Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 07:22 AM EDT

PDB ID	:	3MV3
Title	:	Crystal Structure of a-COP in Complex with e-COP
Authors	:	Hoelz, A.; Hsia, K.C.
Deposited on	:	2010-05-03
Resolution	:	3.25 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:

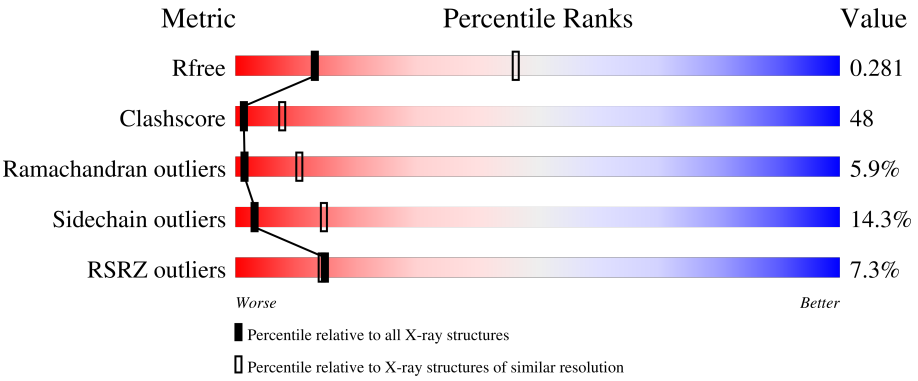
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	325	30% 54% 8% • 7%
1	C	325	31% 53% 8% • 7%
1	E	325	21% 32% 53% 8% • 7%
2	B	310	36% 44% 14% • 5%
2	D	310	34% 45% 14% • 5%

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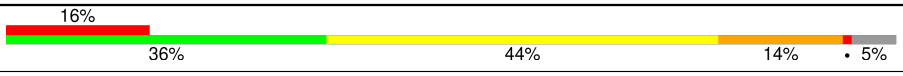
Mol	Chain	Length	Quality of chain
2	F	310	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14256 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 Coatomer subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	Se	0	0	0
			2388	1531	399	447	4	7			
1	C	303	Total	C	N	O	S	Se	0	0	0
			2388	1531	399	447	4	7			
1	E	303	Total	C	N	O	S	Se	0	0	0
			2388	1531	399	447	4	7			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MSE	-	EXPRESSION TAG	UNP P53622
A	-21	GLY	-	EXPRESSION TAG	UNP P53622
A	-20	SER	-	EXPRESSION TAG	UNP P53622
A	-19	SER	-	EXPRESSION TAG	UNP P53622
A	-18	HIS	-	EXPRESSION TAG	UNP P53622
A	-17	HIS	-	EXPRESSION TAG	UNP P53622
A	-16	HIS	-	EXPRESSION TAG	UNP P53622
A	-15	HIS	-	EXPRESSION TAG	UNP P53622
A	-14	HIS	-	EXPRESSION TAG	UNP P53622
A	-13	HIS	-	EXPRESSION TAG	UNP P53622
A	-12	SER	-	EXPRESSION TAG	UNP P53622
A	-11	SER	-	EXPRESSION TAG	UNP P53622
A	-10	GLY	-	EXPRESSION TAG	UNP P53622
A	-9	LEU	-	EXPRESSION TAG	UNP P53622
A	-8	GLU	-	EXPRESSION TAG	UNP P53622
A	-7	VAL	-	EXPRESSION TAG	UNP P53622
A	-6	LEU	-	EXPRESSION TAG	UNP P53622
A	-5	PHE	-	EXPRESSION TAG	UNP P53622
A	-4	GLN	-	EXPRESSION TAG	UNP P53622
A	-3	GLY	-	EXPRESSION TAG	UNP P53622
A	-2	PRO	-	EXPRESSION TAG	UNP P53622
A	-1	HIS	-	EXPRESSION TAG	UNP P53622
A	0	MSE	-	EXPRESSION TAG	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	MSE	-	EXPRESSION TAG	UNP P53622
C	-21	GLY	-	EXPRESSION TAG	UNP P53622
C	-20	SER	-	EXPRESSION TAG	UNP P53622
C	-19	SER	-	EXPRESSION TAG	UNP P53622
C	-18	HIS	-	EXPRESSION TAG	UNP P53622
C	-17	HIS	-	EXPRESSION TAG	UNP P53622
C	-16	HIS	-	EXPRESSION TAG	UNP P53622
C	-15	HIS	-	EXPRESSION TAG	UNP P53622
C	-14	HIS	-	EXPRESSION TAG	UNP P53622
C	-13	HIS	-	EXPRESSION TAG	UNP P53622
C	-12	SER	-	EXPRESSION TAG	UNP P53622
C	-11	SER	-	EXPRESSION TAG	UNP P53622
C	-10	GLY	-	EXPRESSION TAG	UNP P53622
C	-9	LEU	-	EXPRESSION TAG	UNP P53622
C	-8	GLU	-	EXPRESSION TAG	UNP P53622
C	-7	VAL	-	EXPRESSION TAG	UNP P53622
C	-6	LEU	-	EXPRESSION TAG	UNP P53622
C	-5	PHE	-	EXPRESSION TAG	UNP P53622
C	-4	GLN	-	EXPRESSION TAG	UNP P53622
C	-3	GLY	-	EXPRESSION TAG	UNP P53622
C	-2	PRO	-	EXPRESSION TAG	UNP P53622
C	-1	HIS	-	EXPRESSION TAG	UNP P53622
C	0	MSE	-	EXPRESSION TAG	UNP P53622
E	-22	MSE	-	EXPRESSION TAG	UNP P53622
E	-21	GLY	-	EXPRESSION TAG	UNP P53622
E	-20	SER	-	EXPRESSION TAG	UNP P53622
E	-19	SER	-	EXPRESSION TAG	UNP P53622
E	-18	HIS	-	EXPRESSION TAG	UNP P53622
E	-17	HIS	-	EXPRESSION TAG	UNP P53622
E	-16	HIS	-	EXPRESSION TAG	UNP P53622
E	-15	HIS	-	EXPRESSION TAG	UNP P53622
E	-14	HIS	-	EXPRESSION TAG	UNP P53622
E	-13	HIS	-	EXPRESSION TAG	UNP P53622
E	-12	SER	-	EXPRESSION TAG	UNP P53622
E	-11	SER	-	EXPRESSION TAG	UNP P53622
E	-10	GLY	-	EXPRESSION TAG	UNP P53622
E	-9	LEU	-	EXPRESSION TAG	UNP P53622
E	-8	GLU	-	EXPRESSION TAG	UNP P53622
E	-7	VAL	-	EXPRESSION TAG	UNP P53622
E	-6	LEU	-	EXPRESSION TAG	UNP P53622
E	-5	PHE	-	EXPRESSION TAG	UNP P53622
E	-4	GLN	-	EXPRESSION TAG	UNP P53622

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	EXPRESSION TAG	UNP P53622
E	-2	PRO	-	EXPRESSION TAG	UNP P53622
E	-1	HIS	-	EXPRESSION TAG	UNP P53622
E	0	MSE	-	EXPRESSION TAG	UNP P53622

- Molecule 2 is a protein called Coatomer subunit epsilon.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	293	Total	C	N	O	S	Se	0	0	0
			2364	1508	371	480	2	3			
2	D	293	Total	C	N	O	S	Se	0	0	0
			2364	1508	371	480	2	3			
2	F	293	Total	C	N	O	S	Se	0	0	0
			2364	1508	371	480	2	3			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MSE	-	EXPRESSION TAG	UNP P40509
B	-12	GLY	-	EXPRESSION TAG	UNP P40509
B	-11	SER	-	EXPRESSION TAG	UNP P40509
B	-10	SER	-	EXPRESSION TAG	UNP P40509
B	-9	HIS	-	EXPRESSION TAG	UNP P40509
B	-8	HIS	-	EXPRESSION TAG	UNP P40509
B	-7	HIS	-	EXPRESSION TAG	UNP P40509
B	-6	HIS	-	EXPRESSION TAG	UNP P40509
B	-5	HIS	-	EXPRESSION TAG	UNP P40509
B	-4	HIS	-	EXPRESSION TAG	UNP P40509
B	-3	SER	-	EXPRESSION TAG	UNP P40509
B	-2	GLN	-	EXPRESSION TAG	UNP P40509
B	-1	ASP	-	EXPRESSION TAG	UNP P40509
B	0	PRO	-	EXPRESSION TAG	UNP P40509
D	-13	MSE	-	EXPRESSION TAG	UNP P40509
D	-12	GLY	-	EXPRESSION TAG	UNP P40509
D	-11	SER	-	EXPRESSION TAG	UNP P40509
D	-10	SER	-	EXPRESSION TAG	UNP P40509
D	-9	HIS	-	EXPRESSION TAG	UNP P40509
D	-8	HIS	-	EXPRESSION TAG	UNP P40509
D	-7	HIS	-	EXPRESSION TAG	UNP P40509
D	-6	HIS	-	EXPRESSION TAG	UNP P40509
D	-5	HIS	-	EXPRESSION TAG	UNP P40509
D	-4	HIS	-	EXPRESSION TAG	UNP P40509

