCAL COMPLEMENT INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	N	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	P	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	Q	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-6)-beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucop yranose.

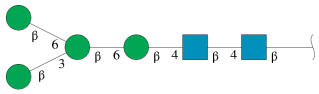
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	R	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	T	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	U	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose -(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acet amido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	S	5	Total	C	N	O	0	0	0
			61	34	2	25			
6	W	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

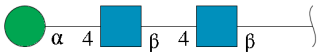


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	V	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	X	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

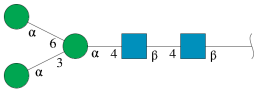


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
9	a	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

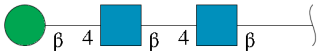
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	Z	2	Total C N O 28 16 2 10	0	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



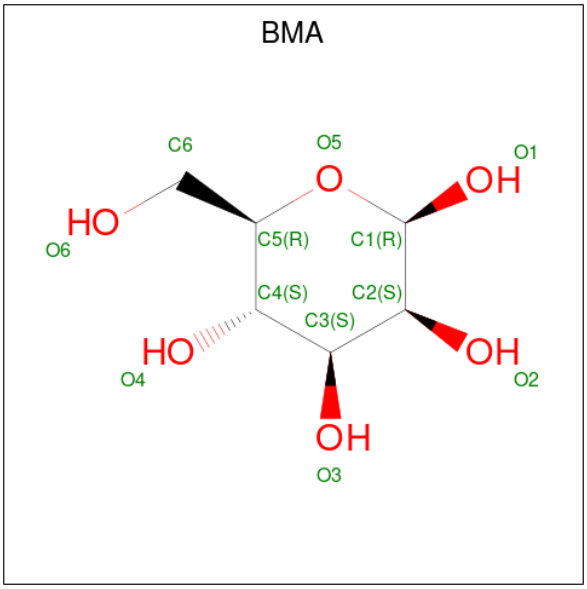
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	b	5	Total C N O 61 34 2 25	0	0	0

- Molecule 12 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



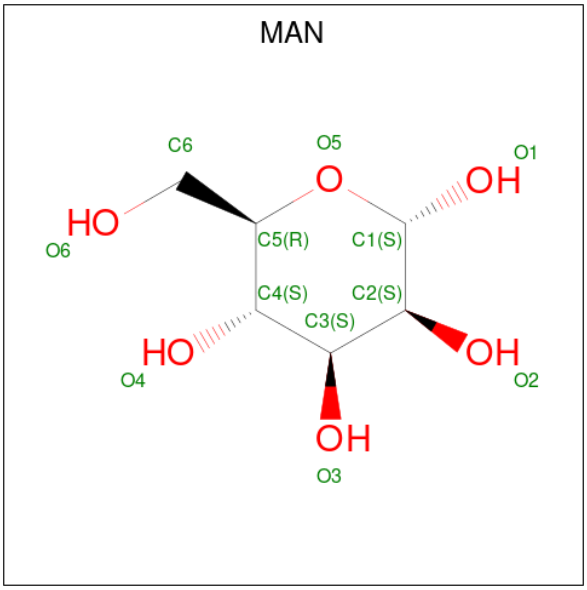
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	c	3	Total C N O 39 22 2 15	0	0	0

- Molecule 13 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C O 11 6 5	0	0
13	K	1	Total C O 11 6 5	0	0

- Molecule 14 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

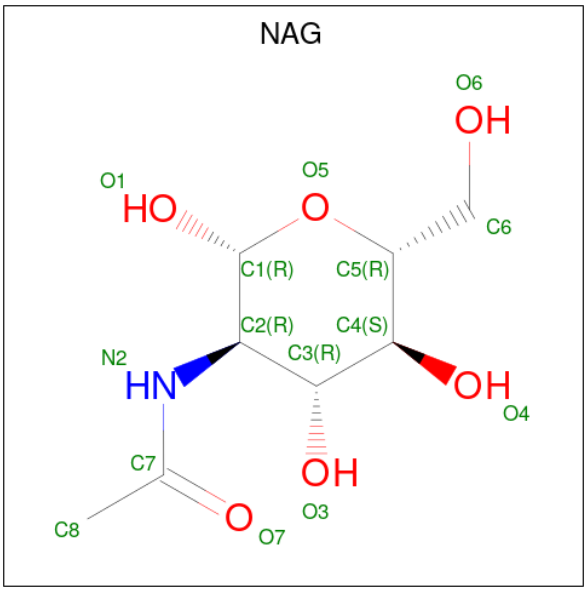


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	G	1	Total C O 11 6 5	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	I	1	Total Mg 1 1	0	0
15	J	1	Total Mg 1 1	0	0
15	K	1	Total Mg 1 1	0	0
15	L	1	Total Mg 1 1	0	0

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	K	1	Total C N O 14 8 1 5	0	0
16	L	1	Total C N O 14 8 1 5	0	0

- Molecule 17 is water.

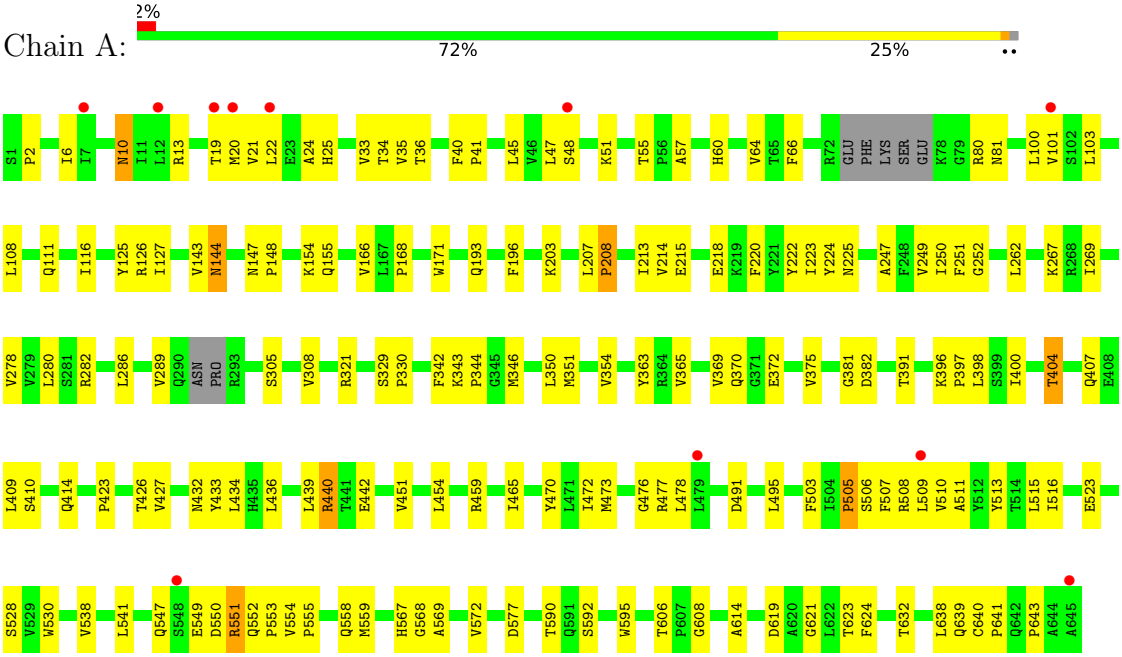
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	1	Total O 1 1	0	0
17	I	2	Total O 2 2	0	0
17	J	2	Total O 2 2	0	0
17	K	2	Total O 2 2	0	0
17	L	1	Total O 1 1	0	0

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.

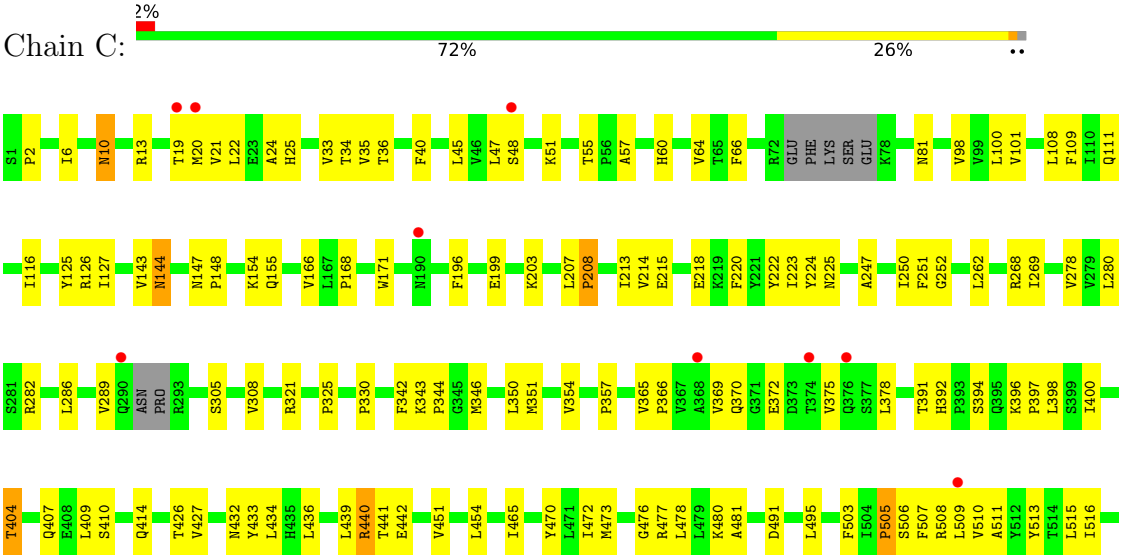
• Molecule 1: COMPLEMENT C3 BETA CHAIN

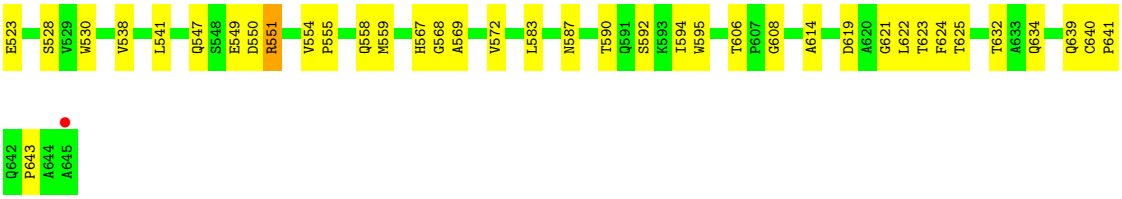
Chain A:



• Molecule 1: COMPLEMENT C3 BETA CHAIN

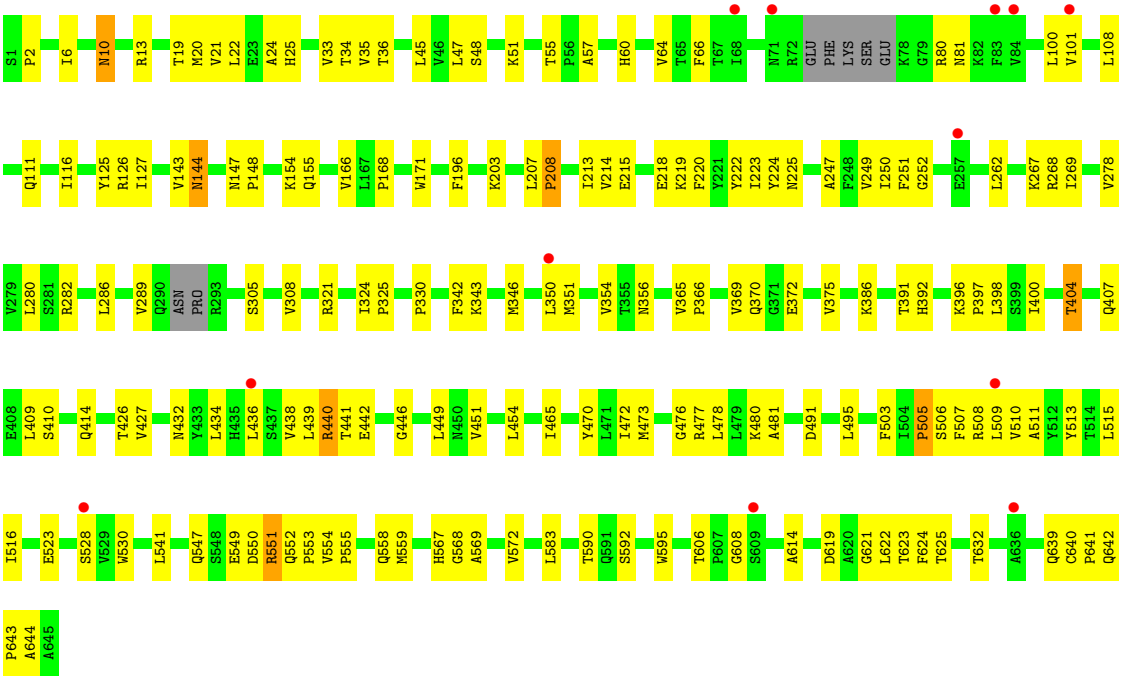
Chain C:





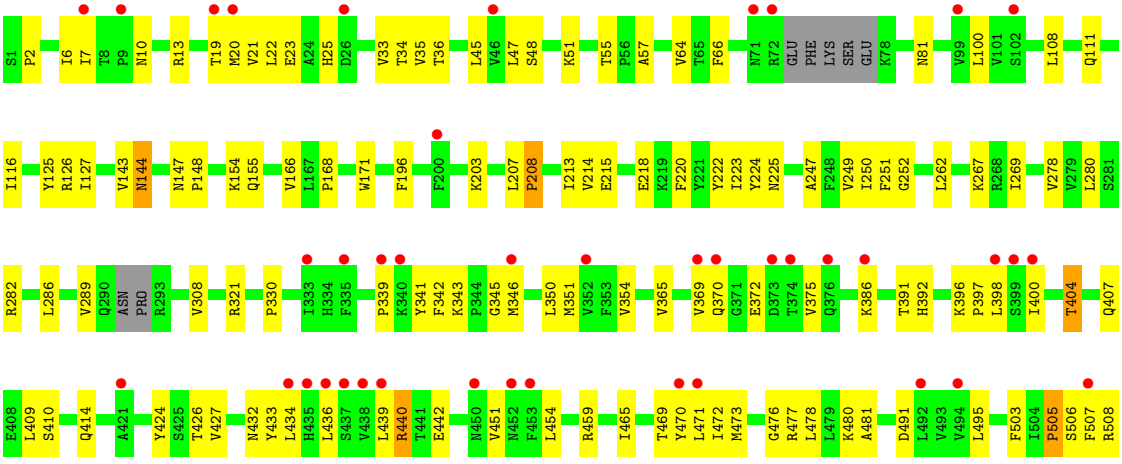
• Molecule 1: COMPLEMENT C3 BETA CHAIN

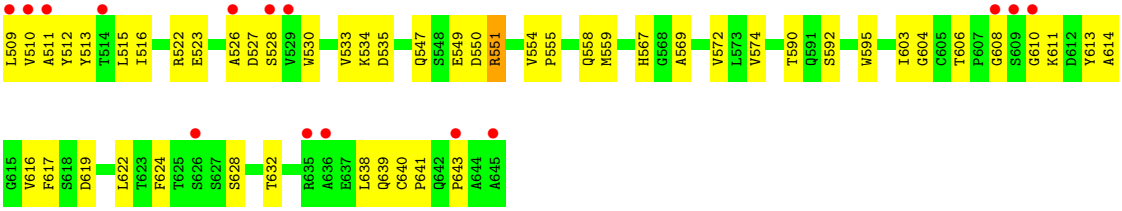
Chain E:



• Molecule 1: COMPLEMENT C3 BETA CHAIN

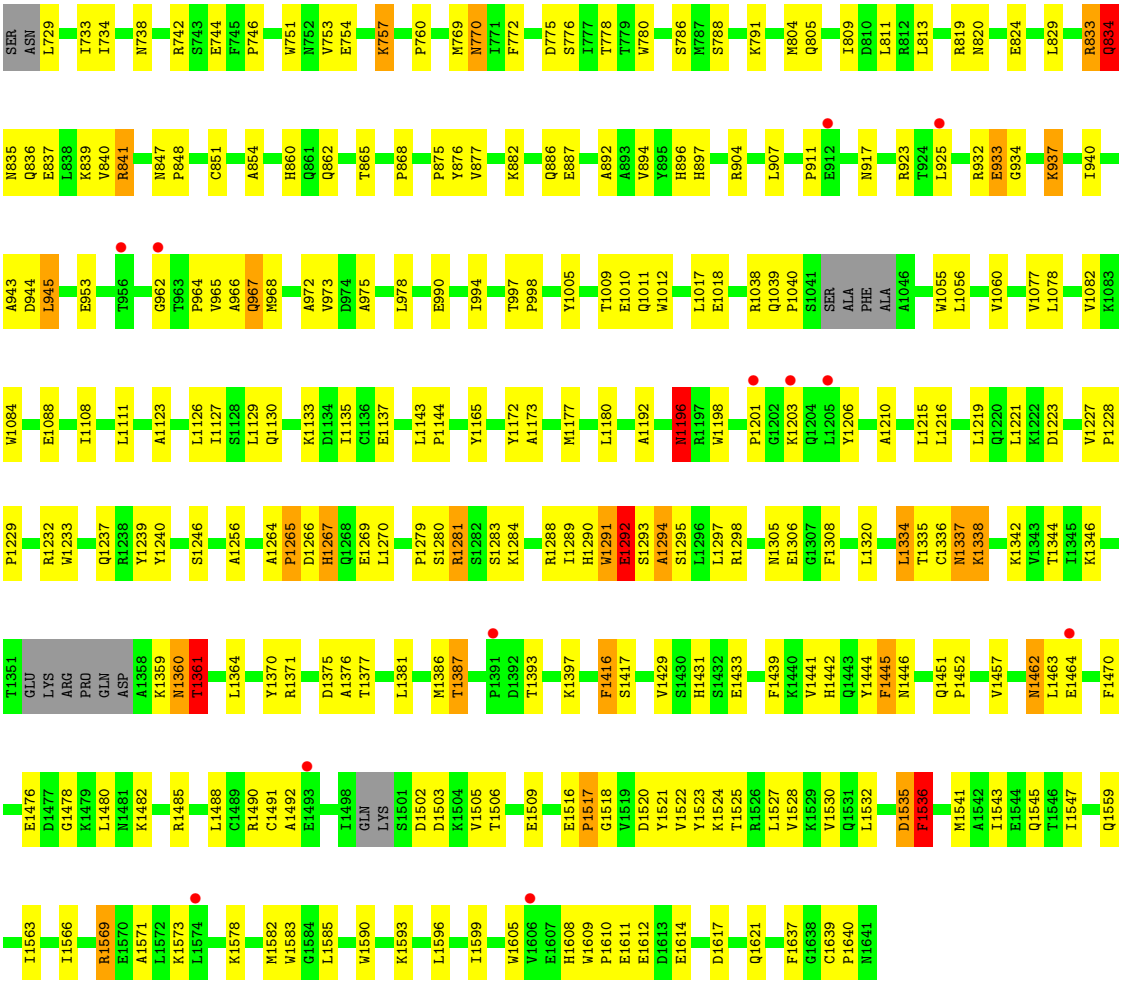
Chain G:





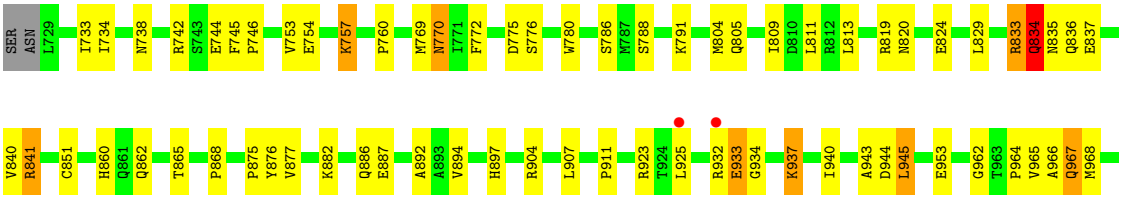
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

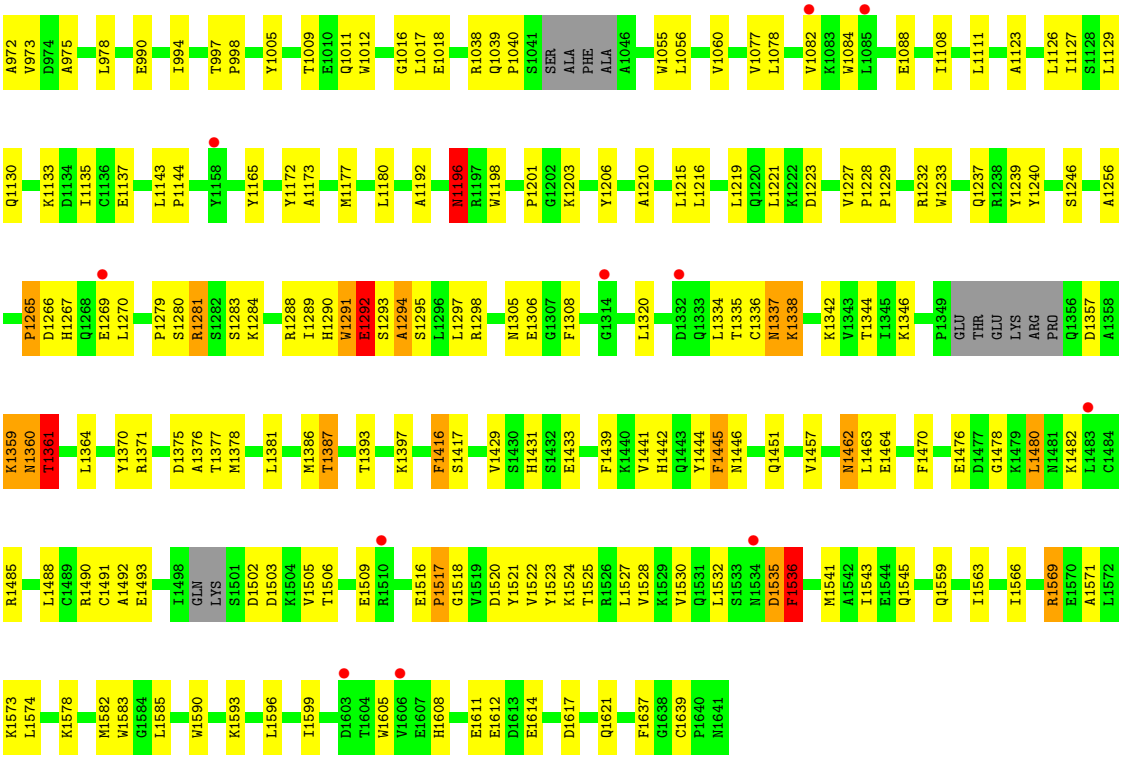
Chain B:



• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

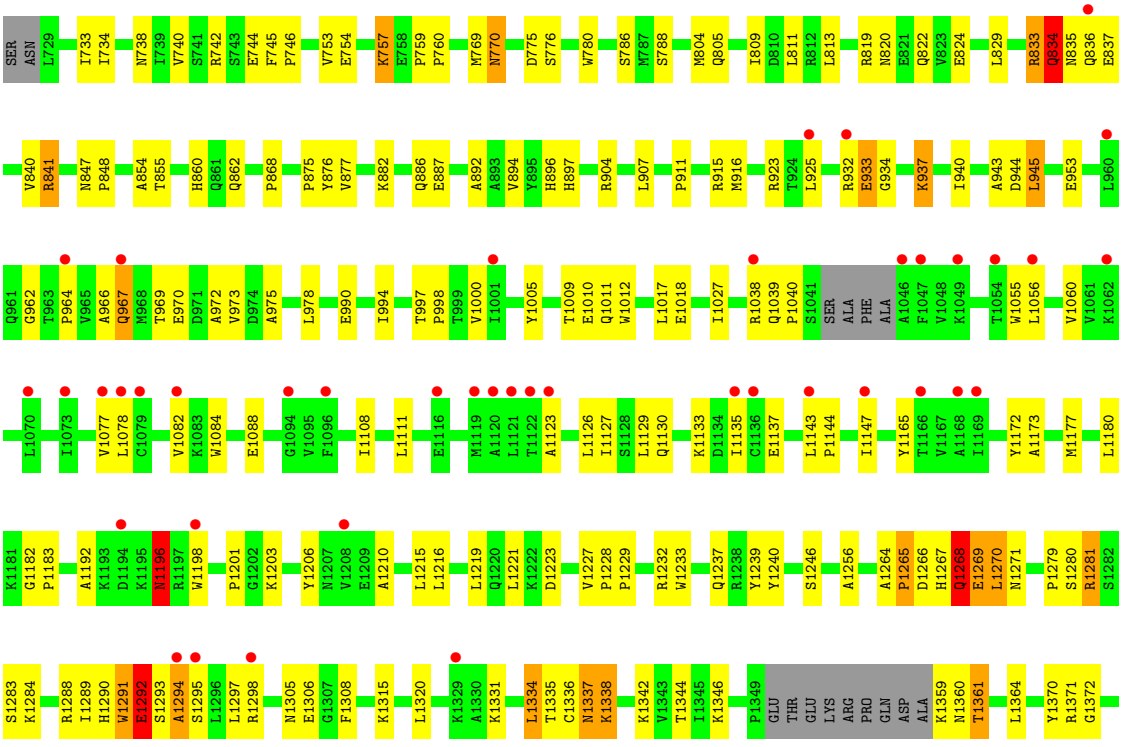
Chain D:

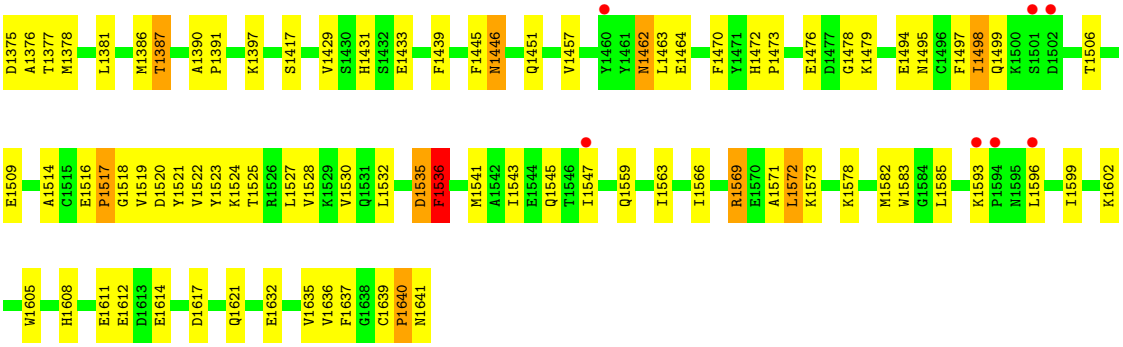




• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

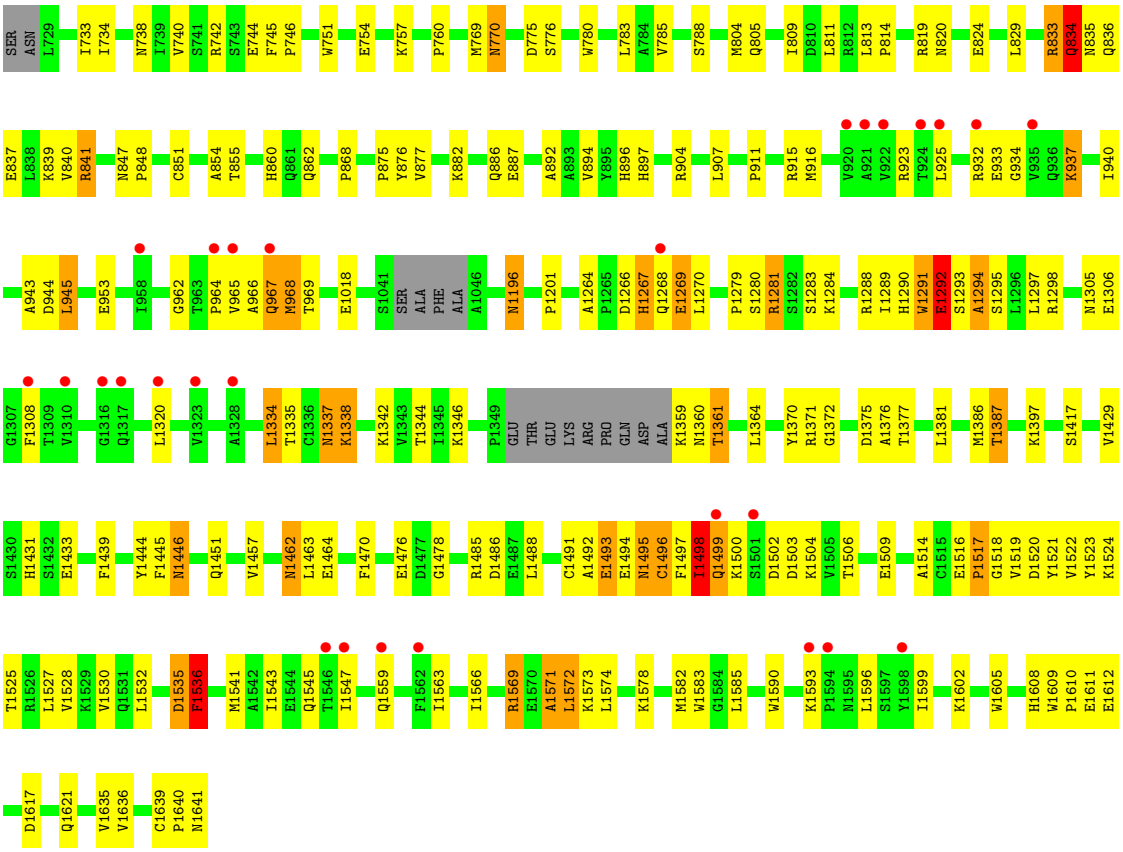
Chain F:





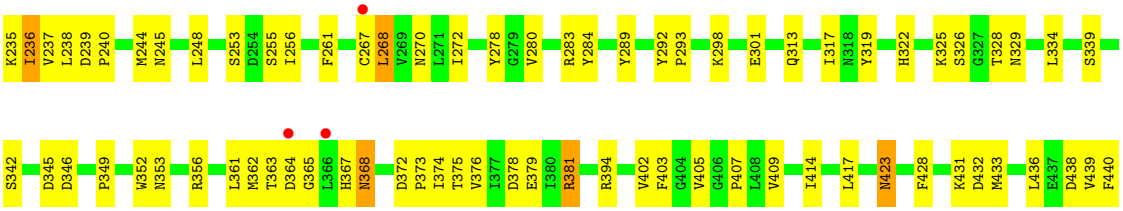
• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

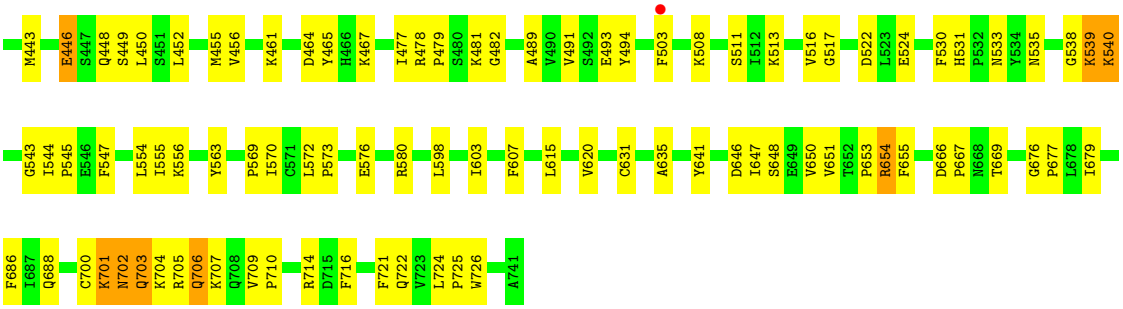
Chain H:



• Molecule 3: COMPLEMENT FACTOR B

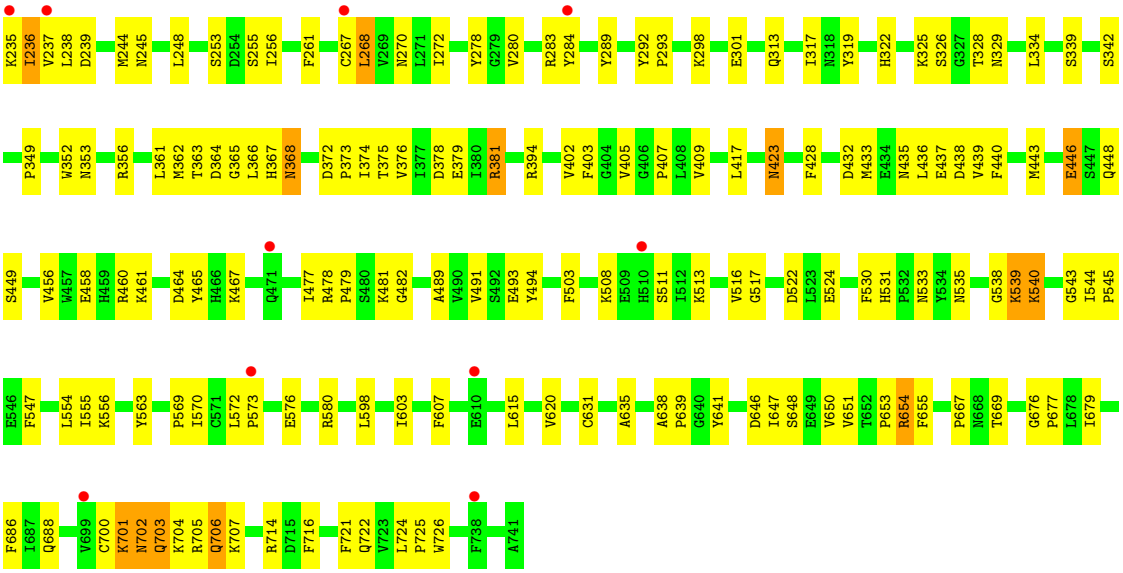
Chain I:





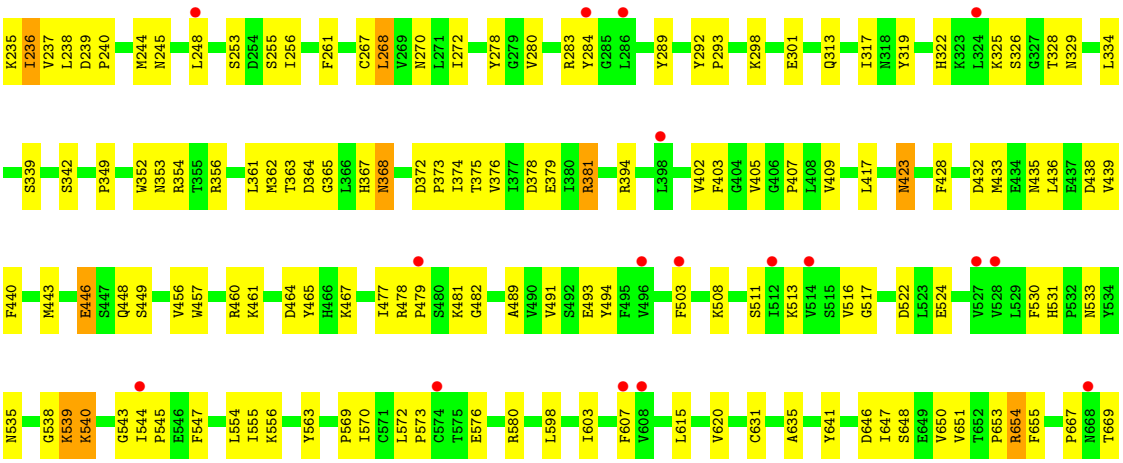
• Molecule 3: COMPLEMENT FACTOR B

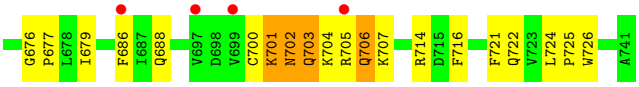
Chain J:



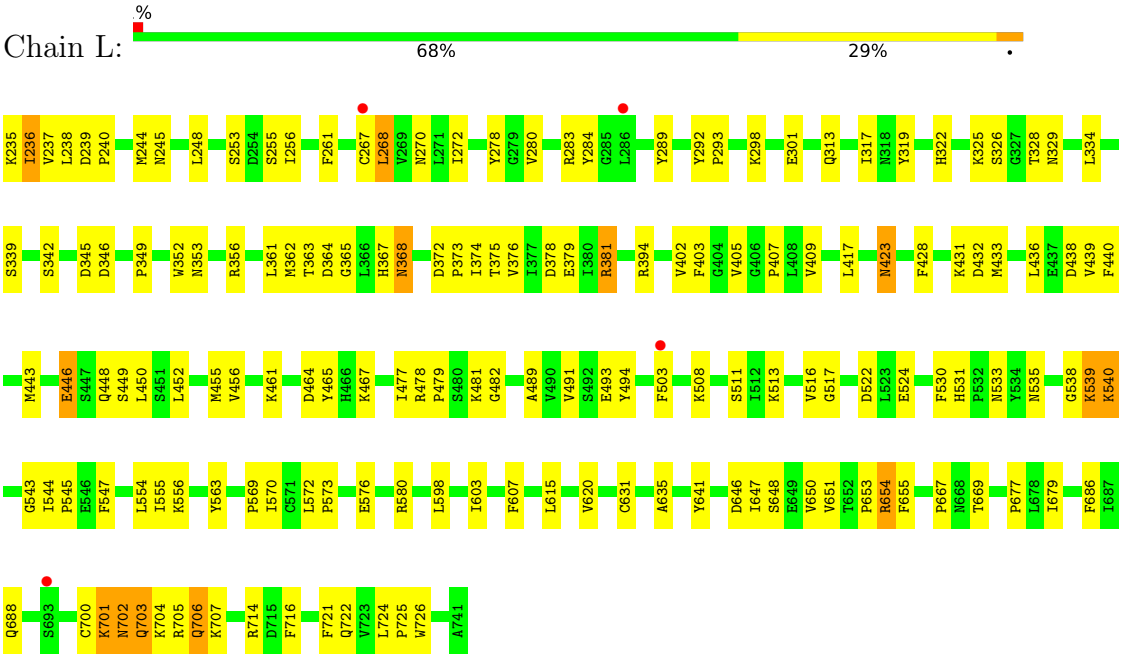
• Molecule 3: COMPLEMENT FACTOR B

Chain K:

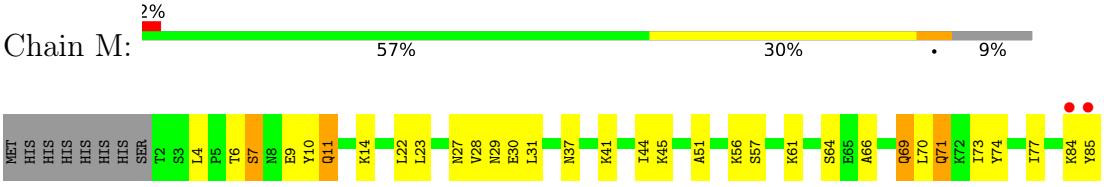




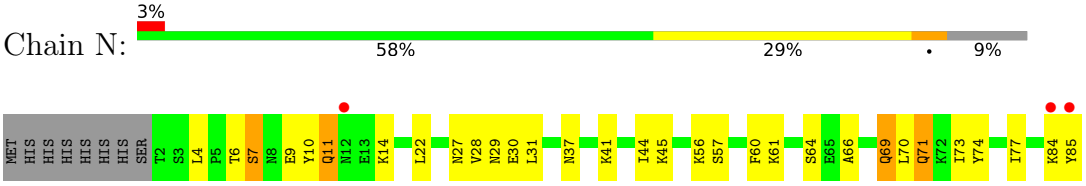
• Molecule 3: COMPLEMENT FACTOR B



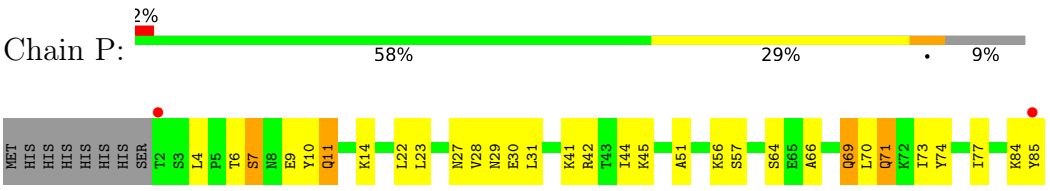
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



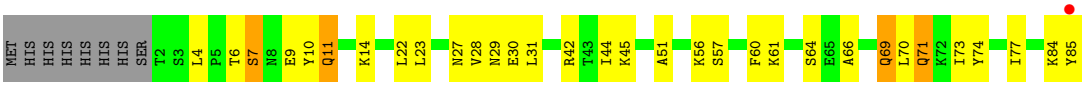
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR

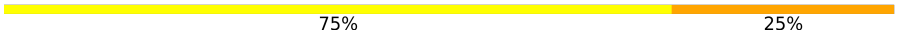


• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



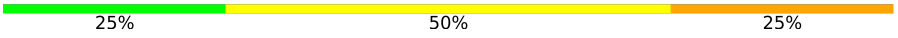
• Molecule 5: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 5: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 5: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

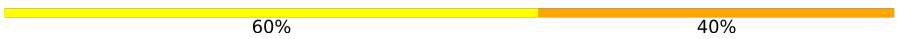
Chain T:

• Molecule 5: beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

• Molecule 6: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• Molecule 6: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

• Molecule 7: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose -(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido -2-deoxy-beta-D-glucopyranose

Chain V: 

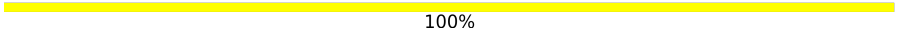
• Molecule 8: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

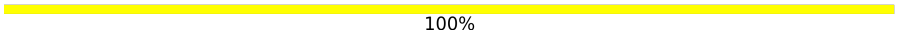
• Molecule 9: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 

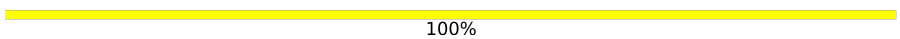
• Molecule 9: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 

• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 

• Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	228.63Å 121.49Å 280.78Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	39.67 – 3.90 39.68 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.67-3.90) 89.7 (39.68-3.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 3.87Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.253 , 0.268 0.247 , 0.261	Depositor DCC
R_{free} test set	2089 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å^2)	125.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 76.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	67989	wwPDB-VP
Average B, all atoms (Å^2)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: MG, MAN, BMA, NAG

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	0.20	0/5056	0.37	0/6870
1	C	0.20	0/5056	0.37	0/6870
1	E	0.20	0/5056	0.37	0/6870
1	G	0.21	0/5056	0.38	0/6870
2	B	0.21	0/7317	0.36	0/9907
2	D	0.21	0/7306	0.36	0/9894
2	F	0.21	0/7314	0.36	0/9905
2	H	0.22	0/7315	0.36	0/9902
3	I	0.20	0/4092	0.37	0/5543
3	J	0.20	0/4092	0.37	0/5543
3	K	0.20	0/4092	0.37	0/5543
3	L	0.20	0/4092	0.37	0/5543
4	M	0.21	0/690	0.33	0/923
4	N	0.21	0/690	0.32	0/923
4	P	0.21	0/690	0.33	0/923
4	Q	0.21	0/690	0.33	0/923
All	All	0.21	0/68604	0.36	0/92952

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	4958	0	5017	127	0
1	C	4958	0	5017	128	0
1	E	4958	0	5017	130	0
1	G	4958	0	5016	144	0
2	B	7177	0	7085	201	0
2	D	7166	0	7062	193	0
2	F	7172	0	7080	220	0
2	H	7175	0	7087	195	0
3	I	4004	0	3966	128	0
3	J	4004	0	3967	129	0
3	K	4004	0	3965	125	0
3	L	4004	0	3966	126	0
4	M	682	0	697	35	0
4	N	682	0	697	38	0
4	P	682	0	697	33	0
4	Q	682	0	697	38	0
5	O	50	0	43	1	0
5	R	50	0	42	1	0
5	T	50	0	43	1	0
5	U	50	0	43	3	0
6	S	61	0	52	1	0
6	W	61	0	52	5	0
7	V	72	0	61	2	0
8	X	50	0	43	2	0
9	Y	39	0	34	2	0
9	a	39	0	34	0	0
10	Z	28	0	25	0	0
11	b	61	0	52	0	0
12	c	39	0	34	0	0
13	B	11	0	10	0	0
13	K	11	0	10	0	0
14	G	11	0	10	1	0
15	I	1	0	0	0	0
15	J	1	0	0	0	0
15	K	1	0	0	0	0
15	L	1	0	0	0	0
16	K	14	0	13	3	0
16	L	14	0	13	0	0
17	B	1	0	0	0	0
17	I	2	0	0	0	0
17	J	2	0	0	1	0
17	K	2	0	0	0	0
17	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	67989	0	67647	1863	0

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 14.