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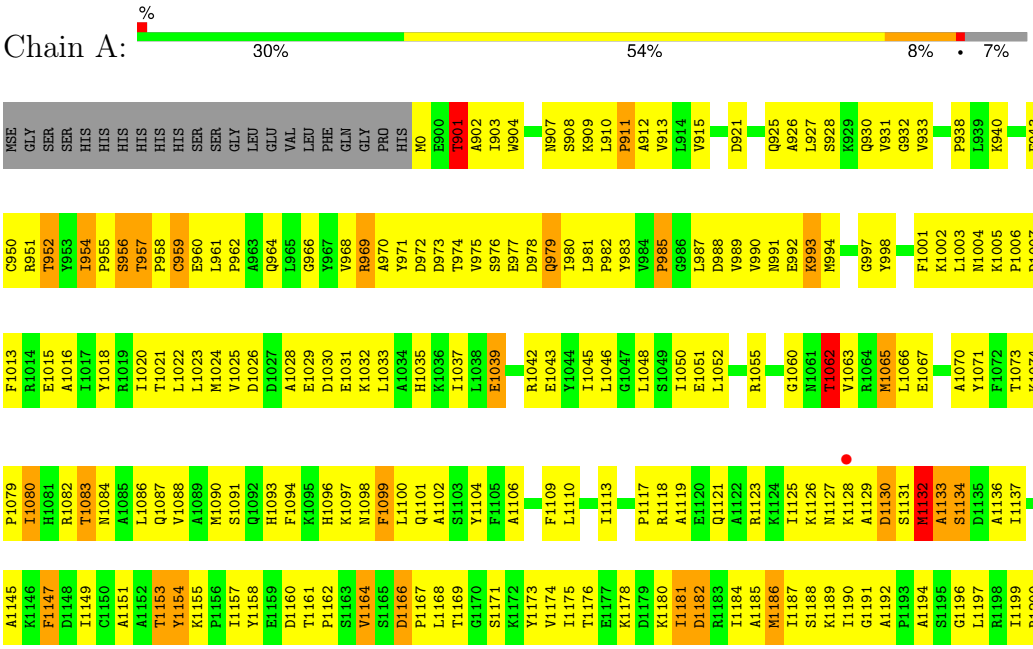
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	SER	-	EXPRESSION TAG	UNP P40509
D	-2	GLN	-	EXPRESSION TAG	UNP P40509
D	-1	ASP	-	EXPRESSION TAG	UNP P40509
D	0	PRO	-	EXPRESSION TAG	UNP P40509
F	-13	MSE	-	EXPRESSION TAG	UNP P40509
F	-12	GLY	-	EXPRESSION TAG	UNP P40509
F	-11	SER	-	EXPRESSION TAG	UNP P40509
F	-10	SER	-	EXPRESSION TAG	UNP P40509
F	-9	HIS	-	EXPRESSION TAG	UNP P40509
F	-8	HIS	-	EXPRESSION TAG	UNP P40509
F	-7	HIS	-	EXPRESSION TAG	UNP P40509
F	-6	HIS	-	EXPRESSION TAG	UNP P40509
F	-5	HIS	-	EXPRESSION TAG	UNP P40509
F	-4	HIS	-	EXPRESSION TAG	UNP P40509
F	-3	SER	-	EXPRESSION TAG	UNP P40509
F	-2	GLN	-	EXPRESSION TAG	UNP P40509
F	-1	ASP	-	EXPRESSION TAG	UNP P40509
F	0	PRO	-	EXPRESSION TAG	UNP P40509

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.

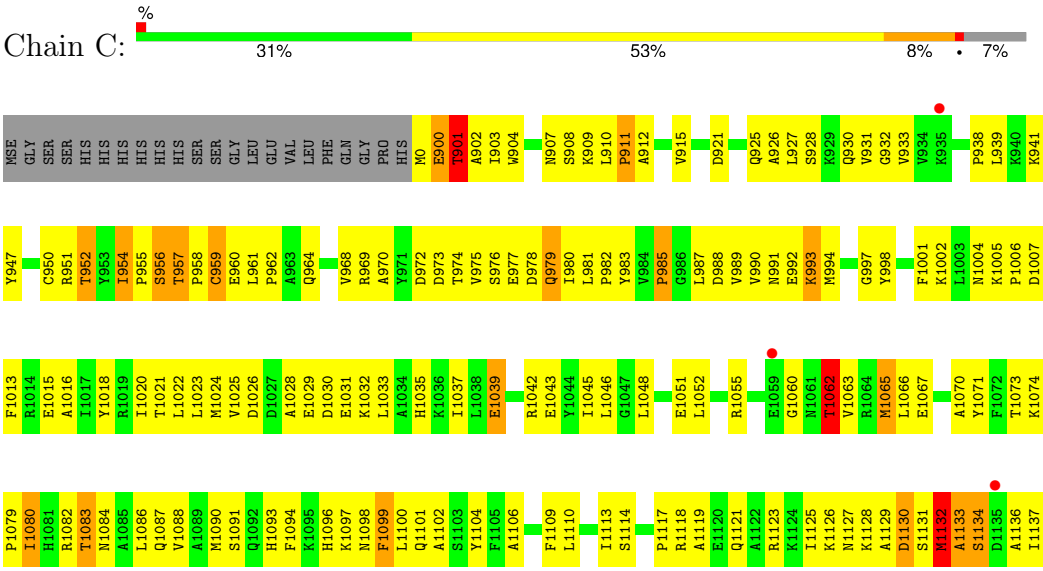
• Molecule 1: Coatomer subunit alpha

Chain A:



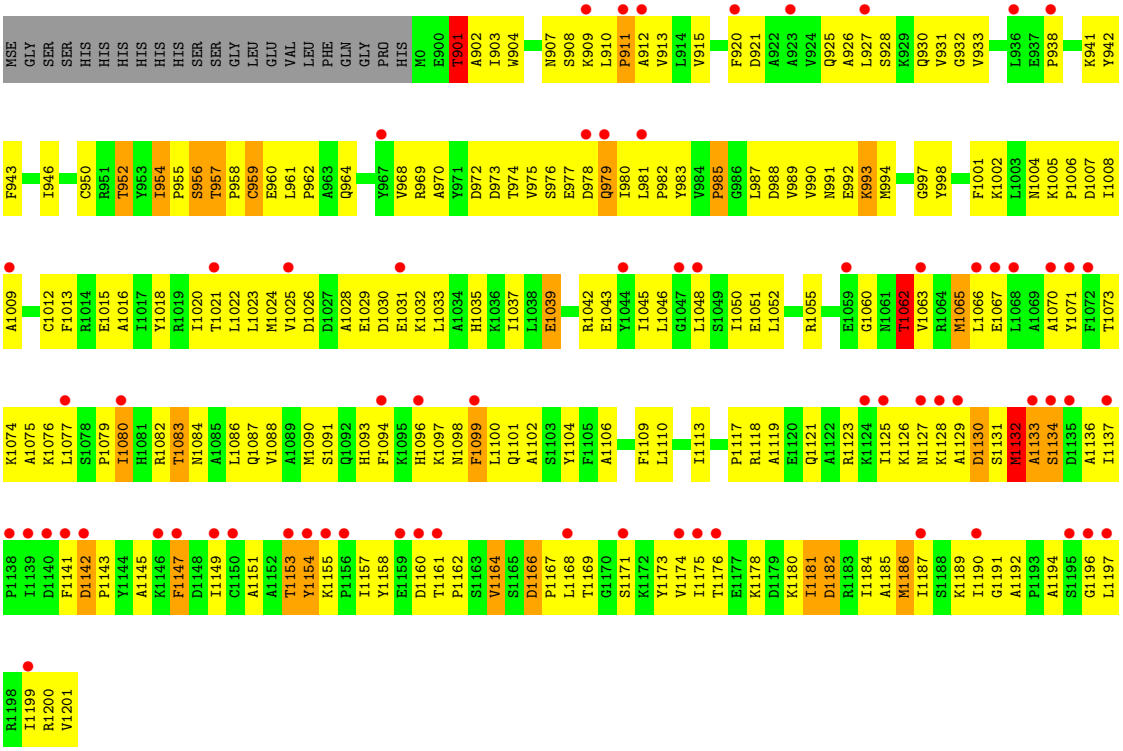
• Molecule 1: Coatomer subunit alpha

Chain C:



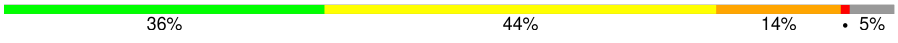
• Molecule 1: Coatomer subunit alpha

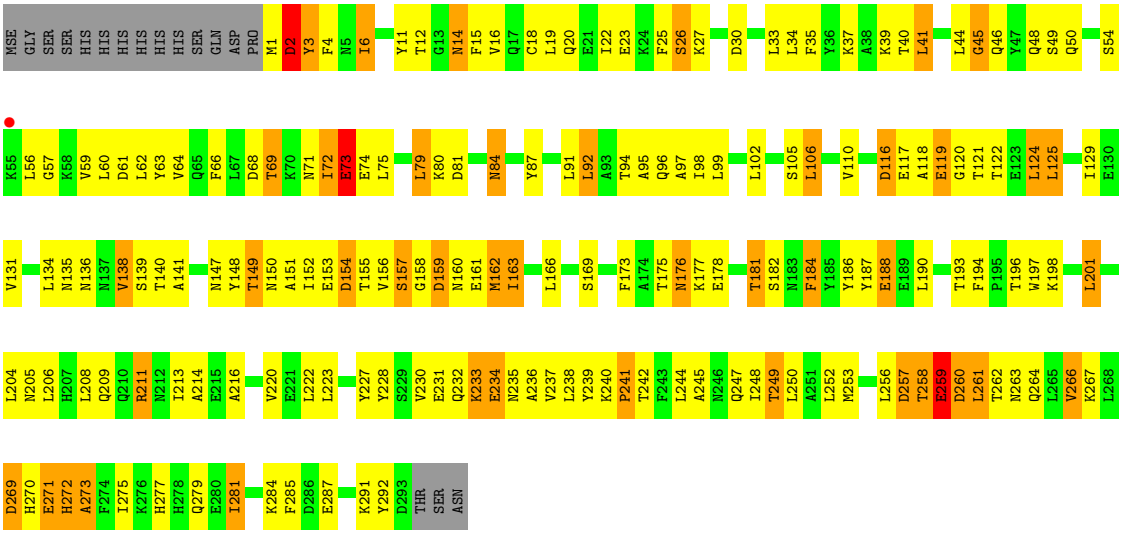
Chain E:



• Molecule 2: Coatomer subunit epsilon

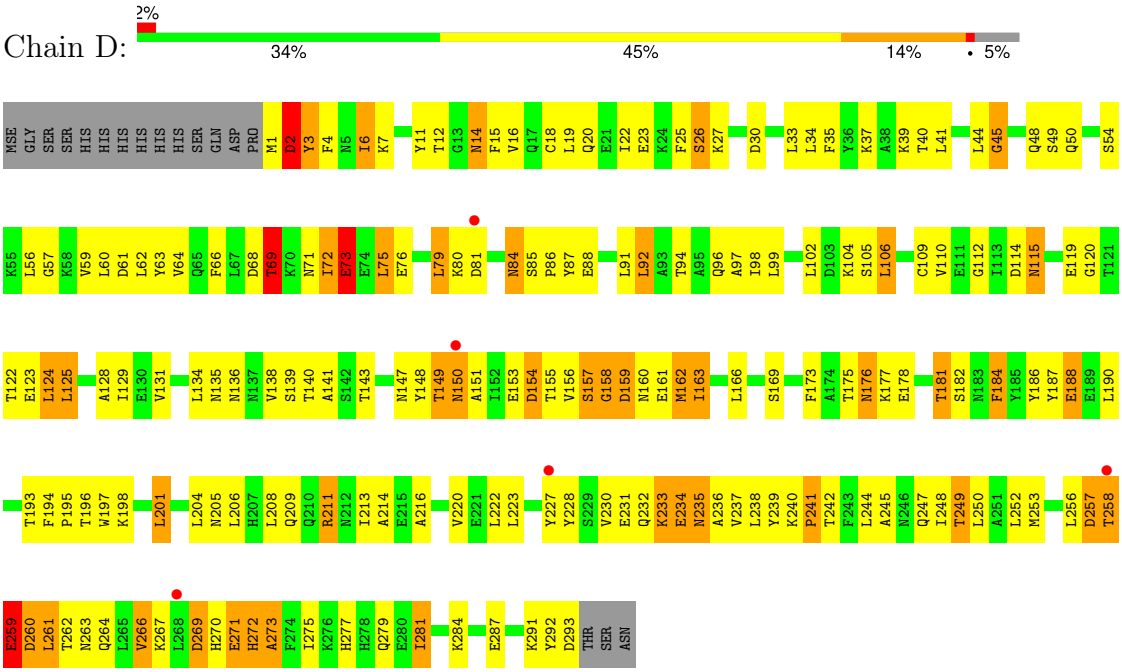
Chain B:





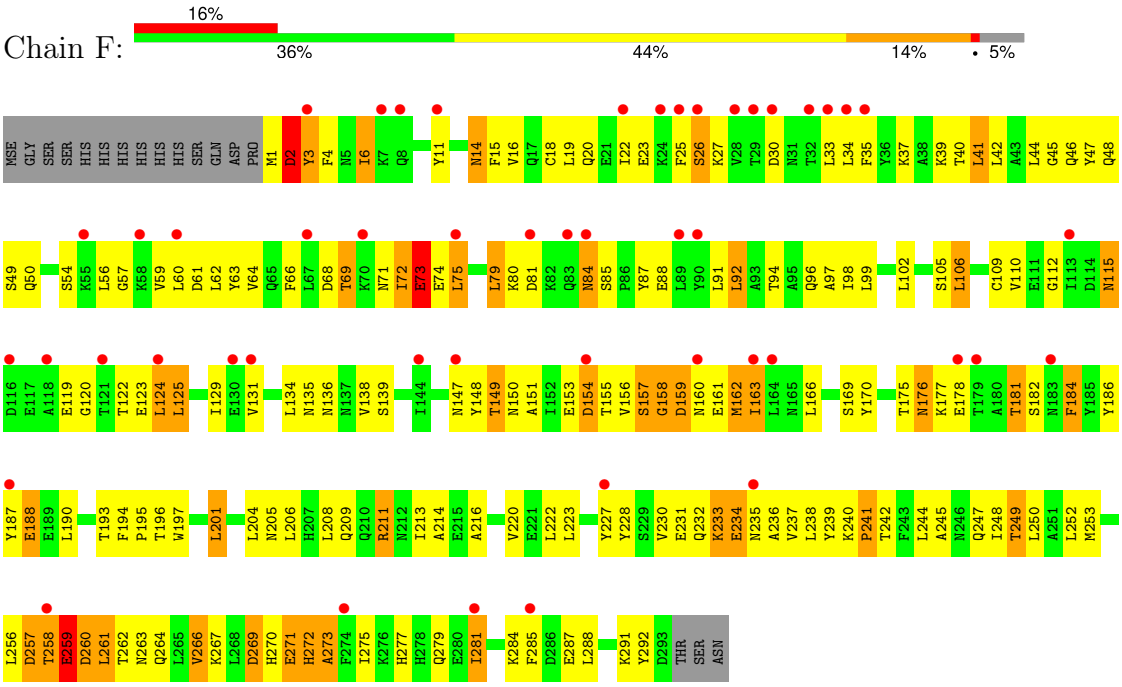
• Molecule 2: Coatomer subunit epsilon

Chain D:



• Molecule 2: Coatomer subunit epsilon

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	328.13Å 74.31Å 96.40Å 90.00° 101.98° 90.00°	Depositor
Resolution (Å)	50.00 – 3.25 48.68 – 3.25	Depositor EDS
% Data completeness (in resolution range)	89.7 (50.00-3.25) 96.1 (48.68-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 3.25Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.287 0.244 , 0.281	Depositor DCC
R_{free} test set	3391 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	85.9	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 125.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14256	wwPDB-VP
Average B, all atoms (Å^2)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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

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	0.50	0/2429	0.79	1/3273 (0.0%)
1	C	0.49	0/2429	0.79	1/3273 (0.0%)
1	E	0.47	0/2429	0.78	1/3273 (0.0%)
2	B	0.51	0/2401	0.76	1/3255 (0.0%)
2	D	0.51	0/2401	0.76	1/3255 (0.0%)
2	F	0.49	0/2401	0.75	1/3255 (0.0%)
All	All	0.49	0/14490	0.77	6/19584 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1155	LYS	N-CA-C	-5.69	95.63	111.00
1	A	1155	LYS	N-CA-C	-5.69	95.65	111.00
1	E	1155	LYS	N-CA-C	-5.68	95.67	111.00
2	F	125	LEU	CA-CB-CG	-5.21	103.31	115.30
2	B	125	LEU	CA-CB-CG	-5.18	103.37	115.30
2	D	125	LEU	CA-CB-CG	-5.13	103.49	115.30

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	2388	0	2441	281	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2388	0	2441	246	0
1	E	2388	0	2441	249	0
2	B	2364	0	2319	214	0
2	D	2364	0	2319	239	0
2	F	2364	0	2319	215	0
All	All	14256	0	14280	1363	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 48.