All (1863) 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:G:426:THR:HG21	1:G:432:ASN:H	1.20	1.07
2:H:1494:GLU:HB3	2:H:1602:LYS:HB3	1.36	1.04
2:D:1569:ARG:HB2	2:D:1569:ARG:HH11	1.32	0.94
2:F:1569:ARG:HB2	2:F:1569:ARG:HH11	1.32	0.94
2:H:1569:ARG:HB2	2:H:1569:ARG:HH11	1.32	0.94
2:B:1569:ARG:HH11	2:B:1569:ARG:HB2	1.32	0.94
2:H:1268:GLN:HG3	2:H:1269:GLU:H	1.34	0.92
1:G:505:PRO:HG3	1:G:595:TRP:CE3	2.08	0.88
3:L:267:CYS:HB2	3:L:433:MET:HE1	1.54	0.87
2:F:1359:LYS:HD2	4:M:4:LEU:HD11	1.58	0.86
1:A:549:GLU:HG2	1:A:550:ASP:H	1.44	0.83
1:G:477:ARG:HG2	1:G:477:ARG:HH11	1.44	0.83
1:C:549:GLU:HG2	1:C:550:ASP:H	1.44	0.82
1:E:477:ARG:HG2	1:E:477:ARG:HH11	1.44	0.82
2:H:1497:PHE:HE2	2:H:1571:ALA:HB1	1.43	0.82
1:E:547:GLN:HE22	1:E:559:MET:HA	1.44	0.82
1:G:549:GLU:HG2	1:G:550:ASP:H	1.44	0.82
3:J:381:ARG:HG2	3:J:381:ARG:HH21	1.45	0.82
1:E:549:GLU:HG2	1:E:550:ASP:H	1.44	0.82
4:Q:6:THR:H	4:Q:9:GLU:HB3	1.45	0.82
4:N:6:THR:H	4:N:9:GLU:HB3	1.45	0.81
4:P:6:THR:H	4:P:9:GLU:HB3	1.45	0.81
1:A:547:GLN:HE22	1:A:559:MET:HA	1.44	0.81
2:H:1485:ARG:HD3	2:H:1536:PHE:CZ	2.16	0.81
1:G:547:GLN:HE22	1:G:559:MET:HA	1.44	0.81
3:K:381:ARG:HH21	3:K:381:ARG:HG2	1.45	0.81
1:C:547:GLN:HE22	1:C:559:MET:HA	1.44	0.81
4:M:6:THR:H	4:M:9:GLU:HB3	1.45	0.81
1:A:477:ARG:HG2	1:A:477:ARG:HH11	1.44	0.80
1:C:477:ARG:HG2	1:C:477:ARG:HH11	1.44	0.80
1:G:508:ARG:CZ	1:G:604:GLY:HA3	2.12	0.80
3:L:381:ARG:HG2	3:L:381:ARG:HH21	1.45	0.80
2:B:819:ARG:HG2	2:B:819:ARG:HH11	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:819:ARG:HG2	2:D:819:ARG:HH11	1.46	0.80
3:I:381:ARG:HH21	3:I:381:ARG:HG2	1.45	0.80
1:C:45:LEU:HD11	1:C:48:SER:HB3	1.64	0.79
2:H:833:ARG:HH11	2:H:833:ARG:HG2	1.48	0.79
2:D:833:ARG:HG2	2:D:833:ARG:HH11	1.48	0.79
2:H:1488:LEU:HG	2:H:1590:TRP:HH2	1.47	0.79
2:F:819:ARG:HG2	2:F:819:ARG:HH11	1.46	0.79
2:H:819:ARG:HG2	2:H:819:ARG:HH11	1.46	0.79
2:D:1532:LEU:HD11	2:D:1569:ARG:HD3	1.65	0.78
3:I:244:MET:HG3	3:I:356:ARG:HB2	1.65	0.78
1:G:45:LEU:HD11	1:G:48:SER:HB3	1.64	0.78
2:H:1532:LEU:HD11	2:H:1569:ARG:HD3	1.65	0.78
2:F:1532:LEU:HD11	2:F:1569:ARG:HD3	1.65	0.78
1:E:45:LEU:HD11	1:E:48:SER:HB3	1.64	0.78
1:A:45:LEU:HD11	1:A:48:SER:HB3	1.64	0.78
2:B:1532:LEU:HD11	2:B:1569:ARG:HD3	1.65	0.78
2:F:738:ASN:HD22	4:P:45:LYS:HE2	1.47	0.78
2:F:833:ARG:HG2	2:F:833:ARG:HH11	1.48	0.78
2:H:966:ALA:O	2:H:967:GLN:HB2	1.83	0.78
2:B:833:ARG:HG2	2:B:833:ARG:HH11	1.48	0.77
2:F:932:ARG:NH1	3:L:339:SER:HB2	1.99	0.77
2:H:738:ASN:HD22	4:Q:45:LYS:HE2	1.49	0.77
2:F:841:ARG:HG2	2:F:841:ARG:HH11	1.50	0.77
3:J:244:MET:HG3	3:J:356:ARG:HB2	1.65	0.77
3:K:244:MET:HG3	3:K:356:ARG:HB2	1.65	0.77
3:L:244:MET:HG3	3:L:356:ARG:HB2	1.65	0.77
2:F:742:ARG:HB3	2:F:775:ASP:HB3	1.67	0.77
1:G:506:SER:HB2	1:G:530:TRP:HE1	1.50	0.77
2:B:841:ARG:HH11	2:B:841:ARG:HG2	1.50	0.76
2:F:740:VAL:HB	4:P:42:ARG:HB2	1.68	0.76
1:A:506:SER:HB2	1:A:530:TRP:HE1	1.50	0.76
1:E:506:SER:HB2	1:E:530:TRP:HE1	1.50	0.76
3:I:705:ARG:O	3:I:706:GLN:HB2	1.86	0.75
3:L:705:ARG:O	3:L:706:GLN:HB2	1.86	0.75
3:K:354:ARG:HB2	16:K:1749:NAG:H81	1.67	0.75
2:D:841:ARG:HG2	2:D:841:ARG:HH11	1.50	0.75
2:H:1498:ILE:HD12	2:H:1605:TRP:HA	1.65	0.75
3:J:705:ARG:O	3:J:706:GLN:HB2	1.86	0.75
2:F:1569:ARG:HH11	2:F:1569:ARG:CB	2.00	0.75
2:H:841:ARG:HG2	2:H:841:ARG:HH11	1.50	0.75
1:C:440:ARG:HG3	1:C:440:ARG:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:SER:HB2	1:C:530:TRP:HE1	1.50	0.75
3:L:446:GLU:O	3:L:450:LEU:HG	1.86	0.74
2:B:1569:ARG:HH11	2:B:1569:ARG:CB	2.00	0.74
1:C:404:THR:HG23	1:C:414:GLN:HE21	1.53	0.74
3:L:489:ALA:HB2	3:L:677:PRO:HG3	1.70	0.74
1:E:440:ARG:O	1:E:440:ARG:HG3	1.85	0.74
3:K:705:ARG:O	3:K:706:GLN:HB2	1.86	0.74
2:H:1569:ARG:HH11	2:H:1569:ARG:CB	2.00	0.74
3:I:464:ASP:HB3	3:I:615:LEU:HB2	1.70	0.74
1:A:440:ARG:HG3	1:A:440:ARG:O	1.86	0.74
1:G:440:ARG:HG3	1:G:440:ARG:O	1.85	0.74
2:H:877:VAL:HG22	2:H:1451:GLN:HE21	1.53	0.74
3:K:464:ASP:HB3	3:K:615:LEU:HB2	1.70	0.74
1:A:404:THR:HG23	1:A:414:GLN:HE21	1.53	0.74
1:E:223:ILE:H	1:E:223:ILE:HD12	1.53	0.74
2:H:740:VAL:HB	4:Q:42:ARG:HB2	1.69	0.74
2:F:834:GLN:NE2	2:F:835:ASN:H	1.86	0.73
2:D:1569:ARG:HH11	2:D:1569:ARG:CB	2.00	0.73
1:G:223:ILE:H	1:G:223:ILE:HD12	1.53	0.73
3:I:248:LEU:HD22	3:I:268:LEU:HD22	1.71	0.73
2:B:834:GLN:NE2	2:B:835:ASN:H	1.86	0.73
1:E:404:THR:HG23	1:E:414:GLN:HE21	1.53	0.73
2:H:742:ARG:HB3	2:H:775:ASP:HB3	1.71	0.73
1:C:223:ILE:HD12	1:C:223:ILE:H	1.53	0.73
1:G:404:THR:HG23	1:G:414:GLN:HE21	1.52	0.73
1:A:223:ILE:H	1:A:223:ILE:HD12	1.53	0.73
3:L:248:LEU:HD22	3:L:268:LEU:HD22	1.71	0.73
2:B:966:ALA:O	2:B:967:GLN:HB2	1.88	0.73
3:I:489:ALA:HB2	3:I:677:PRO:HG3	1.70	0.73
2:D:834:GLN:NE2	2:D:835:ASN:H	1.86	0.73
2:F:966:ALA:O	2:F:967:GLN:HB2	1.89	0.73
2:D:966:ALA:O	2:D:967:GLN:HB2	1.88	0.73
2:D:742:ARG:HB3	2:D:775:ASP:HB3	1.71	0.72
3:L:464:ASP:HB3	3:L:615:LEU:HB2	1.70	0.72
1:G:424:TYR:O	1:G:433:TYR:HE1	1.73	0.72
2:F:1269:GLU:HG3	2:F:1315:LYS:HB3	1.70	0.72
2:F:937:LYS:HG2	3:L:345:ASP:OD1	1.88	0.72
2:H:1497:PHE:CE2	2:H:1571:ALA:HB1	2.24	0.72
3:K:489:ALA:HB2	3:K:677:PRO:HG3	1.70	0.72
3:J:489:ALA:HB2	3:J:677:PRO:HG3	1.70	0.72
1:G:426:THR:HG21	1:G:432:ASN:N	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:635:ALA:HB3	3:K:647:ILE:HD11	1.71	0.72
3:J:248:LEU:HD22	3:J:268:LEU:HD22	1.70	0.72
3:J:464:ASP:HB3	3:J:615:LEU:HB2	1.70	0.72
3:J:653:PRO:HD2	3:J:654:ARG:HH12	1.55	0.72
2:H:834:GLN:NE2	2:H:835:ASN:H	1.86	0.72
1:C:6:ILE:HD13	1:C:22:LEU:HD23	1.72	0.71
1:G:6:ILE:HD13	1:G:22:LEU:HD23	1.72	0.71
3:L:461:LYS:HE2	3:L:461:LYS:HA	1.73	0.71
3:J:539:LYS:HG2	3:J:544:ILE:HD12	1.73	0.71
3:J:576:GLU:HB3	3:J:580:ARG:HH22	1.55	0.71
3:K:539:LYS:HG2	3:K:544:ILE:HD12	1.73	0.71
1:C:13:ARG:HH22	1:C:476:GLY:HA3	1.54	0.71
3:J:635:ALA:HB3	3:J:647:ILE:HD11	1.71	0.71
3:K:461:LYS:HA	3:K:461:LYS:HE2	1.73	0.71
3:I:461:LYS:HE2	3:I:461:LYS:HA	1.73	0.71
3:I:653:PRO:HD2	3:I:654:ARG:HH12	1.55	0.71
3:J:461:LYS:HE2	3:J:461:LYS:HA	1.73	0.71
3:K:576:GLU:HB3	3:K:580:ARG:HH22	1.55	0.71
1:C:439:LEU:HG	1:E:439:LEU:HG	1.71	0.71
3:I:635:ALA:HB3	3:I:647:ILE:HD11	1.71	0.71
3:K:248:LEU:HD22	3:K:268:LEU:HD22	1.70	0.71
3:L:635:ALA:HB3	3:L:647:ILE:HD11	1.71	0.70
1:E:6:ILE:HD13	1:E:22:LEU:HD23	1.72	0.70
1:C:98:VAL:HG11	2:D:1017:LEU:HD13	1.73	0.70
3:K:653:PRO:HD2	3:K:654:ARG:HH12	1.55	0.70
4:Q:71:GLN:HA	4:Q:71:GLN:HE21	1.57	0.70
3:I:539:LYS:HG2	3:I:544:ILE:HD12	1.73	0.70
3:L:576:GLU:HB3	3:L:580:ARG:HH22	1.55	0.70
2:H:1446:ASN:HB2	4:N:4:LEU:HD13	1.74	0.70
4:P:71:GLN:HE21	4:P:71:GLN:HA	1.57	0.70
3:I:576:GLU:HB3	3:I:580:ARG:HH22	1.55	0.70
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.74	0.70
3:L:539:LYS:HG2	3:L:544:ILE:HD12	1.73	0.69
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.72	0.69
2:D:1416:PHE:HZ	2:D:1442:HIS:HB2	1.57	0.69
3:I:381:ARG:HH21	3:I:381:ARG:CG	2.05	0.69
3:J:238:LEU:HD11	3:J:278:TYR:HB3	1.74	0.69
3:L:373:PRO:HB2	3:L:417:LEU:HD21	1.75	0.69
3:I:238:LEU:HD11	3:I:278:TYR:HB3	1.74	0.69
3:K:381:ARG:HH21	3:K:381:ARG:CG	2.06	0.69
3:L:653:PRO:HD2	3:L:654:ARG:HH12	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:962:GLY:O	2:H:964:PRO:HD3	1.92	0.69
1:E:426:THR:HG21	1:E:432:ASN:H	1.57	0.69
2:F:1387:THR:HG22	2:F:1451:GLN:H	1.58	0.69
2:H:1446:ASN:HB2	4:N:4:LEU:CD1	2.21	0.69
3:L:238:LEU:HD11	3:L:278:TYR:HB3	1.74	0.69
1:G:505:PRO:HG3	1:G:595:TRP:HE3	1.55	0.69
2:H:855:THR:HB	2:H:1602:LYS:HZ3	1.56	0.69
4:N:71:GLN:HA	4:N:71:GLN:HE21	1.56	0.69
2:H:1387:THR:HG22	2:H:1451:GLN:H	1.58	0.69
3:J:381:ARG:HH21	3:J:381:ARG:CG	2.05	0.69
2:D:962:GLY:O	2:D:964:PRO:HD3	1.93	0.69
3:L:381:ARG:HH21	3:L:381:ARG:CG	2.05	0.69
2:B:1416:PHE:HZ	2:B:1442:HIS:HB2	1.57	0.68
3:J:705:ARG:O	3:J:705:ARG:HG3	1.93	0.68
2:B:841:ARG:HG2	2:B:841:ARG:NH1	2.08	0.68
2:B:1488:LEU:HG	2:B:1590:TRP:CZ2	2.27	0.68
2:F:841:ARG:HG2	2:F:841:ARG:NH1	2.08	0.68
2:D:1488:LEU:HG	2:D:1590:TRP:CZ2	2.27	0.68
4:M:71:GLN:HA	4:M:71:GLN:HE21	1.56	0.68
2:F:733:ILE:HG12	2:F:734:ILE:H	1.58	0.68
3:I:373:PRO:HB2	3:I:417:LEU:HD21	1.75	0.68
3:J:373:PRO:HB2	3:J:417:LEU:HD21	1.75	0.68
3:K:373:PRO:HB2	3:K:417:LEU:HD21	1.75	0.68
3:J:435:ASN:ND2	3:J:460:ARG:HH21	1.90	0.68
1:G:100:LEU:HD21	1:G:638:LEU:HD23	1.76	0.68
1:G:567:HIS:ND1	2:H:760:PRO:HG3	2.09	0.68
1:C:606:THR:HG22	1:C:608:GLY:H	1.59	0.68
2:D:1445:PHE:CZ	4:P:7:SER:HA	2.28	0.68
2:H:733:ILE:HG12	2:H:734:ILE:H	1.58	0.68
3:J:432:ASP:HA	4:Q:27:ASN:HD21	1.57	0.67
1:C:372:GLU:O	1:C:375:VAL:HG12	1.95	0.67
3:K:446:GLU:HB3	3:K:449:SER:HB2	1.77	0.67
2:D:733:ILE:HG12	2:D:734:ILE:H	1.58	0.67
2:D:1518:GLY:HA3	2:D:1585:LEU:HD22	1.77	0.67
3:K:705:ARG:O	3:K:705:ARG:HG3	1.93	0.67
2:H:841:ARG:HG2	2:H:841:ARG:NH1	2.08	0.67
3:K:238:LEU:HD11	3:K:278:TYR:HB3	1.74	0.67
2:B:733:ILE:HG12	2:B:734:ILE:H	1.58	0.67
3:I:705:ARG:O	3:I:705:ARG:HG3	1.94	0.67
2:B:1518:GLY:HA3	2:B:1585:LEU:HD22	1.77	0.67
1:G:351:MET:SD	1:G:440:ARG:HD2	2.35	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1268:GLN:CG	2:H:1269:GLU:H	2.00	0.67
2:H:1359:LYS:HD2	4:N:4:LEU:HD11	1.75	0.67
3:L:705:ARG:O	3:L:705:ARG:HG3	1.94	0.67
2:D:876:TYR:HA	2:D:1451:GLN:HE22	1.60	0.66
2:F:962:GLY:O	2:F:964:PRO:HD3	1.95	0.66
2:H:1518:GLY:HA3	2:H:1585:LEU:HD22	1.77	0.66
2:D:1337:ASN:O	2:D:1338:LYS:HB2	1.95	0.66
2:H:1499:GLN:HG2	2:H:1500:LYS:HG3	1.77	0.66
1:G:606:THR:HG22	1:G:608:GLY:H	1.59	0.66
1:G:55:THR:HG22	1:G:57:ALA:H	1.61	0.66
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.78	0.66
1:A:606:THR:HG22	1:A:608:GLY:H	1.59	0.66
2:B:877:VAL:HG22	2:B:1451:GLN:HE21	1.59	0.66
2:D:841:ARG:HG2	2:D:841:ARG:NH1	2.08	0.66
2:H:1498:ILE:HG12	2:H:1499:GLN:H	1.60	0.66
1:E:606:THR:HG22	1:E:608:GLY:H	1.59	0.66
2:B:1387:THR:HG22	2:B:1451:GLN:H	1.60	0.66
3:J:446:GLU:HB3	3:J:449:SER:HB2	1.77	0.66
1:G:510:VAL:HG21	1:G:622:LEU:CD1	2.26	0.65
2:H:896:HIS:HB3	4:N:61:LYS:HD3	1.78	0.65
2:B:962:GLY:O	2:B:964:PRO:HD3	1.96	0.65
1:E:473:MET:HB2	1:E:508:ARG:HB2	1.78	0.65
1:A:55:THR:HG22	1:A:57:ALA:H	1.61	0.65
2:B:1417:SER:HB2	4:Q:14:LYS:NZ	2.11	0.65
3:I:446:GLU:HB3	3:I:449:SER:HB2	1.79	0.65
3:I:478:ARG:HG3	3:I:479:PRO:HD2	1.79	0.65
2:F:1518:GLY:HA3	2:F:1585:LEU:HD22	1.77	0.65
1:C:473:MET:HB2	1:C:508:ARG:HB2	1.78	0.65
2:F:829:LEU:HD23	2:F:840:VAL:HG11	1.78	0.65
2:F:1126:LEU:HG	2:F:1130:GLN:HE21	1.61	0.65
2:B:829:LEU:HD23	2:B:840:VAL:HG11	1.78	0.65
2:H:829:LEU:HD23	2:H:840:VAL:HG11	1.78	0.65
1:G:549:GLU:HG2	1:G:550:ASP:N	2.12	0.65
2:B:1337:ASN:O	2:B:1338:LYS:HB2	1.94	0.65
2:B:1126:LEU:HG	2:B:1130:GLN:HE21	1.61	0.64
2:D:829:LEU:HD23	2:D:840:VAL:HG11	1.78	0.64
1:C:55:THR:HG22	1:C:57:ALA:H	1.61	0.64
2:F:1265:PRO:O	2:F:1266:ASP:HB2	1.96	0.64
3:I:446:GLU:O	3:I:450:LEU:HG	1.97	0.64
2:B:1265:PRO:O	2:B:1266:ASP:HB2	1.97	0.64
2:D:1387:THR:HG22	2:D:1451:GLN:H	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:THR:HG22	1:E:57:ALA:H	1.61	0.64
2:D:1126:LEU:HG	2:D:1130:GLN:HE21	1.61	0.64
1:G:473:MET:HB2	1:G:508:ARG:HB2	1.78	0.64
3:J:478:ARG:HG3	3:J:479:PRO:HD2	1.79	0.64
2:F:1268:GLN:O	2:F:1269:GLU:HG2	1.97	0.64
3:K:478:ARG:HG3	3:K:479:PRO:HD2	1.79	0.64
3:L:446:GLU:HB3	3:L:449:SER:HB2	1.79	0.64
2:B:837:GLU:HG2	4:Q:64:SER:OG	1.97	0.64
2:D:1265:PRO:O	2:D:1266:ASP:HB2	1.98	0.64
2:F:1337:ASN:O	2:F:1338:LYS:HB2	1.97	0.64
2:H:1338:LYS:HA	2:H:1371:ARG:HB2	1.80	0.64
1:C:549:GLU:HG2	1:C:550:ASP:N	2.12	0.63
2:D:1527:LEU:HD13	2:D:1541:MET:HG2	1.80	0.63
1:A:551:ARG:HD2	1:A:551:ARG:N	2.13	0.63
2:D:1416:PHE:CZ	2:D:1442:HIS:HB2	2.34	0.63
2:H:837:GLU:HG2	4:N:64:SER:OG	1.98	0.63
3:K:460:ARG:HE	4:P:28:VAL:HG21	1.63	0.63
3:K:513:LYS:HB3	3:K:522:ASP:HB3	1.81	0.63
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.81	0.63
2:H:1498:ILE:HG12	2:H:1499:GLN:N	2.13	0.63
1:C:551:ARG:HD2	1:C:551:ARG:N	2.13	0.63
2:F:1498:ILE:HG22	2:F:1499:GLN:N	2.13	0.63
3:L:478:ARG:HG3	3:L:479:PRO:HD2	1.79	0.63
1:E:551:ARG:N	1:E:551:ARG:HD2	2.13	0.63
1:E:567:HIS:ND1	2:F:760:PRO:HG3	2.13	0.63
1:G:551:ARG:N	1:G:551:ARG:HD2	2.13	0.63
2:H:876:TYR:HA	2:H:1451:GLN:HE22	1.64	0.63
2:H:1337:ASN:O	2:H:1338:LYS:HB2	1.97	0.63
6:S:1:NAG:H61	6:S:2:NAG:C7	2.29	0.63
2:B:1527:LEU:HD13	2:B:1541:MET:HG2	1.80	0.63
1:C:147:ASN:HB2	1:C:148:PRO:HD2	1.80	0.63
1:C:634:GLN:HE22	2:D:1016:GLY:HA2	1.64	0.63
1:A:351:MET:SD	1:A:440:ARG:HD2	2.39	0.63
2:B:1416:PHE:CZ	2:B:1442:HIS:HB2	2.34	0.63
3:J:460:ARG:HE	4:Q:28:VAL:HG21	1.64	0.62
1:E:147:ASN:HB2	1:E:148:PRO:HD2	1.81	0.62
1:G:512:TYR:CZ	1:G:624:PHE:HE1	2.16	0.62
2:H:1527:LEU:HD13	2:H:1541:MET:HG2	1.80	0.62
3:K:432:ASP:HA	4:P:27:ASN:HD21	1.63	0.62
3:L:513:LYS:HB3	3:L:522:ASP:HB3	1.81	0.62
2:B:1295:SER:O	2:B:1297:LEU:HD12	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1295:SER:O	2:D:1297:LEU:HD12	2.00	0.62
2:B:876:TYR:HA	2:B:1451:GLN:HE22	1.63	0.62
3:I:513:LYS:HB3	3:I:522:ASP:HB3	1.81	0.62
3:K:433:MET:HE3	3:K:436:LEU:HD21	1.81	0.62
1:G:147:ASN:HB2	1:G:148:PRO:HD2	1.81	0.62
2:F:877:VAL:HG22	2:F:1451:GLN:HE21	1.65	0.62
2:B:1446:ASN:HB2	4:Q:4:LEU:HB2	1.81	0.62
2:H:1498:ILE:HG13	2:H:1605:TRP:CE3	2.34	0.62
1:A:549:GLU:HG2	1:A:550:ASP:N	2.12	0.62
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.81	0.62
2:H:834:GLN:HE21	2:H:835:ASN:H	1.47	0.62
2:H:855:THR:HB	2:H:1602:LYS:NZ	2.14	0.62
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.35	0.62
2:F:1527:LEU:HD13	2:F:1541:MET:HG2	1.80	0.62
3:J:513:LYS:HB3	3:J:522:ASP:HB3	1.81	0.62
3:I:423:ASN:HD22	3:I:423:ASN:N	1.98	0.61
1:G:19:THR:HB	1:G:478:LEU:HB2	1.81	0.61
2:B:834:GLN:HE21	2:B:835:ASN:H	1.47	0.61
1:E:222:TYR:CE2	1:E:224:TYR:HB2	2.35	0.61
2:F:1295:SER:O	2:F:1297:LEU:HD12	2.00	0.61
2:H:1611:GLU:HG3	2:H:1612:GLU:H	1.66	0.61
3:I:650:VAL:HG23	3:I:651:VAL:HG23	1.83	0.61
1:C:13:ARG:NH2	1:C:476:GLY:HA3	2.15	0.61
2:H:1497:PHE:HB2	2:H:1498:ILE:HD13	1.82	0.61
3:I:267:CYS:HB2	3:I:433:MET:HE1	1.82	0.61
3:K:423:ASN:HD22	3:K:423:ASN:N	1.98	0.61
3:L:461:LYS:HG2	4:N:28:VAL:HG12	1.81	0.61
2:B:1490:ARG:HB3	2:B:1590:TRP:CH2	2.36	0.61
1:E:372:GLU:O	1:E:375:VAL:HG12	1.99	0.61
1:G:372:GLU:O	1:G:375:VAL:HG12	2.01	0.61
1:G:222:TYR:CE2	1:G:224:TYR:HB2	2.35	0.61
3:I:461:LYS:HG2	4:M:28:VAL:HG12	1.82	0.61
3:K:478:ARG:HE	3:K:481:LYS:HD2	1.65	0.61
2:B:1291:TRP:CG	2:B:1292:GLU:N	2.69	0.61
3:L:650:VAL:HG23	3:L:651:VAL:HG23	1.83	0.61
1:C:20:MET:HB3	1:C:64:VAL:HG23	1.83	0.61
2:D:1490:ARG:HB3	2:D:1590:TRP:CH2	2.36	0.61
2:H:1498:ILE:CG1	2:H:1499:GLN:H	2.12	0.61
3:J:423:ASN:HD22	3:J:423:ASN:N	1.98	0.61
1:C:222:TYR:CE2	1:C:224:TYR:HB2	2.35	0.61
2:H:923:ARG:HH22	2:H:940:ILE:HG12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:834:GLN:HE21	2:F:835:ASN:H	1.47	0.61
2:F:1338:LYS:HA	2:F:1371:ARG:HB2	1.81	0.61
2:F:1527:LEU:HD21	2:F:1530:VAL:HG22	1.83	0.61
3:K:650:VAL:HG23	3:K:651:VAL:HG23	1.83	0.61
2:B:1527:LEU:HD21	2:B:1530:VAL:HG22	1.83	0.60
2:F:1611:GLU:HG3	2:F:1612:GLU:H	1.66	0.60
3:I:478:ARG:HE	3:I:481:LYS:HD2	1.65	0.60
1:A:372:GLU:O	1:A:375:VAL:HG12	2.01	0.60
2:D:1611:GLU:HG3	2:D:1612:GLU:H	1.66	0.60
2:F:923:ARG:HH22	2:F:940:ILE:HG12	1.66	0.60
3:J:478:ARG:HE	3:J:481:LYS:HD2	1.65	0.60
2:D:1291:TRP:CG	2:D:1292:GLU:N	2.69	0.60
2:F:837:GLU:HG2	4:M:64:SER:OG	2.00	0.60
1:G:20:MET:HB3	1:G:64:VAL:HG23	1.83	0.60
1:C:426:THR:HG21	1:C:432:ASN:H	1.65	0.60
2:H:1295:SER:O	2:H:1297:LEU:HD12	2.00	0.60
3:L:449:SER:HA	3:L:452:LEU:HD13	1.84	0.60
3:L:478:ARG:HE	3:L:481:LYS:HD2	1.65	0.60
4:P:84:LYS:O	4:P:85:TYR:HB2	2.02	0.60
2:B:973:VAL:HG11	2:B:978:LEU:HD12	1.83	0.60
1:C:572:VAL:HG12	2:D:753:VAL:HG22	1.82	0.60
2:D:772:PHE:HD1	4:M:37:ASN:ND2	1.99	0.60
2:D:973:VAL:HG11	2:D:978:LEU:HD12	1.83	0.60
1:A:20:MET:HB3	1:A:64:VAL:HG23	1.83	0.60
2:B:1532:LEU:HD11	2:B:1569:ARG:CD	2.32	0.60
4:M:84:LYS:O	4:M:85:TYR:HB2	2.02	0.60
2:B:1039:GLN:HB3	2:B:1040:PRO:HD2	1.83	0.60
1:C:10:ASN:HB2	1:C:621:GLY:C	2.21	0.60
3:J:650:VAL:HG23	3:J:651:VAL:HG23	1.83	0.60
3:L:374:ILE:HD13	3:L:417:LEU:HD23	1.84	0.60
2:D:834:GLN:HE21	2:D:835:ASN:H	1.47	0.60
1:E:20:MET:HB3	1:E:64:VAL:HG23	1.83	0.60
2:F:1291:TRP:CD1	2:F:1292:GLU:N	2.70	0.60
2:F:1446:ASN:HB2	4:M:4:LEU:CD1	2.32	0.60
3:J:460:ARG:NE	4:Q:28:VAL:HG21	2.16	0.60
2:D:1532:LEU:HD11	2:D:1569:ARG:CD	2.32	0.59
1:E:220:PHE:CZ	1:E:330:PRO:HB3	2.37	0.59
2:F:876:TYR:HA	2:F:1451:GLN:HE22	1.67	0.59
2:F:1039:GLN:HB3	2:F:1040:PRO:HD2	1.83	0.59
2:D:877:VAL:HG22	2:D:1451:GLN:HE21	1.67	0.59
2:D:1039:GLN:HB3	2:D:1040:PRO:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:570:ILE:HD13	3:J:688:GLN:HB2	1.84	0.59
3:K:436:LEU:HB3	3:K:440:PHE:CE2	2.37	0.59
3:L:423:ASN:HD22	3:L:423:ASN:N	1.98	0.59
2:B:1611:GLU:HG3	2:B:1612:GLU:H	1.66	0.59
2:D:1527:LEU:HD21	2:D:1530:VAL:HG22	1.83	0.59
1:E:549:GLU:HG2	1:E:550:ASP:N	2.12	0.59
1:G:13:ARG:NH2	1:G:476:GLY:HA3	2.18	0.59
2:H:833:ARG:HH11	2:H:833:ARG:CG	2.15	0.59
3:I:563:TYR:CE2	3:I:569:PRO:HG3	2.38	0.59
3:I:570:ILE:HD13	3:I:688:GLN:HB2	1.84	0.59
1:G:555:PRO:HB3	2:H:775:ASP:HA	1.83	0.59
2:D:1337:ASN:O	2:D:1338:LYS:CB	2.51	0.59
2:H:1527:LEU:HD21	2:H:1530:VAL:HG22	1.83	0.59
3:L:570:ILE:HD13	3:L:688:GLN:HB2	1.84	0.59
4:N:84:LYS:O	4:N:85:TYR:HB2	2.02	0.59
3:K:563:TYR:CE2	3:K:569:PRO:HG3	2.38	0.59
1:C:558:GLN:HB3	2:D:770:ASN:HD21	1.68	0.59
1:G:350:LEU:HD21	1:G:400:ILE:HG21	1.83	0.59
3:J:436:LEU:HB3	3:J:440:PHE:CE2	2.37	0.59
3:J:563:TYR:CE2	3:J:569:PRO:HG3	2.38	0.59
3:L:508:LYS:HE2	3:L:508:LYS:HA	1.85	0.59
4:N:22:LEU:HB3	4:N:74:TYR:HE2	1.68	0.59
4:Q:84:LYS:O	4:Q:85:TYR:HB2	2.02	0.59
3:L:563:TYR:CE2	3:L:569:PRO:HG3	2.38	0.59
2:F:973:VAL:HG11	2:F:978:LEU:HD12	1.84	0.58
3:I:374:ILE:HD13	3:I:417:LEU:HD23	1.84	0.58
2:D:833:ARG:HH11	2:D:833:ARG:CG	2.15	0.58
1:E:477:ARG:HH11	1:E:477:ARG:CG	2.16	0.58
2:F:1215:LEU:HD23	2:F:1256:ALA:HB1	1.85	0.58
3:L:436:LEU:HB3	3:L:440:PHE:CE2	2.37	0.58
3:I:436:LEU:HB3	3:I:440:PHE:CE2	2.37	0.58
3:K:374:ILE:HD13	3:K:417:LEU:HD23	1.84	0.58
1:C:40:PHE:CE2	2:D:1017:LEU:HD22	2.38	0.58
2:F:1291:TRP:CG	2:F:1292:GLU:N	2.70	0.58
2:F:1532:LEU:HD11	2:F:1569:ARG:CD	2.34	0.58
3:J:374:ILE:HD13	3:J:417:LEU:HD23	1.84	0.58
4:P:22:LEU:HB3	4:P:74:TYR:HE2	1.68	0.58
2:H:1535:ASP:O	2:H:1536:PHE:HB3	2.04	0.58
4:M:22:LEU:HB3	4:M:74:TYR:HE2	1.68	0.58
3:I:508:LYS:HE2	3:I:508:LYS:HA	1.85	0.58
3:J:508:LYS:HE2	3:J:508:LYS:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:570:ILE:HD13	3:K:688:GLN:HB2	1.84	0.58
2:H:877:VAL:H	2:H:1451:GLN:NE2	2.01	0.58
3:L:477:ILE:O	3:L:511:SER:HB2	2.04	0.58
2:B:833:ARG:HH11	2:B:833:ARG:CG	2.15	0.58
2:B:1215:LEU:HD23	2:B:1256:ALA:HB1	1.85	0.58
2:F:1359:LYS:HD2	4:M:4:LEU:CD1	2.32	0.58
2:H:1532:LEU:HD11	2:H:1569:ARG:CD	2.34	0.58
3:J:477:ILE:O	3:J:511:SER:HB2	2.04	0.58
2:D:1470:PHE:HB2	2:D:1478:GLY:HA3	1.86	0.57
1:G:527:ASP:N	1:G:616:VAL:HG11	2.19	0.57
4:Q:6:THR:H	4:Q:9:GLU:CB	2.16	0.57
1:E:350:LEU:HD21	1:E:400:ILE:HG21	1.86	0.57
1:G:510:VAL:HG11	1:G:622:LEU:HD12	1.86	0.57
2:H:1291:TRP:CD1	2:H:1292:GLU:N	2.70	0.57
2:H:1497:PHE:CZ	2:H:1572:LEU:HD23	2.39	0.57
3:I:477:ILE:O	3:I:511:SER:HB2	2.04	0.57
3:K:477:ILE:O	3:K:511:SER:HB2	2.04	0.57
2:B:1445:PHE:CZ	4:Q:7:SER:HA	2.40	0.57
2:F:1133:LYS:O	2:F:1137:GLU:HG3	2.04	0.57
2:H:1291:TRP:CG	2:H:1292:GLU:N	2.70	0.57
1:A:614:ALA:HB1	1:A:632:THR:HA	1.86	0.57
2:D:809:ILE:HD11	2:D:892:ALA:HB3	1.87	0.57
2:D:1215:LEU:HD23	2:D:1256:ALA:HB1	1.85	0.57
1:G:13:ARG:HH22	1:G:476:GLY:HA3	1.69	0.57
4:Q:22:LEU:HB3	4:Q:74:TYR:HE2	1.68	0.57
2:B:1133:LYS:O	2:B:1137:GLU:HG3	2.04	0.57
2:B:1337:ASN:O	2:B:1338:LYS:CB	2.51	0.57
2:F:1535:ASP:O	2:F:1536:PHE:HB3	2.03	0.57
2:B:809:ILE:HD11	2:B:892:ALA:HB3	1.87	0.57
2:D:962:GLY:C	2:D:964:PRO:HD3	2.24	0.57
2:F:1269:GLU:HG3	2:F:1315:LYS:CB	2.35	0.57
2:F:1446:ASN:HB2	4:M:4:LEU:HD13	1.85	0.57
1:C:567:HIS:ND1	2:D:760:PRO:HG3	2.19	0.57
3:K:460:ARG:NE	4:P:28:VAL:HG21	2.19	0.57
3:K:508:LYS:HE2	3:K:508:LYS:HA	1.85	0.57
2:B:836:GLN:HG2	2:B:897:HIS:HE1	1.70	0.57
1:E:614:ALA:HB1	1:E:632:THR:HA	1.86	0.57
2:B:1470:PHE:HB2	2:B:1478:GLY:HA3	1.86	0.57
2:D:1462:ASN:HD22	2:D:1463:LEU:N	2.03	0.57
2:H:923:ARG:NH2	2:H:940:ILE:HG12	2.19	0.57
2:H:1582:MET:HA	2:H:1605:TRP:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1055:TRP:CZ2	2:F:1108:ILE:HA	2.40	0.57
2:H:819:ARG:HG2	2:H:819:ARG:NH1	2.19	0.57
2:H:1462:ASN:HD22	2:H:1463:LEU:N	2.03	0.57
2:B:965:VAL:O	2:B:1267:HIS:HD2	1.88	0.56
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.86	0.56
1:C:268:ARG:HD3	2:D:1378:MET:SD	2.44	0.56
2:D:1055:TRP:CZ2	2:D:1108:ILE:HA	2.40	0.56
2:D:1143:LEU:HB3	2:D:1144:PRO:HD3	1.86	0.56
3:L:253:SER:HB2	3:L:326:SER:O	2.05	0.56
2:F:809:ILE:HD11	2:F:892:ALA:HB3	1.87	0.56
2:F:833:ARG:HH11	2:F:833:ARG:CG	2.15	0.56
2:F:1582:MET:HA	2:F:1605:TRP:O	2.05	0.56
1:G:614:ALA:HB1	1:G:632:THR:HA	1.86	0.56
2:H:1494:GLU:HG2	2:H:1602:LYS:HD3	1.87	0.56
3:L:461:LYS:HD2	4:N:29:ASN:OD1	2.05	0.56
1:A:558:GLN:HB3	2:B:770:ASN:HD21	1.70	0.56
2:B:923:ARG:HH22	2:B:940:ILE:HG12	1.70	0.56
2:B:925:LEU:HD11	2:B:1320:LEU:HD22	1.87	0.56
2:B:1462:ASN:HD22	2:B:1463:LEU:N	2.03	0.56
2:B:1516:GLU:HB3	2:B:1517:PRO:HD2	1.88	0.56
1:C:614:ALA:HB1	1:C:632:THR:HA	1.86	0.56
2:D:925:LEU:HD11	2:D:1320:LEU:HD22	1.86	0.56
2:D:1133:LYS:O	2:D:1137:GLU:HG3	2.05	0.56
2:D:1535:ASP:O	2:D:1536:PHE:HB3	2.05	0.56
1:E:572:VAL:HG12	2:F:753:VAL:HG22	1.87	0.56
2:F:1462:ASN:HD22	2:F:1463:LEU:N	2.03	0.56
2:H:1337:ASN:O	2:H:1338:LYS:CB	2.53	0.56
2:H:1566:ILE:O	2:H:1569:ARG:HG3	2.06	0.56
3:K:364:ASP:O	3:K:409:VAL:HG23	2.06	0.56
2:F:836:GLN:HG2	2:F:897:HIS:HE1	1.70	0.56
2:H:925:LEU:HD11	2:H:1320:LEU:HD22	1.88	0.56
3:I:353:ASN:HB2	3:I:394:ARG:NH1	2.20	0.56
3:K:253:SER:HB2	3:K:326:SER:O	2.05	0.56
3:L:364:ASP:O	3:L:409:VAL:HG23	2.06	0.56
2:B:1055:TRP:CZ2	2:B:1108:ILE:HA	2.40	0.56
2:B:1180:LEU:HD23	2:B:1221:LEU:HD11	1.88	0.56
2:F:923:ARG:NH2	2:F:940:ILE:HG12	2.19	0.56
2:B:1535:ASP:O	2:B:1536:PHE:HB3	2.05	0.56
1:C:441:THR:HG21	1:E:441:THR:HG21	1.88	0.56
1:E:116:ILE:HD11	1:E:203:LYS:HB3	1.88	0.56
1:G:477:ARG:HH11	1:G:477:ARG:CG	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:836:GLN:HG2	2:H:897:HIS:HE1	1.70	0.56
3:I:253:SER:HB2	3:I:326:SER:O	2.05	0.56
1:A:10:ASN:HB2	1:A:621:GLY:C	2.25	0.56
2:D:1180:LEU:HD23	2:D:1221:LEU:HD11	1.88	0.56
3:J:253:SER:HB2	3:J:326:SER:O	2.06	0.56
3:J:438:ASP:OD2	4:Q:28:VAL:HG13	2.05	0.56
2:D:923:ARG:HH22	2:D:940:ILE:HG12	1.70	0.56
2:D:1279:PRO:HG2	2:D:1306:GLU:HB3	1.88	0.56
2:F:1337:ASN:O	2:F:1338:LYS:CB	2.53	0.56
3:I:364:ASP:O	3:I:409:VAL:HG23	2.06	0.56
3:L:381:ARG:CG	3:L:381:ARG:NH2	2.68	0.56
2:D:1291:TRP:O	2:D:1292:GLU:C	2.45	0.56
2:F:1143:LEU:HB3	2:F:1144:PRO:HD3	1.86	0.56
2:H:809:ILE:HD11	2:H:892:ALA:HB3	1.87	0.56
2:H:964:PRO:HG3	2:H:1270:LEU:HD11	1.88	0.56
3:J:364:ASP:O	3:J:409:VAL:HG23	2.06	0.56
3:L:353:ASN:HB2	3:L:394:ARG:NH1	2.20	0.56
3:L:513:LYS:HZ2	3:L:524:GLU:HG2	1.71	0.56
4:N:6:THR:H	4:N:9:GLU:CB	2.16	0.56
1:A:477:ARG:HH11	1:A:477:ARG:CG	2.16	0.56
2:F:1012:TRP:HB3	2:F:1017:LEU:HD23	1.88	0.56
4:P:6:THR:H	4:P:9:GLU:CB	2.16	0.56
2:B:966:ALA:O	2:B:967:GLN:CB	2.54	0.55
2:F:1566:ILE:O	2:F:1569:ARG:HG3	2.06	0.55
3:I:461:LYS:HG2	4:M:28:VAL:CG1	2.36	0.55
3:K:267:CYS:HB2	3:K:433:MET:HE1	1.87	0.55
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.88	0.55
2:D:1291:TRP:CD1	2:D:1292:GLU:N	2.75	0.55
2:D:1516:GLU:HB3	2:D:1517:PRO:HD2	1.88	0.55
2:F:804:MET:HG2	2:F:805:GLN:H	1.72	0.55
2:F:925:LEU:HD11	2:F:1320:LEU:HD22	1.88	0.55
1:A:569:ALA:HB2	2:B:788:SER:HB2	1.88	0.55
2:B:1338:LYS:HA	2:B:1371:ARG:HB2	1.88	0.55
2:B:1563:ILE:HB	2:B:1599:ILE:HD13	1.88	0.55
2:F:1516:GLU:HB3	2:F:1517:PRO:HD2	1.88	0.55
2:F:1640:PRO:O	2:F:1641:ASN:HB2	2.07	0.55
1:G:143:VAL:C	1:G:144:ASN:HD22	2.10	0.55
2:H:839:LYS:HE2	4:N:60:PHE:CD1	2.41	0.55
1:A:143:VAL:C	1:A:144:ASN:HD22	2.09	0.55
2:B:804:MET:HG2	2:B:805:GLN:H	1.71	0.55
1:C:465:ILE:HD11	1:C:515:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:ARG:HH11	1:C:477:ARG:CG	2.16	0.55
2:F:738:ASN:ND2	4:P:45:LYS:HE2	2.19	0.55
1:G:116:ILE:HD11	1:G:203:LYS:HB3	1.88	0.55
2:H:1525:THR:HG22	2:H:1543:ILE:HA	1.88	0.55
2:H:1563:ILE:HB	2:H:1599:ILE:HD13	1.89	0.55
2:B:1566:ILE:O	2:B:1569:ARG:HG3	2.07	0.55
1:C:350:LEU:HD21	1:C:400:ILE:HG21	1.88	0.55
2:D:836:GLN:HG2	2:D:897:HIS:HE1	1.70	0.55
1:E:13:ARG:HH22	1:E:476:GLY:HA3	1.71	0.55
1:E:143:VAL:C	1:E:144:ASN:HD22	2.10	0.55
2:F:740:VAL:O	4:P:42:ARG:HD3	2.06	0.55
2:F:1498:ILE:HD12	2:F:1498:ILE:N	2.21	0.55
2:H:1338:LYS:CA	2:H:1371:ARG:HB2	2.36	0.55
3:K:353:ASN:HB2	3:K:394:ARG:NH1	2.21	0.55
2:B:1291:TRP:CD1	2:B:1292:GLU:N	2.75	0.55
1:C:252:GLY:HA2	1:C:262:LEU:HG	1.89	0.55
2:D:1012:TRP:HB3	2:D:1017:LEU:HD23	1.88	0.55
2:F:776:SER:HB2	2:F:780:TRP:CZ2	2.42	0.55
2:F:1525:THR:HG22	2:F:1543:ILE:HA	1.88	0.55
2:B:877:VAL:H	2:B:1451:GLN:NE2	2.03	0.55
2:B:1012:TRP:HB3	2:B:1017:LEU:HD23	1.88	0.55
2:F:896:HIS:HB3	4:M:61:LYS:HD3	1.88	0.55
1:G:252:GLY:HA2	1:G:262:LEU:HG	1.89	0.55
2:H:1498:ILE:CD1	2:H:1605:TRP:HA	2.35	0.55
2:B:1417:SER:HB2	4:Q:14:LYS:HZ3	1.71	0.55
1:G:386:LYS:HD3	1:G:440:ARG:HG2	1.87	0.55
1:G:465:ILE:HD11	1:G:515:LEU:HD22	1.89	0.55
1:G:473:MET:CE	1:G:603:ILE:HD11	2.37	0.55
2:H:1516:GLU:HB3	2:H:1517:PRO:HD2	1.88	0.55
1:A:116:ILE:HD11	1:A:203:LYS:HB3	1.88	0.55
2:D:1338:LYS:HA	2:D:1371:ARG:HB2	1.89	0.55
2:F:1084:TRP:CD1	2:F:1088:GLU:HG3	2.42	0.55
2:F:1268:GLN:O	2:F:1269:GLU:CG	2.55	0.55
2:F:1291:TRP:O	2:F:1292:GLU:C	2.44	0.55
1:C:116:ILE:HD11	1:C:203:LYS:HB3	1.88	0.55
2:F:1338:LYS:CA	2:F:1371:ARG:HB2	2.37	0.55
2:H:1641:ASN:HD21	3:J:366:LEU:HB3	1.72	0.55
3:J:353:ASN:HB2	3:J:394:ARG:NH1	2.21	0.55
2:D:776:SER:HB2	2:D:780:TRP:CZ2	2.42	0.54
1:E:10:ASN:HA	1:E:623:THR:HG23	1.89	0.54
2:F:1180:LEU:HD23	2:F:1221:LEU:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1279:PRO:HG2	2:F:1306:GLU:HB3	1.88	0.54
1:G:508:ARG:NH1	1:G:604:GLY:HA3	2.22	0.54
2:D:1525:THR:HG22	2:D:1543:ILE:HA	1.89	0.54
2:H:744:GLU:C	2:H:746:PRO:HD3	2.28	0.54
2:H:1279:PRO:HG2	2:H:1306:GLU:HB3	1.88	0.54
3:L:461:LYS:HG2	4:N:28:VAL:CG1	2.37	0.54
2:B:776:SER:HB2	2:B:780:TRP:CZ2	2.42	0.54
1:C:143:VAL:C	1:C:144:ASN:HD22	2.10	0.54
2:H:1291:TRP:O	2:H:1292:GLU:C	2.45	0.54
2:H:1445:PHE:CE2	4:N:7:SER:HA	2.43	0.54
2:B:1291:TRP:O	2:B:1292:GLU:C	2.45	0.54
1:E:478:LEU:HD21	1:E:622:LEU:HD21	1.88	0.54
2:H:1289:ILE:HD13	2:H:1298:ARG:HE	1.73	0.54
3:J:368:ASN:H	3:J:368:ASN:ND2	2.06	0.54
1:A:465:ILE:HD11	1:A:515:LEU:HD22	1.89	0.54
1:E:252:GLY:HA2	1:E:262:LEU:HG	1.89	0.54
3:I:535:ASN:O	3:I:547:PHE:HB3	2.07	0.54
3:L:535:ASN:O	3:L:547:PHE:HB3	2.07	0.54
2:D:804:MET:HG2	2:D:805:GLN:H	1.71	0.54
2:H:804:MET:HG2	2:H:805:GLN:H	1.72	0.54
3:K:535:ASN:O	3:K:547:PHE:HB3	2.07	0.54
2:B:1084:TRP:CD1	2:B:1088:GLU:HG3	2.42	0.54
2:D:966:ALA:O	2:D:967:GLN:CB	2.54	0.54
2:D:1566:ILE:O	2:D:1569:ARG:HG3	2.07	0.54
1:E:396:LYS:HG3	1:E:397:PRO:HD2	1.90	0.54
1:E:555:PRO:HB3	2:F:775:ASP:HA	1.90	0.54
2:H:1268:GLN:CG	2:H:1269:GLU:N	2.70	0.54
1:A:269:ILE:HD13	1:A:278:VAL:HB	1.90	0.54
2:B:1525:THR:HG22	2:B:1543:ILE:HA	1.89	0.54
2:D:837:GLU:HG2	4:P:64:SER:OG	2.07	0.54
2:D:1563:ILE:HB	2:D:1599:ILE:HD13	1.88	0.54
2:F:1289:ILE:HD13	2:F:1298:ARG:HE	1.73	0.54
1:G:534:LYS:HD2	1:G:535:ASP:H	1.72	0.54
3:J:631:CYS:SG	3:J:714:ARG:HD2	2.48	0.54
3:K:631:CYS:SG	3:K:714:ARG:HD2	2.48	0.54
3:L:478:ARG:NE	3:L:481:LYS:HD2	2.23	0.54
2:F:1563:ILE:HB	2:F:1599:ILE:HD13	1.89	0.54
1:G:396:LYS:HG3	1:G:397:PRO:HD2	1.90	0.54
3:K:478:ARG:NE	3:K:481:LYS:HD2	2.23	0.54
2:B:819:ARG:HG2	2:B:819:ARG:NH1	2.19	0.53
2:B:1582:MET:HA	2:B:1605:TRP:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1084:TRP:CD1	2:D:1088:GLU:HG3	2.41	0.53
3:K:381:ARG:CG	3:K:381:ARG:NH2	2.68	0.53
3:L:436:LEU:HB3	3:L:440:PHE:HE2	1.73	0.53
1:A:13:ARG:HH22	1:A:476:GLY:HA3	1.73	0.53
2:B:923:ARG:NH2	2:B:940:ILE:HG12	2.23	0.53
2:B:1279:PRO:HG2	2:B:1306:GLU:HB3	1.88	0.53
1:C:436:LEU:HD11	1:C:511:ALA:HB3	1.90	0.53
1:C:505:PRO:HG3	1:C:595:TRP:CE3	2.42	0.53
2:D:997:THR:N	2:D:998:PRO:HD2	2.24	0.53
1:E:568:GLY:HA2	2:F:757:LYS:HE2	1.89	0.53
2:F:804:MET:HG2	2:F:805:GLN:N	2.23	0.53
1:G:451:VAL:HB	1:G:495:LEU:HB3	1.91	0.53
1:A:472:ILE:HD13	1:A:509:LEU:HD23	1.90	0.53
2:D:804:MET:HG2	2:D:805:GLN:N	2.23	0.53
3:J:535:ASN:O	3:J:547:PHE:HB3	2.07	0.53
2:F:744:GLU:C	2:F:746:PRO:HD3	2.29	0.53
3:K:435:ASN:ND2	3:K:460:ARG:HH21	2.06	0.53
3:L:631:CYS:SG	3:L:714:ARG:HD2	2.48	0.53
1:A:252:GLY:HA2	1:A:262:LEU:HG	1.89	0.53
1:A:436:LEU:HD11	1:A:511:ALA:HB3	1.90	0.53
1:E:465:ILE:HD11	1:E:515:LEU:HD22	1.89	0.53
2:F:940:ILE:HD12	2:F:1308:PHE:CE1	2.44	0.53
2:D:1289:ILE:HD13	2:D:1298:ARG:HE	1.74	0.53
2:D:1582:MET:HA	2:D:1605:TRP:O	2.08	0.53
1:E:219:LYS:NZ	1:E:356:ASN:HD22	2.07	0.53
1:G:269:ILE:HD13	1:G:278:VAL:HB	1.90	0.53
3:J:478:ARG:NE	3:J:481:LYS:HD2	2.23	0.53
1:A:451:VAL:HB	1:A:495:LEU:HB3	1.91	0.53
2:B:997:THR:N	2:B:998:PRO:HD2	2.24	0.53
1:C:269:ILE:HD13	1:C:278:VAL:HB	1.90	0.53
2:D:923:ARG:NH2	2:D:940:ILE:HG12	2.23	0.53
2:D:967:GLN:O	2:D:968:MET:HB2	2.08	0.53
2:H:940:ILE:HD12	2:H:1308:PHE:CE1	2.43	0.53
2:B:804:MET:HG2	2:B:805:GLN:N	2.23	0.53
1:E:477:ARG:HG2	1:E:477:ARG:NH1	2.21	0.53
2:H:1521:TYR:HB2	2:H:1523:TYR:CE2	2.44	0.53
3:I:478:ARG:NE	3:I:481:LYS:HD2	2.23	0.53
3:K:456:VAL:HG13	3:K:467:LYS:HA	1.91	0.53
1:A:506:SER:CB	1:A:530:TRP:HE1	2.21	0.53
2:F:937:LYS:HD2	2:F:937:LYS:O	2.09	0.53
2:H:776:SER:HB2	2:H:780:TRP:CZ2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:456:VAL:HG13	3:I:467:LYS:HA	1.91	0.53
3:J:456:VAL:HG13	3:J:467:LYS:HA	1.91	0.53
3:L:438:ASP:OD2	4:N:28:VAL:HG13	2.09	0.53
4:M:6:THR:H	4:M:9:GLU:CB	2.16	0.53
2:D:865:THR:OG1	4:P:11:GLN:HG2	2.08	0.53
2:D:877:VAL:H	2:D:1451:GLN:NE2	2.07	0.53
2:D:1470:PHE:CB	2:D:1478:GLY:HA3	2.39	0.53
1:E:505:PRO:HG3	1:E:595:TRP:CE3	2.44	0.53
2:F:822:GLN:OE1	2:F:1479:LYS:HA	2.09	0.53
2:F:973:VAL:HG12	2:F:975:ALA:H	1.73	0.53
2:F:997:THR:N	2:F:998:PRO:HD2	2.24	0.53
2:F:1387:THR:CG2	2:F:1451:GLN:H	2.21	0.53
3:I:631:CYS:SG	3:I:714:ARG:HD2	2.48	0.53
3:J:436:LEU:HB3	3:J:440:PHE:HE2	1.73	0.53
3:K:436:LEU:HB3	3:K:440:PHE:HE2	1.73	0.53
2:B:1289:ILE:HD13	2:B:1298:ARG:HE	1.73	0.52
1:C:439:LEU:H	1:C:439:LEU:HD12	1.74	0.52
1:E:590:THR:HG22	1:E:592:SER:H	1.75	0.52
1:G:569:ALA:HB2	2:H:788:SER:HB2	1.90	0.52
2:H:740:VAL:O	4:Q:42:ARG:HD3	2.09	0.52
2:B:962:GLY:C	2:B:964:PRO:HD3	2.29	0.52
2:D:1196:ASN:HD22	2:D:1196:ASN:N	2.07	0.52
2:F:978:LEU:HG	2:F:1240:TYR:HB3	1.91	0.52
1:G:342:PHE:CE1	1:G:391:THR:HG21	2.45	0.52
1:G:472:ILE:HD13	1:G:509:LEU:HD23	1.90	0.52
3:K:438:ASP:OD2	4:P:28:VAL:HG13	2.09	0.52
3:K:654:ARG:HA	3:K:722:GLN:HG3	1.91	0.52
3:L:368:ASN:ND2	3:L:368:ASN:H	2.08	0.52
2:B:1387:THR:CG2	2:B:1451:GLN:H	2.22	0.52
2:B:1446:ASN:CB	4:Q:4:LEU:HB2	2.40	0.52
2:B:1470:PHE:CB	2:B:1478:GLY:HA3	2.39	0.52
1:C:19:THR:HB	1:C:478:LEU:HB2	1.91	0.52
1:C:396:LYS:HG3	1:C:397:PRO:HD2	1.90	0.52
1:C:569:ALA:HB2	2:D:788:SER:HB2	1.89	0.52
2:D:1387:THR:CG2	2:D:1451:GLN:H	2.22	0.52
1:E:439:LEU:H	1:E:439:LEU:HD12	1.74	0.52
1:G:527:ASP:CA	1:G:616:VAL:HG11	2.40	0.52
2:H:804:MET:HG2	2:H:805:GLN:N	2.23	0.52
3:K:461:LYS:HD2	4:P:29:ASN:OD1	2.10	0.52
3:K:598:LEU:HA	3:K:603:ILE:HD13	1.91	0.52
2:B:973:VAL:HG12	2:B:975:ALA:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:978:LEU:HG	2:B:1240:TYR:HB3	1.91	0.52
2:D:1360:ASN:O	2:D:1361:THR:C	2.48	0.52
1:E:451:VAL:HB	1:E:495:LEU:HB3	1.91	0.52
3:J:654:ARG:HA	3:J:722:GLN:HG3	1.91	0.52
2:B:1344:THR:HG21	2:B:1346:LYS:HE2	1.92	0.52
2:D:973:VAL:HG12	2:D:975:ALA:H	1.73	0.52
2:F:932:ARG:HH11	3:L:339:SER:HB2	1.73	0.52
3:I:461:LYS:HD2	4:M:29:ASN:OD1	2.09	0.52
1:A:344:PRO:HD2	1:A:433:TYR:CE1	2.44	0.52
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.75	0.52
1:C:451:VAL:HB	1:C:495:LEU:HB3	1.91	0.52
2:D:1521:TYR:HB2	2:D:1523:TYR:CE2	2.44	0.52
1:E:434:LEU:HB2	1:E:513:TYR:HE2	1.75	0.52
1:G:339:PRO:HB3	1:G:608:GLY:O	2.09	0.52
1:G:436:LEU:HD11	1:G:511:ALA:HB3	1.90	0.52
2:H:1578:LYS:HD3	2:H:1608:HIS:HE1	1.74	0.52
3:J:598:LEU:HA	3:J:603:ILE:HD13	1.91	0.52
3:K:531:HIS:CD2	3:K:533:ASN:H	2.27	0.52
8:X:2:NAG:H82	8:X:2:NAG:O3	2.10	0.52
1:C:434:LEU:HB2	1:C:513:TYR:HE2	1.75	0.52
1:E:472:ILE:HD13	1:E:509:LEU:HD23	1.90	0.52
2:F:1196:ASN:HD22	2:F:1196:ASN:N	2.07	0.52
2:F:1521:TYR:HB2	2:F:1523:TYR:CE2	2.44	0.52
2:H:1470:PHE:HB2	2:H:1478:GLY:HA3	1.92	0.52
3:I:313:GLN:O	3:I:317:ILE:HG13	2.10	0.52
3:I:513:LYS:HZ2	3:I:524:GLU:HG2	1.75	0.52
3:I:531:HIS:CD2	3:I:533:ASN:H	2.27	0.52
3:L:256:ILE:HD12	3:L:405:VAL:HG23	1.92	0.52
1:A:214:VAL:HG23	1:A:321:ARG:HB2	1.92	0.52
1:C:472:ILE:HD13	1:C:509:LEU:HD23	1.90	0.52
3:I:292:TYR:HD1	3:I:325:LYS:HD3	1.74	0.52
3:I:368:ASN:ND2	3:I:368:ASN:H	2.08	0.52
3:I:654:ARG:HA	3:I:722:GLN:HG3	1.91	0.52
3:J:531:HIS:CD2	3:J:533:ASN:H	2.27	0.52
3:L:292:TYR:HD1	3:L:325:LYS:HD3	1.74	0.52
2:B:1521:TYR:HB2	2:B:1523:TYR:CE2	2.44	0.52
2:D:978:LEU:HG	2:D:1240:TYR:HB3	1.91	0.52
2:F:1470:PHE:HB2	2:F:1478:GLY:HA3	1.92	0.52
1:G:214:VAL:HG23	1:G:321:ARG:HB2	1.92	0.52
1:G:506:SER:CB	1:G:530:TRP:HE1	2.21	0.52
2:H:1359:LYS:HD2	4:N:4:LEU:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1387:THR:CG2	2:H:1451:GLN:H	2.21	0.52
2:H:1641:ASN:O	3:J:368:ASN:ND2	2.43	0.52
3:J:239:ASP:HB3	3:J:448:GLN:HB2	1.92	0.52
3:J:256:ILE:HD12	3:J:405:VAL:HG23	1.92	0.52
3:J:381:ARG:CG	3:J:381:ARG:NH2	2.68	0.52
3:L:598:LEU:HA	3:L:603:ILE:HD13	1.91	0.52
1:A:396:LYS:HG3	1:A:397:PRO:HD2	1.90	0.52
1:A:404:THR:HG23	1:A:414:GLN:HB3	1.92	0.52
1:E:269:ILE:HD13	1:E:278:VAL:HB	1.90	0.52
1:E:436:LEU:HD11	1:E:511:ALA:HB3	1.90	0.52
1:G:424:TYR:O	1:G:433:TYR:CE1	2.59	0.52
3:I:436:LEU:HB3	3:I:440:PHE:HE2	1.73	0.52
3:L:654:ARG:HA	3:L:722:GLN:HG3	1.91	0.52
4:P:30:GLU:HA	4:P:44:ILE:HD13	1.92	0.52
2:B:1196:ASN:HD22	2:B:1196:ASN:N	2.07	0.51
2:F:1228:PRO:HB2	2:F:1229:PRO:HD3	1.92	0.51
3:L:239:ASP:HB3	3:L:448:GLN:HB2	1.92	0.51
1:A:439:LEU:H	1:A:439:LEU:HD12	1.74	0.51
2:B:1360:ASN:O	2:B:1361:THR:C	2.48	0.51
2:H:860:HIS:CE1	2:H:862:GLN:HE22	2.29	0.51
3:K:313:GLN:O	3:K:317:ILE:HG13	2.10	0.51
3:K:368:ASN:ND2	3:K:368:ASN:H	2.07	0.51
3:L:531:HIS:CD2	3:L:533:ASN:H	2.27	0.51
4:N:30:GLU:HA	4:N:44:ILE:HD13	1.92	0.51
1:C:126:ARG:HG2	1:C:168:PRO:HA	1.93	0.51
1:E:214:VAL:HG23	1:E:321:ARG:HB2	1.92	0.51
1:A:590:THR:HG22	1:A:592:SER:H	1.75	0.51
2:D:972:ALA:HB1	2:D:1005:TYR:OH	2.10	0.51
2:D:1228:PRO:HB2	2:D:1229:PRO:HD3	1.92	0.51
2:D:1344:THR:HG21	2:D:1346:LYS:HE2	1.92	0.51
1:E:410:SER:O	1:E:414:GLN:HG2	2.11	0.51
2:F:754:GLU:HG3	2:F:769:MET:SD	2.51	0.51
3:I:598:LEU:HA	3:I:603:ILE:HD13	1.91	0.51
3:J:292:TYR:HD1	3:J:325:LYS:HD3	1.74	0.51
3:L:313:GLN:O	3:L:317:ILE:HG13	2.10	0.51
1:C:568:GLY:HA2	2:D:757:LYS:HE2	1.93	0.51
2:D:1381:LEU:HD23	2:D:1457:VAL:HG12	1.92	0.51
2:F:972:ALA:HB1	2:F:1005:TYR:OH	2.09	0.51
2:F:1578:LYS:HD3	2:F:1608:HIS:HE1	1.74	0.51
3:K:256:ILE:HD12	3:K:405:VAL:HG23	1.92	0.51
4:M:70:LEU:HG	4:M:74:TYR:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:972:ALA:HB1	2:B:1005:TYR:OH	2.10	0.51
1:C:478:LEU:HD21	1:C:622:LEU:HD21	1.91	0.51
2:D:754:GLU:HG3	2:D:769:MET:SD	2.51	0.51
3:J:461:LYS:HD2	4:Q:29:ASN:OD1	2.10	0.51
3:K:292:TYR:HD1	3:K:325:LYS:HD3	1.74	0.51
1:A:640:CYS:HB3	1:A:641:PRO:HD2	1.93	0.51
2:B:754:GLU:HG3	2:B:769:MET:SD	2.51	0.51
2:B:1126:LEU:HD23	2:B:1173:ALA:HB1	1.93	0.51
2:B:1381:LEU:HD23	2:B:1457:VAL:HG12	1.92	0.51
2:D:1233:TRP:O	2:D:1237:GLN:HG2	2.11	0.51
1:E:19:THR:HB	1:E:478:LEU:HB2	1.93	0.51
1:E:506:SER:CB	1:E:530:TRP:HE1	2.21	0.51
1:G:36:THR:HG23	1:G:48:SER:HA	1.93	0.51
1:G:439:LEU:HD12	1:G:439:LEU:H	1.74	0.51
1:G:590:THR:HG22	1:G:592:SER:H	1.74	0.51
2:H:937:LYS:O	2:H:937:LYS:HD2	2.10	0.51
3:L:235:LYS:O	3:L:236:ILE:HB	2.11	0.51
3:L:456:VAL:HG13	3:L:467:LYS:HA	1.91	0.51
1:A:36:THR:HG23	1:A:48:SER:HA	1.93	0.51
1:A:410:SER:O	1:A:414:GLN:HG2	2.11	0.51
2:B:860:HIS:CE1	2:B:862:GLN:HE22	2.29	0.51
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.91	0.51
1:C:214:VAL:HG23	1:C:321:ARG:HB2	1.93	0.51
2:D:1126:LEU:HD23	2:D:1173:ALA:HB1	1.93	0.51
2:D:1480:LEU:HB3	2:D:1493:GLU:OE2	2.10	0.51
1:G:404:THR:HG23	1:G:414:GLN:HB3	1.92	0.51
1:G:640:CYS:HB3	1:G:641:PRO:HD2	1.93	0.51
2:B:839:LYS:HE2	4:Q:60:PHE:CD1	2.46	0.51
1:C:590:THR:HG22	1:C:592:SER:H	1.75	0.51
2:D:819:ARG:HG2	2:D:819:ARG:NH1	2.19	0.51
1:G:126:ARG:HG2	1:G:168:PRO:HA	1.93	0.51
4:Q:30:GLU:HA	4:Q:44:ILE:HD13	1.92	0.51
4:Q:70:LEU:HG	4:Q:74:TYR:CE2	2.46	0.51
2:B:1578:LYS:HD3	2:B:1608:HIS:HE1	1.75	0.51
1:C:640:CYS:HB3	1:C:641:PRO:HD2	1.93	0.51
2:D:772:PHE:CD1	4:M:37:ASN:ND2	2.78	0.51
2:F:860:HIS:CE1	2:F:862:GLN:HE22	2.29	0.51
2:F:966:ALA:O	2:F:967:GLN:CB	2.57	0.51
2:F:1126:LEU:HD23	2:F:1173:ALA:HB1	1.93	0.51
2:F:1233:TRP:O	2:F:1237:GLN:HG2	2.11	0.51
1:G:434:LEU:HB2	1:G:513:TYR:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:738:ASN:ND2	4:Q:45:LYS:HE2	2.22	0.51
2:H:754:GLU:HG3	2:H:769:MET:SD	2.51	0.51
3:I:334:LEU:HB3	3:I:376:VAL:HG11	1.93	0.51
3:I:381:ARG:CG	3:I:381:ARG:NH2	2.68	0.51
3:L:339:SER:HA	3:L:342:SER:HB3	1.93	0.51
3:L:724:LEU:HB3	3:L:725:PRO:HD3	1.92	0.51
1:E:36:THR:HG23	1:E:48:SER:HA	1.93	0.50
3:I:256:ILE:HD12	3:I:405:VAL:HG23	1.92	0.50
3:J:563:TYR:CZ	3:J:569:PRO:HG3	2.47	0.50
3:K:724:LEU:HB3	3:K:725:PRO:HD3	1.92	0.50
4:P:70:LEU:HG	4:P:74:TYR:CE2	2.46	0.50
1:C:36:THR:HG23	1:C:48:SER:HA	1.93	0.50
2:D:1593:LYS:HG2	2:D:1596:LEU:HD11	1.94	0.50
1:E:404:THR:HG23	1:E:414:GLN:HB3	1.92	0.50
1:E:640:CYS:HB3	1:E:641:PRO:HD2	1.93	0.50
2:F:882:LYS:HG3	2:F:886:GLN:NE2	2.27	0.50
2:H:1381:LEU:HD23	2:H:1457:VAL:HG12	1.93	0.50
3:I:724:LEU:HB3	3:I:725:PRO:HD3	1.92	0.50
3:L:334:LEU:HB3	3:L:376:VAL:HG11	1.93	0.50
2:B:772:PHE:HD1	4:N:37:ASN:ND2	2.10	0.50
2:B:1233:TRP:O	2:B:1237:GLN:HG2	2.11	0.50
1:C:410:SER:O	1:C:414:GLN:HG2	2.11	0.50
2:F:1344:THR:HG21	2:F:1346:LYS:HE2	1.93	0.50
3:J:313:GLN:O	3:J:317:ILE:HG13	2.10	0.50
3:K:239:ASP:HB3	3:K:448:GLN:HB2	1.92	0.50
3:L:439:VAL:HG22	4:N:31:LEU:HD21	1.91	0.50
1:G:554:VAL:HG13	1:G:555:PRO:HD2	1.94	0.50
3:I:239:ASP:HB3	3:I:448:GLN:HB2	1.92	0.50
3:J:334:LEU:HB3	3:J:376:VAL:HG11	1.93	0.50
3:L:278:TYR:HA	3:L:455:MET:HE1	1.92	0.50
3:L:465:TYR:CD1	3:L:517:GLY:HA2	2.46	0.50
3:L:641:TYR:HE2	3:L:650:VAL:HB	1.77	0.50
2:B:940:ILE:HD12	2:B:1308:PHE:CE1	2.47	0.50
2:B:964:PRO:HG3	2:B:1270:LEU:HD11	1.92	0.50
2:B:1569:ARG:HH11	2:B:1569:ARG:CG	2.25	0.50
1:C:404:THR:HG23	1:C:414:GLN:HB3	1.92	0.50
2:D:860:HIS:CE1	2:D:862:GLN:HE22	2.29	0.50
2:D:1578:LYS:HD3	2:D:1608:HIS:HE1	1.75	0.50
2:F:819:ARG:HH11	2:F:819:ARG:CG	2.22	0.50
1:G:369:VAL:HG12	1:G:370:GLN:H	1.77	0.50
1:G:410:SER:O	1:G:414:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:882:LYS:HG3	2:H:886:GLN:NE2	2.27	0.50
3:I:563:TYR:CZ	3:I:569:PRO:HG3	2.46	0.50
3:I:641:TYR:HE2	3:I:650:VAL:HB	1.77	0.50
3:J:235:LYS:O	3:J:236:ILE:HB	2.11	0.50
3:J:724:LEU:HB3	3:J:725:PRO:HD3	1.92	0.50
2:B:882:LYS:HG3	2:B:886:GLN:NE2	2.27	0.50
2:B:1593:LYS:HG2	2:B:1596:LEU:HD11	1.94	0.50
3:J:339:SER:HA	3:J:342:SER:HB3	1.93	0.50
3:J:465:TYR:CD1	3:J:517:GLY:HA2	2.46	0.50
3:K:641:TYR:HE2	3:K:650:VAL:HB	1.77	0.50
3:L:513:LYS:NZ	3:L:524:GLU:HG2	2.27	0.50
4:M:30:GLU:HA	4:M:44:ILE:HD13	1.92	0.50
1:A:126:ARG:HG2	1:A:168:PRO:HA	1.93	0.50
1:E:126:ARG:HG2	1:E:168:PRO:HA	1.93	0.50
1:E:268:ARG:HD3	2:F:1378:MET:SD	2.51	0.50
2:F:964:PRO:HG3	2:F:1270:LEU:HD11	1.93	0.50
2:H:1617:ASP:O	2:H:1621:GLN:HG3	2.12	0.50
3:K:339:SER:HA	3:K:342:SER:HB3	1.93	0.50
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.94	0.50
2:D:907:LEU:HD23	2:D:907:LEU:H	1.77	0.50
2:F:855:THR:HB	2:F:1602:LYS:HZ3	1.76	0.50
2:F:1617:ASP:O	2:F:1621:GLN:HG3	2.12	0.50
2:H:839:LYS:HE2	4:N:60:PHE:CE1	2.47	0.50
2:H:907:LEU:H	2:H:907:LEU:HD23	1.77	0.50
2:H:962:GLY:C	2:H:964:PRO:HD3	2.31	0.50
3:I:339:SER:HA	3:I:342:SER:HB3	1.93	0.50
3:J:478:ARG:CG	3:J:479:PRO:HD2	2.42	0.50
1:C:10:ASN:HA	1:C:623:THR:HG23	1.93	0.50
1:C:222:TYR:HB3	1:C:225:ASN:HB2	1.94	0.50
1:E:222:TYR:HB3	1:E:225:ASN:HB2	1.94	0.50
2:F:1268:GLN:O	2:F:1269:GLU:CB	2.59	0.50
3:K:334:LEU:HB3	3:K:376:VAL:HG11	1.93	0.50
3:K:563:TYR:CZ	3:K:569:PRO:HG3	2.47	0.50
3:L:431:LYS:HG3	4:N:27:ASN:ND2	2.27	0.50
1:A:103:LEU:HB3	1:A:193:GLN:HE21	1.77	0.49
1:A:568:GLY:HA2	2:B:757:LYS:HE2	1.94	0.49
2:B:1617:ASP:O	2:B:1621:GLN:HG3	2.12	0.49
2:H:1488:LEU:HG	2:H:1590:TRP:CH2	2.35	0.49
3:J:267:CYS:HB2	3:J:433:MET:HE1	1.94	0.49
3:J:641:TYR:HE2	3:J:650:VAL:HB	1.77	0.49
1:A:426:THR:HG21	1:A:432:ASN:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:733:ILE:HG12	2:D:734:ILE:N	2.26	0.49
2:F:1593:LYS:HG2	2:F:1596:LEU:HD11	1.94	0.49
3:I:465:TYR:CD1	3:I:517:GLY:HA2	2.46	0.49
3:K:465:TYR:CD1	3:K:517:GLY:HA2	2.46	0.49
1:C:351:MET:SD	1:C:440:ARG:HD2	2.53	0.49
2:D:841:ARG:HH11	2:D:841:ARG:CG	2.23	0.49
2:D:882:LYS:HG3	2:D:886:GLN:NE2	2.27	0.49
2:D:940:ILE:HD12	2:D:1308:PHE:CE1	2.47	0.49
2:D:1617:ASP:O	2:D:1621:GLN:HG3	2.12	0.49
1:G:572:VAL:CG2	2:H:785:VAL:HB	2.42	0.49
3:I:438:ASP:OD2	4:M:28:VAL:HG13	2.12	0.49
3:J:435:ASN:HD21	3:J:460:ARG:HH21	1.57	0.49
2:B:1505:VAL:HG23	2:B:1505:VAL:O	2.12	0.49
2:D:1505:VAL:O	2:D:1505:VAL:HG23	2.12	0.49
1:E:554:VAL:HG13	1:E:555:PRO:HD2	1.94	0.49
2:F:1495:ASN:O	2:F:1602:LYS:HA	2.13	0.49
3:I:328:THR:HB	3:I:367:HIS:HA	1.94	0.49
3:K:235:LYS:O	3:K:236:ILE:HB	2.11	0.49
3:L:478:ARG:CG	3:L:479:PRO:HD2	2.42	0.49
4:N:70:LEU:HG	4:N:74:TYR:CE2	2.46	0.49
2:B:1239:TYR:OH	2:B:1246:SER:HB2	2.13	0.49
2:F:841:ARG:HH11	2:F:841:ARG:CG	2.23	0.49
2:F:1569:ARG:HH11	2:F:1569:ARG:CG	2.26	0.49
1:G:439:LEU:HD12	1:G:439:LEU:N	2.28	0.49
2:H:733:ILE:HG12	2:H:734:ILE:N	2.26	0.49
2:H:1593:LYS:HG2	2:H:1596:LEU:HD11	1.94	0.49
3:J:513:LYS:NZ	3:J:524:GLU:HG2	2.27	0.49
3:L:328:THR:HB	3:L:367:HIS:HA	1.94	0.49
2:H:1344:THR:HG21	2:H:1346:LYS:HE2	1.93	0.49
2:H:1635:VAL:HG23	2:H:1636:VAL:H	1.78	0.49
2:D:1485:ARG:HD3	2:D:1536:PHE:HZ	1.78	0.49
1:E:108:LEU:HB2	1:E:196:PHE:CD1	2.48	0.49
2:F:1381:LEU:HD23	2:F:1457:VAL:HG12	1.93	0.49
3:I:573:PRO:HB3	3:I:721:PHE:CZ	2.48	0.49
3:K:328:THR:HB	3:K:367:HIS:HA	1.95	0.49
3:L:563:TYR:CZ	3:L:569:PRO:HG3	2.47	0.49
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.48	0.49
1:C:554:VAL:HG13	1:C:555:PRO:HD2	1.94	0.49
2:D:1569:ARG:HH11	2:D:1569:ARG:CG	2.24	0.49
2:F:907:LEU:HD23	2:F:907:LEU:H	1.77	0.49
1:G:369:VAL:HG12	1:G:370:GLN:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:268:LEU:O	3:L:272:ILE:HG13	2.13	0.49
1:A:222:TYR:HB3	1:A:225:ASN:HB2	1.94	0.49
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.48	0.49
1:A:567:HIS:ND1	2:B:760:PRO:HG3	2.27	0.49
2:B:813:LEU:HD23	2:B:907:LEU:HB3	1.95	0.49
3:I:235:LYS:O	3:I:236:ILE:HB	2.11	0.49
2:B:738:ASN:HD22	4:N:45:LYS:HE2	1.78	0.49
1:A:477:ARG:CG	1:A:477:ARG:NH1	2.76	0.48
2:B:907:LEU:HD23	2:B:907:LEU:H	1.77	0.48
2:D:813:LEU:HD23	2:D:907:LEU:HB3	1.95	0.48
2:D:833:ARG:CG	2:D:833:ARG:NH1	2.76	0.48
2:D:1239:TYR:OH	2:D:1246:SER:HB2	2.13	0.48
2:D:1417:SER:HB2	4:P:14:LYS:NZ	2.27	0.48
1:G:454:LEU:HA	1:G:491:ASP:O	2.13	0.48
1:G:477:ARG:CG	1:G:477:ARG:NH1	2.76	0.48
2:H:813:LEU:HD23	2:H:907:LEU:HB3	1.95	0.48
3:J:268:LEU:O	3:J:272:ILE:HG13	2.13	0.48
3:J:573:PRO:HB3	3:J:721:PHE:CZ	2.48	0.48
3:L:372:ASP:O	3:L:375:THR:HG22	2.13	0.48
3:L:573:PRO:HB3	3:L:721:PHE:CZ	2.48	0.48
1:C:477:ARG:CG	1:C:477:ARG:NH1	2.76	0.48
2:H:1446:ASN:HB2	4:N:4:LEU:HB2	1.94	0.48
2:H:1492:ALA:O	2:H:1494:GLU:N	2.46	0.48
3:I:620:VAL:HG12	3:I:667:PRO:HD2	1.95	0.48
3:K:372:ASP:O	3:K:375:THR:HG22	2.13	0.48
3:K:513:LYS:NZ	3:K:524:GLU:HG2	2.27	0.48
3:L:620:VAL:HG12	3:L:667:PRO:HD2	1.95	0.48
2:F:1635:VAL:HG23	2:F:1636:VAL:H	1.78	0.48
2:H:1338:LYS:H	2:H:1371:ARG:HD2	1.78	0.48
2:H:1499:GLN:HG2	2:H:1500:LYS:N	2.27	0.48
3:I:372:ASP:O	3:I:375:THR:HG22	2.13	0.48
3:I:513:LYS:NZ	3:I:524:GLU:HG2	2.27	0.48
3:J:328:THR:HB	3:J:367:HIS:HA	1.95	0.48
3:J:372:ASP:O	3:J:375:THR:HG22	2.13	0.48
3:K:268:LEU:O	3:K:272:ILE:HG13	2.13	0.48
3:K:478:ARG:CG	3:K:479:PRO:HD2	2.42	0.48
1:A:439:LEU:HD12	1:A:439:LEU:N	2.28	0.48
1:C:108:LEU:HB2	1:C:196:PHE:CD1	2.48	0.48
3:I:268:LEU:O	3:I:272:ILE:HG13	2.13	0.48
3:I:270:ASN:HD22	3:I:270:ASN:N	2.12	0.48
3:J:493:GLU:HG3	3:J:563:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:620:VAL:HG12	3:J:667:PRO:HD2	1.95	0.48
5:U:1:NAG:H61	5:U:2:NAG:H83	1.94	0.48
2:D:744:GLU:C	2:D:746:PRO:HD3	2.34	0.48
2:F:1239:TYR:OH	2:F:1246:SER:HB2	2.13	0.48
2:F:1445:PHE:CE2	4:M:7:SER:HA	2.48	0.48
1:G:108:LEU:HB2	1:G:196:PHE:CD1	2.48	0.48
2:H:1569:ARG:HH11	2:H:1569:ARG:CG	2.26	0.48
3:I:478:ARG:CG	3:I:479:PRO:HD2	2.42	0.48
2:B:1485:ARG:HD3	2:B:1536:PHE:HZ	1.78	0.48
3:J:270:ASN:HD22	3:J:270:ASN:N	2.11	0.48
3:K:267:CYS:HB2	3:K:433:MET:CE	2.44	0.48
3:K:362:MET:HG2	3:K:403:PHE:HB2	1.95	0.48
4:N:11:GLN:NE2	4:N:11:GLN:H	2.11	0.48
2:D:738:ASN:HD22	4:M:45:LYS:HE2	1.77	0.48
3:L:493:GLU:HG3	3:L:563:TYR:OH	2.14	0.48
4:P:11:GLN:NE2	4:P:11:GLN:H	2.11	0.48
4:Q:11:GLN:NE2	4:Q:11:GLN:H	2.11	0.48
1:C:506:SER:CB	1:C:530:TRP:HE1	2.21	0.48
1:E:369:VAL:HG12	1:E:370:GLN:H	1.78	0.48
1:G:222:TYR:HB3	1:G:225:ASN:HB2	1.94	0.48
3:I:439:VAL:HG22	4:M:31:LEU:HD21	1.95	0.48
3:I:465:TYR:CE1	3:I:517:GLY:HA2	2.49	0.48
3:I:493:GLU:HG3	3:I:563:TYR:OH	2.14	0.48
3:K:378:ASP:HA	3:K:381:ARG:HB2	1.96	0.48
3:K:573:PRO:HB3	3:K:721:PHE:CZ	2.48	0.48
2:D:1291:TRP:O	2:D:1294:ALA:N	2.47	0.48
2:D:1361:THR:HA	2:D:1441:VAL:O	2.14	0.48
1:G:624:PHE:HB3	1:G:632:THR:HG23	1.96	0.48
3:J:465:TYR:CE1	3:J:517:GLY:HA2	2.49	0.48
3:K:465:TYR:CE1	3:K:517:GLY:HA2	2.49	0.48
3:L:328:THR:O	3:L:367:HIS:HB2	2.14	0.48
3:L:544:ILE:HD13	3:L:650:VAL:HG12	1.96	0.48
4:M:11:GLN:NE2	4:M:11:GLN:H	2.11	0.48
1:A:624:PHE:HB3	1:A:632:THR:HG23	1.96	0.48
2:B:865:THR:OG1	4:Q:11:GLN:HG2	2.14	0.48
1:C:439:LEU:HD12	1:C:439:LEU:N	2.28	0.48
1:E:606:THR:HB	1:E:619:ASP:HB3	1.96	0.48
2:F:819:ARG:HG2	2:F:819:ARG:NH1	2.19	0.48
1:G:528:SER:N	1:G:616:VAL:HG13	2.29	0.48
2:H:932:ARG:O	2:H:934:GLY:N	2.47	0.48
3:K:493:GLU:HG3	3:K:563:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:TYR:HA	1:A:510:VAL:O	2.14	0.47
2:B:1361:THR:HA	2:B:1441:VAL:O	2.14	0.47
2:D:964:PRO:HB3	2:D:1270:LEU:HD11	1.95	0.47
1:E:439:LEU:HD12	1:E:439:LEU:N	2.28	0.47
2:F:733:ILE:HG12	2:F:734:ILE:N	2.26	0.47
1:G:35:VAL:HG21	1:G:64:VAL:HG21	1.96	0.47
3:J:267:CYS:HB2	3:J:433:MET:CE	2.44	0.47
3:J:539:LYS:HD2	3:J:539:LYS:N	2.30	0.47
3:K:328:THR:O	3:K:367:HIS:HB2	2.14	0.47
3:L:361:LEU:O	3:L:402:VAL:HA	2.14	0.47
3:L:465:TYR:CE1	3:L:517:GLY:HA2	2.49	0.47
1:A:382:ASP:OD2	1:A:440:ARG:NH2	2.47	0.47
1:C:35:VAL:HG21	1:C:64:VAL:HG21	1.96	0.47
2:F:877:VAL:H	2:F:1451:GLN:NE2	2.12	0.47
2:F:1338:LYS:H	2:F:1371:ARG:HD2	1.79	0.47
1:G:470:TYR:HA	1:G:510:VAL:O	2.14	0.47
1:G:510:VAL:HG21	1:G:622:LEU:HD12	1.96	0.47
3:I:278:TYR:HA	3:I:455:MET:HE1	1.97	0.47
5:O:1:NAG:H4	5:O:2:NAG:H2	1.61	0.47
1:A:6:ILE:HD12	1:A:21:VAL:O	2.15	0.47
2:D:1521:TYR:HB2	2:D:1523:TYR:CZ	2.50	0.47
1:G:345:GLY:HA2	1:G:391:THR:O	2.14	0.47
3:I:544:ILE:HD13	3:I:650:VAL:HG12	1.96	0.47
3:K:620:VAL:HG12	3:K:667:PRO:HD2	1.95	0.47
2:B:1291:TRP:O	2:B:1294:ALA:N	2.47	0.47
1:C:555:PRO:HB3	2:D:775:ASP:HA	1.96	0.47
2:D:965:VAL:O	2:D:1267:HIS:HD2	1.97	0.47
2:F:813:LEU:HD23	2:F:907:LEU:HB3	1.95	0.47
3:J:362:MET:HG2	3:J:403:PHE:HB2	1.95	0.47
3:J:378:ASP:HA	3:J:381:ARG:HB2	1.96	0.47
3:L:334:LEU:HD12	3:L:373:PRO:HB3	1.97	0.47
4:N:10:TYR:HE2	4:N:14:LYS:HE3	1.80	0.47
2:B:1521:TYR:HB2	2:B:1523:TYR:CZ	2.50	0.47
1:C:624:PHE:HB3	1:C:632:THR:HG23	1.96	0.47
1:E:13:ARG:NH2	1:E:476:GLY:HA3	2.28	0.47
1:E:369:VAL:HG12	1:E:370:GLN:N	2.29	0.47
1:E:624:PHE:HB3	1:E:632:THR:HG23	1.96	0.47
2:H:1270:LEU:O	2:H:1290:HIS:HA	2.15	0.47
3:I:378:ASP:HA	3:I:381:ARG:HB2	1.96	0.47
3:I:538:GLY:C	3:I:539:LYS:HD2	2.35	0.47
3:K:334:LEU:HD12	3:K:373:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:10:TYR:HE2	4:M:14:LYS:HE3	1.79	0.47
1:C:166:VAL:O	1:C:168:PRO:HD3	2.15	0.47
1:E:35:VAL:HG21	1:E:64:VAL:HG21	1.96	0.47
2:F:932:ARG:O	2:F:934:GLY:N	2.47	0.47
1:G:606:THR:HB	1:G:619:ASP:HB3	1.96	0.47
3:I:334:LEU:HD12	3:I:373:PRO:HB3	1.97	0.47
3:I:349:PRO:O	3:I:352:TRP:HD1	1.98	0.47
3:I:361:LEU:O	3:I:402:VAL:HA	2.14	0.47
3:I:362:MET:HG2	3:I:403:PHE:HB2	1.95	0.47
3:J:349:PRO:O	3:J:352:TRP:HD1	1.98	0.47
3:J:538:GLY:C	3:J:539:LYS:HD2	2.35	0.47
1:A:35:VAL:HG21	1:A:64:VAL:HG21	1.96	0.47
1:C:10:ASN:HB2	1:C:621:GLY:HA2	1.95	0.47
1:C:470:TYR:HA	1:C:510:VAL:O	2.14	0.47
2:F:1269:GLU:HG3	2:F:1269:GLU:O	2.15	0.47
2:F:1270:LEU:O	2:F:1290:HIS:HA	2.15	0.47
2:H:1359:LYS:HD2	4:N:4:LEU:CG	2.45	0.47
2:H:1521:TYR:HB2	2:H:1523:TYR:CZ	2.49	0.47
3:J:236:ILE:HG21	3:J:443:MET:O	2.15	0.47
3:J:513:LYS:HZ2	3:J:524:GLU:HG2	1.78	0.47
3:K:544:ILE:HD13	3:K:650:VAL:HG12	1.96	0.47
3:L:362:MET:HG2	3:L:403:PHE:HB2	1.95	0.47
3:L:539:LYS:HD2	3:L:539:LYS:N	2.30	0.47
1:A:606:THR:HB	1:A:619:ASP:HB3	1.96	0.47
2:B:967:GLN:O	2:B:968:MET:HB2	2.13	0.47
2:H:1446:ASN:CB	4:N:4:LEU:HB2	2.44	0.47
3:I:236:ILE:HG23	3:I:236:ILE:O	2.15	0.47
3:J:328:THR:O	3:J:367:HIS:HB2	2.15	0.47
3:J:544:ILE:HD13	3:J:650:VAL:HG12	1.96	0.47
3:K:363:THR:HG23	3:K:365:GLY:H	1.80	0.47
3:K:538:GLY:C	3:K:539:LYS:HD2	2.35	0.47
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.97	0.47
1:C:510:VAL:HG12	1:C:528:SER:HB3	1.97	0.47
1:E:6:ILE:HG22	1:E:625:THR:O	2.14	0.47
1:E:219:LYS:HZ2	1:E:356:ASN:HD22	1.63	0.47
2:F:1521:TYR:HB2	2:F:1523:TYR:CZ	2.49	0.47
1:G:522:ARG:HG2	1:G:628:SER:CB	2.44	0.47
2:H:1291:TRP:O	2:H:1294:ALA:N	2.48	0.47
2:H:1498:ILE:HG13	2:H:1605:TRP:CZ3	2.50	0.47
3:K:236:ILE:HG21	3:K:443:MET:O	2.15	0.47
1:C:325:PRO:HG2	1:C:357:PRO:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:470:TYR:HA	1:E:510:VAL:O	2.14	0.47
3:K:270:ASN:N	3:K:270:ASN:HD22	2.12	0.47
3:K:539:LYS:HD2	3:K:539:LYS:N	2.30	0.47
3:L:236:ILE:O	3:L:236:ILE:HG23	2.15	0.47
2:B:733:ILE:HD13	2:B:841:ARG:HD3	1.98	0.46
2:B:1640:PRO:HA	3:L:326:SER:OG	2.14	0.46
1:C:378:LEU:HD13	1:E:446:GLY:O	2.16	0.46
1:C:541:LEU:HD22	2:D:786:SER:HB3	1.96	0.46
2:D:1524:LYS:HB3	2:D:1545:GLN:HG2	1.97	0.46
1:E:34:THR:HG22	1:E:51:LYS:HE3	1.97	0.46
2:F:1269:GLU:CG	2:F:1315:LYS:HB3	2.40	0.46
2:F:1524:LYS:HB3	2:F:1545:GLN:HG2	1.97	0.46
3:L:236:ILE:HG21	3:L:443:MET:O	2.15	0.46
1:A:166:VAL:O	1:A:168:PRO:HD3	2.15	0.46
1:A:213:ILE:HG22	1:A:215:GLU:HG3	1.97	0.46
2:B:1524:LYS:HB3	2:B:1545:GLN:HG2	1.97	0.46
1:C:6:ILE:HD12	1:C:21:VAL:O	2.14	0.46
1:C:369:VAL:HG12	1:C:370:GLN:N	2.31	0.46
2:D:990:GLU:O	2:D:994:ILE:HG13	2.16	0.46
2:D:1172:TYR:CE1	2:D:1216:LEU:HB3	2.51	0.46
2:F:733:ILE:HD13	2:F:841:ARG:HD3	1.97	0.46
2:F:1265:PRO:O	2:F:1266:ASP:CB	2.64	0.46
3:I:328:THR:O	3:I:367:HIS:HB2	2.14	0.46
3:L:270:ASN:HD22	3:L:270:ASN:N	2.11	0.46
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.51	0.46
1:E:6:ILE:HD12	1:E:21:VAL:O	2.14	0.46
1:E:207:LEU:HA	1:E:208:PRO:HD2	1.82	0.46
2:F:990:GLU:O	2:F:994:ILE:HG13	2.16	0.46
2:F:1291:TRP:O	2:F:1294:ALA:N	2.48	0.46
1:G:34:THR:HG22	1:G:51:LYS:HE3	1.97	0.46
1:G:477:ARG:HG2	1:G:477:ARG:NH1	2.21	0.46
2:H:1444:TYR:HB2	4:N:10:TYR:CE1	2.50	0.46
3:I:700:CYS:O	3:I:701:LYS:C	2.53	0.46
3:J:361:LEU:O	3:J:402:VAL:HA	2.14	0.46
3:L:538:GLY:C	3:L:539:LYS:HD2	2.35	0.46
3:L:679:ILE:HG21	3:L:686:PHE:HB3	1.97	0.46
3:L:700:CYS:O	3:L:701:LYS:C	2.53	0.46
1:A:34:THR:HG22	1:A:51:LYS:HE3	1.97	0.46
2:B:733:ILE:HG12	2:B:734:ILE:N	2.26	0.46
2:B:990:GLU:O	2:B:994:ILE:HG13	2.16	0.46
1:E:80:ARG:HD2	2:F:1010:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:VAL:O	1:E:168:PRO:HD3	2.15	0.46
3:K:361:LEU:O	3:K:402:VAL:HA	2.14	0.46
3:K:700:CYS:O	3:K:701:LYS:C	2.53	0.46
3:L:378:ASP:HA	3:L:381:ARG:HB2	1.96	0.46
4:Q:10:TYR:HE2	4:Q:14:LYS:HE3	1.79	0.46
4:Q:73:ILE:O	4:Q:77:ILE:HG13	2.16	0.46
2:F:740:VAL:CB	4:P:42:ARG:HB2	2.43	0.46
1:G:154:LYS:HD2	1:G:171:TRP:CD1	2.51	0.46
2:H:833:ARG:CG	2:H:833:ARG:NH1	2.75	0.46
3:I:236:ILE:HG21	3:I:443:MET:O	2.15	0.46
3:I:363:THR:HG23	3:I:365:GLY:H	1.80	0.46
3:I:539:LYS:HD2	3:I:539:LYS:N	2.30	0.46
3:J:236:ILE:HG23	3:J:236:ILE:O	2.15	0.46
3:J:700:CYS:O	3:J:701:LYS:C	2.53	0.46
3:K:349:PRO:O	3:K:352:TRP:HD1	1.98	0.46
3:L:349:PRO:O	3:L:352:TRP:HD1	1.98	0.46
1:A:154:LYS:HD2	1:A:171:TRP:CD1	2.51	0.46
1:C:213:ILE:HG22	1:C:215:GLU:HG3	1.97	0.46
1:C:639:GLN:NE2	1:C:639:GLN:H	2.14	0.46
2:F:1172:TYR:CE1	2:F:1216:LEU:HB3	2.51	0.46
1:G:6:ILE:HD12	1:G:21:VAL:O	2.15	0.46
3:I:531:HIS:HD2	3:I:533:ASN:H	1.64	0.46
3:K:236:ILE:HG23	3:K:236:ILE:O	2.15	0.46
4:M:73:ILE:O	4:M:77:ILE:HG13	2.16	0.46
8:X:3:MAN:H62	8:X:4:MAN:H2	1.43	0.46
1:C:606:THR:HB	1:C:619:ASP:HB3	1.96	0.46
1:E:342:PHE:CE1	1:E:391:THR:HG21	2.50	0.46
2:F:1494:GLU:HB2	2:F:1602:LYS:HB3	1.97	0.46
1:G:247:ALA:HB2	1:G:308:VAL:HG22	1.97	0.46
2:H:837:GLU:HB3	2:H:868:PRO:HD3	1.97	0.46
3:J:531:HIS:HD2	3:J:533:ASN:H	1.64	0.46
3:K:292:TYR:CD1	3:K:325:LYS:HD3	2.51	0.46
3:L:363:THR:HG23	3:L:365:GLY:H	1.80	0.46
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.97	0.46
2:B:744:GLU:C	2:B:746:PRO:HD3	2.35	0.46
2:B:1393:THR:O	2:B:1397:LYS:HD3	2.16	0.46
1:C:47:LEU:HD13	1:C:66:PHE:HB2	1.97	0.46
1:C:154:LYS:HD2	1:C:171:TRP:CD1	2.51	0.46
2:D:1393:THR:O	2:D:1397:LYS:HD3	2.16	0.46
1:G:354:VAL:HG11	1:G:365:VAL:HG11	1.98	0.46
3:J:363:THR:HG23	3:J:365:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:261:PHE:HB3	3:K:319:TYR:HD1	1.81	0.46
3:K:679:ILE:HG21	3:K:686:PHE:HB3	1.97	0.46
3:L:345:ASP:HB3	3:L:346:ASP:H	1.49	0.46
3:L:531:HIS:HD2	3:L:533:ASN:H	1.64	0.46
4:N:73:ILE:O	4:N:77:ILE:HG13	2.15	0.46
1:A:639:GLN:NE2	1:A:639:GLN:H	2.14	0.46
1:C:6:ILE:HG22	1:C:625:THR:O	2.16	0.46
1:E:10:ASN:HB2	1:E:621:GLY:C	2.36	0.46
2:F:811:LEU:HG	2:F:813:LEU:HD13	1.98	0.46
2:F:1290:HIS:O	2:F:1291:TRP:O	2.34	0.46
3:I:700:CYS:HA	3:I:704:LYS:O	2.16	0.46
3:J:334:LEU:HD12	3:J:373:PRO:HB3	1.97	0.46
3:L:261:PHE:HB3	3:L:319:TYR:HD1	1.81	0.46
4:P:73:ILE:O	4:P:77:ILE:HG13	2.16	0.46
7:V:4:BMA:H62	7:V:6:BMA:H2	1.36	0.46
1:E:147:ASN:HB2	1:E:148:PRO:CD	2.46	0.46
1:E:354:VAL:HG11	1:E:365:VAL:HG11	1.98	0.46
1:G:47:LEU:HD13	1:G:66:PHE:HB2	1.97	0.46
1:G:144:ASN:HD22	1:G:144:ASN:N	2.14	0.46
1:G:166:VAL:O	1:G:168:PRO:HD3	2.15	0.46
3:I:267:CYS:HB2	3:I:433:MET:CE	2.44	0.46
4:M:66:ALA:HA	4:M:69:GLN:HB2	1.98	0.46
2:B:819:ARG:HH11	2:B:819:ARG:CG	2.22	0.45
1:C:34:THR:HG22	1:C:51:LYS:HE3	1.97	0.45
1:G:213:ILE:HG22	1:G:215:GLU:HG3	1.97	0.45
3:J:679:ILE:HG21	3:J:686:PHE:HB3	1.97	0.45
3:K:646:ASP:OD2	3:K:648:SER:HB3	2.17	0.45
4:N:66:ALA:HA	4:N:69:GLN:HB2	1.98	0.45
4:P:10:TYR:HE2	4:P:14:LYS:HE3	1.79	0.45
1:A:369:VAL:HG12	1:A:370:GLN:N	2.31	0.45
1:A:426:THR:HG22	1:A:427:VAL:N	2.31	0.45
3:I:646:ASP:OD2	3:I:648:SER:HB3	2.16	0.45
3:L:653:PRO:CD	3:L:654:ARG:HH12	2.27	0.45
1:A:144:ASN:HD22	1:A:144:ASN:N	2.14	0.45
1:A:427:VAL:HB	1:A:523:GLU:HG3	1.99	0.45
1:A:538:VAL:HB	2:B:791:LYS:O	2.16	0.45
1:E:47:LEU:HD13	1:E:66:PHE:HB2	1.97	0.45
1:E:351:MET:SD	1:E:440:ARG:HD2	2.57	0.45
1:G:639:GLN:NE2	1:G:639:GLN:H	2.14	0.45
2:H:1524:LYS:HB3	2:H:1545:GLN:HG2	1.97	0.45
3:I:261:PHE:HB3	3:I:319:TYR:HD1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:700:CYS:HA	3:J:704:LYS:O	2.16	0.45
3:L:292:TYR:CD1	3:L:325:LYS:HD3	2.51	0.45
2:B:819:ARG:O	2:B:820:ASN:HB2	2.17	0.45
2:B:837:GLU:HB3	2:B:868:PRO:HD3	1.97	0.45
1:E:154:LYS:HD2	1:E:171:TRP:CD1	2.51	0.45
2:F:837:GLU:HB3	2:F:868:PRO:HD3	1.97	0.45
1:G:473:MET:HE2	1:G:603:ILE:HD11	1.98	0.45
2:H:733:ILE:HD13	2:H:841:ARG:HD3	1.98	0.45
3:K:239:ASP:HA	3:K:240:PRO:HD3	1.86	0.45
3:K:702:ASN:O	3:K:703:GLN:HG3	2.17	0.45
3:L:702:ASN:O	3:L:703:GLN:HG3	2.17	0.45
2:B:1264:ALA:HA	2:B:1265:PRO:HD3	1.73	0.45
2:D:1223:ASP:O	2:D:1227:VAL:HG23	2.17	0.45
2:D:1280:SER:O	2:D:1281:ARG:C	2.55	0.45
2:D:1288:ARG:HD3	2:D:1290:HIS:NE2	2.32	0.45
2:D:1364:LEU:HD23	2:D:1439:PHE:CZ	2.52	0.45
1:E:569:ALA:HB2	2:F:788:SER:HB2	1.99	0.45