All (1363) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1090:MSE:HE2	1:C:1106:ALA:HA	1.30	1.12
1:E:1090:MSE:HE2	1:E:1106:ALA:HA	1.29	1.12
2:B:211:ARG:HH11	2:B:211:ARG:HB2	1.11	1.10
1:C:1028:ALA:HB2	1:C:1200:ARG:CZ	1.80	1.10
1:A:1090:MSE:HE2	1:A:1106:ALA:HA	1.30	1.08
2:D:211:ARG:HH11	2:D:211:ARG:HB2	1.11	1.08
1:A:1113:ILE:HG23	2:D:150:ASN:ND2	1.69	1.06
2:F:211:ARG:HH11	2:F:211:ARG:HB2	1.11	1.05
2:D:195:PRO:HG3	1:E:1079:PRO:HG3	1.40	1.03
1:C:957:THR:HB	1:C:958:PRO:CD	1.93	0.99
1:A:957:THR:HB	1:A:958:PRO:CD	1.92	0.99
1:E:957:THR:HB	1:E:958:PRO:CD	1.94	0.98
2:D:1:MSE:HG2	2:D:2:ASP:H	1.29	0.97
1:C:1028:ALA:HB2	1:C:1200:ARG:NH1	1.78	0.97
1:C:990:VAL:HG11	1:C:1020:ILE:HD11	1.46	0.97
1:E:1097:LYS:HG3	1:E:1099:PHE:HE1	1.29	0.97
2:B:1:MSE:HG2	2:B:2:ASP:H	1.29	0.96
1:A:990:VAL:HG11	1:A:1020:ILE:HD11	1.46	0.95
1:E:990:VAL:HG11	1:E:1020:ILE:HD11	1.45	0.95
1:A:1083:THR:HG21	1:A:1118:ARG:NH1	1.84	0.93
1:A:1097:LYS:HG3	1:A:1099:PHE:HE1	1.29	0.93
1:C:1097:LYS:HG3	1:C:1099:PHE:HE1	1.29	0.93
2:F:1:MSE:HG2	2:F:2:ASP:H	1.29	0.92
1:C:1025:VAL:HG11	1:C:1030:ASP:HB2	1.51	0.92
1:E:1025:VAL:HG11	1:E:1030:ASP:HB2	1.51	0.92
1:E:1083:THR:HG21	1:E:1118:ARG:NH1	1.84	0.92
1:A:1080:ILE:HG13	2:D:147:ASN:OD1	1.71	0.91
1:C:1083:THR:HG21	1:C:1118:ARG:NH1	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:ILE:HD12	2:B:6:ILE:H	1.36	0.91
1:A:1003:LEU:HD21	2:D:110:VAL:HG21	1.53	0.91
1:C:1079:PRO:HG3	2:F:195:PRO:HG3	1.54	0.90
2:D:6:ILE:H	2:D:6:ILE:HD12	1.36	0.90
2:F:6:ILE:HD12	2:F:6:ILE:H	1.36	0.90
1:A:1025:VAL:HG11	1:A:1030:ASP:HB2	1.51	0.90
1:C:994:MSE:HE3	1:C:1016:ALA:CB	2.02	0.90
2:B:11:TYR:CE1	2:B:163:ILE:HD11	2.08	0.88
2:B:211:ARG:HH11	2:B:211:ARG:CB	1.87	0.88
1:A:994:MSE:HE3	1:A:1016:ALA:CB	2.02	0.88
1:E:994:MSE:HE3	1:E:1016:ALA:CB	2.02	0.88
2:D:211:ARG:HH11	2:D:211:ARG:CB	1.87	0.88
2:F:211:ARG:HH11	2:F:211:ARG:CB	1.87	0.88
1:E:1028:ALA:HB2	1:E:1200:ARG:CZ	2.02	0.87
1:C:1025:VAL:HG23	1:C:1199:ILE:HG22	1.54	0.87
1:E:1166:ASP:OD2	1:E:1169:THR:HB	1.76	0.86
1:A:1028:ALA:HB2	1:A:1200:ARG:CZ	2.05	0.86
1:A:1166:ASP:OD2	1:A:1169:THR:HB	1.76	0.86
1:C:1166:ASP:OD2	1:C:1169:THR:HB	1.76	0.85
2:F:11:TYR:CE1	2:F:163:ILE:HD11	2.10	0.85
2:D:112:GLY:O	2:D:115:ASN:HB2	1.75	0.84
1:C:1174:VAL:HG23	1:C:1176:THR:HB	1.58	0.84
1:A:1174:VAL:HG23	1:A:1176:THR:HB	1.58	0.84
1:E:1174:VAL:HG23	1:E:1176:THR:HB	1.58	0.84
2:D:195:PRO:HG3	1:E:1079:PRO:CG	2.06	0.84
1:A:1113:ILE:HG23	2:D:150:ASN:HD21	1.43	0.83
2:D:87:TYR:HE1	2:D:119:GLU:HG2	1.42	0.83
2:B:72:ILE:HD12	2:B:72:ILE:H	1.43	0.83
1:E:1097:LYS:HG3	1:E:1099:PHE:CE1	2.14	0.83
1:C:1097:LYS:HG3	1:C:1099:PHE:CE1	2.14	0.83
2:F:211:ARG:HA	2:F:253:MSE:HE1	1.61	0.83
1:A:976:SER:C	1:A:978:ASP:H	1.82	0.82
2:B:211:ARG:HA	2:B:253:MSE:HE1	1.61	0.82
1:A:0:MSE:HE1	2:B:138:VAL:HG11	1.60	0.82
1:A:1097:LYS:HG3	1:A:1099:PHE:CE1	2.14	0.82
1:A:1189:LYS:HE3	1:A:1192:ALA:HB2	1.61	0.82
2:F:72:ILE:H	2:F:72:ILE:HD12	1.43	0.82
1:A:1045:ILE:HD12	1:A:1184:ILE:HG23	1.60	0.82
1:C:1189:LYS:HE3	1:C:1192:ALA:HB2	1.61	0.82
2:F:125:LEU:HD22	2:F:148:TYR:CD2	2.15	0.82
2:B:125:LEU:HD22	2:B:148:TYR:CD2	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:ILE:HD12	2:D:72:ILE:H	1.43	0.82
2:D:211:ARG:HA	2:D:253:MSE:HE1	1.61	0.82
2:B:20:GLN:HA	2:B:23:GLU:HG3	1.61	0.81
2:B:264:GLN:OE1	2:B:264:GLN:HA	1.79	0.81
2:F:20:GLN:HA	2:F:23:GLU:HG3	1.61	0.81
2:D:264:GLN:HA	2:D:264:GLN:OE1	1.80	0.81
1:E:1045:ILE:HD12	1:E:1184:ILE:HG23	1.60	0.81
2:B:275:ILE:O	2:B:279:GLN:HG2	1.80	0.81
2:D:20:GLN:HA	2:D:23:GLU:HG3	1.61	0.81
2:F:264:GLN:HA	2:F:264:GLN:OE1	1.80	0.81
2:D:94:THR:O	2:D:98:ILE:HG13	1.81	0.80
2:F:94:THR:O	2:F:98:ILE:HG13	1.80	0.80
2:D:35:PHE:CD1	2:D:87:TYR:HD2	1.99	0.80
1:E:1189:LYS:HE3	1:E:1192:ALA:HB2	1.62	0.80
2:F:211:ARG:HB2	2:F:211:ARG:NH1	1.96	0.80
2:F:275:ILE:O	2:F:279:GLN:HG2	1.80	0.80
1:E:976:SER:C	1:E:978:ASP:H	1.82	0.80
1:C:976:SER:C	1:C:978:ASP:H	1.82	0.80
2:D:125:LEU:HD22	2:D:148:TYR:CD2	2.15	0.80
2:D:275:ILE:O	2:D:279:GLN:HG2	1.80	0.80
2:B:94:THR:O	2:B:98:ILE:HG13	1.81	0.79
1:C:1074:LYS:HE3	1:C:1147:PHE:CE1	2.17	0.79
2:B:181:THR:HG22	2:B:182:SER:N	1.98	0.79
2:B:211:ARG:HB2	2:B:211:ARG:NH1	1.95	0.79
2:D:181:THR:HG22	2:D:182:SER:H	1.48	0.79
1:C:1104:TYR:CE2	1:C:1143:PRO:HB3	2.17	0.79
2:D:181:THR:HG22	2:D:182:SER:N	1.99	0.78
2:B:181:THR:HG22	2:B:182:SER:H	1.48	0.78
1:A:1099:PHE:HD1	1:A:1134:SER:HB3	1.47	0.78
2:F:206:LEU:O	2:F:209:GLN:HB2	1.84	0.78
2:B:71:ASN:HB2	2:B:73:GLU:CG	2.14	0.78
2:F:71:ASN:HB2	2:F:73:GLU:HG2	1.65	0.78
2:D:206:LEU:O	2:D:209:GLN:HB2	1.84	0.78
2:D:71:ASN:HB2	2:D:73:GLU:HG2	1.65	0.78
1:E:983:TYR:CE2	2:F:253:MSE:HG2	2.19	0.78
1:A:983:TYR:CE2	2:B:253:MSE:HG2	2.19	0.77
2:B:206:LEU:O	2:B:209:GLN:HB2	1.84	0.77
2:D:71:ASN:HB2	2:D:73:GLU:CG	2.14	0.77
2:F:181:THR:HG22	2:F:182:SER:H	1.48	0.77