1:G:100:LEU:HD21	1:G:638:LEU:CD2	2.44	0.45
1:G:567:HIS:CG	2:H:760:PRO:HG3	2.52	0.45
3:I:679:ILE:HG21	3:I:686:PHE:HB3	1.97	0.45
3:J:646:ASP:OD2	3:J:648:SER:HB3	2.17	0.45
3:J:705:ARG:O	3:J:706:GLN:CB	2.60	0.45
5:T:1:NAG:H61	5:T:2:NAG:C7	2.46	0.45
2:B:1123:ALA:O	2:B:1127:ILE:HG13	2.17	0.45
2:B:1288:ARG:HD3	2:B:1290:HIS:NE2	2.32	0.45
1:C:342:PHE:CE1	1:C:391:THR:HG21	2.52	0.45
1:C:427:VAL:HB	1:C:523:GLU:HG3	1.99	0.45
2:D:1192:ALA:HB2	2:D:1198:TRP:CZ2	2.52	0.45
1:E:510:VAL:HG12	1:E:528:SER:HB3	1.97	0.45
1:G:424:TYR:OH	1:G:613:TYR:HB3	2.16	0.45
2:H:1492:ALA:O	2:H:1493:GLU:C	2.55	0.45
2:H:1495:ASN:O	2:H:1496:CYS:C	2.54	0.45
3:I:292:TYR:CD1	3:I:325:LYS:HD3	2.51	0.45
3:J:261:PHE:HB3	3:J:319:TYR:HD1	1.81	0.45
3:L:646:ASP:OD2	3:L:648:SER:HB3	2.16	0.45
2:B:1192:ALA:HB2	2:B:1198:TRP:CZ2	2.52	0.45
2:B:1203:LYS:HD2	2:B:1206:TYR:CE2	2.52	0.45
2:F:1470:PHE:CB	2:F:1478:GLY:HA3	2.47	0.45
2:H:819:ARG:O	2:H:820:ASN:HB2	2.17	0.45
3:I:653:PRO:CD	3:I:654:ARG:HH12	2.27	0.45
3:K:428:PHE:CE1	4:P:31:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:653:PRO:CD	3:K:654:ARG:HH12	2.27	0.45
4:P:66:ALA:HA	4:P:69:GLN:HB2	1.98	0.45
1:A:354:VAL:HG11	1:A:365:VAL:HG11	1.98	0.45
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.98	0.45
2:B:729:LEU:O	2:B:729:LEU:HD22	2.17	0.45
2:B:851:CYS:HB2	2:B:1491:CYS:HB2	1.90	0.45
2:B:1280:SER:O	2:B:1281:ARG:C	2.55	0.45
2:D:811:LEU:HG	2:D:813:LEU:HD13	1.98	0.45
2:D:837:GLU:HB3	2:D:868:PRO:HD3	1.97	0.45
2:D:1123:ALA:O	2:D:1127:ILE:HG13	2.17	0.45
2:F:1182:GLY:HA3	2:F:1183:PRO:HD2	1.82	0.45
1:G:516:ILE:N	1:G:516:ILE:HD12	2.32	0.45
2:H:1497:PHE:C	2:H:1498:ILE:HD13	2.37	0.45
3:J:292:TYR:CD1	3:J:325:LYS:HD3	2.51	0.45
2:D:937:LYS:HD2	2:D:937:LYS:O	2.17	0.45
1:E:213:ILE:HG22	1:E:215:GLU:HG3	1.97	0.45
1:E:639:GLN:NE2	1:E:639:GLN:H	2.14	0.45
2:F:962:GLY:C	2:F:964:PRO:HD3	2.37	0.45
2:F:1203:LYS:HD2	2:F:1206:TYR:CE2	2.52	0.45
2:F:1280:SER:O	2:F:1281:ARG:C	2.55	0.45
2:F:1288:ARG:HD3	2:F:1290:HIS:NE2	2.32	0.45
2:F:1364:LEU:HD23	2:F:1439:PHE:CZ	2.52	0.45
14:G:1651:MAN:C1	6:W:3:BMA:H3	2.46	0.45
2:H:811:LEU:HG	2:H:813:LEU:HD13	1.98	0.45
1:A:369:VAL:HG12	1:A:370:GLN:H	1.82	0.45
2:D:733:ILE:HD13	2:D:841:ARG:HD3	1.98	0.45
2:D:1126:LEU:HD21	2:D:1177:MET:HE3	1.99	0.45
2:D:1444:TYR:HB2	4:P:10:TYR:CE1	2.52	0.45
2:F:1506:THR:OG1	2:F:1509:GLU:HG2	2.17	0.45
2:H:734:ILE:N	2:H:734:ILE:HD12	2.32	0.45
2:H:1498:ILE:HD13	2:H:1498:ILE:N	2.32	0.45
3:J:702:ASN:O	3:J:703:GLN:HG3	2.17	0.45
3:K:554:LEU:H	3:K:726:TRP:HH2	1.65	0.45
3:L:272:ILE:HG12	3:L:284:TYR:CE1	2.52	0.45
3:L:432:ASP:HA	4:N:27:ASN:HD21	1.82	0.45
2:B:1126:LEU:HD21	2:B:1177:MET:HE3	1.99	0.44
2:B:1223:ASP:O	2:B:1227:VAL:HG23	2.17	0.44
1:C:344:PRO:HD2	1:C:433:TYR:CE1	2.51	0.44
1:C:354:VAL:HG11	1:C:365:VAL:HG11	1.98	0.44
1:E:477:ARG:CG	1:E:477:ARG:NH1	2.76	0.44
2:F:1192:ALA:HB2	2:F:1198:TRP:CZ2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1290:HIS:O	2:H:1291:TRP:O	2.34	0.44
3:K:238:LEU:HD22	3:K:280:VAL:HG21	1.99	0.44
3:K:531:HIS:HD2	3:K:533:ASN:H	1.64	0.44
3:L:700:CYS:HA	3:L:704:LYS:O	2.16	0.44
3:L:705:ARG:O	3:L:706:GLN:CB	2.60	0.44
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.46	0.44
1:A:516:ILE:N	1:A:516:ILE:HD12	2.32	0.44
1:C:369:VAL:HG12	1:C:370:GLN:H	1.82	0.44
2:F:1126:LEU:O	2:F:1130:GLN:HG3	2.17	0.44
2:F:1223:ASP:O	2:F:1227:VAL:HG23	2.17	0.44
1:G:526:ALA:HB2	1:G:617:PHE:CE2	2.52	0.44
2:H:1497:PHE:O	2:H:1498:ILE:C	2.56	0.44
3:J:272:ILE:HG12	3:J:284:TYR:CE1	2.52	0.44
3:J:554:LEU:H	3:J:726:TRP:HH2	1.65	0.44
3:K:491:VAL:HB	3:K:572:LEU:HD11	1.99	0.44
3:L:554:LEU:H	3:L:726:TRP:HH2	1.65	0.44
1:A:100:LEU:HD21	1:A:638:LEU:HD23	2.00	0.44
2:B:734:ILE:N	2:B:734:ILE:HD12	2.33	0.44
2:B:1126:LEU:O	2:B:1130:GLN:HG3	2.17	0.44
2:B:1283:SER:O	2:B:1284:LYS:HG2	2.18	0.44
2:D:819:ARG:O	2:D:820:ASN:HB2	2.17	0.44
2:D:1203:LYS:HD2	2:D:1206:TYR:CE2	2.52	0.44
2:F:1360:ASN:O	2:F:1361:THR:O	2.36	0.44
2:H:1470:PHE:CB	2:H:1478:GLY:HA3	2.47	0.44
3:I:433:MET:HE3	3:I:433:MET:HB3	1.83	0.44
3:K:489:ALA:HB2	3:K:677:PRO:CG	2.45	0.44
6:W:2:NAG:H3	6:W:4:BMA:O3	2.17	0.44
1:A:459:ARG:HH21	1:G:459:ARG:HE	1.66	0.44
2:B:847:ASN:HA	2:B:848:PRO:HD2	1.83	0.44
1:C:250:ILE:HG22	1:C:305:SER:HB3	2.00	0.44
1:E:144:ASN:HD22	1:E:144:ASN:N	2.14	0.44
1:E:247:ALA:HB2	1:E:308:VAL:HG22	1.98	0.44
1:E:427:VAL:HB	1:E:523:GLU:HG3	1.99	0.44
2:F:734:ILE:N	2:F:734:ILE:HD12	2.33	0.44
2:F:943:ALA:O	2:F:1305:ASN:ND2	2.49	0.44
2:H:943:ALA:O	2:H:1305:ASN:ND2	2.49	0.44
2:H:1288:ARG:HD3	2:H:1290:HIS:NE2	2.32	0.44
2:H:1360:ASN:O	2:H:1361:THR:O	2.36	0.44
2:H:1364:LEU:HD23	2:H:1439:PHE:CZ	2.52	0.44
1:A:342:PHE:CE1	1:A:391:THR:HG21	2.53	0.44
1:A:555:PRO:HB3	2:B:775:ASP:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1364:LEU:HD23	2:B:1439:PHE:CZ	2.52	0.44
2:B:1639:CYS:HB2	3:L:368:ASN:OD1	2.18	0.44
2:H:847:ASN:HA	2:H:848:PRO:HD2	1.83	0.44
2:H:1280:SER:O	2:H:1281:ARG:C	2.55	0.44
3:I:272:ILE:HG12	3:I:284:TYR:CE1	2.52	0.44
3:I:554:LEU:H	3:I:726:TRP:HH2	1.65	0.44
3:K:238:LEU:HD11	3:K:278:TYR:CB	2.46	0.44
3:L:491:VAL:HB	3:L:572:LEU:HD11	1.99	0.44
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.98	0.44
2:D:1265:PRO:O	2:D:1266:ASP:CB	2.65	0.44
2:D:1292:GLU:HG2	2:D:1293:SER:H	1.83	0.44
2:D:1639:CYS:HB2	3:I:368:ASN:OD1	2.18	0.44
2:F:847:ASN:HA	2:F:848:PRO:HD2	1.83	0.44
3:I:375:THR:O	3:I:379:GLU:HG3	2.18	0.44
3:K:446:GLU:OE2	3:K:457:TRP:NE1	2.50	0.44
3:L:375:THR:O	3:L:379:GLU:HG3	2.18	0.44
4:Q:66:ALA:HA	4:Q:69:GLN:HB2	1.98	0.44
1:A:459:ARG:HE	1:G:459:ARG:NH2	2.16	0.44
2:B:840:VAL:HG22	2:B:894:VAL:HG12	2.00	0.44
2:B:937:LYS:O	2:B:937:LYS:HD2	2.17	0.44
1:C:22:LEU:HD13	1:C:33:VAL:HG11	2.00	0.44
2:D:1446:ASN:HB2	4:P:4:LEU:HB2	1.99	0.44
1:E:516:ILE:HD12	1:E:516:ILE:N	2.32	0.44
1:E:558:GLN:HB3	2:F:770:ASN:HD21	1.82	0.44
1:E:567:HIS:CG	2:F:760:PRO:HG3	2.53	0.44
2:F:1370:TYR:CD1	2:F:1376:ALA:HB2	2.52	0.44
1:G:147:ASN:HB2	1:G:148:PRO:CD	2.46	0.44
3:J:375:THR:O	3:J:379:GLU:HG3	2.18	0.44
1:A:329:SER:HA	1:A:330:PRO:HD3	1.78	0.44
2:B:1462:ASN:HD22	2:B:1462:ASN:C	2.21	0.44
2:D:1283:SER:O	2:D:1284:LYS:HG2	2.18	0.44
2:F:1126:LEU:HD21	2:F:1177:MET:HE3	1.99	0.44
2:F:1264:ALA:HA	2:F:1265:PRO:HD3	1.74	0.44
2:F:1375:ASP:OD1	2:F:1431:HIS:HD2	2.01	0.44
2:H:1283:SER:O	2:H:1284:LYS:HG2	2.18	0.44
2:H:1375:ASP:OD1	2:H:1431:HIS:HD2	2.01	0.44
3:I:543:GLY:O	3:I:545:PRO:HD3	2.18	0.44
3:J:366:LEU:HB2	17:J:2002:HOH:O	2.18	0.44
3:J:433:MET:HE1	3:J:436:LEU:HD21	1.99	0.44
3:K:245:ASN:OD1	3:K:283:ARG:HB2	2.18	0.44
1:A:407:GLN:C	1:A:409:LEU:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ASN:HB2	1:C:621:GLY:CA	2.48	0.44
2:D:734:ILE:N	2:D:734:ILE:HD12	2.33	0.44
2:D:1338:LYS:H	2:D:1371:ARG:HD2	1.83	0.44
2:D:1375:ASP:OD1	2:D:1431:HIS:HD2	2.01	0.44
2:D:1462:ASN:HD21	2:D:1464:GLU:HB2	1.83	0.44
2:F:1123:ALA:O	2:F:1127:ILE:HG13	2.17	0.44
1:G:407:GLN:C	1:G:409:LEU:H	2.21	0.44
1:G:510:VAL:HG12	1:G:528:SER:HB3	1.99	0.44
2:H:1292:GLU:HG2	2:H:1293:SER:H	1.83	0.44
3:I:702:ASN:O	3:I:703:GLN:HG3	2.17	0.44
3:J:238:LEU:HD22	3:J:280:VAL:HG21	1.99	0.44
3:J:491:VAL:HB	3:J:572:LEU:HD11	1.99	0.44
3:J:654:ARG:HG3	3:J:722:GLN:CB	2.48	0.44
3:K:272:ILE:HG12	3:K:284:TYR:CE1	2.52	0.44
3:K:375:THR:O	3:K:379:GLU:HG3	2.18	0.44
1:A:207:LEU:HA	1:A:208:PRO:HD2	1.81	0.43
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.18	0.43
1:C:144:ASN:HD22	1:C:144:ASN:N	2.14	0.43
2:D:1126:LEU:O	2:D:1130:GLN:HG3	2.17	0.43
1:E:407:GLN:C	1:E:409:LEU:H	2.21	0.43
2:F:819:ARG:O	2:F:820:ASN:HB2	2.17	0.43
2:F:1497:PHE:CZ	2:F:1572:LEU:HD23	2.52	0.43
3:I:491:VAL:HB	3:I:572:LEU:HD11	1.99	0.43
3:K:654:ARG:HG3	3:K:722:GLN:CB	2.48	0.43
3:K:700:CYS:HA	3:K:704:LYS:O	2.16	0.43
1:A:19:THR:HB	1:A:478:LEU:HB2	1.99	0.43
1:A:247:ALA:HB2	1:A:308:VAL:HG22	1.99	0.43
2:B:1038:ARG:NH1	2:B:1077:VAL:HG22	2.33	0.43
1:E:343:LYS:HB2	1:E:346:MET:HB2	2.00	0.43
2:F:1283:SER:O	2:F:1284:LYS:HG2	2.18	0.43
2:F:1359:LYS:HB2	4:M:4:LEU:HD21	2.00	0.43
2:F:1462:ASN:HD21	2:F:1464:GLU:HB2	1.84	0.43
2:H:840:VAL:HG22	2:H:894:VAL:HG12	2.00	0.43
2:H:1370:TYR:CD1	2:H:1376:ALA:HB2	2.52	0.43
9:Y:1:NAG:H61	9:Y:2:NAG:C7	2.48	0.43
2:D:887:GLU:OE2	2:D:904:ARG:HD2	2.19	0.43
2:D:1056:LEU:O	2:D:1060:VAL:HG23	2.19	0.43
2:F:1038:ARG:NH1	2:F:1077:VAL:HG22	2.33	0.43
1:G:343:LYS:N	1:G:343:LYS:HD2	2.33	0.43
2:H:887:GLU:OE2	2:H:904:ARG:HD2	2.18	0.43
3:J:543:GLY:O	3:J:545:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:653:PRO:CD	3:J:654:ARG:HH12	2.27	0.43
3:K:513:LYS:HZ2	3:K:524:GLU:HG2	1.82	0.43
3:L:654:ARG:HG3	3:L:722:GLN:CB	2.48	0.43
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.54	0.43
1:E:208:PRO:CD	1:E:583:LEU:HD11	2.48	0.43
2:F:833:ARG:CG	2:F:833:ARG:NH1	2.75	0.43
2:F:1639:CYS:HA	2:F:1640:PRO:HD3	1.69	0.43
1:G:341:TYR:CE1	1:G:611:LYS:HB3	2.53	0.43
1:G:427:VAL:HB	1:G:523:GLU:HG3	1.99	0.43
1:G:473:MET:HE1	1:G:603:ILE:HD11	1.99	0.43
3:I:245:ASN:OD1	3:I:283:ARG:HB2	2.18	0.43
6:W:2:NAG:H61	6:W:3:BMA:H2	1.99	0.43
1:A:22:LEU:HD13	1:A:33:VAL:HG11	2.00	0.43
2:B:1338:LYS:H	2:B:1371:ARG:HD2	1.83	0.43
2:B:1482:LYS:HA	2:B:1492:ALA:HB3	2.00	0.43
1:C:407:GLN:C	1:C:409:LEU:H	2.21	0.43
1:C:516:ILE:HD12	1:C:516:ILE:N	2.32	0.43
1:E:22:LEU:HD13	1:E:33:VAL:HG11	2.00	0.43
1:E:250:ILE:HG12	1:E:251:PHE:H	1.84	0.43
1:E:343:LYS:N	1:E:343:LYS:HD2	2.33	0.43
2:F:1462:ASN:HD22	2:F:1462:ASN:C	2.21	0.43
3:L:238:LEU:HD22	3:L:280:VAL:HG21	1.99	0.43
2:B:1290:HIS:O	2:B:1291:TRP:O	2.37	0.43
2:B:1336:CYS:O	2:B:1337:ASN:O	2.37	0.43
2:B:1375:ASP:OD1	2:B:1431:HIS:HD2	2.01	0.43
2:D:840:VAL:HG22	2:D:894:VAL:HG12	2.00	0.43
2:D:1336:CYS:O	2:D:1337:ASN:O	2.36	0.43
1:G:2:PRO:HA	1:G:25:HIS:O	2.19	0.43
2:H:1506:THR:OG1	2:H:1509:GLU:HG2	2.17	0.43
3:I:654:ARG:HG3	3:I:722:GLN:CB	2.48	0.43
3:J:245:ASN:OD1	3:J:283:ARG:HB2	2.18	0.43
2:B:944:ASP:O	2:B:945:LEU:C	2.57	0.43
1:C:343:LYS:HD2	1:C:343:LYS:N	2.33	0.43
2:D:944:ASP:O	2:D:945:LEU:C	2.57	0.43
1:E:282:ARG:CZ	1:E:286:LEU:HD11	2.49	0.43
2:F:840:VAL:HG22	2:F:894:VAL:HG12	2.00	0.43
2:F:1078:LEU:HD23	2:F:1135:ILE:HG21	2.01	0.43
1:G:572:VAL:HG23	2:H:785:VAL:HB	2.01	0.43
3:I:238:LEU:HD22	3:I:280:VAL:HG21	1.99	0.43
3:K:543:GLY:O	3:K:545:PRO:HD3	2.18	0.43
3:K:655:PHE:HD2	3:K:716:PHE:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:543:GLY:O	3:L:545:PRO:HD3	2.18	0.43
1:A:343:LYS:HD2	1:A:343:LYS:N	2.33	0.43
1:C:2:PRO:HA	1:C:25:HIS:O	2.19	0.43
1:E:2:PRO:HA	1:E:25:HIS:O	2.19	0.43
1:E:251:PHE:CG	1:E:280:LEU:HD22	2.54	0.43
1:G:526:ALA:O	1:G:616:VAL:HG21	2.19	0.43
3:I:655:PHE:HD2	3:I:716:PHE:HB3	1.84	0.43
1:C:282:ARG:CZ	1:C:286:LEU:HD11	2.49	0.43
1:C:503:PHE:HD1	1:C:507:PHE:CG	2.37	0.43
1:G:250:ILE:HG12	1:G:251:PHE:H	1.84	0.43
1:G:343:LYS:HB2	1:G:346:MET:HB2	2.00	0.43
2:H:1528:VAL:HG21	2:H:1559:GLN:HE21	1.84	0.43
3:I:431:LYS:HG3	4:M:27:ASN:ND2	2.34	0.43
3:I:446:GLU:H	3:I:446:GLU:HG3	1.66	0.43
2:B:824:GLU:OE2	2:B:875:PRO:HB3	2.19	0.43
2:B:887:GLU:OE2	2:B:904:ARG:HD2	2.18	0.43
2:B:896:HIS:HB3	4:Q:61:LYS:HD3	2.00	0.43
2:B:1386:MET:O	2:B:1387:THR:C	2.57	0.43
2:B:1462:ASN:HD21	2:B:1464:GLU:HB2	1.83	0.43
2:B:1523:TYR:HB3	2:B:1543:ILE:HG23	2.01	0.43
1:C:506:SER:HB2	1:C:530:TRP:NE1	2.27	0.43
2:D:1038:ARG:NH1	2:D:1077:VAL:HG22	2.33	0.43
2:D:1523:TYR:HB3	2:D:1543:ILE:HG23	2.01	0.43
2:F:1056:LEU:O	2:F:1060:VAL:HG23	2.19	0.43
2:F:1227:VAL:HB	2:F:1228:PRO:HD3	2.01	0.43
2:H:1376:ALA:HB3	2:H:1429:VAL:CG2	2.49	0.43
3:L:238:LEU:HD11	3:L:278:TYR:CB	2.46	0.43
1:A:251:PHE:CG	1:A:280:LEU:HD22	2.54	0.42
1:A:577:ASP:CG	2:B:778:THR:HG21	2.40	0.42
2:B:1334:LEU:HA	2:B:1334:LEU:HD13	1.80	0.42
1:C:251:PHE:CG	1:C:280:LEU:HD22	2.54	0.42
1:C:538:VAL:HB	2:D:791:LYS:O	2.18	0.42
1:G:282:ARG:CZ	1:G:286:LEU:HD11	2.49	0.42
2:H:851:CYS:HB2	2:H:1491:CYS:HB2	1.81	0.42
2:H:1462:ASN:HD21	2:H:1464:GLU:HB2	1.84	0.42
3:J:607:PHE:CE1	3:J:669:THR:HG22	2.54	0.42
3:K:503:PHE:HB2	3:K:530:PHE:CZ	2.54	0.42
3:K:607:PHE:CE1	3:K:669:THR:HG22	2.54	0.42
2:B:772:PHE:CD1	4:N:37:ASN:ND2	2.87	0.42
2:B:1215:LEU:O	2:B:1219:LEU:HG	2.19	0.42
1:C:247:ALA:HB2	1:C:308:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:819:ARG:NH1	2:D:819:ARG:CG	2.80	0.42
2:F:745:PHE:N	2:F:746:PRO:HD3	2.32	0.42
2:F:1292:GLU:HG2	2:F:1293:SER:H	1.83	0.42
2:H:824:GLU:OE2	2:H:875:PRO:HB3	2.19	0.42
3:I:238:LEU:HD11	3:I:278:TYR:CB	2.46	0.42
3:J:446:GLU:H	3:J:446:GLU:HG3	1.66	0.42
3:L:245:ASN:OD1	3:L:283:ARG:HB2	2.18	0.42
1:A:439:LEU:H	1:A:439:LEU:CD1	2.32	0.42
2:B:932:ARG:O	2:B:933:GLU:C	2.57	0.42
2:B:1265:PRO:O	2:B:1266:ASP:CB	2.64	0.42
2:B:1292:GLU:HG2	2:B:1293:SER:H	1.83	0.42
1:C:343:LYS:HB2	1:C:346:MET:HB2	2.00	0.42
2:D:824:GLU:OE2	2:D:875:PRO:HB3	2.19	0.42
2:D:1482:LYS:HA	2:D:1492:ALA:HB3	2.01	0.42
1:E:111:GLN:O	1:E:125:TYR:HA	2.20	0.42
1:G:22:LEU:HD13	1:G:33:VAL:HG11	2.00	0.42
2:H:1500:LYS:NZ	2:H:1504:LYS:HB2	2.34	0.42
3:I:449:SER:HA	3:I:452:LEU:HD13	2.01	0.42
3:J:437:GLU:CD	3:J:458:GLU:HB2	2.40	0.42
3:J:655:PHE:HD2	3:J:716:PHE:HB3	1.84	0.42
3:L:655:PHE:HD2	3:L:716:PHE:HB3	1.84	0.42
6:W:2:NAG:N2	6:W:4:BMA:O3	2.52	0.42
1:A:503:PHE:HD1	1:A:507:PHE:CG	2.37	0.42
1:A:549:GLU:O	1:A:550:ASP:HB2	2.20	0.42
2:B:1446:ASN:HB2	4:Q:4:LEU:CD1	2.49	0.42
2:D:932:ARG:O	2:D:933:GLU:C	2.57	0.42
1:G:127:ILE:N	1:G:127:ILE:HD12	2.35	0.42
3:I:607:PHE:CE1	3:I:669:THR:HG22	2.55	0.42
3:L:607:PHE:CE1	3:L:669:THR:HG22	2.54	0.42
1:A:10:ASN:HB2	1:A:621:GLY:HA2	2.01	0.42
1:A:127:ILE:HD12	1:A:127:ILE:N	2.35	0.42
1:A:282:ARG:CZ	1:A:286:LEU:HD11	2.49	0.42
1:C:111:GLN:O	1:C:125:TYR:HA	2.20	0.42
2:D:1078:LEU:HD23	2:D:1135:ILE:HG21	2.01	0.42
2:D:1082:VAL:HG13	2:D:1129:LEU:HD22	2.01	0.42
2:F:969:THR:O	2:F:970:GLU:C	2.57	0.42
2:F:1528:VAL:HG21	2:F:1559:GLN:HE21	1.84	0.42
2:H:745:PHE:N	2:H:746:PRO:HD3	2.35	0.42
3:I:432:ASP:HA	4:M:27:ASN:HD21	1.84	0.42
3:I:709:VAL:HA	3:I:710:PRO:HD3	1.92	0.42
3:K:354:ARG:HB2	16:K:1749:NAG:C8	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Y:2:NAG:H82	9:Y:2:NAG:H2	1.91	0.42
1:A:40:PHE:HA	1:A:41:PRO:HA	1.84	0.42
2:B:1506:THR:OG1	2:B:1509:GLU:HG2	2.20	0.42
2:D:1215:LEU:O	2:D:1219:LEU:HG	2.19	0.42
2:D:1290:HIS:O	2:D:1291:TRP:O	2.37	0.42
2:D:1506:THR:OG1	2:D:1509:GLU:HG2	2.20	0.42
1:E:454:LEU:HA	1:E:491:ASP:O	2.19	0.42
1:G:251:PHE:CG	1:G:280:LEU:HD22	2.54	0.42
3:I:289:TYR:HA	3:I:293:PRO:HA	2.01	0.42
3:K:353:ASN:OD1	16:K:1749:NAG:C7	2.67	0.42
3:L:489:ALA:HB2	3:L:677:PRO:CG	2.45	0.42
2:B:1227:VAL:HB	2:B:1228:PRO:HD3	2.01	0.42
1:C:147:ASN:HB2	1:C:148:PRO:CD	2.46	0.42
1:C:218:GLU:C	1:C:220:PHE:H	2.23	0.42
1:E:127:ILE:HD12	1:E:127:ILE:N	2.35	0.42
1:G:439:LEU:H	1:G:439:LEU:CD1	2.32	0.42
2:H:1485:ARG:HH21	2:H:1590:TRP:HE1	1.67	0.42
2:H:1516:GLU:HB3	2:H:1517:PRO:CD	2.50	0.42
3:J:531:HIS:CD2	3:J:533:ASN:HB2	2.55	0.42
1:A:218:GLU:C	1:A:220:PHE:H	2.23	0.42
2:B:1078:LEU:HD23	2:B:1135:ILE:HG21	2.01	0.42
1:C:127:ILE:HD12	1:C:127:ILE:N	2.35	0.42
2:D:943:ALA:O	2:D:1305:ASN:ND2	2.53	0.42
1:E:6:ILE:HD11	1:E:20:MET:CG	2.50	0.42
1:E:219:LYS:NZ	1:E:356:ASN:ND2	2.68	0.42
2:F:887:GLU:OE2	2:F:904:ARG:HD2	2.19	0.42
2:F:944:ASP:O	2:F:945:LEU:C	2.57	0.42
2:F:1215:LEU:O	2:F:1219:LEU:HG	2.19	0.42
2:F:1216:LEU:HD21	2:F:1256:ALA:HA	2.02	0.42
1:G:512:TYR:CE1	1:G:624:PHE:HE1	2.37	0.42
2:H:944:ASP:O	2:H:945:LEU:C	2.57	0.42
2:H:1386:MET:O	2:H:1387:THR:C	2.58	0.42
3:I:531:HIS:CD2	3:I:533:ASN:HB2	2.55	0.42
3:L:289:TYR:HA	3:L:293:PRO:HA	2.02	0.42
3:L:503:PHE:HB2	3:L:530:PHE:CZ	2.54	0.42
3:L:531:HIS:CD2	3:L:533:ASN:HB2	2.55	0.42
1:A:250:ILE:HG22	1:A:305:SER:HB3	2.01	0.42
2:B:1376:ALA:HB3	2:B:1429:VAL:CG2	2.49	0.42
1:C:330:PRO:HG2	1:C:409:LEU:HD21	2.01	0.42
2:D:1386:MET:O	2:D:1387:THR:C	2.58	0.42
1:G:111:GLN:O	1:G:125:TYR:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:574:VAL:HG13	2:H:783:LEU:HB3	2.01	0.42
2:H:1334:LEU:HA	2:H:1334:LEU:HD13	1.80	0.42
3:I:676:GLY:HA2	3:I:677:PRO:HD3	1.83	0.42
3:I:705:ARG:O	3:I:706:GLN:CB	2.60	0.42
3:J:443:MET:HB3	3:J:443:MET:HE2	1.86	0.42
3:K:244:MET:HG2	3:K:245:ASN:N	2.35	0.42
4:Q:84:LYS:O	4:Q:84:LYS:HG3	2.20	0.42
1:C:250:ILE:HG12	1:C:251:PHE:H	1.84	0.42
2:D:1009:THR:HB	2:D:1011:GLN:HE21	1.85	0.42
2:D:1462:ASN:HD22	2:D:1462:ASN:C	2.21	0.42
2:D:1518:GLY:CA	2:D:1585:LEU:HD22	2.48	0.42
2:F:1009:THR:HB	2:F:1011:GLN:HE21	1.85	0.42
2:F:1269:GLU:O	2:F:1271:ASN:N	2.52	0.42
2:F:1522:VAL:HG22	2:F:1583:TRP:HB3	2.02	0.42
1:G:19:THR:HG22	1:G:20:MET:N	2.35	0.42
1:G:503:PHE:HD1	1:G:507:PHE:CG	2.37	0.42
3:I:503:PHE:HB2	3:I:530:PHE:CZ	2.54	0.42
3:J:503:PHE:HB2	3:J:530:PHE:CZ	2.54	0.42
3:L:298:LYS:HB2	3:L:301:GLU:HG3	2.02	0.42
3:L:443:MET:HB3	3:L:443:MET:HE2	1.87	0.42
2:B:1082:VAL:HG13	2:B:1129:LEU:HD22	2.02	0.41
1:C:6:ILE:HD11	1:C:20:MET:CG	2.50	0.41
1:C:439:LEU:H	1:C:439:LEU:CD1	2.32	0.41
2:D:1227:VAL:HB	2:D:1228:PRO:HD3	2.01	0.41
2:F:1336:CYS:O	2:F:1337:ASN:C	2.59	0.41
2:F:1390:ALA:HA	2:F:1391:PRO:HD3	1.91	0.41
1:G:6:ILE:HD11	1:G:20:MET:CG	2.50	0.41
1:G:526:ALA:CB	1:G:617:PHE:CE2	3.03	0.41
2:H:841:ARG:HH11	2:H:841:ARG:CG	2.23	0.41
2:H:854:ALA:HB2	2:H:860:HIS:HB3	2.02	0.41
2:H:877:VAL:H	2:H:1451:GLN:HE21	1.68	0.41
2:H:1338:LYS:N	2:H:1371:ARG:HB2	2.34	0.41
4:M:23:LEU:HD21	4:M:51:ALA:HB3	2.02	0.41
4:N:56:LYS:HG3	4:N:57:SER:N	2.34	0.41
1:A:80:ARG:HD2	2:B:1010:GLU:HG3	2.01	0.41
1:A:330:PRO:HG2	1:A:409:LEU:HD21	2.00	0.41
2:B:932:ARG:O	2:B:934:GLY:N	2.53	0.41
2:B:943:ALA:O	2:B:1305:ASN:ND2	2.53	0.41
2:B:1165:TYR:HD1	2:B:1210:ALA:HB2	1.85	0.41
2:D:932:ARG:O	2:D:934:GLY:N	2.53	0.41
2:D:1528:VAL:HG21	2:D:1559:GLN:HE21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:350:LEU:CD2	1:G:400:ILE:HG21	2.50	0.41
3:J:489:ALA:HB2	3:J:677:PRO:CG	2.45	0.41
3:K:540:LYS:NZ	3:K:540:LYS:HB2	2.36	0.41
3:L:239:ASP:HA	3:L:240:PRO:HD3	1.86	0.41
4:M:56:LYS:HG3	4:M:57:SER:N	2.34	0.41
4:Q:23:LEU:HD21	4:Q:51:ALA:HB3	2.02	0.41
1:A:111:GLN:O	1:A:125:TYR:HA	2.20	0.41
1:A:249:VAL:HG13	1:A:267:LYS:HB2	2.02	0.41
2:B:1009:THR:HB	2:B:1011:GLN:HE21	1.85	0.41
2:B:1528:VAL:HG21	2:B:1559:GLN:HE21	1.84	0.41
2:B:1541:MET:HB2	2:B:1541:MET:HE3	1.96	0.41
1:C:19:THR:HG22	1:C:20:MET:N	2.35	0.41
2:D:1370:TYR:CG	2:D:1376:ALA:HB2	2.55	0.41
2:D:1376:ALA:HB3	2:D:1429:VAL:CG2	2.49	0.41
1:E:126:ARG:CZ	1:E:572:VAL:HB	2.50	0.41
1:E:365:VAL:HA	1:E:366:PRO:HD2	1.80	0.41
1:E:386:LYS:HD3	1:E:440:ARG:HG2	2.02	0.41
2:F:915:ARG:O	2:F:916:MET:HG3	2.21	0.41
2:F:1165:TYR:HD1	2:F:1210:ALA:HB2	1.85	0.41
2:F:1472:HIS:HA	2:F:1473:PRO:HD3	1.94	0.41
1:G:341:TYR:CD2	1:G:610:GLY:HA2	2.56	0.41
1:G:481:ALA:O	6:W:1:NAG:H82	2.20	0.41
2:H:1611:GLU:HG3	2:H:1612:GLU:N	2.34	0.41
3:I:666:ASP:HA	3:I:667:PRO:HD3	1.95	0.41
3:J:244:MET:HG2	3:J:245:ASN:N	2.35	0.41
3:J:298:LYS:HB2	3:J:301:GLU:HG3	2.02	0.41
3:J:433:MET:HB3	3:J:433:MET:HE3	1.82	0.41
3:K:443:MET:HB3	3:K:443:MET:HE2	1.87	0.41
3:K:531:HIS:CD2	3:K:533:ASN:HB2	2.55	0.41
3:L:494:TYR:O	3:L:556:LYS:HA	2.21	0.41
3:L:503:PHE:CZ	3:L:555:ILE:HD11	2.55	0.41
3:L:540:LYS:HB2	3:L:540:LYS:NZ	2.36	0.41
4:N:84:LYS:O	4:N:84:LYS:HG3	2.20	0.41
4:Q:56:LYS:HG3	4:Q:57:SER:N	2.34	0.41
7:V:3:BMA:H5	7:V:4:BMA:H2	2.01	0.41
1:A:343:LYS:HB2	1:A:346:MET:HB2	2.00	0.41
1:A:454:LEU:HA	1:A:491:ASP:O	2.21	0.41
2:B:1055:TRP:CD1	2:B:1111:LEU:HD22	2.56	0.41
1:C:100:LEU:HD12	1:C:101:VAL:H	1.86	0.41
2:F:932:ARG:HH11	3:L:339:SER:CB	2.34	0.41
2:F:1055:TRP:CD1	2:F:1111:LEU:HD22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1518:GLY:CA	2:F:1585:LEU:HD22	2.48	0.41
1:G:218:GLU:C	1:G:220:PHE:H	2.23	0.41
2:H:740:VAL:CB	4:Q:42:ARG:HB2	2.45	0.41
2:H:1514:ALA:O	2:H:1519:VAL:HG11	2.20	0.41
3:I:503:PHE:CZ	3:I:555:ILE:HD11	2.55	0.41
3:J:494:TYR:O	3:J:556:LYS:HA	2.21	0.41
3:L:278:TYR:CE2	3:L:455:MET:SD	3.13	0.41
4:N:41:LYS:O	4:N:45:LYS:HG3	2.21	0.41
4:P:84:LYS:O	4:P:84:LYS:HG3	2.20	0.41
1:A:2:PRO:HA	1:A:25:HIS:O	2.19	0.41
1:A:13:ARG:NH2	1:A:476:GLY:HA3	2.35	0.41
1:A:250:ILE:HG12	1:A:251:PHE:H	1.84	0.41
2:B:1451:GLN:HA	2:B:1452:PRO:HD3	1.94	0.41
2:D:1055:TRP:CD1	2:D:1111:LEU:HD22	2.56	0.41
2:D:1516:GLU:HB3	2:D:1517:PRO:CD	2.50	0.41
2:F:759:PRO:HA	2:F:760:PRO:HD3	1.84	0.41
2:F:932:ARG:O	2:F:933:GLU:C	2.58	0.41
2:F:1082:VAL:HG13	2:F:1129:LEU:HD22	2.02	0.41
2:H:1359:LYS:CB	4:N:4:LEU:HD21	2.50	0.41
2:H:1462:ASN:HD22	2:H:1462:ASN:C	2.21	0.41
3:I:244:MET:HG2	3:I:245:ASN:N	2.35	0.41
3:J:289:TYR:HA	3:J:293:PRO:HA	2.02	0.41
3:J:461:LYS:HG2	4:Q:28:VAL:HG12	2.03	0.41
3:J:676:GLY:HA2	3:J:677:PRO:HD3	1.83	0.41
3:K:446:GLU:H	3:K:446:GLU:HG3	1.66	0.41
3:K:503:PHE:CZ	3:K:555:ILE:HD11	2.55	0.41
2:B:813:LEU:HD23	2:B:907:LEU:HD22	2.02	0.41
1:C:549:GLU:O	1:C:550:ASP:HB2	2.20	0.41
2:D:1357:ASP:C	2:D:1359:LYS:H	2.24	0.41
2:F:824:GLU:OE2	2:F:875:PRO:HB3	2.19	0.41
2:F:1334:LEU:HD13	2:F:1334:LEU:HA	1.80	0.41
1:G:549:GLU:O	1:G:550:ASP:HB2	2.20	0.41
2:H:1500:LYS:HE3	2:H:1504:LYS:O	2.21	0.41
3:J:368:ASN:ND2	3:J:368:ASN:N	2.69	0.41
3:J:540:LYS:NZ	3:J:540:LYS:HB2	2.35	0.41
4:M:84:LYS:O	4:M:84:LYS:HG3	2.20	0.41
4:P:56:LYS:HG3	4:P:57:SER:N	2.34	0.41
1:A:10:ASN:HA	1:A:623:THR:HG23	2.03	0.41
1:A:459:ARG:NH2	1:G:459:ARG:HE	2.19	0.41
2:B:854:ALA:HB2	2:B:860:HIS:HB3	2.02	0.41
2:B:1522:VAL:HG22	2:B:1583:TRP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:851:CYS:HB2	2:D:1491:CYS:HB2	1.78	0.41
2:D:1522:VAL:HG22	2:D:1583:TRP:HB3	2.02	0.41
2:D:1611:GLU:HG3	2:D:1612:GLU:N	2.34	0.41
1:E:481:ALA:N	5:U:1:NAG:H81	2.35	0.41
1:E:503:PHE:HD1	1:E:507:PHE:CG	2.37	0.41
2:F:1386:MET:O	2:F:1387:THR:C	2.58	0.41
2:F:1514:ALA:O	2:F:1519:VAL:HG11	2.20	0.41
1:G:7:ILE:HG21	1:G:471:LEU:HD22	2.02	0.41
2:H:1518:GLY:CA	2:H:1585:LEU:HD22	2.48	0.41
3:I:494:TYR:O	3:I:556:LYS:HA	2.21	0.41
3:K:298:LYS:HB2	3:K:301:GLU:HG3	2.02	0.41
1:A:6:ILE:HD11	1:A:20:MET:CG	2.50	0.41
1:A:363:TYR:CD2	1:A:381:GLY:HA2	2.56	0.41
2:B:841:ARG:HH11	2:B:841:ARG:CG	2.23	0.41
2:B:1216:LEU:HD21	2:B:1256:ALA:HA	2.02	0.41
2:B:1444:TYR:HB2	4:Q:10:TYR:CE1	2.55	0.41
2:B:1522:VAL:HG12	2:B:1547:ILE:HD12	2.03	0.41
1:C:207:LEU:HA	1:C:208:PRO:HD2	1.82	0.41
1:E:549:GLU:O	1:E:550:ASP:HB2	2.20	0.41
2:F:1338:LYS:N	2:F:1371:ARG:HB2	2.36	0.41
1:G:23:GLU:OE1	1:G:469:THR:HG21	2.21	0.41
1:G:249:VAL:HG13	1:G:267:LYS:HB2	2.02	0.41
2:H:813:LEU:HA	2:H:814:PRO:HD3	1.97	0.41
2:H:1639:CYS:HA	2:H:1640:PRO:HD3	1.76	0.41
3:L:428:PHE:CE1	3:L:439:VAL:HG13	2.56	0.41
1:A:24:ALA:HB3	1:A:60:HIS:HB3	2.03	0.41
1:A:250:ILE:HG12	1:A:251:PHE:N	2.36	0.41
1:A:506:SER:HB2	1:A:530:TRP:NE1	2.27	0.41
1:A:552:GLN:HA	1:A:553:PRO:HD3	1.81	0.41
2:B:1192:ALA:HB2	2:B:1198:TRP:CE2	2.56	0.41
2:B:1370:TYR:CG	2:B:1376:ALA:HB2	2.55	0.41
2:B:1611:GLU:HB3	2:B:1614:GLU:HG3	2.03	0.41
1:C:10:ASN:HB2	1:C:622:LEU:N	2.36	0.41
1:C:454:LEU:HA	1:C:491:ASP:O	2.21	0.41
2:D:1165:TYR:HD1	2:D:1210:ALA:HB2	1.85	0.41
2:D:1611:GLU:HB3	2:D:1614:GLU:HG3	2.03	0.41
1:E:19:THR:HG22	1:E:20:MET:N	2.35	0.41
1:E:218:GLU:C	1:E:220:PHE:H	2.23	0.41
1:E:250:ILE:HG12	1:E:251:PHE:N	2.36	0.41
1:E:250:ILE:HG22	1:E:305:SER:HB3	2.03	0.41
1:E:324:ILE:HA	1:E:325:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:640:CYS:HB3	1:E:641:PRO:CD	2.51	0.41
2:F:745:PHE:HA	2:F:776:SER:OG	2.21	0.41
2:F:1376:ALA:HB3	2:F:1429:VAL:CG2	2.49	0.41
1:G:207:LEU:HA	1:G:208:PRO:HD2	1.82	0.41
2:H:1522:VAL:HG22	2:H:1583:TRP:HB3	2.02	0.41
2:H:1523:TYR:HB3	2:H:1543:ILE:HG23	2.02	0.41
2:H:1541:MET:HB2	2:H:1541:MET:HE3	1.96	0.41
3:I:239:ASP:HA	3:I:240:PRO:HD3	1.86	0.41
3:J:238:LEU:HD11	3:J:278:TYR:CB	2.46	0.41
3:J:423:ASN:N	3:J:423:ASN:ND2	2.68	0.41
3:J:428:PHE:CE1	4:Q:31:LEU:HD11	2.55	0.41
3:J:503:PHE:CZ	3:J:555:ILE:HD11	2.55	0.41
3:J:638:ALA:HA	3:J:639:PRO:HD3	1.98	0.41
3:K:289:TYR:HA	3:K:293:PRO:HA	2.02	0.41
3:K:676:GLY:HA2	3:K:677:PRO:HD3	1.83	0.41
4:M:69:GLN:HE21	4:M:69:GLN:HB3	1.68	0.41
4:P:23:LEU:HD21	4:P:51:ALA:HB3	2.02	0.41
1:A:19:THR:HG22	1:A:20:MET:N	2.35	0.41
1:A:100:LEU:HD12	1:A:101:VAL:H	1.86	0.41
2:B:729:LEU:C	2:B:729:LEU:HD13	2.41	0.41
2:B:1229:PRO:HA	2:B:1232:ARG:NH1	2.36	0.41
1:C:477:ARG:HG2	1:C:477:ARG:NH1	2.21	0.41
2:D:745:PHE:N	2:D:746:PRO:HD3	2.35	0.41
2:D:1216:LEU:HD21	2:D:1256:ALA:HA	2.02	0.41
1:E:438:VAL:HG13	1:E:449:LEU:HD11	2.03	0.41
1:E:439:LEU:H	1:E:439:LEU:CD1	2.32	0.41
2:F:813:LEU:HD23	2:F:907:LEU:HD22	2.02	0.41
2:F:1522:VAL:HG12	2:F:1547:ILE:HD12	2.03	0.41
1:G:391:THR:HG22	1:G:392:HIS:N	2.36	0.41
2:H:1635:VAL:HG23	2:H:1636:VAL:N	2.36	0.41
3:I:503:PHE:HB2	3:I:530:PHE:HZ	1.86	0.41
3:J:428:PHE:CE1	3:J:439:VAL:HG13	2.56	0.41
3:K:244:MET:HG2	3:K:245:ASN:H	1.86	0.41
1:A:400:ILE:N	1:A:400:ILE:HD12	2.36	0.40
2:B:917:ASN:OD1	5:R:1:NAG:O5	2.38	0.40
1:C:365:VAL:HA	1:C:366:PRO:HD2	1.81	0.40
2:D:1192:ALA:HB2	2:D:1198:TRP:CE2	2.56	0.40
1:E:249:VAL:HG13	1:E:267:LYS:HB2	2.03	0.40
1:E:541:LEU:HD22	2:F:786:SER:HB3	2.02	0.40
2:F:819:ARG:CG	2:F:819:ARG:NH1	2.80	0.40
2:F:854:ALA:HB2	2:F:860:HIS:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1229:PRO:HA	2:F:1232:ARG:NH1	2.36	0.40
2:F:1516:GLU:HB3	2:F:1517:PRO:CD	2.50	0.40
1:G:400:ILE:HD12	1:G:400:ILE:N	2.36	0.40
2:H:915:ARG:O	2:H:916:MET:HG3	2.21	0.40
2:H:965:VAL:HG23	2:H:1268:GLN:OE1	2.22	0.40
2:H:1522:VAL:HG12	2:H:1547:ILE:HD12	2.03	0.40
3:K:428:PHE:CE1	3:K:439:VAL:HG13	2.56	0.40
3:K:439:VAL:HA	4:P:31:LEU:HD21	2.02	0.40
4:M:41:LYS:O	4:M:45:LYS:HG3	2.21	0.40
4:P:41:LYS:O	4:P:45:LYS:HG3	2.21	0.40
1:A:344:PRO:HG3	1:A:423:PRO:HB3	2.02	0.40
1:E:24:ALA:HB3	1:E:60:HIS:HB3	2.03	0.40
1:E:391:THR:HG22	1:E:392:HIS:N	2.36	0.40
1:E:552:GLN:HA	1:E:553:PRO:HD3	1.81	0.40
2:F:1000:VAL:HG22	2:F:1027:ILE:HG23	2.04	0.40
2:F:1192:ALA:HB2	2:F:1198:TRP:CE2	2.56	0.40
2:F:1370:TYR:CE2	2:F:1372:GLY:HA3	2.56	0.40
2:F:1611:GLU:HB3	2:F:1614:GLU:HG3	2.03	0.40
1:G:558:GLN:HB3	2:H:770:ASN:HD21	1.86	0.40
2:H:813:LEU:HD23	2:H:907:LEU:HD22	2.02	0.40
2:H:877:VAL:HG22	2:H:1451:GLN:NE2	2.28	0.40
2:H:1370:TYR:CG	2:H:1376:ALA:HB2	2.56	0.40
2:H:1503:ASP:O	2:H:1504:LYS:HG3	2.21	0.40
1:C:109:PHE:CZ	1:C:594:ILE:HG23	2.56	0.40
2:D:813:LEU:HD23	2:D:907:LEU:HD22	2.02	0.40
1:E:480:LYS:HG2	1:E:481:ALA:N	2.36	0.40
2:F:1523:TYR:HB3	2:F:1543:ILE:HG23	2.02	0.40
1:G:126:ARG:HG3	2:H:751:TRP:CZ2	2.56	0.40
1:G:480:LYS:HG2	1:G:481:ALA:N	2.37	0.40
1:G:505:PRO:O	1:G:533:VAL:HB	2.21	0.40
1:G:506:SER:HB2	1:G:530:TRP:NE1	2.27	0.40
2:H:809:ILE:HD11	2:H:892:ALA:CB	2.52	0.40
2:H:1527:LEU:HD22	2:H:1574:LEU:HB3	2.04	0.40
3:I:345:ASP:HB3	3:I:346:ASP:H	1.49	0.40
3:I:654:ARG:HG3	3:I:722:GLN:HB3	2.03	0.40
5:U:3:BMA:H62	5:U:4:BMA:H2	1.58	0.40
1:A:342:PHE:CZ	1:A:423:PRO:HG3	2.56	0.40
1:A:363:TYR:HD2	1:A:381:GLY:HA2	1.86	0.40
2:B:1446:ASN:HB2	4:Q:4:LEU:HD12	2.03	0.40
1:C:391:THR:HG22	1:C:392:HIS:N	2.36	0.40
1:C:392:HIS:C	1:C:394:SER:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:LEU:HD12	1:C:583:LEU:N	2.36	0.40
2:D:776:SER:HB2	2:D:780:TRP:HZ2	1.86	0.40
2:D:1229:PRO:HA	2:D:1232:ARG:NH1	2.36	0.40
1:E:100:LEU:HD12	1:E:101:VAL:H	1.86	0.40
1:E:583:LEU:HD12	1:E:583:LEU:N	2.36	0.40
2:H:1370:TYR:CE2	2:H:1372:GLY:HA3	2.56	0.40
2:H:1609:TRP:HD1	2:H:1610:PRO:O	2.04	0.40
3:I:298:LYS:HB2	3:I:301:GLU:HG3	2.02	0.40
3:I:402:VAL:HG11	3:I:414:ILE:HG23	2.04	0.40
3:I:428:PHE:CE1	3:I:439:VAL:HG13	2.56	0.40
3:I:461:LYS:CG	4:M:28:VAL:HG12	2.51	0.40
3:I:540:LYS:HB2	3:I:540:LYS:NZ	2.35	0.40
3:K:328:THR:N	3:K:368:ASN:HD21	2.20	0.40
3:K:494:TYR:O	3:K:556:LYS:HA	2.21	0.40
3:L:244:MET:HG2	3:L:245:ASN:N	2.35	0.40
2:B:1609:TRP:HD1	2:B:1610:PRO:O	2.04	0.40
1:C:24:ALA:HB3	1:C:60:HIS:HB3	2.03	0.40
1:C:199:GLU:HB2	1:C:587:ASN:OD1	2.22	0.40
1:C:400:ILE:HD12	1:C:400:ILE:N	2.36	0.40
1:C:480:LYS:HG2	1:C:481:ALA:N	2.37	0.40
2:D:1527:LEU:HD22	2:D:1574:LEU:HB3	2.04	0.40
1:E:642:GLN:O	1:E:644:ALA:N	2.54	0.40
2:F:1143:LEU:O	2:F:1147:ILE:HG13	2.22	0.40
2:F:1632:GLU:HA	2:F:1635:VAL:HG22	2.04	0.40
1:G:220:PHE:CZ	1:G:330:PRO:HB3	2.56	0.40
3:J:292:TYR:HA	3:J:293:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

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	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	25	63
1	C	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	25	63
1	E	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	25	63
1	G	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	25	63
2	B	893/915 (98%)	785 (88%)	80 (9%)	28 (3%)	4	32
2	D	893/915 (98%)	784 (88%)	82 (9%)	27 (3%)	4	33
2	F	894/915 (98%)	786 (88%)	78 (9%)	30 (3%)	3	31
2	H	890/915 (97%)	782 (88%)	75 (8%)	33 (4%)	3	29
3	I	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	9	44
3	J	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	9	44
3	K	505/507 (100%)	445 (88%)	52 (10%)	8 (2%)	9	44
3	L	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	9	44
4	M	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	13	49
4	N	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	13	49
4	P	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	13	49
4	Q	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	13	49
All	All	8446/8636 (98%)	7530 (89%)	746 (9%)	170 (2%)	7	40

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	933	GLU
2	B	967	GLN
2	B	1269	GLU
2	B	1281	ARG
2	B	1291	TRP
2	B	1292	GLU
2	B	1294	ALA
2	B	1337	ASN
2	B	1338	LYS
2	B	1359	LYS
2	B	1377	THR
2	B	1503	ASP
2	D	933	GLU
2	D	967	GLN
2	D	1281	ARG
2	D	1291	TRP

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Mol	Chain	Res	Type
2	D	1292	GLU
2	D	1294	ALA
2	D	1337	ASN
2	D	1338	LYS
2	D	1359	LYS
2	D	1377	THR
2	D	1503	ASP
2	F	933	GLU
2	F	967	GLN
2	F	1269	GLU
2	F	1281	ARG
2	F	1291	TRP
2	F	1292	GLU
2	F	1337	ASN
2	F	1338	LYS
2	F	1361	THR
2	F	1377	THR
2	F	1417	SER
2	F	1446	ASN
2	H	933	GLU
2	H	968	MET
2	H	1281	ARG
2	H	1291	TRP
2	H	1292	GLU
2	H	1337	ASN
2	H	1338	LYS
2	H	1361	THR
2	H	1377	THR
2	H	1417	SER
2	H	1446	ASN
2	H	1493	GLU
3	I	236	ILE
3	I	407	PRO
3	I	701	LYS
3	I	706	GLN
3	J	236	ILE
3	J	407	PRO
3	J	701	LYS
3	J	706	GLN
3	K	236	ILE
3	K	407	PRO
3	K	701	LYS

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Mol	Chain	Res	Type
3	K	706	GLN
3	L	236	ILE
3	L	407	PRO
3	L	701	LYS
3	L	706	GLN
2	B	911	PRO
2	B	1360	ASN
2	B	1361	THR
2	B	1476	GLU
2	B	1571	ALA
2	D	911	PRO
2	D	1360	ASN
2	D	1361	THR
2	D	1476	GLU
2	D	1480	LEU
2	D	1571	ALA
2	F	911	PRO
2	F	1267	HIS
2	F	1294	ALA
2	F	1476	GLU
2	F	1498	ILE
2	F	1571	ALA
2	H	1266	ASP
2	H	1269	GLU
2	H	1294	ALA
2	H	1476	GLU
2	H	1496	CYS
2	H	1498	ILE
2	H	1571	ALA
1	A	442	GLU
1	A	643	PRO
2	B	1387	THR
2	B	1502	ASP
2	B	1573	LYS
1	C	442	GLU
1	C	643	PRO
2	D	1387	THR
2	D	1502	ASP
2	D	1573	LYS
1	E	442	GLU
1	E	643	PRO
2	F	1387	THR

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Mol	Chain	Res	Type
2	F	1573	LYS
1	G	442	GLU
2	H	911	PRO
2	H	1387	THR
2	H	1573	LYS
3	I	707	LYS
3	J	516	VAL
3	J	707	LYS
3	K	516	VAL
3	K	707	LYS
3	L	707	LYS
1	A	505	PRO
2	B	1196	ASN
2	B	1265	PRO
2	B	1480	LEU
1	C	505	PRO
2	D	1196	ASN
2	D	1265	PRO
2	D	1269	GLU
1	E	505	PRO
2	F	1196	ASN
2	F	1265	PRO
2	F	1268	GLN
2	F	1331	LYS
2	F	1637	PHE
1	G	505	PRO
2	H	967	GLN
2	H	1267	HIS
2	H	1486	ASP
2	H	1495	ASN
2	H	1502	ASP
3	I	516	VAL
3	L	516	VAL
4	M	7	SER
4	N	7	SER
4	P	7	SER
4	Q	7	SER
2	B	834	GLN
2	B	1201	PRO
2	B	1267	HIS
2	B	1536	PHE
2	D	834	GLN