2:D:11:TYR:CE1	2:D:163:ILE:HD11	2.19	0.77
2:D:211:ARG:HB2	2:D:211:ARG:NH1	1.95	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:60:LEU:O	2:F:64:VAL:HG23	1.84	0.77
2:F:181:THR:HG22	2:F:182:SER:N	1.99	0.77
2:D:60:LEU:O	2:D:64:VAL:HG23	1.84	0.77
2:B:71:ASN:HB2	2:B:73:GLU:HG2	1.65	0.77
2:B:6:ILE:H	2:B:6:ILE:CD1	1.98	0.76
1:E:1099:PHE:HD1	1:E:1134:SER:HB3	1.50	0.76
1:A:957:THR:HB	1:A:958:PRO:HD2	1.68	0.76
2:F:71:ASN:HB2	2:F:73:GLU:CG	2.14	0.76
2:D:6:ILE:HD12	2:D:6:ILE:N	2.01	0.76
1:E:1002:LYS:NZ	1:E:1080:ILE:HD11	2.01	0.76
1:C:994:MSE:HE3	1:C:1016:ALA:HB3	1.68	0.75
2:B:60:LEU:O	2:B:64:VAL:HG23	1.84	0.75
2:F:157:SER:HB2	2:F:161:GLU:HB2	1.67	0.75
1:C:957:THR:HB	1:C:958:PRO:HD2	1.68	0.75
2:D:6:ILE:H	2:D:6:ILE:CD1	1.98	0.75
2:F:6:ILE:H	2:F:6:ILE:CD1	1.98	0.75
2:D:87:TYR:CE1	2:D:119:GLU:HG2	2.22	0.75
2:F:6:ILE:HD12	2:F:6:ILE:N	2.01	0.74
1:A:1002:LYS:NZ	1:A:1080:ILE:HD11	2.01	0.74
1:C:1002:LYS:NZ	1:C:1080:ILE:HD11	2.01	0.74
1:E:994:MSE:HE3	1:E:1016:ALA:HB3	1.68	0.74
1:A:994:MSE:HE3	1:A:1016:ALA:HB3	1.68	0.74
1:A:1045:ILE:HB	1:A:1184:ILE:HD12	1.68	0.74
1:E:957:THR:HB	1:E:958:PRO:HD2	1.68	0.74
1:A:931:VAL:HG13	1:A:1168:LEU:HB2	1.67	0.74
1:E:954:ILE:HD13	1:E:955:PRO:N	2.03	0.74
1:C:1079:PRO:CG	2:F:195:PRO:HG3	2.18	0.74
1:C:954:ILE:HD13	1:C:955:PRO:N	2.03	0.73
2:F:35:PHE:CD1	2:F:87:TYR:HD2	2.05	0.73
2:F:69:THR:HB	2:F:71:ASN:OD1	1.89	0.73
1:A:954:ILE:HD13	1:A:955:PRO:N	2.03	0.73
1:C:933:VAL:HG13	1:C:1187:ILE:HG23	1.69	0.73
2:F:3:TYR:CB	2:F:6:ILE:HD13	2.19	0.73
2:F:257:ASP:O	2:F:259:GLU:N	2.21	0.73
2:F:63:TYR:O	2:F:66:PHE:HB3	1.89	0.73
2:B:6:ILE:HD12	2:B:6:ILE:N	2.01	0.73
2:B:3:TYR:CB	2:B:6:ILE:HD13	2.19	0.73
2:D:63:TYR:O	2:D:66:PHE:HB3	1.89	0.73
2:B:257:ASP:O	2:B:259:GLU:N	2.21	0.73
2:D:257:ASP:O	2:D:259:GLU:N	2.21	0.72
1:E:1045:ILE:HB	1:E:1184:ILE:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:TYR:CB	2:D:6:ILE:HD13	2.19	0.72
2:F:159:ASP:O	2:F:162:MSE:HE2	1.89	0.72
2:B:63:TYR:O	2:B:66:PHE:HB3	1.89	0.72
2:B:125:LEU:O	2:B:129:ILE:HD13	1.90	0.72
1:A:1113:ILE:HD12	2:D:150:ASN:HD22	1.52	0.72
2:B:159:ASP:O	2:B:162:MSE:HE2	1.89	0.72
2:D:125:LEU:O	2:D:129:ILE:HD13	1.90	0.72
2:D:159:ASP:O	2:D:162:MSE:HE2	1.89	0.71
1:A:1117:PRO:HB2	2:D:177:LYS:HZ3	1.56	0.71
1:C:978:ASP:O	1:C:980:ILE:N	2.23	0.71
2:B:30:ASP:HB3	2:B:33:LEU:HD12	1.73	0.71
1:E:978:ASP:O	1:E:980:ILE:N	2.23	0.71
2:F:30:ASP:HB3	2:F:33:LEU:HD12	1.73	0.71
1:E:1074:LYS:HE3	1:E:1147:PHE:CE1	2.25	0.71
2:F:125:LEU:O	2:F:129:ILE:HD13	1.90	0.71
1:A:1099:PHE:HA	1:A:1102:ALA:HB3	1.73	0.71
2:F:258:THR:HG22	2:F:262:THR:OG1	1.91	0.70
2:D:156:VAL:C	2:D:158:GLY:H	1.92	0.70
1:E:1174:VAL:CG2	1:E:1176:THR:HB	2.22	0.70
2:D:30:ASP:HB3	2:D:33:LEU:HD12	1.73	0.70
1:E:1099:PHE:HA	1:E:1102:ALA:HB3	1.73	0.70
1:E:1185:ALA:O	1:E:1187:ILE:N	2.25	0.70
2:B:57:GLY:HA2	2:B:60:LEU:HD12	1.73	0.70
2:B:106:LEU:HD23	2:B:106:LEU:O	1.92	0.70
1:A:1185:ALA:O	1:A:1187:ILE:N	2.25	0.70
1:E:957:THR:CB	1:E:958:PRO:CD	2.70	0.70
1:A:1074:LYS:HE3	1:A:1147:PHE:CE1	2.27	0.70
2:B:258:THR:HG22	2:B:262:THR:OG1	1.92	0.70
1:C:1174:VAL:CG2	1:C:1176:THR:HB	2.22	0.70
2:D:106:LEU:O	2:D:106:LEU:HD23	1.92	0.70
1:E:1023:LEU:HD23	1:E:1024:MSE:H	1.57	0.70
1:A:957:THR:CB	1:A:958:PRO:CD	2.69	0.70
1:A:978:ASP:O	1:A:980:ILE:N	2.23	0.70
1:A:1174:VAL:CG2	1:A:1176:THR:HB	2.22	0.70
1:A:1023:LEU:HD23	1:A:1024:MSE:H	1.56	0.69
1:C:957:THR:CB	1:C:958:PRO:CD	2.69	0.69
1:C:1045:ILE:HD12	1:C:1184:ILE:HG23	1.74	0.69
2:F:57:GLY:HA2	2:F:60:LEU:HD12	1.73	0.69
1:A:1113:ILE:HD12	2:D:150:ASN:ND2	2.07	0.69
1:E:1090:MSE:HG3	1:E:1106:ALA:HB2	1.75	0.69
1:A:926:ALA:O	1:A:930:GLN:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:LEU:O	2:B:222:LEU:HD23	1.92	0.69
1:A:940:LYS:HB2	2:B:285:PHE:CE2	2.28	0.69
1:A:961:LEU:HD21	2:B:134:LEU:HD11	1.72	0.69
1:C:1185:ALA:O	1:C:1187:ILE:N	2.25	0.69
1:E:926:ALA:O	1:E:930:GLN:HG3	1.92	0.69
2:F:112:GLY:O	2:F:115:ASN:HB2	1.92	0.69
1:C:1099:PHE:HA	1:C:1102:ALA:HB3	1.73	0.69
1:A:1090:MSE:HG3	1:A:1106:ALA:HB2	1.75	0.69
1:C:1023:LEU:HD23	1:C:1024:MSE:H	1.57	0.69
1:C:1090:MSE:HG3	1:C:1106:ALA:HB2	1.74	0.69
1:E:994:MSE:CE	1:E:1013:PHE:HD2	2.05	0.69
1:A:1002:LYS:NZ	2:D:147:ASN:HB3	2.08	0.69
2:D:57:GLY:HA2	2:D:60:LEU:HD12	1.73	0.69
2:F:106:LEU:O	2:F:106:LEU:HD23	1.92	0.69
1:A:933:VAL:HG13	1:A:1187:ILE:HG23	1.75	0.69
1:C:926:ALA:O	1:C:930:GLN:HG3	1.92	0.69
1:C:1181:ILE:HD12	1:C:1181:ILE:H	1.58	0.69
2:D:222:LEU:HD23	2:D:222:LEU:O	1.92	0.69
2:D:231:GLU:HB3	1:E:1113:ILE:HD12	1.74	0.69
2:F:222:LEU:HD23	2:F:222:LEU:O	1.92	0.69
1:E:1025:VAL:HG23	1:E:1199:ILE:HG22	1.74	0.69
1:E:1181:ILE:H	1:E:1181:ILE:HD12	1.58	0.69
1:A:1117:PRO:CA	2:D:177:LYS:HZ1	2.05	0.69
2:B:175:THR:HG21	2:B:177:LYS:HD3	1.75	0.68
2:F:175:THR:HG21	2:F:177:LYS:HD3	1.75	0.68
1:A:1099:PHE:CD1	1:A:1134:SER:HB3	2.27	0.68
2:D:227:TYR:O	2:D:231:GLU:HB2	1.94	0.68