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Mol	Chain	Res	Type
2	D	1201	PRO
2	D	1536	PHE
2	F	834	GLN
2	F	1201	PRO
2	F	1270	LEU
2	F	1536	PHE
1	G	643	PRO
2	H	834	GLN
2	H	1196	ASN
2	H	1201	PRO
2	H	1264	ALA
2	H	1536	PHE
3	I	268	LEU
3	J	268	LEU
3	K	268	LEU
3	L	268	LEU
3	I	482	GLY
3	J	482	GLY
3	K	482	GLY
3	L	482	GLY
2	B	1517	PRO
2	D	1517	PRO
2	F	1517	PRO
2	H	1517	PRO
1	A	208	PRO
1	C	208	PRO
1	E	208	PRO
1	G	208	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	558/567 (98%)	549 (98%)	9 (2%)	62 79
1	C	558/567 (98%)	549 (98%)	9 (2%)	62 79
1	E	558/567 (98%)	549 (98%)	9 (2%)	62 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	558/567 (98%)	549 (98%)	9 (2%)	62	79
2	B	793/810 (98%)	769 (97%)	24 (3%)	41	64
2	D	790/810 (98%)	766 (97%)	24 (3%)	41	64
2	F	793/810 (98%)	769 (97%)	24 (3%)	41	64
2	H	793/810 (98%)	766 (97%)	27 (3%)	37	62
3	I	442/446 (99%)	429 (97%)	13 (3%)	42	65
3	J	442/446 (99%)	429 (97%)	13 (3%)	42	65
3	K	442/446 (99%)	429 (97%)	13 (3%)	42	65
3	L	442/446 (99%)	429 (97%)	13 (3%)	42	65
4	M	76/84 (90%)	73 (96%)	3 (4%)	32	59
4	N	76/84 (90%)	73 (96%)	3 (4%)	32	59
4	P	76/84 (90%)	73 (96%)	3 (4%)	32	59
4	Q	76/84 (90%)	73 (96%)	3 (4%)	32	59
All	All	7473/7628 (98%)	7274 (97%)	199 (3%)	44	67

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	81	ASN
1	A	144	ASN
1	A	155	GLN
1	A	289	VAL
1	A	398	LEU
1	A	404	THR
1	A	440	ARG
1	A	551	ARG
2	B	757	LYS
2	B	770	ASN
2	B	833	ARG
2	B	834	GLN
2	B	841	ARG
2	B	937	LYS
2	B	945	LEU
2	B	953	GLU
2	B	1018	GLU
2	B	1196	ASN

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Mol	Chain	Res	Type
2	B	1292	GLU
2	B	1334	LEU
2	B	1335	THR
2	B	1342	LYS
2	B	1361	THR
2	B	1416	PHE
2	B	1433	GLU
2	B	1445	PHE
2	B	1462	ASN
2	B	1520	ASP
2	B	1535	ASP
2	B	1536	PHE
2	B	1569	ARG
2	B	1637	PHE
1	C	10	ASN
1	C	81	ASN
1	C	144	ASN
1	C	155	GLN
1	C	289	VAL
1	C	398	LEU
1	C	404	THR
1	C	440	ARG
1	C	551	ARG
2	D	757	LYS
2	D	770	ASN
2	D	833	ARG
2	D	834	GLN
2	D	841	ARG
2	D	937	LYS
2	D	945	LEU
2	D	953	GLU
2	D	1018	GLU
2	D	1196	ASN
2	D	1292	GLU
2	D	1334	LEU
2	D	1335	THR
2	D	1342	LYS
2	D	1361	THR
2	D	1416	PHE
2	D	1433	GLU
2	D	1445	PHE
2	D	1462	ASN

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Mol	Chain	Res	Type
2	D	1520	ASP
2	D	1535	ASP
2	D	1536	PHE
2	D	1569	ARG
2	D	1637	PHE
1	E	10	ASN
1	E	81	ASN
1	E	144	ASN
1	E	155	GLN
1	E	289	VAL
1	E	398	LEU
1	E	404	THR
1	E	440	ARG
1	E	551	ARG
2	F	757	LYS
2	F	770	ASN
2	F	833	ARG
2	F	834	GLN
2	F	841	ARG
2	F	937	LYS
2	F	945	LEU
2	F	953	GLU
2	F	1018	GLU
2	F	1196	ASN
2	F	1268	GLN
2	F	1292	GLU
2	F	1334	LEU
2	F	1335	THR
2	F	1342	LYS
2	F	1397	LYS
2	F	1433	GLU
2	F	1462	ASN
2	F	1520	ASP
2	F	1535	ASP
2	F	1536	PHE
2	F	1569	ARG
2	F	1572	LEU
2	F	1640	PRO
1	G	10	ASN
1	G	81	ASN
1	G	144	ASN
1	G	155	GLN

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Mol	Chain	Res	Type
1	G	289	VAL
1	G	398	LEU
1	G	404	THR
1	G	440	ARG
1	G	551	ARG
2	H	757	LYS
2	H	770	ASN
2	H	833	ARG
2	H	834	GLN
2	H	841	ARG
2	H	937	LYS
2	H	945	LEU
2	H	953	GLU
2	H	968	MET
2	H	969	THR
2	H	1018	GLU
2	H	1196	ASN
2	H	1267	HIS
2	H	1292	GLU
2	H	1334	LEU
2	H	1335	THR
2	H	1342	LYS
2	H	1397	LYS
2	H	1433	GLU
2	H	1462	ASN
2	H	1498	ILE
2	H	1499	GLN
2	H	1520	ASP
2	H	1535	ASP
2	H	1536	PHE
2	H	1569	ARG
2	H	1572	LEU
3	I	237	VAL
3	I	255	SER
3	I	322	HIS
3	I	329	ASN
3	I	368	ASN
3	I	381	ARG
3	I	423	ASN
3	I	446	GLU
3	I	539	LYS
3	I	540	LYS

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Mol	Chain	Res	Type
3	I	654	ARG
3	I	702	ASN
3	I	703	GLN
3	J	237	VAL
3	J	255	SER
3	J	322	HIS
3	J	329	ASN
3	J	368	ASN
3	J	381	ARG
3	J	423	ASN
3	J	446	GLU
3	J	539	LYS
3	J	540	LYS
3	J	654	ARG
3	J	702	ASN
3	J	703	GLN
3	K	237	VAL
3	K	255	SER
3	K	322	HIS
3	K	329	ASN
3	K	368	ASN
3	K	381	ARG
3	K	423	ASN
3	K	446	GLU
3	K	539	LYS
3	K	540	LYS
3	K	654	ARG
3	K	702	ASN
3	K	703	GLN
3	L	237	VAL
3	L	255	SER
3	L	322	HIS
3	L	329	ASN
3	L	368	ASN
3	L	381	ARG
3	L	423	ASN
3	L	446	GLU
3	L	539	LYS
3	L	540	LYS
3	L	654	ARG
3	L	702	ASN
3	L	703	GLN

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Mol	Chain	Res	Type
4	M	11	GLN
4	M	69	GLN
4	M	71	GLN
4	N	11	GLN
4	N	69	GLN
4	N	71	GLN
4	P	11	GLN
4	P	69	GLN
4	P	71	GLN
4	Q	11	GLN
4	Q	69	GLN
4	Q	71	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (256) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	87	GLN
1	A	104	GLN
1	A	144	ASN
1	A	155	GLN
1	A	161	GLN
1	A	162	ASN
1	A	163	GLN
1	A	370	GLN
1	A	380	GLN
1	A	390	ASN
1	A	414	GLN
1	A	490	GLN
1	A	558	GLN
1	A	567	HIS
1	A	634	GLN
1	A	639	GLN
2	B	738	ASN
2	B	752	ASN
2	B	762	ASN
2	B	770	ASN
2	B	820	ASN
2	B	834	GLN
2	B	860	HIS
2	B	886	GLN
2	B	896	HIS

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Mol	Chain	Res	Type
2	B	897	HIS
2	B	1011	GLN
2	B	1069	ASN
2	B	1076	GLN
2	B	1114	ASN
2	B	1130	GLN
2	B	1141	ASN
2	B	1160	ASN
2	B	1196	ASN
2	B	1204	GLN
2	B	1267	HIS
2	B	1277	GLN
2	B	1333	GLN
2	B	1337	ASN
2	B	1401	ASN
2	B	1431	HIS
2	B	1451	GLN
2	B	1462	ASN
2	B	1559	GLN
2	B	1579	HIS
2	B	1608	HIS
2	B	1620	ASN
1	C	10	ASN
1	C	60	HIS
1	C	87	GLN
1	C	104	GLN
1	C	132	HIS
1	C	144	ASN
1	C	155	GLN
1	C	161	GLN
1	C	162	ASN
1	C	163	GLN
1	C	356	ASN
1	C	370	GLN
1	C	380	GLN
1	C	390	ASN
1	C	414	GLN
1	C	450	ASN
1	C	490	GLN
1	C	558	GLN
1	C	567	HIS
1	C	634	GLN

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Mol	Chain	Res	Type
1	C	639	GLN
2	D	738	ASN
2	D	752	ASN
2	D	762	ASN
2	D	770	ASN
2	D	820	ASN
2	D	834	GLN
2	D	860	HIS
2	D	897	HIS
2	D	1011	GLN
2	D	1069	ASN
2	D	1076	GLN
2	D	1114	ASN
2	D	1130	GLN
2	D	1141	ASN
2	D	1160	ASN
2	D	1196	ASN
2	D	1204	GLN
2	D	1267	HIS
2	D	1277	GLN
2	D	1333	GLN
2	D	1337	ASN
2	D	1401	ASN
2	D	1431	HIS
2	D	1451	GLN
2	D	1462	ASN
2	D	1559	GLN
2	D	1579	HIS
2	D	1608	HIS
2	D	1620	ASN
1	E	60	HIS
1	E	87	GLN
1	E	104	GLN
1	E	132	HIS
1	E	144	ASN
1	E	155	GLN
1	E	161	GLN
1	E	162	ASN
1	E	163	GLN
1	E	356	ASN
1	E	370	GLN
1	E	380	GLN

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Mol	Chain	Res	Type
1	E	390	ASN
1	E	414	GLN
1	E	450	ASN
1	E	490	GLN
1	E	558	GLN
1	E	567	HIS
1	E	639	GLN
2	F	738	ASN
2	F	752	ASN
2	F	762	ASN
2	F	770	ASN
2	F	820	ASN
2	F	834	GLN
2	F	860	HIS
2	F	897	HIS
2	F	1011	GLN
2	F	1069	ASN
2	F	1076	GLN
2	F	1114	ASN
2	F	1130	GLN
2	F	1141	ASN
2	F	1160	ASN
2	F	1196	ASN
2	F	1204	GLN
2	F	1267	HIS
2	F	1277	GLN
2	F	1333	GLN
2	F	1337	ASN
2	F	1401	ASN
2	F	1431	HIS
2	F	1451	GLN
2	F	1462	ASN
2	F	1559	GLN
2	F	1579	HIS
2	F	1608	HIS
2	F	1620	ASN
2	F	1641	ASN
1	G	60	HIS
1	G	87	GLN
1	G	104	GLN
1	G	132	HIS
1	G	144	ASN

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Mol	Chain	Res	Type
1	G	155	GLN
1	G	161	GLN
1	G	162	ASN
1	G	163	GLN
1	G	356	ASN
1	G	370	GLN
1	G	380	GLN
1	G	390	ASN
1	G	414	GLN
1	G	490	GLN
1	G	558	GLN
1	G	587	ASN
1	G	634	GLN
1	G	639	GLN
2	H	738	ASN
2	H	752	ASN
2	H	762	ASN
2	H	770	ASN
2	H	820	ASN
2	H	834	GLN
2	H	860	HIS
2	H	896	HIS
2	H	897	HIS
2	H	1277	GLN
2	H	1333	GLN
2	H	1337	ASN
2	H	1401	ASN
2	H	1431	HIS
2	H	1451	GLN
2	H	1462	ASN
2	H	1559	GLN
2	H	1579	HIS
2	H	1608	HIS
2	H	1620	ASN
3	I	270	ASN
3	I	329	ASN
3	I	368	ASN
3	I	392	ASN
3	I	411	GLN
3	I	413	ASN
3	I	423	ASN
3	I	466	HIS

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Mol	Chain	Res	Type
3	I	531	HIS
3	I	533	ASN
3	I	591	GLN
3	I	703	GLN
3	J	270	ASN
3	J	329	ASN
3	J	368	ASN
3	J	392	ASN
3	J	411	GLN
3	J	413	ASN
3	J	423	ASN
3	J	435	ASN
3	J	466	HIS
3	J	531	HIS
3	J	533	ASN
3	J	591	GLN
3	J	703	GLN
3	K	270	ASN
3	K	329	ASN
3	K	368	ASN
3	K	392	ASN
3	K	411	GLN
3	K	413	ASN
3	K	423	ASN
3	K	435	ASN
3	K	466	HIS
3	K	531	HIS
3	K	533	ASN
3	K	591	GLN
3	K	703	GLN
3	L	270	ASN
3	L	329	ASN
3	L	368	ASN
3	L	392	ASN
3	L	411	GLN
3	L	413	ASN
3	L	423	ASN
3	L	466	HIS
3	L	531	HIS
3	L	533	ASN
3	L	591	GLN
3	L	703	GLN

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Mol	Chain	Res	Type
4	M	11	GLN
4	M	27	ASN
4	M	49	GLN
4	M	69	GLN
4	M	71	GLN
4	N	11	GLN
4	N	27	ASN
4	N	49	GLN
4	N	69	GLN
4	N	71	GLN
4	P	11	GLN
4	P	27	ASN
4	P	49	GLN
4	P	69	GLN
4	P	71	GLN
4	Q	11	GLN
4	Q	27	ASN
4	Q	49	GLN
4	Q	69	GLN
4	Q	71	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

52 monosaccharides 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	$\#\|Z\|>2$
5	NAG	O	1	1,5	14,14,15	0.46	0	17,19,21	0.79	0
5	NAG	O	2	5	14,14,15	0.65	0	17,19,21	1.80	4 (23%)
5	BMA	O	3	5	11,11,12	0.57	0	15,15,17	1.40	2 (13%)
5	BMA	O	4	5	11,11,12	0.67	0	15,15,17	1.38	2 (13%)
5	NAG	R	1	5,2	14,14,15	0.55	0	17,19,21	1.11	2 (11%)
5	NAG	R	2	5	14,14,15	0.54	0	17,19,21	2.19	3 (17%)
5	BMA	R	3	5	11,11,12	0.95	0	15,15,17	1.97	6 (40%)
5	BMA	R	4	5	11,11,12	0.73	0	15,15,17	0.81	0
6	NAG	S	1	1,6	14,14,15	0.62	0	17,19,21	1.17	2 (11%)
6	NAG	S	2	6	14,14,15	0.67	0	17,19,21	1.13	2 (11%)
6	BMA	S	3	6	11,11,12	0.68	0	15,15,17	1.14	1 (6%)
6	BMA	S	4	6	11,11,12	0.77	0	15,15,17	1.54	3 (20%)
6	BMA	S	5	6	11,11,12	0.67	0	15,15,17	1.76	4 (26%)
5	NAG	T	1	5,2	14,14,15	0.50	0	17,19,21	0.83	0
5	NAG	T	2	5	14,14,15	0.58	0	17,19,21	1.05	2 (11%)
5	BMA	T	3	5	11,11,12	0.64	0	15,15,17	1.37	2 (13%)
5	BMA	T	4	5	11,11,12	0.67	0	15,15,17	1.30	2 (13%)
5	NAG	U	1	1,5	14,14,15	0.56	0	17,19,21	0.87	1 (5%)
5	NAG	U	2	5	14,14,15	0.60	0	17,19,21	1.16	2 (11%)
5	BMA	U	3	5	11,11,12	0.70	0	15,15,17	1.07	1 (6%)
5	BMA	U	4	5	11,11,12	0.94	1 (9%)	15,15,17	1.70	3 (20%)
7	NAG	V	1	7,2	14,14,15	0.39	0	17,19,21	1.28	3 (17%)
7	NAG	V	2	7	14,14,15	0.44	0	17,19,21	1.66	4 (23%)
7	BMA	V	3	7	11,11,12	0.60	0	15,15,17	1.60	4 (26%)
7	BMA	V	4	7	11,11,12	1.00	1 (9%)	15,15,17	1.68	4 (26%)
7	BMA	V	5	7	11,11,12	0.67	0	15,15,17	1.86	4 (26%)
7	BMA	V	6	7	11,11,12	0.71	0	15,15,17	1.05	1 (6%)
6	NAG	W	1	1,6	14,14,15	0.45	0	17,19,21	1.17	1 (5%)
6	NAG	W	2	6	14,14,15	0.50	0	17,19,21	2.17	4 (23%)
6	BMA	W	3	6	11,11,12	0.52	0	15,15,17	2.97	6 (40%)
6	BMA	W	4	6	11,11,12	0.57	0	15,15,17	4.54	6 (40%)
6	BMA	W	5	6	11,11,12	0.65	0	15,15,17	1.41	2 (13%)
8	NAG	X	1	2,8	14,14,15	0.59	0	17,19,21	0.80	0
8	NAG	X	2	8	14,14,15	0.49	0	17,19,21	0.79	0
8	MAN	X	3	8	11,11,12	0.78	0	15,15,17	1.39	2 (13%)
8	MAN	X	4	8	11,11,12	0.77	0	15,15,17	1.06	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	Y	1	9,3	14,14,15	0.57	0	17,19,21	1.00	2 (11%)
9	NAG	Y	2	9	14,14,15	0.63	0	17,19,21	1.03	1 (5%)
9	MAN	Y	3	9	11,11,12	0.65	0	15,15,17	1.05	1 (6%)
10	NAG	Z	1	3,10	14,14,15	0.55	0	17,19,21	1.12	2 (11%)
10	NAG	Z	2	10	14,14,15	0.55	0	17,19,21	0.93	1 (5%)
9	NAG	a	1	9,3	14,14,15	0.52	0	17,19,21	1.01	1 (5%)
9	NAG	a	2	9	14,14,15	0.61	0	17,19,21	1.05	1 (5%)
9	MAN	a	3	9	11,11,12	0.65	0	15,15,17	0.99	1 (6%)
11	NAG	b	1	11,3	14,14,15	0.63	0	17,19,21	1.04	2 (11%)
11	NAG	b	2	11	14,14,15	0.71	0	17,19,21	1.39	3 (17%)
11	MAN	b	3	11	11,11,12	0.57	0	15,15,17	1.91	5 (33%)
11	MAN	b	4	11	11,11,12	0.61	0	15,15,17	1.15	3 (20%)
11	MAN	b	5	11	11,11,12	0.76	0	15,15,17	1.64	3 (20%)
12	NAG	c	1	3,12	14,14,15	0.49	0	17,19,21	0.89	0
12	NAG	c	2	12	14,14,15	0.61	0	17,19,21	1.06	1 (5%)
12	BMA	c	3	12	11,11,12	0.65	0	15,15,17	0.90	1 (6%)

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
5	NAG	O	1	1,5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	4/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1
5	BMA	O	4	5	-	0/2/19/22	0/1/1/1
5	NAG	R	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	BMA	R	4	5	-	0/2/19/22	0/1/1/1
6	NAG	S	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	S	2	6	-	4/6/23/26	0/1/1/1
6	BMA	S	3	6	-	2/2/19/22	0/1/1/1
6	BMA	S	4	6	-	0/2/19/22	0/1/1/1
6	BMA	S	5	6	-	0/2/19/22	0/1/1/1
5	NAG	T	1	5,2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
5	BMA	T	4	5	-	0/2/19/22	0/1/1/1
5	NAG	U	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
5	BMA	U	3	5	-	2/2/19/22	0/1/1/1
5	BMA	U	4	5	-	0/2/19/22	0/1/1/1
7	NAG	V	1	7,2	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	V	2	7	-	4/6/23/26	0/1/1/1
7	BMA	V	3	7	-	2/2/19/22	0/1/1/1
7	BMA	V	4	7	-	2/2/19/22	0/1/1/1
7	BMA	V	5	7	-	1/2/19/22	0/1/1/1
7	BMA	V	6	7	-	0/2/19/22	0/1/1/1
6	NAG	W	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	BMA	W	3	6	-	0/2/19/22	0/1/1/1
6	BMA	W	4	6	-	0/2/19/22	0/1/1/1
6	BMA	W	5	6	-	0/2/19/22	0/1/1/1
8	NAG	X	1	2,8	-	3/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1
8	MAN	X	3	8	1/1/4/5	2/2/19/22	0/1/1/1
8	MAN	X	4	8	1/1/4/5	2/2/19/22	0/1/1/1
9	NAG	Y	1	9,3	-	3/6/23/26	0/1/1/1
9	NAG	Y	2	9	-	2/6/23/26	0/1/1/1
9	MAN	Y	3	9	1/1/4/5	0/2/19/22	0/1/1/1
10	NAG	Z	1	3,10	1/1/5/7	3/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	2/6/23/26	0/1/1/1
9	NAG	a	1	9,3	-	3/6/23/26	0/1/1/1
9	NAG	a	2	9	-	2/6/23/26	0/1/1/1
9	MAN	a	3	9	1/1/4/5	0/2/19/22	0/1/1/1
11	NAG	b	1	11,3	1/1/5/7	4/6/23/26	0/1/1/1
11	NAG	b	2	11	-	4/6/23/26	0/1/1/1
11	MAN	b	3	11	1/1/4/5	0/2/19/22	0/1/1/1
11	MAN	b	4	11	1/1/4/5	0/2/19/22	0/1/1/1
11	MAN	b	5	11	1/1/4/5	2/2/19/22	0/1/1/1
12	NAG	c	1	3,12	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	c	2	12	-	2/6/23/26	0/1/1/1
12	BMA	c	3	12	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	4	BMA	O5-C1	-2.34	1.40	1.43
7	V	4	BMA	O5-C1	-2.22	1.40	1.43

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	W	4	BMA	C1-C2-C3	-10.68	96.54	109.67
6	W	4	BMA	C3-C4-C5	-7.10	97.58	110.24
5	R	2	NAG	C1-O5-C5	7.08	121.79	112.19
6	W	4	BMA	C1-O5-C5	-6.98	102.74	112.19
6	W	4	BMA	O5-C5-C6	6.86	117.96	107.20
6	W	3	BMA	O5-C5-C6	6.61	117.57	107.20
6	W	4	BMA	O3-C3-C4	6.14	124.55	110.35
6	W	2	NAG	C1-O5-C5	5.96	120.26	112.19
6	W	3	BMA	C1-C2-C3	-5.51	102.89	109.67
5	O	2	NAG	C4-C3-C2	4.96	118.29	111.02
5	U	4	BMA	C1-O5-C5	-4.45	106.16	112.19
7	V	5	BMA	C1-C2-C3	-4.45	104.20	109.67
5	R	3	BMA	C1-C2-C3	4.44	115.13	109.67
6	W	3	BMA	C6-C5-C4	-4.37	102.77	113.00
6	S	5	BMA	C1-C2-C3	-4.23	104.46	109.67
11	b	3	MAN	O5-C5-C6	4.23	113.83	107.20
6	W	3	BMA	C1-O5-C5	-4.03	106.73	112.19
8	X	3	MAN	C1-C2-C3	3.90	114.46	109.67
7	V	4	BMA	C1-C2-C3	3.88	114.44	109.67
5	R	2	NAG	O5-C1-C2	3.79	117.27	111.29
5	R	3	BMA	C1-O5-C5	-3.74	107.13	112.19
5	T	3	BMA	C1-O5-C5	-3.73	107.14	112.19
11	b	3	MAN	C1-O5-C5	-3.72	107.16	112.19
11	b	5	MAN	C3-C4-C5	3.72	116.87	110.24
11	b	2	NAG	C4-C3-C2	3.67	116.40	111.02
5	O	3	BMA	O5-C5-C6	3.63	112.90	107.20
7	V	3	BMA	O5-C1-C2	-3.63	105.17	110.77
7	V	2	NAG	C1-O5-C5	3.52	116.97	112.19
6	W	2	NAG	C4-C3-C2	-3.48	105.92	111.02
7	V	5	BMA	O5-C1-C2	-3.39	105.53	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	2	NAG	C4-C3-C2	-3.30	106.18	111.02
5	O	2	NAG	C1-O5-C5	3.28	116.63	112.19
6	S	4	BMA	O3-C3-C4	-3.27	102.78	110.35
6	W	5	BMA	C1-C2-C3	-3.25	105.68	109.67
6	W	2	NAG	O4-C4-C5	3.20	117.25	109.30
6	W	3	BMA	C3-C4-C5	3.15	115.85	110.24
5	O	4	BMA	O5-C1-C2	-3.13	105.94	110.77
5	O	3	BMA	C1-O5-C5	-3.10	107.99	112.19
6	W	5	BMA	O5-C1-C2	-3.07	106.03	110.77
6	S	4	BMA	C3-C4-C5	3.06	115.70	110.24
5	U	4	BMA	O5-C1-C2	-3.02	106.11	110.77
5	T	3	BMA	O5-C5-C6	3.02	111.93	107.20
5	O	4	BMA	C1-C2-C3	-2.98	106.00	109.67
6	S	5	BMA	O5-C1-C2	-2.98	106.17	110.77
6	S	1	NAG	C3-C4-C5	2.97	115.54	110.24
5	T	4	BMA	O5-C1-C2	-2.97	106.19	110.77
11	b	5	MAN	O5-C1-C2	-2.96	106.21	110.77
5	R	1	NAG	C1-O5-C5	2.93	116.17	112.19
9	Y	3	MAN	C1-O5-C5	-2.91	108.24	112.19
7	V	4	BMA	C2-C3-C4	2.90	115.91	110.89
5	U	4	BMA	C1-C2-C3	-2.88	106.13	109.67
7	V	2	NAG	O4-C4-C3	2.82	116.87	110.35
6	W	1	NAG	C4-C3-C2	2.82	115.15	111.02
11	b	2	NAG	C3-C4-C5	2.78	115.19	110.24
5	T	4	BMA	C1-C2-C3	-2.77	106.25	109.67
11	b	3	MAN	C1-C2-C3	-2.77	106.26	109.67
11	b	3	MAN	O3-C3-C2	2.75	115.25	109.99
11	b	1	NAG	C3-C4-C5	2.70	115.05	110.24
6	S	5	BMA	C1-O5-C5	-2.69	108.54	112.19
12	c	2	NAG	C4-C3-C2	2.64	114.89	111.02
9	a	1	NAG	C1-O5-C5	2.61	115.73	112.19
7	V	5	BMA	C3-C4-C5	2.61	114.89	110.24
7	V	2	NAG	O5-C5-C6	2.60	111.27	107.20
5	O	2	NAG	C3-C4-C5	2.60	114.87	110.24
10	Z	1	NAG	C3-C4-C5	2.58	114.84	110.24
9	a	2	NAG	C4-C3-C2	2.58	114.79	111.02
6	S	3	BMA	C1-O5-C5	-2.56	108.72	112.19
9	a	3	MAN	C1-O5-C5	-2.56	108.73	112.19
9	Y	2	NAG	C4-C3-C2	2.55	114.76	111.02
7	V	4	BMA	C1-O5-C5	-2.54	108.75	112.19
6	W	3	BMA	O6-C6-C5	2.50	119.86	111.29
6	W	2	NAG	O5-C1-C2	2.48	115.21	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	1	NAG	O5-C1-C2	-2.48	107.37	111.29
5	U	2	NAG	C1-O5-C5	2.46	115.53	112.19
10	Z	2	NAG	C1-O5-C5	2.46	115.53	112.19
7	V	5	BMA	C1-O5-C5	-2.45	108.87	112.19
6	S	4	BMA	C1-O5-C5	-2.44	108.88	112.19
11	b	4	MAN	O5-C5-C6	2.44	111.02	107.20
10	Z	1	NAG	C4-C3-C2	2.43	114.57	111.02
5	U	2	NAG	O5-C1-C2	2.42	115.11	111.29
5	U	3	BMA	C1-O5-C5	-2.42	108.92	112.19
6	S	5	BMA	C3-C4-C5	2.39	114.50	110.24
5	R	3	BMA	O5-C5-C6	2.38	110.93	107.20
7	V	3	BMA	C2-C3-C4	-2.36	106.81	110.89
5	R	3	BMA	C2-C3-C4	2.36	114.97	110.89
8	X	4	MAN	C1-O5-C5	-2.34	109.03	112.19
6	S	2	NAG	C4-C3-C2	2.31	114.41	111.02
7	V	3	BMA	C1-C2-C3	-2.30	106.84	109.67
6	S	1	NAG	C1-O5-C5	2.29	115.30	112.19
7	V	1	NAG	O4-C4-C5	2.29	114.99	109.30
5	T	2	NAG	C1-O5-C5	2.29	115.29	112.19
5	R	3	BMA	O5-C5-C4	-2.28	105.29	110.83
5	O	2	NAG	O4-C4-C3	-2.27	105.10	110.35
7	V	6	BMA	O5-C1-C2	-2.26	107.29	110.77
11	b	5	MAN	C6-C5-C4	-2.22	107.81	113.00
7	V	1	NAG	C4-C3-C2	-2.21	107.77	111.02
6	W	4	BMA	O3-C3-C2	2.20	114.21	109.99
9	Y	1	NAG	C3-C4-C5	2.17	114.11	110.24
8	X	4	MAN	O5-C1-C2	-2.17	107.43	110.77
8	X	3	MAN	O5-C5-C6	2.16	110.58	107.20
12	c	3	BMA	C1-O5-C5	-2.16	109.27	112.19
9	Y	1	NAG	C1-O5-C5	2.15	115.11	112.19
7	V	3	BMA	C6-C5-C4	-2.12	108.03	113.00
7	V	4	BMA	C3-C4-C5	2.12	114.02	110.24
5	R	1	NAG	C3-C4-C5	2.11	113.99	110.24
11	b	3	MAN	C2-C3-C4	-2.10	107.26	110.89
6	S	2	NAG	O5-C1-C2	2.09	114.58	111.29
11	b	4	MAN	C3-C4-C5	2.07	113.94	110.24
5	R	2	NAG	C6-C5-C4	-2.07	108.15	113.00
5	R	3	BMA	C6-C5-C4	2.05	117.80	113.00
11	b	2	NAG	O4-C4-C3	-2.04	105.62	110.35
11	b	4	MAN	C1-O5-C5	2.04	114.96	112.19
5	T	2	NAG	C4-C3-C2	2.03	114.00	111.02
11	b	1	NAG	C4-C3-C2	2.02	113.98	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	U	1	NAG	C3-C4-C5	2.00	113.81	110.24

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	O	1	NAG	C1
7	V	1	NAG	C1
8	X	3	MAN	C1
8	X	4	MAN	C1
9	Y	3	MAN	C1
9	a	3	MAN	C1
10	Z	1	NAG	C1
11	b	1	NAG	C1
11	b	3	MAN	C1
11	b	4	MAN	C1
11	b	5	MAN	C1

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	O	2	NAG	C8-C7-N2-C2
5	O	2	NAG	O7-C7-N2-C2
5	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	T	1	NAG	C8-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	U	1	NAG	C8-C7-N2-C2
5	U	1	NAG	O7-C7-N2-C2
6	S	1	NAG	C1-C2-N2-C7
6	S	1	NAG	C8-C7-N2-C2
6	S	1	NAG	O7-C7-N2-C2
6	W	1	NAG	C8-C7-N2-C2
6	W	1	NAG	O7-C7-N2-C2
7	V	1	NAG	C8-C7-N2-C2
7	V	1	NAG	O7-C7-N2-C2
8	X	1	NAG	C3-C2-N2-C7
8	X	1	NAG	C8-C7-N2-C2
8	X	1	NAG	O7-C7-N2-C2
12	c	1	NAG	O7-C7-N2-C2
12	c	2	NAG	C8-C7-N2-C2
9	Y	2	NAG	C8-C7-N2-C2
9	a	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
12	c	1	NAG	C8-C7-N2-C2
12	c	2	NAG	O7-C7-N2-C2
5	U	3	BMA	O5-C5-C6-O6
9	Y	1	NAG	C8-C7-N2-C2
9	Y	1	NAG	O7-C7-N2-C2
9	Y	2	NAG	O7-C7-N2-C2
9	a	2	NAG	O7-C7-N2-C2
10	Z	1	NAG	C8-C7-N2-C2
10	Z	1	NAG	O7-C7-N2-C2
7	V	4	BMA	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
7	V	2	NAG	C4-C5-C6-O6
7	V	3	BMA	O5-C5-C6-O6
11	b	2	NAG	O5-C5-C6-O6
5	O	1	NAG	C8-C7-N2-C2
6	S	2	NAG	C8-C7-N2-C2
6	S	2	NAG	O7-C7-N2-C2
11	b	1	NAG	C8-C7-N2-C2
5	R	1	NAG	C1-C2-N2-C7
5	T	1	NAG	C1-C2-N2-C7
5	U	1	NAG	C1-C2-N2-C7
6	W	1	NAG	C1-C2-N2-C7
7	V	1	NAG	C1-C2-N2-C7
6	S	3	BMA	C4-C5-C6-O6
11	b	2	NAG	C4-C5-C6-O6
11	b	5	MAN	C4-C5-C6-O6
5	U	3	BMA	C4-C5-C6-O6
5	O	1	NAG	O7-C7-N2-C2
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
5	T	2	NAG	C8-C7-N2-C2
5	T	2	NAG	O7-C7-N2-C2
5	U	2	NAG	C8-C7-N2-C2
5	U	2	NAG	O7-C7-N2-C2
6	W	2	NAG	C8-C7-N2-C2
6	W	2	NAG	O7-C7-N2-C2
7	V	2	NAG	C8-C7-N2-C2
7	V	2	NAG	O7-C7-N2-C2
8	X	2	NAG	C8-C7-N2-C2
8	X	2	NAG	O7-C7-N2-C2
9	a	1	NAG	C8-C7-N2-C2
10	Z	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
10	Z	2	NAG	O7-C7-N2-C2
11	b	1	NAG	O7-C7-N2-C2
11	b	2	NAG	C8-C7-N2-C2
11	b	2	NAG	O7-C7-N2-C2
5	O	2	NAG	C4-C5-C6-O6
5	O	3	BMA	C4-C5-C6-O6
9	Y	1	NAG	C1-C2-N2-C7
10	Z	1	NAG	C1-C2-N2-C7
12	c	1	NAG	C1-C2-N2-C7
9	a	1	NAG	O7-C7-N2-C2
7	V	3	BMA	C4-C5-C6-O6
6	S	3	BMA	O5-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
7	V	4	BMA	C4-C5-C6-O6
11	b	5	MAN	O5-C5-C6-O6
8	X	3	MAN	O5-C5-C6-O6
11	b	1	NAG	C1-C2-N2-C7
9	a	1	NAG	C1-C2-N2-C7
5	T	3	BMA	C4-C5-C6-O6
8	X	3	MAN	C4-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
8	X	4	MAN	C4-C5-C6-O6
5	R	3	BMA	C4-C5-C6-O6
8	X	4	MAN	O5-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
6	S	2	NAG	C4-C5-C6-O6
11	b	1	NAG	C4-C5-C6-O6
7	V	5	BMA	C4-C5-C6-O6

There are no ring outliers.

23 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	1	NAG	1	0
7	V	6	BMA	1	0
6	S	2	NAG	1	0
6	W	4	BMA	2	0
8	X	4	MAN	1	0
8	X	3	MAN	1	0
6	W	1	NAG	1	0

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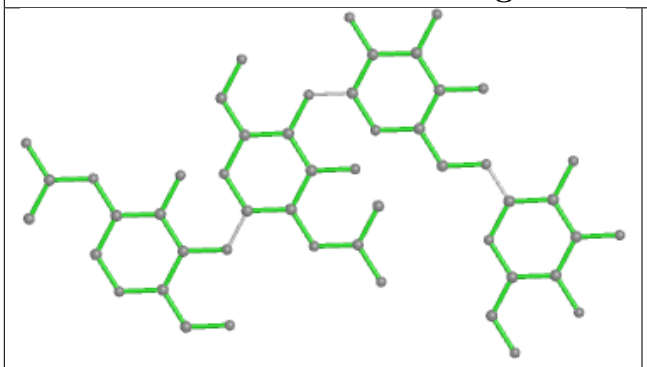
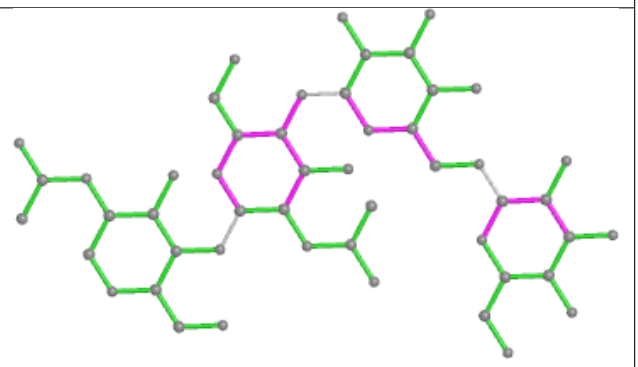
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	W	2	NAG	3	0
9	Y	2	NAG	2	0
6	W	3	BMA	2	0
6	S	1	NAG	1	0
5	U	3	BMA	1	0
8	X	2	NAG	1	0
7	V	3	BMA	1	0
5	O	2	NAG	1	0
5	T	2	NAG	1	0
5	T	1	NAG	1	0
9	Y	1	NAG	1	0
5	U	1	NAG	2	0
5	U	4	BMA	1	0
5	U	2	NAG	1	0
7	V	4	BMA	2	0
5	R	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

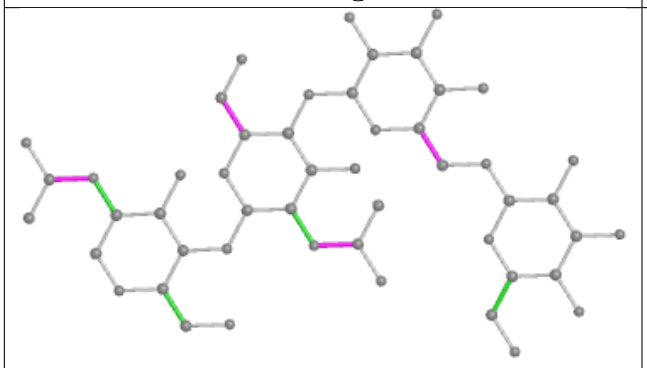
Oligosaccharide Chain O



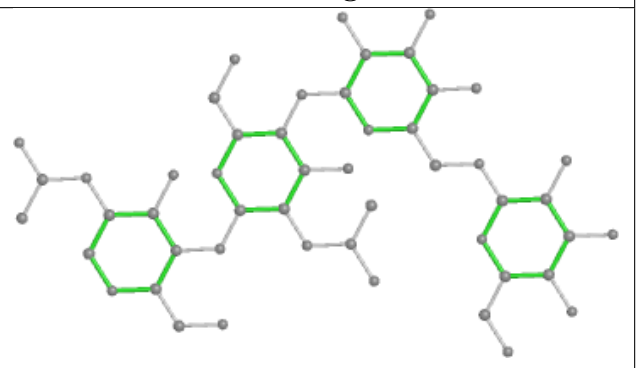
Bond lengths



Bond angles

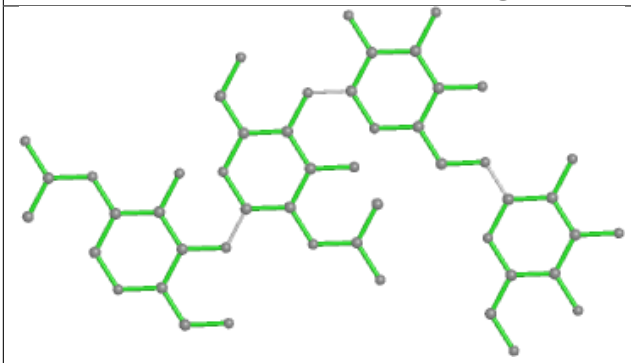


Torsions

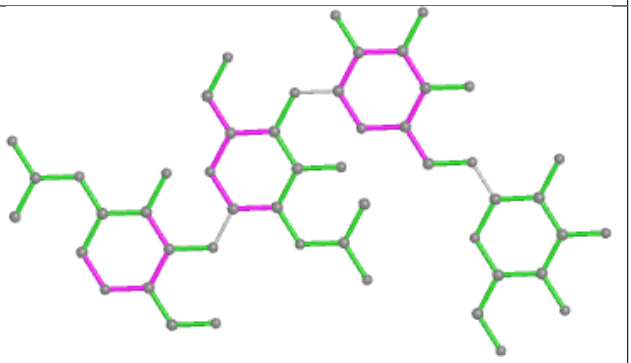


Rings

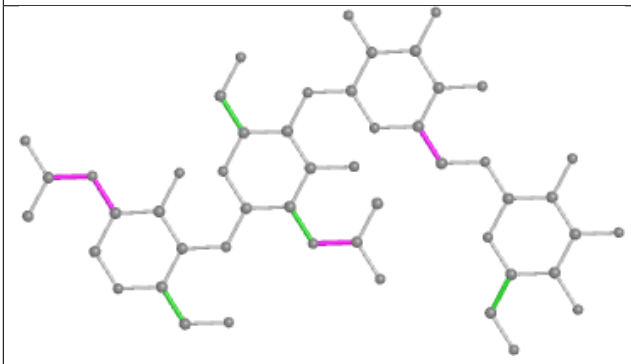
Oligosaccharide Chain R



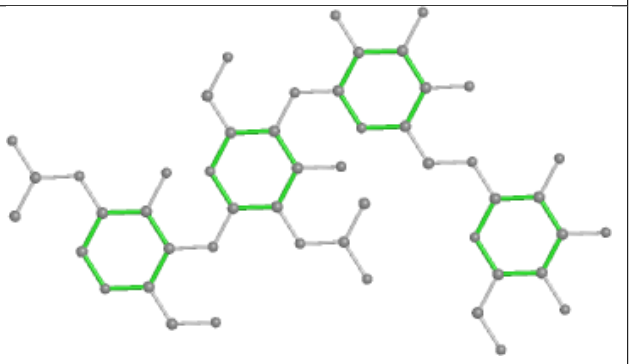
Bond lengths



Bond angles

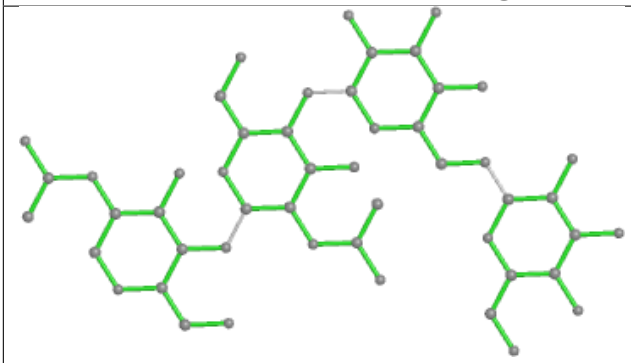


Torsions

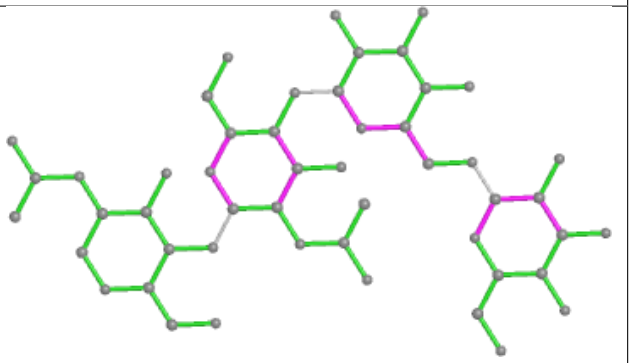


Rings

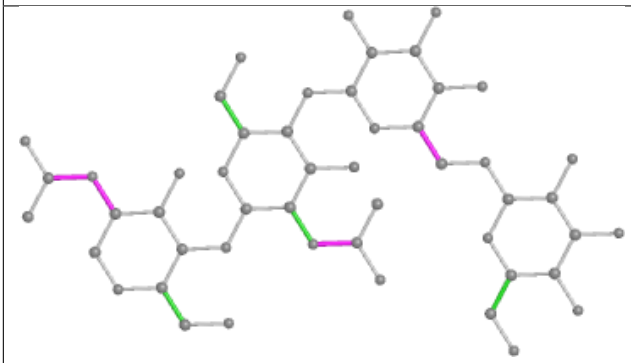
Oligosaccharide Chain T



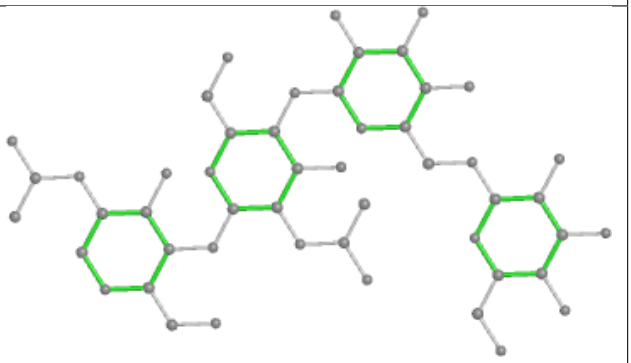
Bond lengths



Bond angles

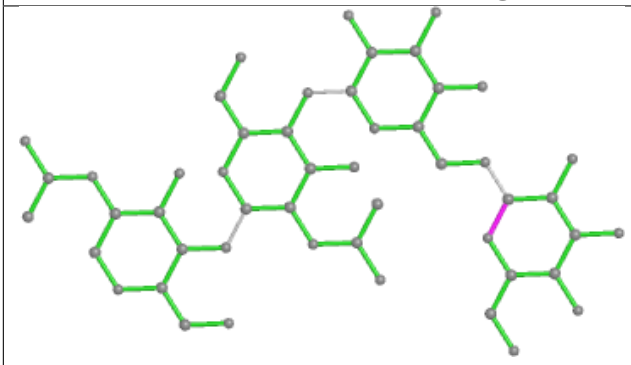


Torsions

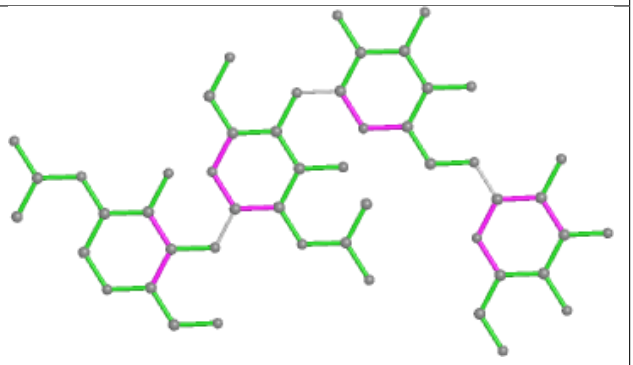


Rings

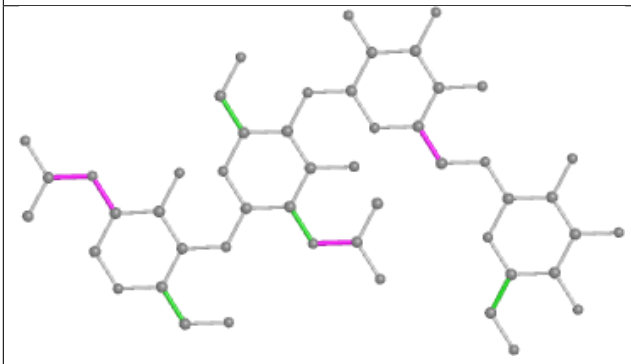
Oligosaccharide Chain U



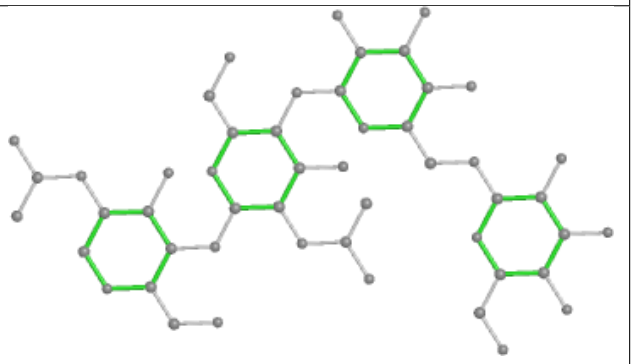
Bond lengths



Bond angles

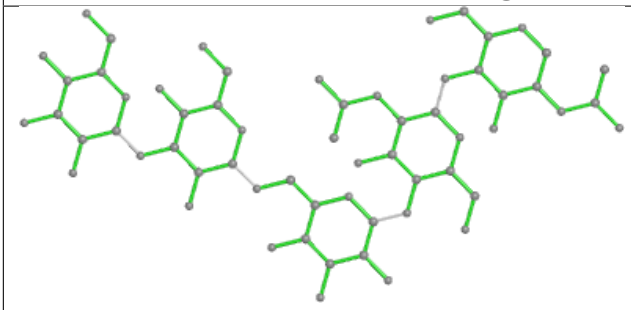


Torsions

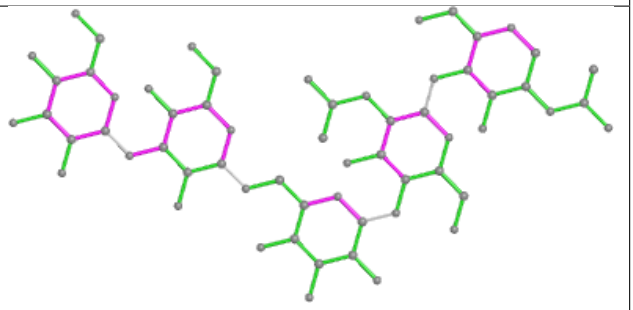


Rings

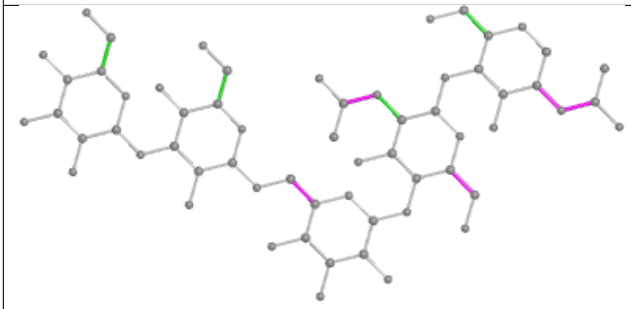
Oligosaccharide Chain S



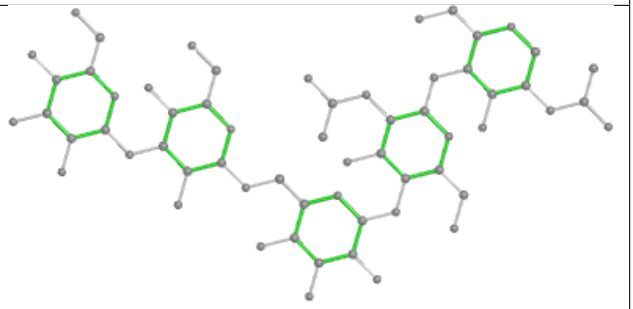
Bond lengths



Bond angles

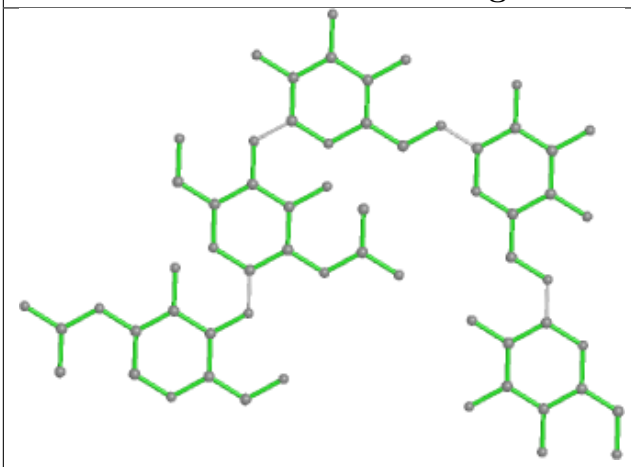


Torsions

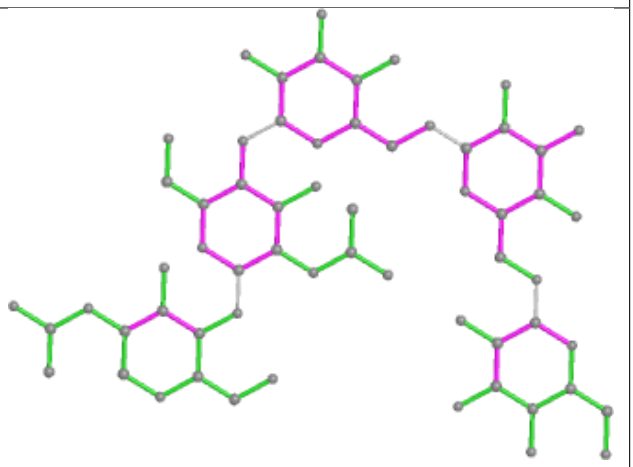


Rings

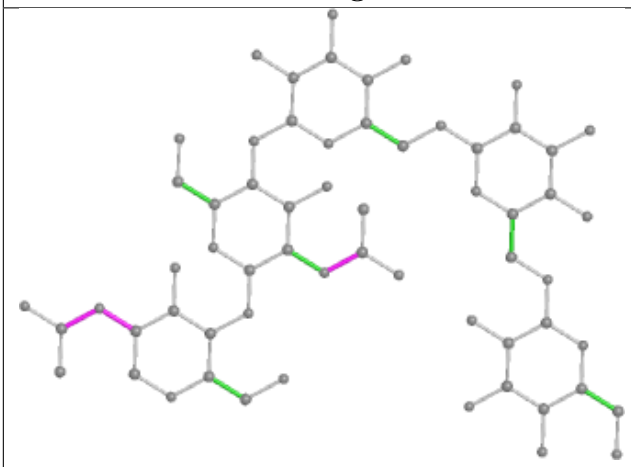
Oligosaccharide Chain W



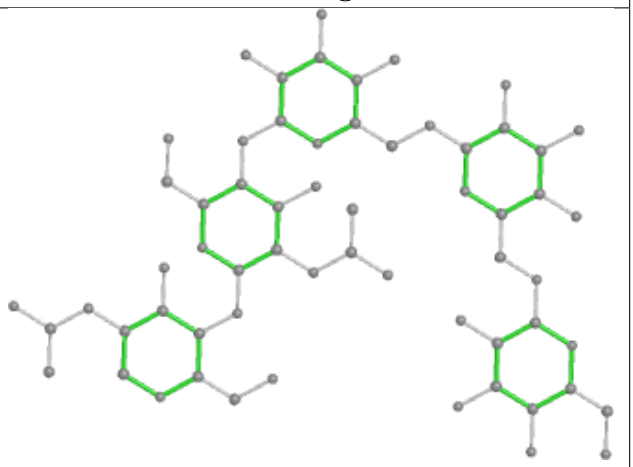
Bond lengths



Bond angles

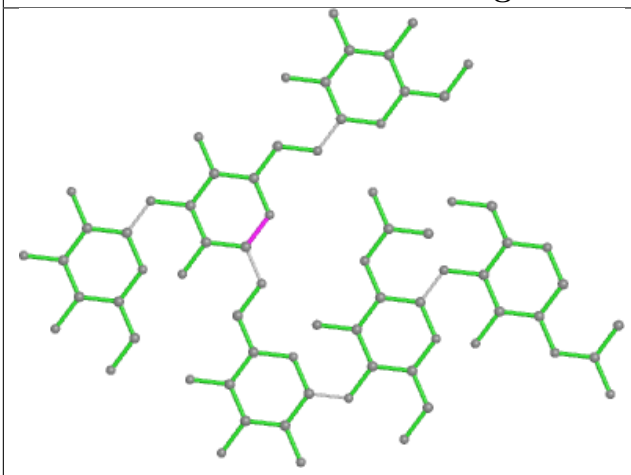


Torsions

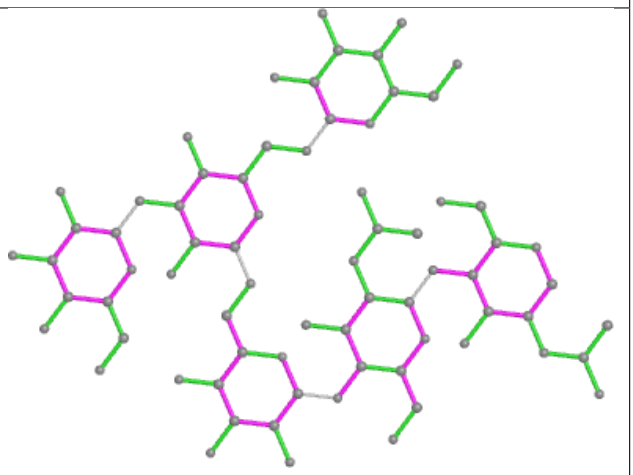


Rings

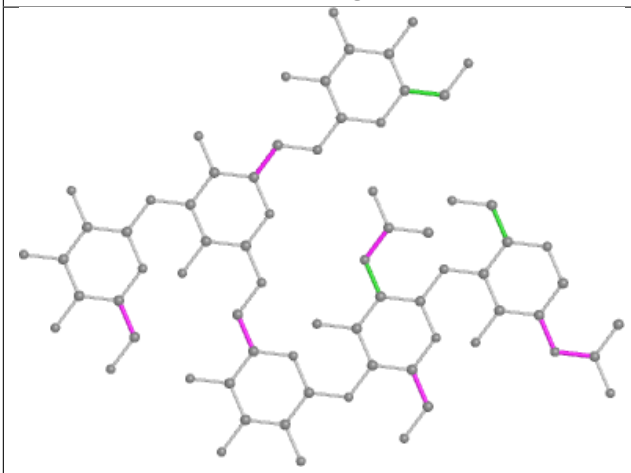
Oligosaccharide Chain V



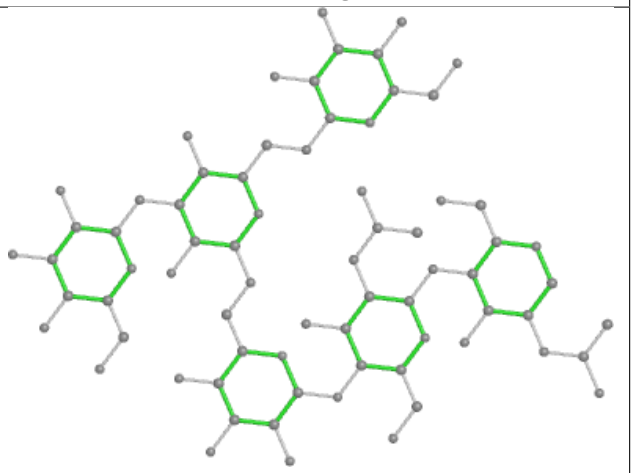
Bond lengths



Bond angles

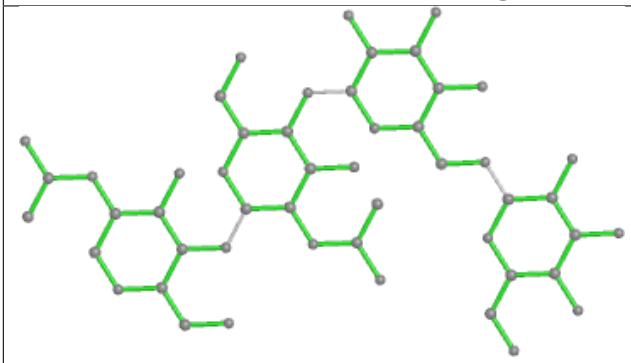


Torsions

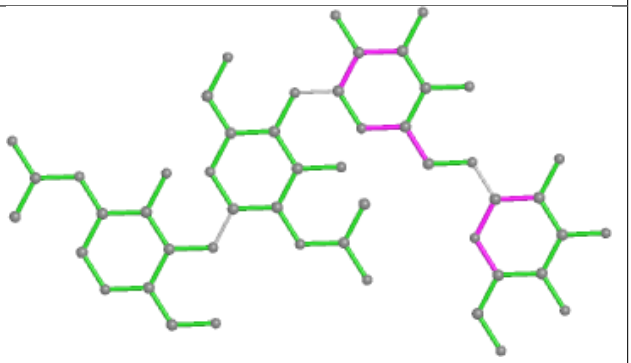


Rings

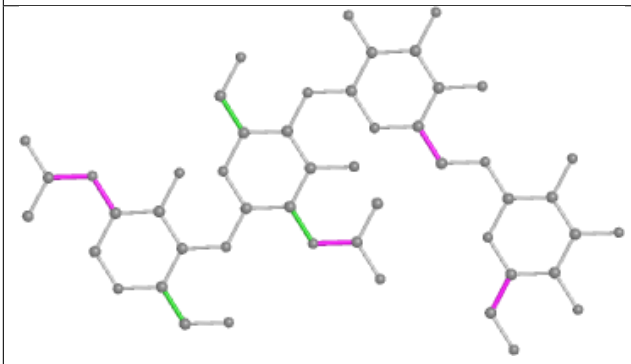
Oligosaccharide Chain X



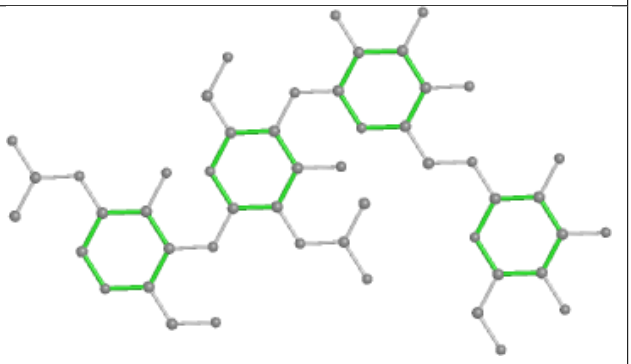
Bond lengths



Bond angles

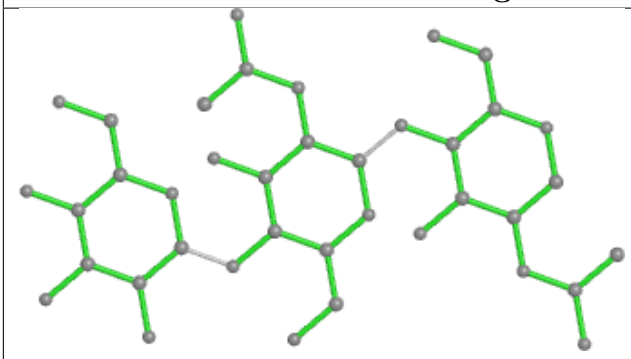


Torsions

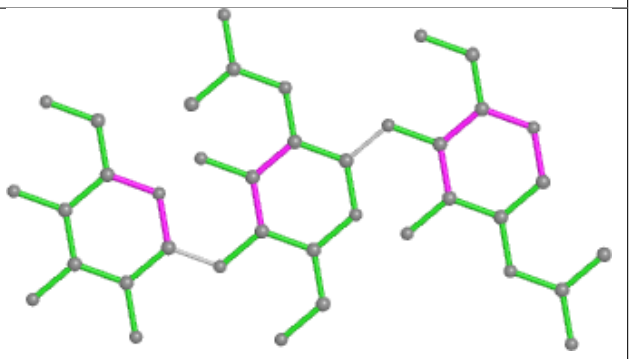


Rings

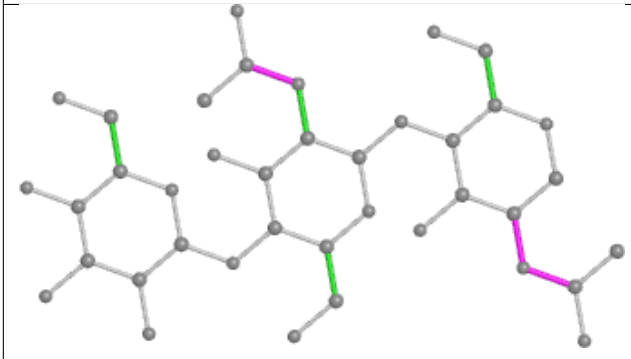
Oligosaccharide Chain Y



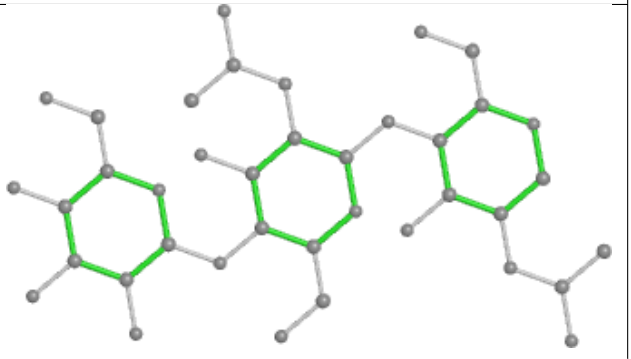
Bond lengths



Bond angles

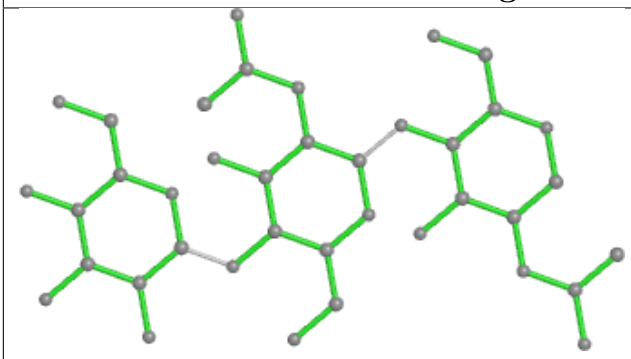


Torsions

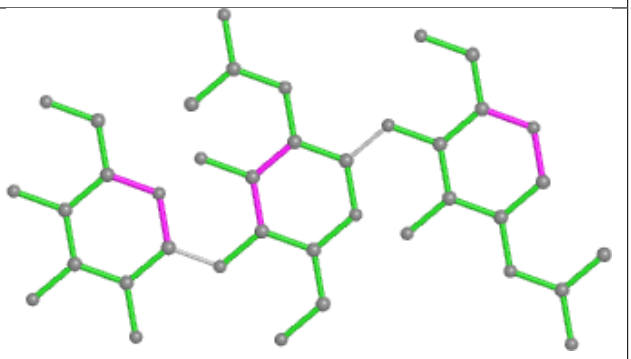


Rings

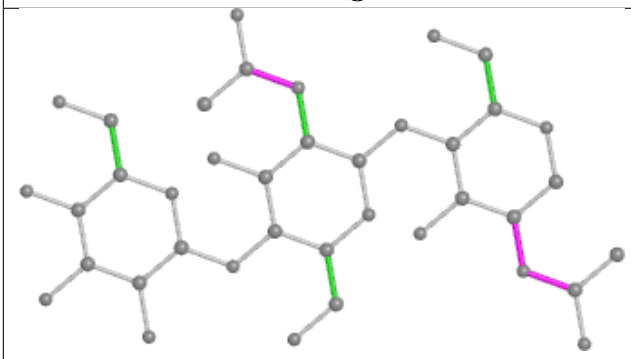
Oligosaccharide Chain a



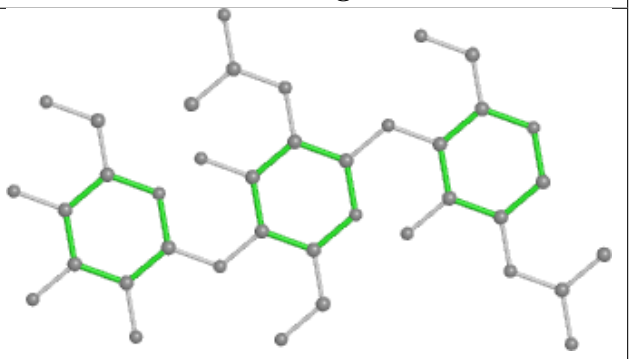
Bond lengths



Bond angles

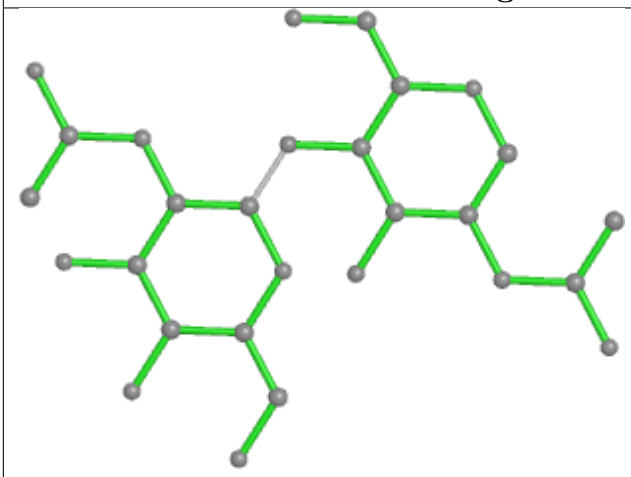


Torsions

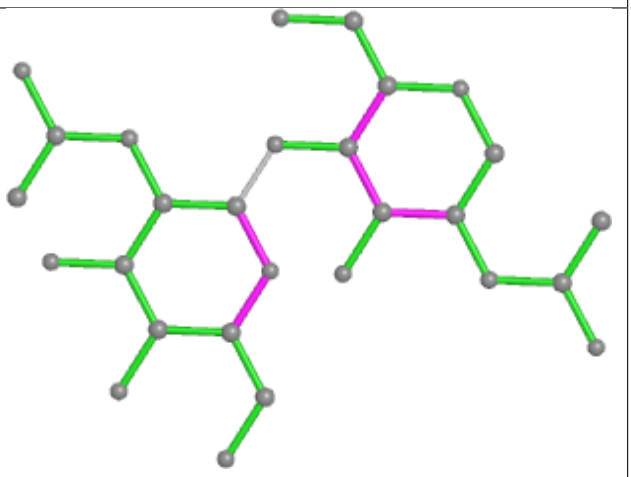


Rings

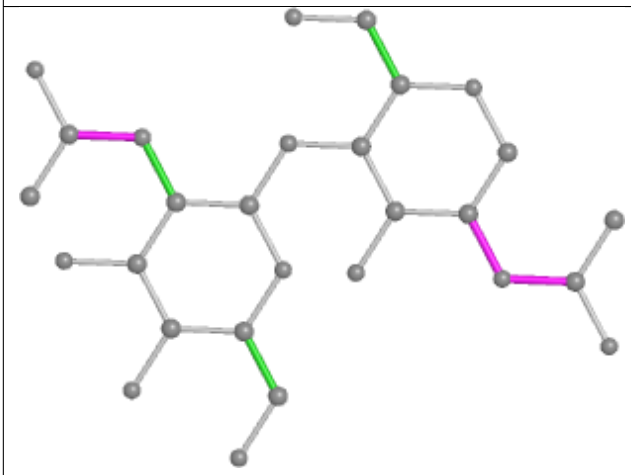
Oligosaccharide Chain Z



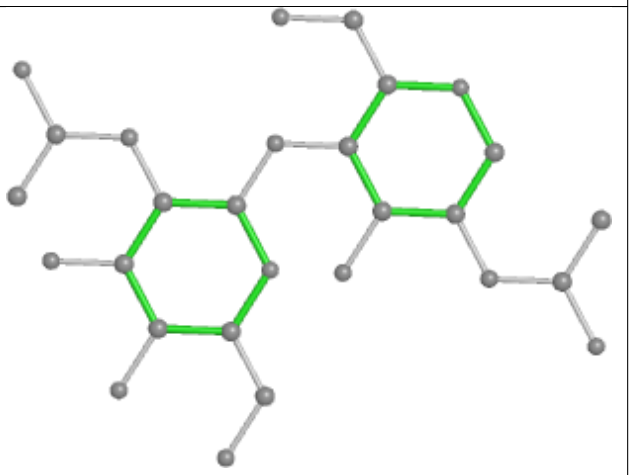
Bond lengths



Bond angles

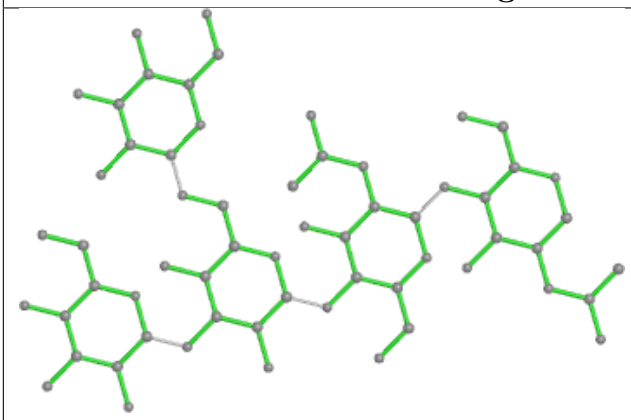


Torsions

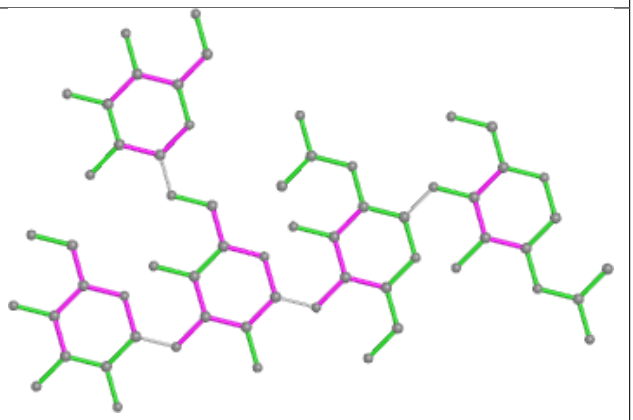


Rings

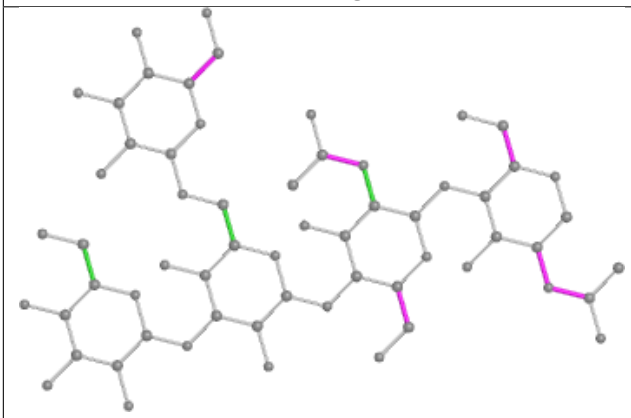
Oligosaccharide Chain b



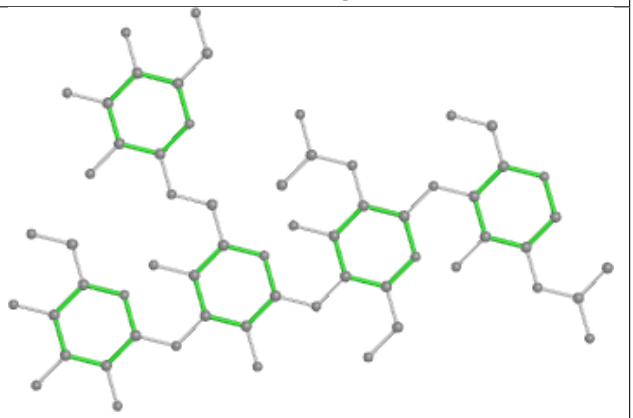
Bond lengths



Bond angles

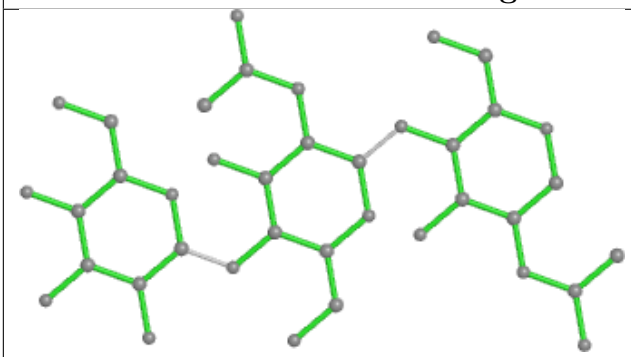


Torsions

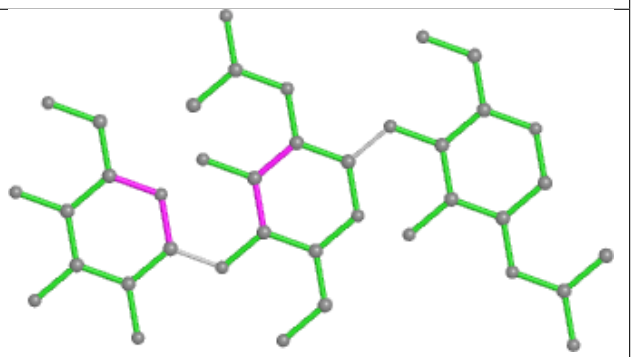


Rings

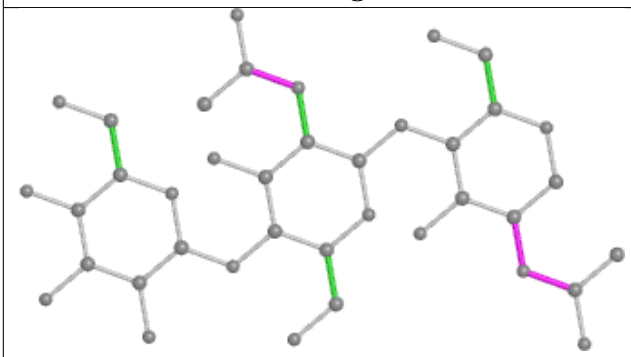
Oligosaccharide Chain c



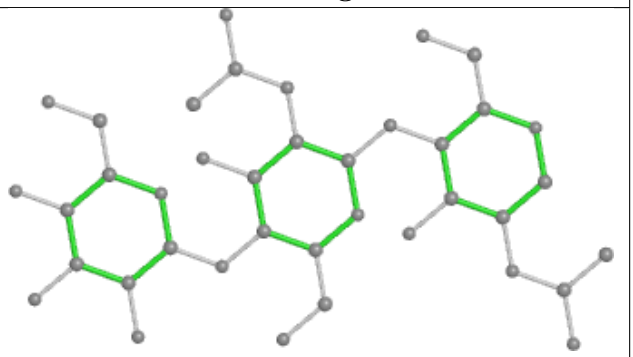
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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	$\#\|Z\| > 2$
14	MAN	G	1651	-	11,11,12	0.83	1 (9%)	15,15,17	1.71	4 (26%)
16	NAG	K	1749	3	14,14,15	0.52	0	17,19,21	1.79	2 (11%)
13	BMA	B	2646	-	11,11,12	0.74	0	15,15,17	1.42	3 (20%)
16	NAG	L	1746	3	14,14,15	0.52	0	17,19,21	0.69	0
13	BMA	K	1747	-	11,11,12	0.81	0	15,15,17	1.93	4 (26%)

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
14	MAN	G	1651	-	-	0/2/19/22	0/1/1/1
16	NAG	K	1749	3	1/1/5/7	3/6/23/26	0/1/1/1
13	BMA	B	2646	-	-	0/2/19/22	0/1/1/1
16	NAG	L	1746	3	1/1/5/7	3/6/23/26	0/1/1/1
13	BMA	K	1747	-	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	1651	MAN	O5-C1	-2.03	1.40	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	K	1747	BMA	C1-O5-C5	-5.03	105.37	112.19
16	K	1749	NAG	O5-C1-C2	-4.75	103.78	111.29
14	G	1651	MAN	C1-C2-C3	-4.04	104.70	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	K	1749	NAG	C1-C2-N2	3.83	117.04	110.49
13	K	1747	BMA	C1-C2-C3	-3.78	105.01	109.67
13	B	2646	BMA	C1-C2-C3	-3.38	105.52	109.67
14	G	1651	MAN	O5-C1-C2	3.00	115.41	110.77
14	G	1651	MAN	C1-O5-C5	-3.00	108.12	112.19
13	K	1747	BMA	O5-C1-C2	2.67	114.90	110.77
14	G	1651	MAN	C3-C4-C5	2.65	114.96	110.24
13	B	2646	BMA	O5-C1-C2	2.63	114.83	110.77
13	B	2646	BMA	C1-O5-C5	-2.15	109.28	112.19
13	K	1747	BMA	C3-C4-C5	2.13	114.03	110.24

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	K	1749	NAG	C1
16	L	1746	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	K	1749	NAG	C8-C7-N2-C2
16	K	1749	NAG	O7-C7-N2-C2
16	L	1746	NAG	C8-C7-N2-C2
16	L	1746	NAG	O7-C7-N2-C2
16	K	1749	NAG	C1-C2-N2-C7
16	L	1746	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	1651	MAN	1	0
16	K	1749	NAG	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	1500:LYS	C	1501:SER	N	3.64
1	H	988:CYS	C	989:GLY	N	2.97

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	638/645 (98%)	0.24	11 (1%)	70	60	87, 142, 190, 237	0
1	C	638/645 (98%)	0.27	10 (1%)	72	62	80, 127, 176, 228	0
1	E	638/645 (98%)	0.28	12 (1%)	66	57	84, 142, 196, 245	0
1	G	638/645 (98%)	0.53	56 (8%)	10	7	93, 180, 241, 267	0
2	B	901/915 (98%)	0.17	12 (1%)	77	68	91, 167, 229, 260	0
2	D	901/915 (98%)	0.23	13 (1%)	75	66	81, 155, 216, 266	0
2	F	900/915 (98%)	0.40	49 (5%)	25	21	96, 179, 284, 329	0
2	H	605/915 (66%)	0.38	28 (4%)	32	26	98, 162, 231, 294	0
3	I	507/507 (100%)	0.17	4 (0%)	86	79	93, 142, 197, 240	0
3	J	507/507 (100%)	0.15	10 (1%)	65	55	127, 170, 220, 261	0
3	K	507/507 (100%)	0.20	21 (4%)	37	29	132, 183, 230, 284	0
3	L	507/507 (100%)	0.15	4 (0%)	86	79	101, 144, 194, 239	0
4	M	84/92 (91%)	0.34	2 (2%)	59	48	87, 110, 186, 221	0
4	N	84/92 (91%)	0.33	3 (3%)	42	33	97, 116, 189, 227	0
4	P	84/92 (91%)	0.23	2 (2%)	59	48	100, 124, 176, 211	0
4	Q	84/92 (91%)	0.20	1 (1%)	79	70	100, 119, 186, 200	0
All	All	8223/8636 (95%)	0.27	238 (2%)	51	40	80, 154, 228, 329	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	421	ALA	8.9
1	G	529	VAL	7.9
1	G	509	LEU	7.7
1	G	437	SER	7.0
1	C	645	ALA	6.4