2:D:258:THR:HG22	2:D:262:THR:OG1	1.92	0.68
2:B:162:MSE:HE3	2:B:163:ILE:CD1	2.24	0.68
2:F:248:ILE:HD11	2:F:263:ASN:HB3	1.76	0.68
1:E:931:VAL:HG13	1:E:1168:LEU:HB2	1.74	0.68
2:D:162:MSE:HE3	2:D:163:ILE:CD1	2.24	0.68
2:F:227:TYR:O	2:F:231:GLU:HB2	1.94	0.68
1:C:994:MSE:CE	1:C:1013:PHE:HD2	2.05	0.68
1:A:1153:THR:O	1:A:1154:TYR:HB2	1.94	0.68
1:C:1002:LYS:HZ1	1:C:1080:ILE:HD11	1.58	0.68
1:C:1153:THR:O	1:C:1154:TYR:HB2	1.94	0.68
1:C:911:PRO:HB3	1:C:927:LEU:HD21	1.76	0.67
2:D:175:THR:HG21	2:D:177:LYS:HD3	1.75	0.67
1:C:1025:VAL:HG23	1:C:1199:ILE:CG2	2.24	0.67
1:C:1033:LEU:HD23	1:C:1037:ILE:HG13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:248:ILE:HD11	2:D:263:ASN:HB3	1.76	0.67
2:B:157:SER:HB2	2:B:161:GLU:HB2	1.77	0.67
1:E:904:TRP:CH2	1:E:982:PRO:HB3	2.29	0.67
1:E:1109:PHE:CZ	1:E:1118:ARG:HD3	2.30	0.67
1:E:1153:THR:O	1:E:1154:TYR:HB2	1.95	0.67
2:F:162:MSE:HE3	2:F:163:ILE:CD1	2.23	0.67
2:B:227:TYR:O	2:B:231:GLU:HB2	1.93	0.67
1:E:913:VAL:CG2	1:E:1024:MSE:HE3	2.24	0.67
1:A:994:MSE:CE	1:A:1013:PHE:HD2	2.05	0.67
1:A:1033:LEU:HD23	1:A:1037:ILE:HG13	1.76	0.67
1:A:954:ILE:HD13	1:A:955:PRO:CD	2.25	0.67
1:A:1104:TYR:CE2	1:A:1143:PRO:HB3	2.30	0.67
1:A:1109:PHE:CZ	1:A:1118:ARG:HD3	2.30	0.67
2:B:35:PHE:CD1	2:B:87:TYR:HD2	2.12	0.67
1:E:911:PRO:HB3	1:E:927:LEU:HD21	1.76	0.67
1:E:1002:LYS:HZ3	1:E:1080:ILE:HD11	1.60	0.67
1:A:1181:ILE:HD12	1:A:1181:ILE:H	1.58	0.67
2:B:186:TYR:CZ	2:B:190:LEU:HD11	2.30	0.67
1:C:1109:PHE:CZ	1:C:1118:ARG:HD3	2.30	0.67
2:D:186:TYR:CZ	2:D:190:LEU:HD11	2.30	0.67
2:B:248:ILE:HD11	2:B:263:ASN:HB3	1.76	0.67
1:A:911:PRO:HB3	1:A:927:LEU:HD21	1.76	0.67
1:C:931:VAL:HG13	1:C:1168:LEU:HB2	1.77	0.67
2:D:15:PHE:HB2	2:D:44:LEU:HD21	1.77	0.67
1:E:1162:PRO:O	1:E:1175:ILE:HG12	1.95	0.67
2:F:186:TYR:CZ	2:F:190:LEU:HD11	2.30	0.67
2:F:156:VAL:C	2:F:158:GLY:H	1.99	0.66
2:F:15:PHE:HB2	2:F:44:LEU:HD21	1.77	0.66
1:A:976:SER:O	1:A:978:ASP:N	2.29	0.66
2:D:72:ILE:H	2:D:72:ILE:CD1	2.03	0.66
1:E:1033:LEU:HD23	1:E:1037:ILE:HG13	1.76	0.66
1:C:954:ILE:HD13	1:C:955:PRO:CD	2.26	0.66
1:A:1147:PHE:HD1	1:A:1147:PHE:O	1.79	0.66
1:E:1008:ILE:HD12	1:E:1008:ILE:H	1.61	0.66
1:A:981:LEU:HD13	1:A:1024:MSE:HE2	1.78	0.66
1:C:1008:ILE:HD12	1:C:1008:ILE:H	1.61	0.66
2:B:15:PHE:HB2	2:B:44:LEU:HD21	1.78	0.66
1:C:1147:PHE:HD1	1:C:1147:PHE:O	1.79	0.66
1:A:1162:PRO:O	1:A:1175:ILE:HG12	1.95	0.65
1:C:1162:PRO:O	1:C:1175:ILE:HG12	1.95	0.65
2:D:54:SER:C	2:D:56:LEU:H	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:961:LEU:HD21	2:F:134:LEU:HD11	1.79	0.65
2:B:54:SER:C	2:B:56:LEU:H	1.99	0.65
2:D:19:LEU:O	2:D:23:GLU:HG2	1.97	0.65
2:D:80:LYS:O	2:D:81:ASP:HB2	1.96	0.65
1:E:976:SER:O	1:E:978:ASP:N	2.30	0.65
1:A:957:THR:HB	1:A:958:PRO:HD3	1.78	0.65
2:B:19:LEU:O	2:B:23:GLU:HG2	1.97	0.65
1:C:976:SER:O	1:C:978:ASP:N	2.29	0.65
1:E:954:ILE:HD13	1:E:955:PRO:CD	2.26	0.65
1:E:1104:TYR:CE2	1:E:1143:PRO:HB3	2.32	0.65
1:A:1008:ILE:HD12	1:A:1008:ILE:H	1.61	0.64
1:E:1147:PHE:HD1	1:E:1147:PHE:O	1.79	0.64
2:F:87:TYR:HE1	2:F:119:GLU:HG2	1.62	0.64
2:F:72:ILE:H	2:F:72:ILE:CD1	2.03	0.64
2:F:80:LYS:O	2:F:81:ASP:HB2	1.97	0.64
2:D:181:THR:CG2	2:D:182:SER:H	2.07	0.64
2:F:19:LEU:O	2:F:23:GLU:HG2	1.97	0.64
2:B:3:TYR:HB2	2:B:6:ILE:HD13	1.80	0.64
1:C:1074:LYS:HE3	1:C:1147:PHE:HE1	1.62	0.64
1:A:976:SER:C	1:A:978:ASP:N	2.51	0.64
1:C:1099:PHE:HD1	1:C:1134:SER:HB3	1.62	0.64
1:E:1099:PHE:CD1	1:E:1134:SER:HB3	2.31	0.64
1:A:0:MSE:HE2	2:B:138:VAL:HG21	1.79	0.64
2:F:54:SER:C	2:F:56:LEU:H	1.99	0.64
1:A:1084:ASN:HD21	2:D:143:THR:HG21	1.62	0.63
1:A:1166:ASP:OD2	1:A:1169:THR:CB	2.46	0.63
2:F:181:THR:CG2	2:F:182:SER:H	2.07	0.63
1:A:1025:VAL:HG23	1:A:1199:ILE:HG22	1.79	0.63
1:C:1181:ILE:H	1:C:1181:ILE:CD1	2.09	0.63
1:E:957:THR:HB	1:E:958:PRO:HD3	1.79	0.63
1:E:1166:ASP:OD2	1:E:1169:THR:CB	2.47	0.63
2:F:63:TYR:HD1	2:F:91:LEU:HB3	1.64	0.63
2:B:80:LYS:O	2:B:81:ASP:HB2	1.96	0.63
2:D:157:SER:O	2:D:159:ASP:N	2.32	0.63
1:E:1197:LEU:HD21	1:E:1199:ILE:HD11	1.80	0.63
2:F:162:MSE:HE3	2:F:163:ILE:HD12	1.81	0.63
1:A:1197:LEU:HD21	1:A:1199:ILE:HD11	1.80	0.63
1:A:1117:PRO:CB	2:D:177:LYS:NZ	2.62	0.62
1:C:957:THR:HB	1:C:958:PRO:HD3	1.78	0.62
1:E:1181:ILE:H	1:E:1181:ILE:CD1	2.09	0.62
2:D:162:MSE:HE3	2:D:163:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1074:LYS:HE3	1:C:1147:PHE:CD1	2.34	0.62
2:D:1:MSE:HG2	2:D:2:ASP:N	2.10	0.62
2:D:157:SER:HB2	2:D:161:GLU:HB2	1.80	0.62
2:D:208:LEU:HD21	2:D:250:LEU:HB2	1.81	0.62
1:A:1117:PRO:HB2	2:D:177:LYS:NZ	2.14	0.62
2:B:162:MSE:HE3	2:B:163:ILE:HD12	1.81	0.62
2:F:1:MSE:HG2	2:F:2:ASP:N	2.10	0.62
2:F:63:TYR:CD1	2:F:91:LEU:HB3	2.34	0.62
1:C:1166:ASP:OD2	1:C:1169:THR:CB	2.47	0.62
1:C:1197:LEU:HD21	1:C:1199:ILE:HD11	1.80	0.62
2:D:3:TYR:HB2	2:D:6:ILE:HD13	1.80	0.62
1:E:976:SER:C	1:E:978:ASP:N	2.51	0.62
1:E:1042:ARG:HG3	1:E:1043:GLU:N	2.15	0.62
2:B:20:GLN:HA	2:B:23:GLU:CG	2.30	0.62
1:C:990:VAL:HG11	1:C:1020:ILE:CD1	2.27	0.62
2:F:3:TYR:HB2	2:F:6:ILE:HD13	1.80	0.61
2:F:20:GLN:HA	2:F:23:GLU:CG	2.30	0.61
2:F:156:VAL:O	2:F:158:GLY:N	2.33	0.61
1:A:1002:LYS:HZ1	1:A:1080:ILE:HD11	1.63	0.61
1:A:1083:THR:HG21	1:A:1118:ARG:HH12	1.63	0.61
2:F:248:ILE:CD1	2:F:263:ASN:HB3	2.30	0.61
1:A:1042:ARG:HG3	1:A:1043:GLU:N	2.15	0.61
1:A:1181:ILE:H	1:A:1181:ILE:CD1	2.09	0.61
2:F:240:LYS:N	2:F:241:PRO:HD2	2.15	0.61
2:B:208:LEU:HD21	2:B:250:LEU:HB2	1.81	0.61
2:D:240:LYS:N	2:D:241:PRO:HD2	2.15	0.61
1:C:976:SER:C	1:C:978:ASP:N	2.51	0.61
1:C:1083:THR:HG21	1:C:1118:ARG:HH12	1.63	0.61
2:F:197:TRP:CZ3	2:F:223:LEU:HD22	2.36	0.61
2:F:208:LEU:HD21	2:F:250:LEU:HB2	1.81	0.61
1:E:957:THR:O	1:E:959:CYS:N	2.34	0.61
1:E:994:MSE:HE1	1:E:1013:PHE:HD2	1.66	0.61
1:A:971:TYR:CA	2:B:211:ARG:HH21	2.13	0.61
1:C:1042:ARG:HG3	1:C:1043:GLU:N	2.15	0.61
1:A:961:LEU:HD23	1:A:962:PRO:CD	2.31	0.61
1:E:1083:THR:HG21	1:E:1118:ARG:HH12	1.63	0.61
1:C:957:THR:O	1:C:959:CYS:N	2.34	0.61
2:B:79:LEU:HD23	2:B:84:ASN:OD1	2.01	0.60
1:C:954:ILE:HA	2:D:205:ASN:ND2	2.15	0.60
1:C:1025:VAL:O	1:C:1201:VAL:HG23	2.01	0.60
2:D:248:ILE:CD1	2:D:263:ASN:HB3	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:204:LEU:O	2:F:204:LEU:HD12	2.01	0.60
2:B:248:ILE:CD1	2:B:263:ASN:HB3	2.30	0.60
2:D:197:TRP:CZ3	2:D:223:LEU:HD22	2.36	0.60
2:B:240:LYS:N	2:B:241:PRO:HD2	2.15	0.60
1:C:961:LEU:HG	1:C:962:PRO:HD2	1.83	0.60
2:D:72:ILE:HG13	2:D:99:LEU:HD11	1.82	0.60
1:E:915:VAL:HG11	1:E:943:PHE:HA	1.84	0.60
1:A:957:THR:O	1:A:959:CYS:N	2.34	0.60
1:C:915:VAL:HG11	1:C:943:PHE:HA	1.84	0.60
1:E:961:LEU:HD23	1:E:962:PRO:CD	2.31	0.60
2:F:79:LEU:HD23	2:F:84:ASN:OD1	2.01	0.60
1:A:961:LEU:HD23	1:A:961:LEU:C	2.22	0.60
1:C:910:LEU:HB2	1:C:911:PRO:HD2	1.84	0.60
1:C:1005:LYS:HB3	1:C:1008:ILE:HD13	1.84	0.60
1:C:1023:LEU:HD23	1:C:1024:MSE:N	2.17	0.60
2:D:79:LEU:HD23	2:D:84:ASN:OD1	2.01	0.60
1:E:1023:LEU:HD23	1:E:1024:MSE:N	2.17	0.60
1:C:994:MSE:HE1	1:C:1013:PHE:HD2	1.66	0.59
1:C:1045:ILE:HB	1:C:1184:ILE:HD12	1.84	0.59
2:D:195:PRO:CG	1:E:1079:PRO:HG3	2.25	0.59
1:E:910:LEU:HB2	1:E:911:PRO:HD2	1.84	0.59
1:E:961:LEU:HG	1:E:962:PRO:HD2	1.84	0.59
1:E:1071:TYR:HE2	1:E:1141:PHE:HB2	1.67	0.59
2:D:20:GLN:HA	2:D:23:GLU:CG	2.30	0.59
2:F:15:PHE:HB3	2:F:40:THR:HG23	1.83	0.59
2:B:197:TRP:CZ3	2:B:223:LEU:HD22	2.36	0.59
2:B:204:LEU:HD12	2:B:204:LEU:O	2.02	0.59
1:C:961:LEU:HD23	1:C:961:LEU:C	2.23	0.59
1:A:1005:LYS:HB3	1:A:1008:ILE:HD13	1.84	0.59
1:A:915:VAL:HG11	1:A:943:PHE:HA	1.84	0.59
1:A:1002:LYS:HZ2	2:D:147:ASN:HB3	1.68	0.59
2:B:15:PHE:HB3	2:B:40:THR:HG23	1.83	0.59
1:E:990:VAL:HG11	1:E:1020:ILE:CD1	2.27	0.59
1:A:994:MSE:HE1	1:A:1013:PHE:HD2	1.66	0.59
1:A:1018:TYR:HE2	1:A:1187:ILE:CG1	2.15	0.59
1:A:1132:MSE:O	1:A:1134:SER:N	2.35	0.59
1:A:961:LEU:HG	1:A:962:PRO:HD2	1.84	0.59
2:B:63:TYR:CD1	2:B:91:LEU:HB3	2.38	0.59
1:C:1162:PRO:HB2	1:C:1175:ILE:HG13	1.85	0.59
1:E:1162:PRO:HB2	1:E:1175:ILE:HG13	1.85	0.59
1:A:910:LEU:HB2	1:A:911:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:LEU:HD23	1:A:1024:MSE:N	2.17	0.59
1:A:1117:PRO:HA	2:D:177:LYS:HZ1	1.68	0.59
1:C:1084:ASN:O	1:C:1088:VAL:HG23	2.03	0.59
1:E:1005:LYS:HB3	1:E:1008:ILE:HD13	1.84	0.59
2:B:193:THR:HB	2:B:194:PHE:CD1	2.38	0.59
1:C:961:LEU:HD21	2:D:134:LEU:HD11	1.84	0.59
1:A:1084:ASN:O	1:A:1088:VAL:HG23	2.03	0.58
2:D:193:THR:HB	2:D:194:PHE:CD1	2.38	0.58
2:D:216:ALA:O	2:D:220:VAL:HG23	2.03	0.58
2:D:204:LEU:HD12	2:D:204:LEU:O	2.02	0.58
1:A:1162:PRO:HB2	1:A:1175:ILE:HG13	1.85	0.58
2:D:15:PHE:HB3	2:D:40:THR:HG23	1.83	0.58
2:F:193:THR:HB	2:F:194:PHE:CD1	2.37	0.58
1:A:981:LEU:HB3	1:A:1024:MSE:HE1	1.84	0.58
1:C:961:LEU:CG	1:C:962:PRO:HD2	2.34	0.58
1:C:1025:VAL:CG1	1:C:1030:ASP:HB2	2.31	0.58
2:B:69:THR:HB	2:B:71:ASN:OD1	2.04	0.58
1:C:961:LEU:HD23	1:C:962:PRO:CD	2.32	0.58
1:E:961:LEU:HD23	1:E:961:LEU:C	2.23	0.58
1:A:1033:LEU:HD23	1:A:1033:LEU:O	2.04	0.58
2:D:35:PHE:CG	2:D:87:TYR:CD2	2.92	0.58
1:C:1028:ALA:CB	1:C:1200:ARG:CZ	2.70	0.58
2:D:149:THR:O	2:D:151:ALA:N	2.37	0.58
1:A:1003:LEU:CD2	2:D:106:LEU:HD22	2.34	0.57
1:E:1033:LEU:HD23	1:E:1033:LEU:O	2.04	0.57
2:D:72:ILE:HD12	2:D:72:ILE:N	2.18	0.57
1:E:1025:VAL:CG1	1:E:1030:ASP:HB2	2.31	0.57
2:F:149:THR:O	2:F:151:ALA:N	2.38	0.57
2:F:59:VAL:O	2:F:62:LEU:HB2	2.05	0.57
1:C:1033:LEU:HD23	1:C:1033:LEU:O	2.04	0.57
2:F:72:ILE:HD12	2:F:72:ILE:N	2.18	0.57
2:B:71:ASN:HB2	2:B:73:GLU:CD	2.25	0.57
2:B:92:LEU:HD22	2:B:96:GLN:HG3	1.87	0.57
2:B:222:LEU:HD21	2:B:228:TYR:HE1	1.68	0.57
1:E:1084:ASN:O	1:E:1088:VAL:HG23	2.03	0.57
2:F:216:ALA:O	2:F:220:VAL:HG23	2.03	0.57
2:B:149:THR:O	2:B:151:ALA:N	2.38	0.57
1:E:921:ASP:OD2	2:F:288:LEU:HD22	2.04	0.57
1:E:1123:ARG:HH11	1:E:1123:ARG:HG2	1.70	0.57
1:A:940:LYS:HA	2:B:285:PHE:CZ	2.40	0.57
1:A:954:ILE:HD13	1:A:955:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:VAL:O	2:B:62:LEU:HB2	2.05	0.57