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Mol	Chain	Res	Type	RSRZ
1	G	609	SER	5.5
1	G	373	ASP	5.4
1	A	645	ALA	5.2
4	M	85	TYR	4.9
1	G	400	ILE	4.8
1	G	511	ALA	4.7
1	G	608	GLY	4.7
2	F	1501	SER	4.7
2	F	1120	ALA	4.6
1	G	436	LEU	4.5
1	G	626	SER	4.5
2	F	1078	LEU	4.5
3	J	235	LYS	4.5
4	N	85	TYR	4.4
1	G	528	SER	4.4
2	H	1593	LYS	4.3
1	G	374	THR	4.3
2	F	1122	THR	4.3
1	G	510	VAL	4.3
2	F	1049	LYS	4.1
1	G	399	SER	4.1
1	G	71	ASN	4.0
1	G	339	PRO	4.0
2	H	1501	SER	3.9
2	F	1077	VAL	3.9
2	H	1547	ILE	3.9
2	F	1593	LYS	3.8
2	H	1268	GLN	3.8
1	G	514	THR	3.7
1	C	48	SER	3.7
1	G	452	ASN	3.6
2	F	1166	THR	3.6
2	F	925	LEU	3.6
2	D	1603	ASP	3.6
1	C	376	GLN	3.5
2	H	935	VAL	3.5
2	F	1169	ILE	3.5
2	H	1316	GLY	3.5
1	G	645	ALA	3.5
1	G	7	ILE	3.5
1	G	20	MET	3.5
1	G	610	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	71	ASN	3.5
3	I	366	LEU	3.4
4	P	2	THR	3.4
2	D	925	LEU	3.4
2	F	1038	ARG	3.3
3	L	267	CYS	3.3
1	G	470	TYR	3.3
2	B	1201	PRO	3.3
1	C	19	THR	3.3
1	A	20	MET	3.3
2	F	1329	LYS	3.2
1	A	22	LEU	3.2
2	F	1143	LEU	3.2
1	E	509	LEU	3.2
2	H	967	GLN	3.2
2	H	921	ALA	3.2
1	A	19	THR	3.2
2	F	1070	LEU	3.1
1	G	72	ARG	3.1
2	F	1168	ALA	3.1
1	G	471	LEU	3.1
3	K	608	VAL	3.1
1	A	48	SER	3.1
1	G	398	LEU	3.1
2	H	1308	PHE	3.1
1	G	438	VAL	3.0
3	K	479	PRO	3.0
3	K	284	TYR	3.0
1	G	494	VAL	3.0
1	G	453	PHE	3.0
3	K	324	LEU	3.0
1	G	636	ALA	3.0
2	F	1047	PHE	3.0
1	G	333	ILE	3.0
1	E	636	ALA	3.0
1	E	83	PHE	3.0
2	F	932	ARG	3.0
2	H	1317	GLN	2.9
1	A	12	LEU	2.9
2	F	1054	THR	2.9
2	H	925	LEU	2.9
1	G	435	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	1121	LEU	2.9
2	H	964	PRO	2.9
2	F	1082	VAL	2.9
2	D	1269	GLU	2.8
2	F	1119	MET	2.8
3	K	286	LEU	2.8
1	C	374	THR	2.8
2	B	1606	VAL	2.8
1	G	352	VAL	2.8
2	B	1205	LEU	2.8
3	K	527	VAL	2.8
2	H	932	ARG	2.8
1	G	507	PHE	2.7
3	K	699	VAL	2.7
2	F	1198	TRP	2.7
2	F	1116	GLU	2.7
2	F	1001	ILE	2.7
2	B	1574	LEU	2.7
4	N	84	LYS	2.7
1	E	436	LEU	2.7
1	G	99	VAL	2.7
1	G	369	VAL	2.6
2	H	1328	ALA	2.6
3	J	284	TYR	2.6
2	F	1147	ILE	2.6
2	B	925	LEU	2.6
2	D	1332	ASP	2.6
1	E	528	SER	2.6
2	F	1096	PHE	2.6
1	G	200	PHE	2.6
2	F	1547	ILE	2.6
1	C	290	GLN	2.6
3	J	510	HIS	2.6
3	J	267	CYS	2.6
2	D	1158	TYR	2.6
1	G	102	SER	2.6
3	J	738	PHE	2.6
2	B	1203	LYS	2.6
3	K	686	PHE	2.5
2	F	1136	CYS	2.5
2	B	962	GLY	2.5
2	D	1314	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	1073	ILE	2.5
3	K	503	PHE	2.5
1	G	643	PRO	2.5
2	F	1094	GLY	2.5
2	H	1323	VAL	2.5
1	G	335	PHE	2.5
1	G	376	GLN	2.5
1	E	68	ILE	2.4
3	K	705	ARG	2.4
1	G	439	LEU	2.4
2	B	912	GLU	2.4
1	C	20	MET	2.4
2	F	1594	PRO	2.4
2	H	1546	THR	2.4
2	F	960	LEU	2.4
1	G	386	LYS	2.4
3	K	528	VAL	2.4
2	F	1062	LYS	2.4
2	D	1483	LEU	2.4
1	E	101	VAL	2.4
3	K	544	ILE	2.4
2	D	1534	ASN	2.4
2	H	1594	PRO	2.4
3	K	512	ILE	2.4
3	K	398	LEU	2.3
3	J	610	GLU	2.3
2	F	967	GLN	2.3
2	H	920	VAL	2.3
2	F	1079	CYS	2.3
2	F	1460	TYR	2.3
1	A	7	ILE	2.3
2	F	1294	ALA	2.3
2	H	965	VAL	2.3
3	J	471	GLN	2.3
2	F	1298	ARG	2.3
1	G	346	MET	2.3
2	F	836	GLN	2.3
2	F	1123	ALA	2.3
3	K	514	VAL	2.3
2	B	1464	GLU	2.3
3	K	668	ASN	2.3
2	F	1295	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	1194	ASP	2.3
2	H	1598	TYR	2.2
1	G	635	ARG	2.2
2	H	1559	GLN	2.2
2	H	924	THR	2.2
1	G	526	ALA	2.2
3	L	286	LEU	2.2
2	H	1320	LEU	2.2
3	I	364	ASP	2.2
2	F	964	PRO	2.2
1	A	509	LEU	2.2
1	G	26	ASP	2.2
2	H	922	VAL	2.2
4	Q	85	TYR	2.2
3	L	693	SER	2.2
3	J	573	PRO	2.2
3	K	496	VAL	2.2
3	L	503	PHE	2.2
1	A	479	LEU	2.2
2	B	1391	PRO	2.2
2	H	1562	PHE	2.2
4	N	12	ASN	2.2
4	M	84	LYS	2.1
1	C	190	ASN	2.1
2	F	1056	LEU	2.1
2	H	1310	VAL	2.1
3	I	267	CYS	2.1
1	A	101	VAL	2.1
1	E	350	LEU	2.1
1	G	450	ASN	2.1
1	E	609	SER	2.1
1	G	340	LYS	2.1
2	F	1208	VAL	2.1
2	H	958	ILE	2.1
2	F	1596	LEU	2.1
1	G	19	THR	2.1
3	J	237	VAL	2.1
1	G	492	LEU	2.1
3	K	607	PHE	2.1
1	G	9	PRO	2.1
3	K	574	CYS	2.1
2	F	1135	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	956	THR	2.0
2	F	1046	ALA	2.0
4	P	85	TYR	2.0
3	J	699	VAL	2.0
1	E	257	GLU	2.0
3	I	503	PHE	2.0
2	D	1606	VAL	2.0
1	G	370	GLN	2.0
2	B	1493	GLU	2.0
2	H	1499	GLN	2.0
1	C	368	ALA	2.0
1	G	46	VAL	2.0
3	K	248	LEU	2.0
2	D	1510	ARG	2.0
1	E	84	VAL	2.0
2	D	1082	VAL	2.0
2	D	1085	LEU	2.0
3	K	697	VAL	2.0
1	A	548	SER	2.0
2	F	1502	ASP	2.0
1	C	509	LEU	2.0
1	G	434	LEU	2.0
2	D	932	ARG	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)

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
5	BMA	R	4	11/12	0.29	0.30	237,239,240,241	0
5	BMA	R	3	11/12	0.56	0.23	218,220,222,223	0
6	BMA	S	4	11/12	0.58	0.21	235,237,239,240	0
6	BMA	W	5	11/12	0.62	0.41	229,231,232,232	0
7	BMA	V	6	11/12	0.66	0.39	214,215,217,217	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MAN	X	4	11/12	0.67	0.37	234,236,237,238	0
10	NAG	Z	2	14/15	0.70	0.37	222,223,224,224	0
6	BMA	S	3	11/12	0.72	0.19	219,220,222,223	0
9	MAN	a	3	11/12	0.73	0.21	206,210,211,212	0
9	MAN	Y	3	11/12	0.73	0.28	205,207,208,209	0
6	BMA	W	3	11/12	0.74	0.32	247,249,250,251	0
7	BMA	V	4	11/12	0.75	0.17	248,249,249,250	0
11	MAN	b	3	11/12	0.75	0.16	249,252,253,254	0
12	BMA	c	3	11/12	0.75	0.21	197,201,202,202	0
6	BMA	W	4	11/12	0.76	0.18	226,228,229,230	0
7	BMA	V	5	11/12	0.76	0.23	221,222,224,224	0
6	BMA	S	5	11/12	0.76	0.23	231,233,235,235	0
5	BMA	T	3	11/12	0.77	0.19	220,221,223,223	0
6	NAG	S	1	14/15	0.79	0.28	163,191,192,193	0
6	NAG	S	2	14/15	0.80	0.21	200,202,203,203	0
10	NAG	Z	1	14/15	0.81	0.33	198,225,227,227	0
5	BMA	U	4	11/12	0.81	0.17	209,212,214,215	0
7	BMA	V	3	11/12	0.83	0.18	232,233,234,234	0
5	NAG	O	2	14/15	0.84	0.19	199,200,201,203	0
5	NAG	U	1	14/15	0.84	0.17	174,204,206,206	0
8	MAN	X	3	11/12	0.84	0.19	229,230,231,232	0
6	NAG	W	1	14/15	0.84	0.14	198,201,208,215	0
11	MAN	b	4	11/12	0.84	0.22	230,232,235,235	0
5	BMA	O	3	11/12	0.84	0.17	212,214,215,216	0
11	NAG	b	2	14/15	0.85	0.16	196,199,201,202	0
9	NAG	a	2	14/15	0.85	0.18	177,179,180,180	0
5	BMA	T	4	11/12	0.85	0.13	229,232,233,234	0
11	MAN	b	5	11/12	0.85	0.25	229,230,232,232	0
11	NAG	b	1	14/15	0.85	0.19	174,204,206,207	0
5	BMA	U	3	11/12	0.86	0.19	229,230,231,232	0
8	NAG	X	2	14/15	0.86	0.17	221,222,224,225	0
12	NAG	c	2	14/15	0.86	0.26	185,187,189,189	0
5	NAG	O	1	14/15	0.86	0.24	156,185,187,188	0
7	NAG	V	1	14/15	0.87	0.24	169,193,194,194	0
5	BMA	O	4	11/12	0.87	0.24	226,227,228,228	0
5	NAG	R	1	14/15	0.88	0.23	163,194,194,195	0
9	NAG	a	1	14/15	0.89	0.21	158,188,189,189	0
12	NAG	c	1	14/15	0.89	0.27	122,147,148,148	0
5	NAG	T	1	14/15	0.89	0.23	147,176,178,179	0
5	NAG	U	2	14/15	0.89	0.17	223,225,227,227	0
7	NAG	V	2	14/15	0.90	0.14	200,202,204,204	0
6	NAG	W	2	14/15	0.90	0.12	213,216,216,217	0

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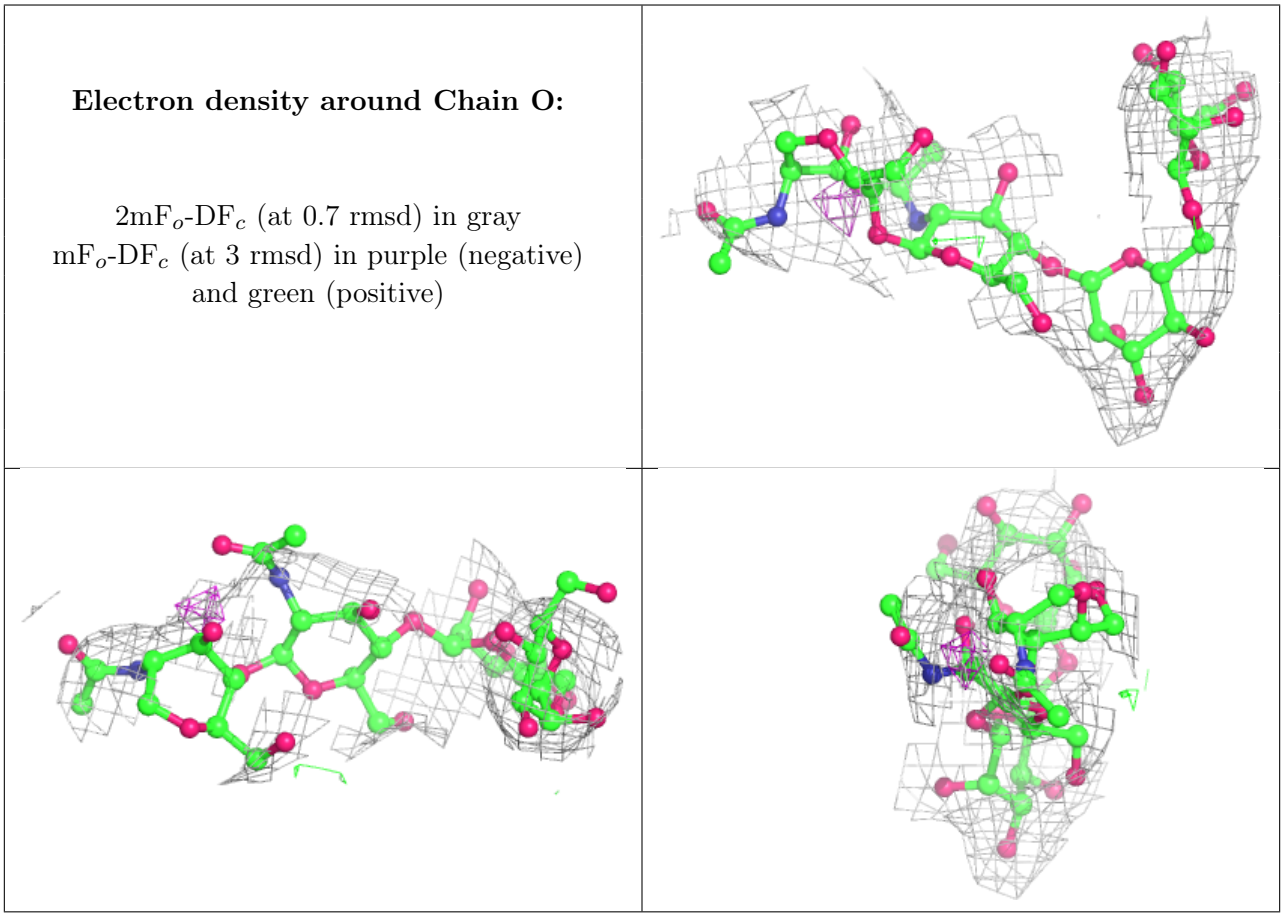
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	T	2	14/15	0.91	0.17	200,201,202,203	0
5	NAG	R	2	14/15	0.91	0.14	193,196,196,197	0
8	NAG	X	1	14/15	0.92	0.17	183,213,214,215	0
9	NAG	Y	1	14/15	0.93	0.26	122,149,151,152	0
9	NAG	Y	2	14/15	0.93	0.21	178,180,181,182	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

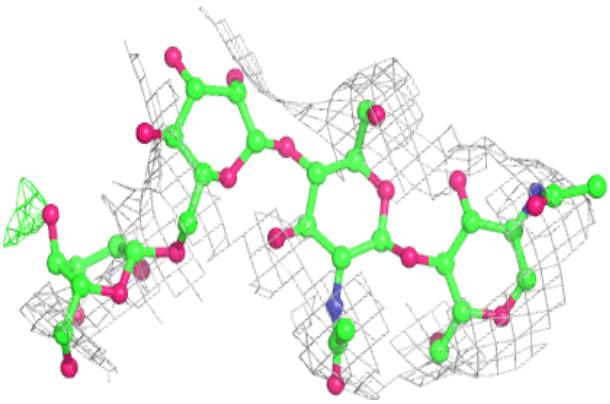
Electron density around Chain O:

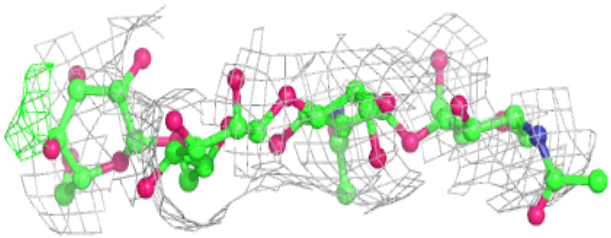
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

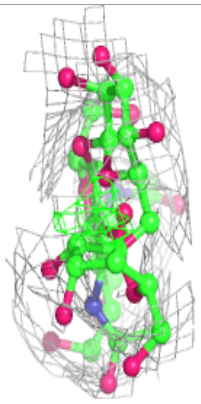


Electron density around Chain R:

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

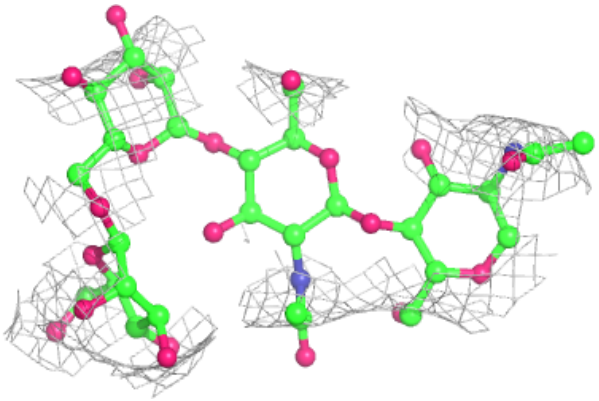


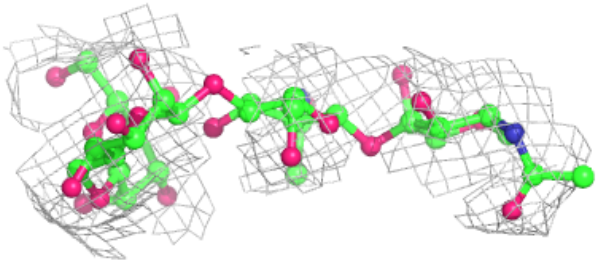


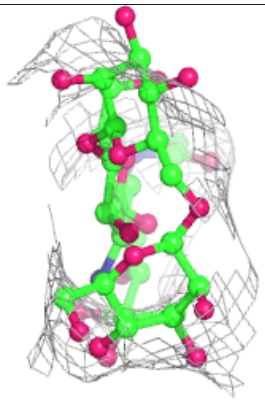


Electron density around Chain T:

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

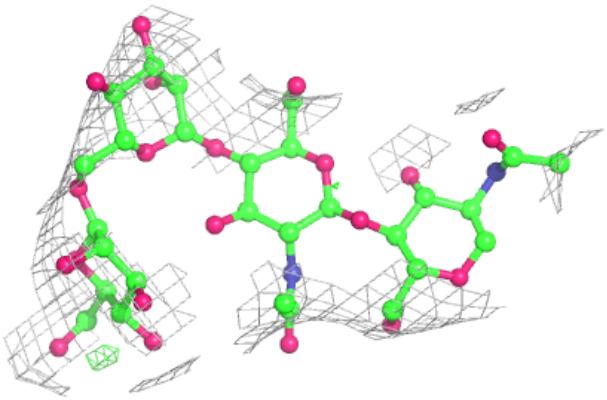


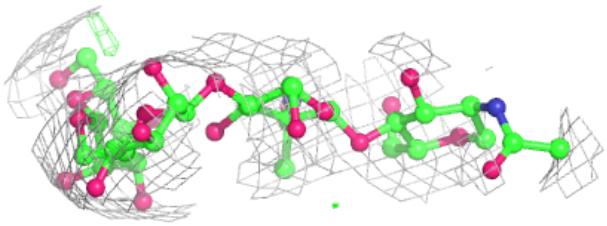


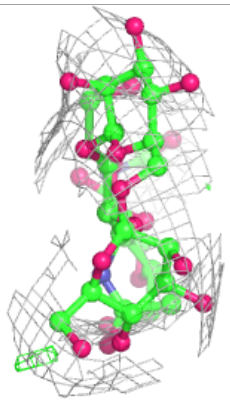


Electron density around Chain U:

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

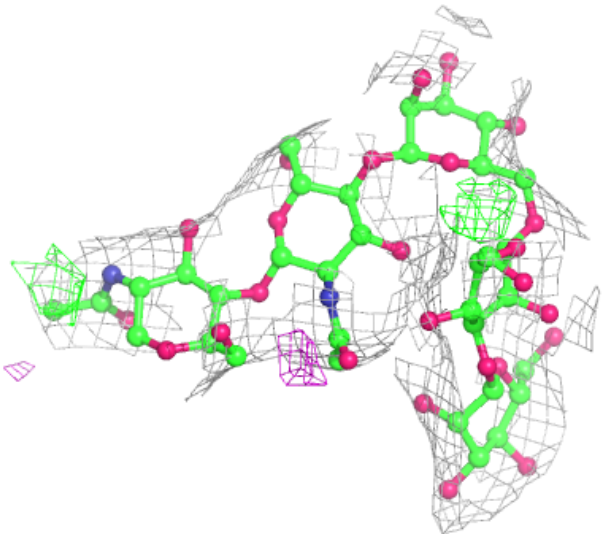


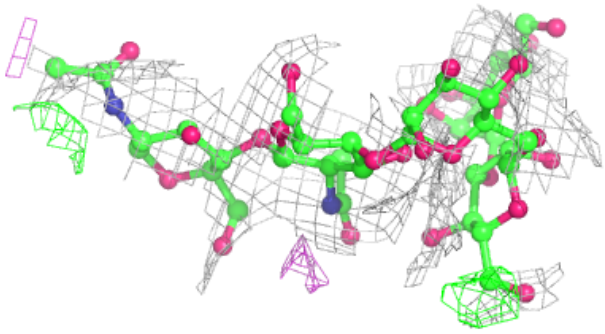


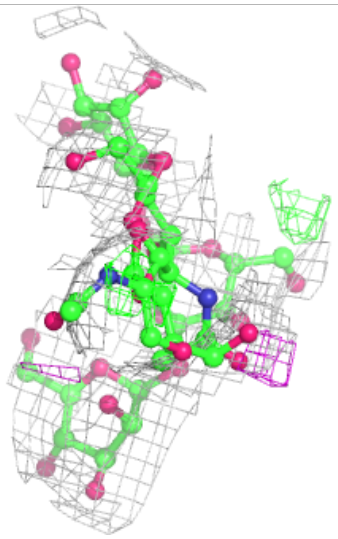


Electron density around Chain S:

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

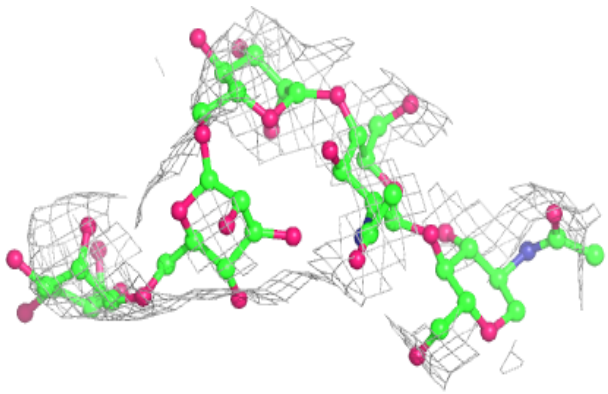


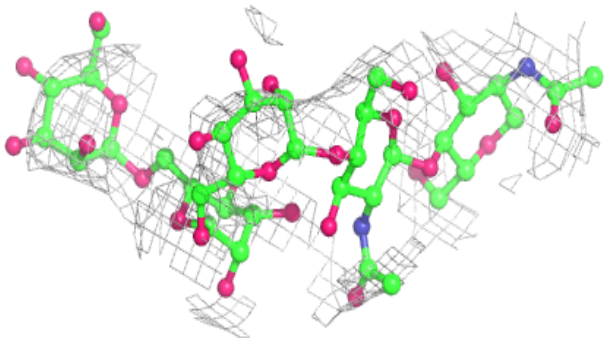


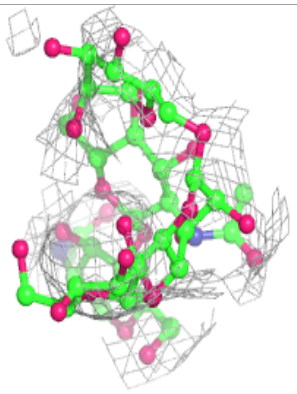


Electron density around Chain W:

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

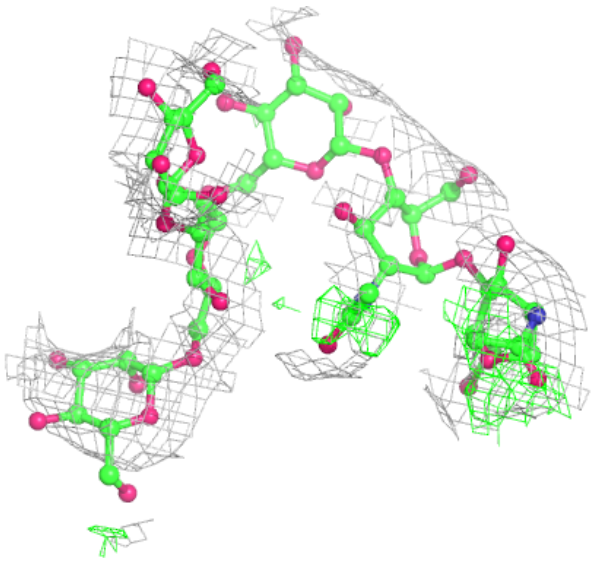


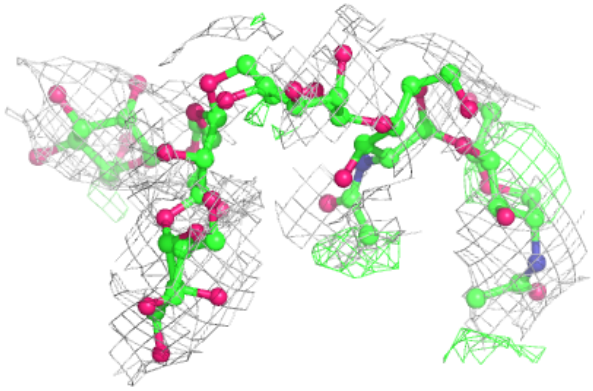


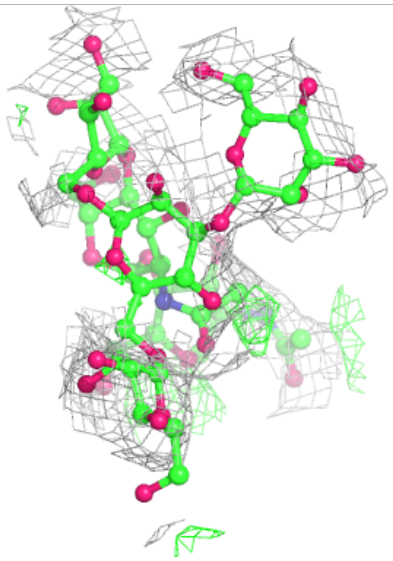


Electron density around Chain V:

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

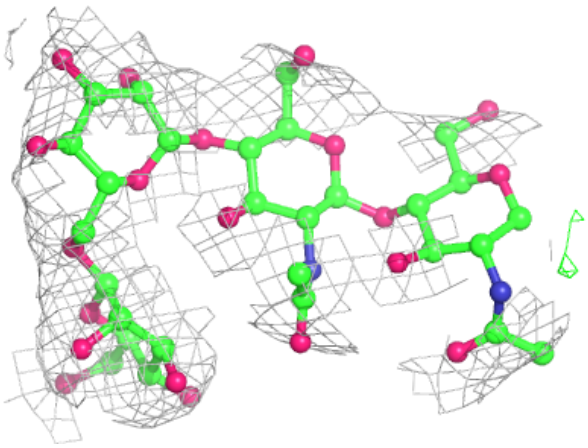


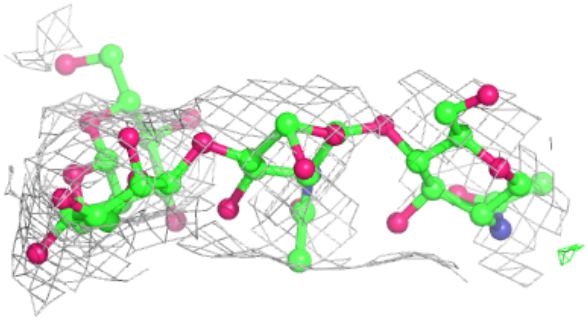


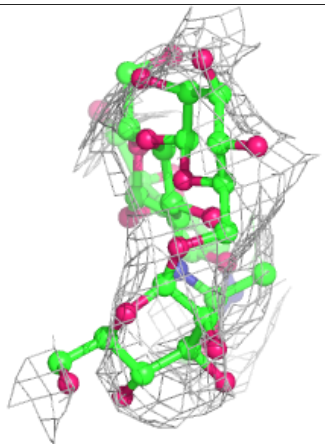


Electron density around Chain X:

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

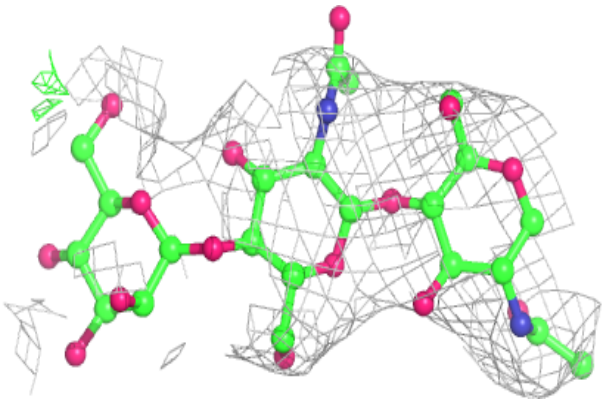


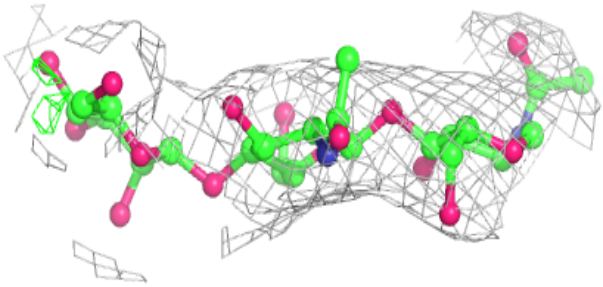


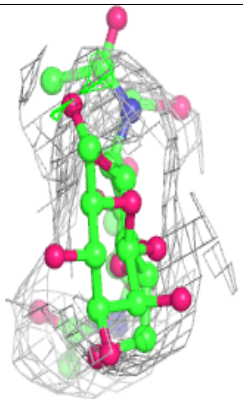


Electron density around Chain Y:

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

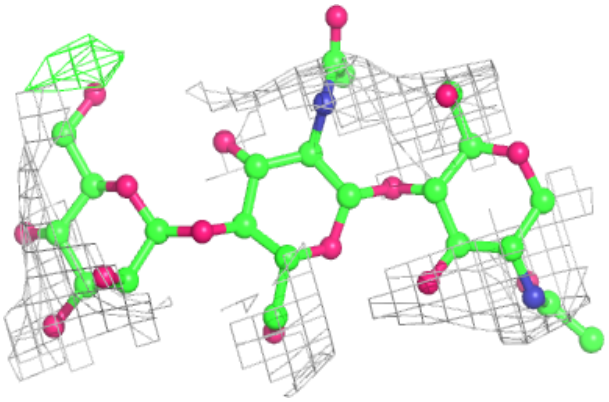


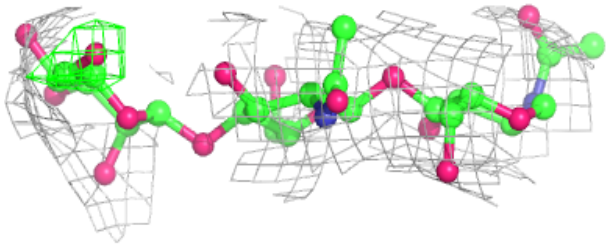


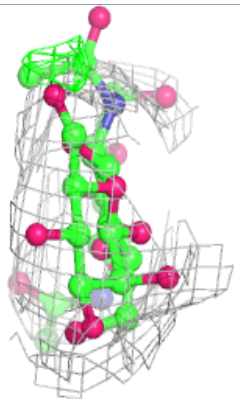


Electron density around Chain a:

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

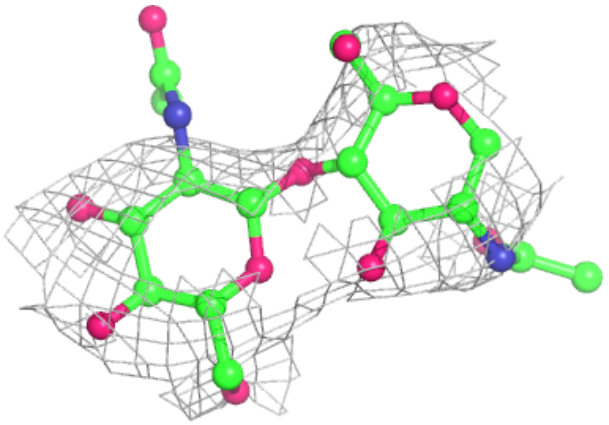


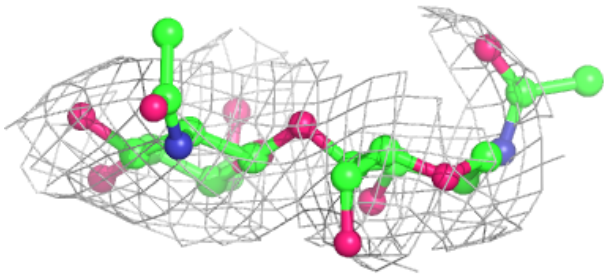


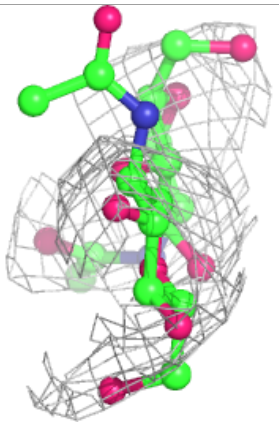


Electron density around Chain Z:

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

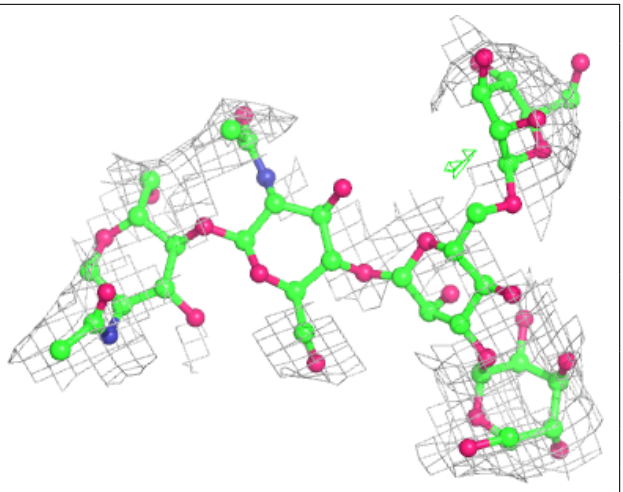


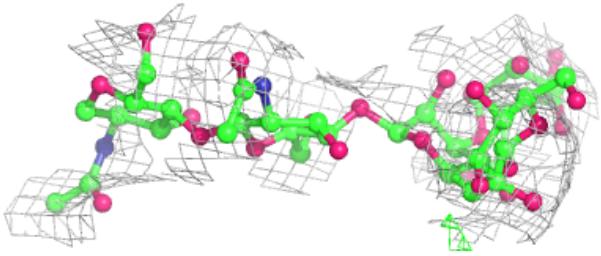


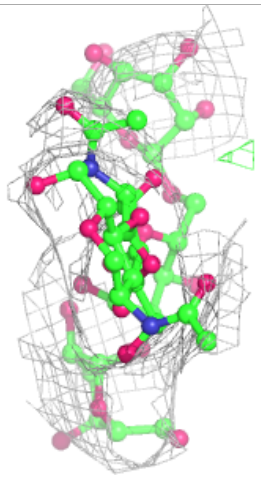


Electron density around Chain b:

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

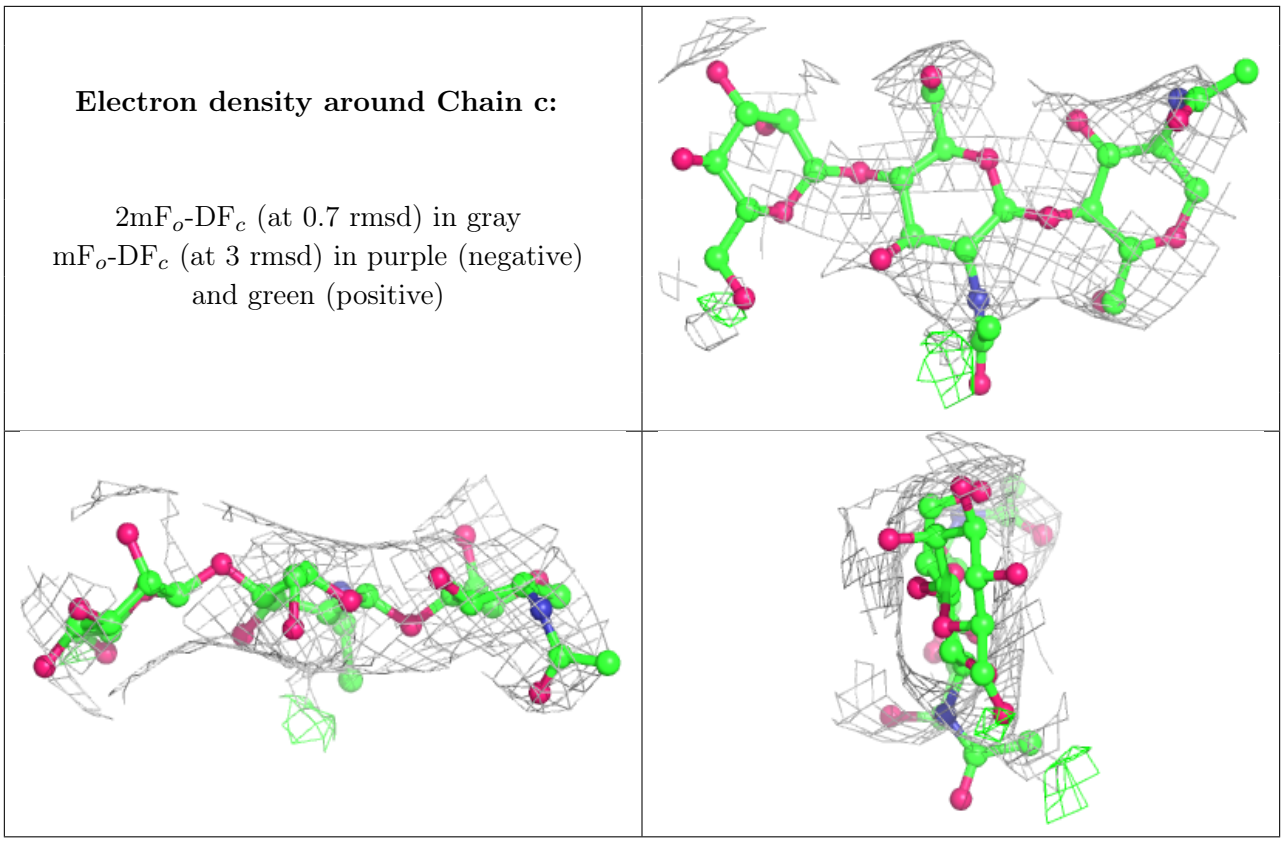






Electron density around Chain c:

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



6.4 Ligands

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
14	MAN	G	1651	11/12	0.55	0.25	222,225,227,228	0
13	BMA	B	2646	11/12	0.65	0.29	198,200,200,201	0
15	MG	I	1742	1/1	0.71	0.20	120,120,120,120	0
16	NAG	K	1749	14/15	0.78	0.24	184,214,216,217	0
13	BMA	K	1747	11/12	0.79	0.35	194,195,196,196	0
15	MG	J	1742	1/1	0.80	0.14	148,148,148,148	0
15	MG	K	1742	1/1	0.87	0.14	138,138,138,138	0
16	NAG	L	1746	14/15	0.88	0.26	176,204,205,205	0
15	MG	L	1742	1/1	0.93	0.24	127,127,127,127	0

6.5 Other polymers

There are no such residues in this entry.