1:E:961:LEU:CG	1:E:962:PRO:HD2	2.34	0.57
1:E:1110:LEU:HD11	1:E:1123:ARG:HA	1.87	0.57
1:C:1110:LEU:HD11	1:C:1123:ARG:HA	1.87	0.57
1:C:1131:SER:OG	1:C:1132:MSE:HE2	2.05	0.57
2:D:92:LEU:HD22	2:D:96:GLN:HG3	1.87	0.57
1:E:1001:PHE:CE1	1:E:1048:LEU:HD21	2.40	0.57
2:B:230:VAL:O	2:B:233:LYS:HG3	2.05	0.57
2:D:59:VAL:O	2:D:62:LEU:HB2	2.05	0.57
1:E:974:THR:HG22	1:E:974:THR:O	2.04	0.57
1:A:990:VAL:HG11	1:A:1020:ILE:CD1	2.27	0.56
2:D:222:LEU:HD21	2:D:228:TYR:HE1	1.68	0.56
2:D:230:VAL:O	2:D:233:LYS:HG3	2.05	0.56
1:E:1074:LYS:HE3	1:E:1147:PHE:HE1	1.67	0.56
1:A:930:GLN:HB3	1:A:1196:GLY:O	2.05	0.56
1:A:961:LEU:CG	1:A:962:PRO:HD2	2.35	0.56
2:B:216:ALA:O	2:B:220:VAL:HG23	2.03	0.56
2:D:71:ASN:HB2	2:D:73:GLU:CD	2.25	0.56
1:E:1065:MSE:HG3	1:E:1066:LEU:N	2.19	0.56
1:E:1131:SER:OG	1:E:1132:MSE:HE2	2.05	0.56
1:A:1001:PHE:CE1	1:A:1048:LEU:HD21	2.40	0.56
1:A:1074:LYS:HE3	1:A:1147:PHE:HE1	1.70	0.56
2:B:1:MSE:HG2	2:B:2:ASP:N	2.10	0.56
2:B:72:ILE:HD12	2:B:72:ILE:N	2.18	0.56
2:D:106:LEU:O	2:D:110:VAL:HG23	2.06	0.56
2:D:252:LEU:HD21	2:D:259:GLU:HG3	1.87	0.56
2:F:35:PHE:CG	2:F:87:TYR:CD2	2.94	0.56
2:F:92:LEU:HD22	2:F:96:GLN:HG3	1.87	0.56
2:F:252:LEU:HD21	2:F:259:GLU:HG3	1.87	0.56
1:C:1123:ARG:HG2	1:C:1123:ARG:HH11	1.70	0.56
1:E:930:GLN:C	1:E:1194:ALA:HB1	2.26	0.56
2:B:252:LEU:HD21	2:B:259:GLU:HG3	1.87	0.56
1:C:983:TYR:CE2	2:D:253:MSE:HG2	2.40	0.56
1:C:1099:PHE:CD1	1:C:1134:SER:HB3	2.40	0.56
2:F:230:VAL:O	2:F:233:LYS:HG3	2.05	0.56
2:D:181:THR:CG2	2:D:182:SER:N	2.64	0.56
1:E:1083:THR:HG23	1:E:1109:PHE:CE1	2.41	0.56
1:A:1002:LYS:HZ3	1:A:1080:ILE:HD11	1.70	0.56
1:A:1123:ARG:HG2	1:A:1123:ARG:HH11	1.70	0.56
1:C:1001:PHE:CE1	1:C:1048:LEU:HD21	2.40	0.56
2:D:156:VAL:O	2:D:158:GLY:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:222:LEU:HD21	2:F:228:TYR:HE1	1.69	0.56
1:A:981:LEU:HD13	1:A:1024:MSE:CE	2.36	0.56
1:A:1083:THR:HG23	1:A:1109:PHE:CE1	2.41	0.56
1:C:974:THR:HG22	1:C:974:THR:O	2.04	0.56
1:C:1083:THR:HG23	1:C:1109:PHE:CE1	2.41	0.56
2:D:149:THR:C	2:D:151:ALA:H	2.09	0.56
1:E:1018:TYR:HE2	1:E:1187:ILE:CG1	2.18	0.56
1:A:1131:SER:OG	1:A:1132:MSE:HE2	2.05	0.56
1:C:1113:ILE:HD12	2:F:231:GLU:HB3	1.88	0.56
2:F:37:LYS:HE2	2:F:50:GLN:HE22	1.71	0.56
2:F:71:ASN:HB2	2:F:73:GLU:CD	2.25	0.56
1:A:974:THR:HG22	1:A:974:THR:O	2.04	0.56
2:B:63:TYR:HD1	2:B:91:LEU:HB3	1.70	0.56
2:B:106:LEU:O	2:B:110:VAL:HG23	2.05	0.56
2:B:270:HIS:CD2	2:B:272:HIS:HB3	2.41	0.56
1:C:954:ILE:HD13	1:C:955:PRO:HD2	1.88	0.56
1:C:1151:ALA:HB3	1:C:1173:TYR:CE2	2.41	0.56
1:A:932:GLY:O	1:A:1188:SER:HB2	2.06	0.55
2:D:270:HIS:CD2	2:D:272:HIS:HB3	2.41	0.55
1:E:1151:ALA:HB3	1:E:1173:TYR:CE2	2.41	0.55
2:B:148:TYR:O	2:B:151:ALA:HB3	2.07	0.55
1:C:1065:MSE:HG3	1:C:1066:LEU:N	2.19	0.55
1:E:954:ILE:HD13	1:E:955:PRO:HD2	1.88	0.55
2:F:106:LEU:O	2:F:110:VAL:HG23	2.06	0.55
2:B:1:MSE:CG	2:B:2:ASP:H	2.10	0.55
2:D:35:PHE:CG	2:D:87:TYR:HD2	2.23	0.55
1:E:930:GLN:O	1:E:1194:ALA:HB1	2.07	0.55
1:E:1094:PHE:C	1:E:1096:HIS:H	2.10	0.55
1:A:1065:MSE:HG3	1:A:1066:LEU:N	2.20	0.55
1:E:946:ILE:HD11	1:E:1022:LEU:HB3	1.88	0.55
1:A:1110:LEU:HD11	1:A:1123:ARG:HA	1.87	0.55
2:B:270:HIS:CG	2:B:271:GLU:H	2.25	0.55
1:A:954:ILE:HA	2:B:205:ASN:ND2	2.22	0.55
1:A:1153:THR:O	1:A:1154:TYR:CB	2.55	0.55
2:B:6:ILE:CD1	2:B:6:ILE:N	2.67	0.55
2:B:35:PHE:CG	2:B:87:TYR:HD2	2.24	0.55
1:C:1028:ALA:HA	1:C:1200:ARG:HD2	1.88	0.55
1:A:931:VAL:HG11	1:A:1168:LEU:HD13	1.89	0.54
1:A:961:LEU:HD23	1:A:962:PRO:N	2.22	0.54
2:F:149:THR:C	2:F:151:ALA:H	2.09	0.54
2:F:270:HIS:CG	2:F:271:GLU:H	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:270:HIS:CD2	2:F:272:HIS:HB3	2.41	0.54
2:D:149:THR:C	2:D:151:ALA:N	2.59	0.54
1:E:1153:THR:O	1:E:1154:TYR:CB	2.55	0.54
2:F:148:TYR:O	2:F:151:ALA:HB3	2.07	0.54
1:A:1151:ALA:HB3	1:A:1173:TYR:CE2	2.41	0.54
2:D:148:TYR:O	2:D:151:ALA:HB3	2.07	0.54
2:F:162:MSE:HE3	2:F:163:ILE:HD13	1.90	0.54
1:A:1117:PRO:CB	2:D:177:LYS:HZ1	2.18	0.54
1:C:975:VAL:O	1:C:976:SER:C	2.46	0.54
1:A:1066:LEU:HB3	1:A:1093:HIS:CE1	2.43	0.54
2:B:4:PHE:HD1	2:B:159:ASP:HB2	1.71	0.54
2:B:149:THR:C	2:B:151:ALA:H	2.09	0.54
1:C:981:LEU:HD13	1:C:1024:MSE:CE	2.38	0.54
2:D:76:GLU:OE2	2:D:104:LYS:NZ	2.40	0.54
1:E:930:GLN:HB3	1:E:1196:GLY:O	2.07	0.54
1:E:933:VAL:HG13	1:E:1187:ILE:HG23	1.90	0.54
1:E:1181:ILE:HD12	1:E:1181:ILE:N	2.22	0.54
1:C:1153:THR:O	1:C:1154:TYR:CB	2.55	0.54
2:D:270:HIS:CG	2:D:271:GLU:H	2.25	0.54
2:D:291:LYS:O	2:D:291:LYS:HG2	2.08	0.54
2:D:291:LYS:HD2	2:D:292:TYR:CE1	2.43	0.54
1:E:938:PRO:HG2	1:E:1187:ILE:HD11	1.89	0.54
1:E:1006:PRO:HG2	1:E:1007:ASP:H	1.73	0.54
1:E:1066:LEU:HB3	1:E:1093:HIS:CE1	2.43	0.54
1:A:1003:LEU:HD21	2:D:110:VAL:CG2	2.33	0.54
1:A:1006:PRO:HG2	1:A:1007:ASP:H	1.73	0.54
1:A:1065:MSE:SE	1:A:1066:LEU:HD23	2.58	0.54
1:A:1136:ALA:C	1:A:1137:ILE:HG13	2.28	0.54
2:B:291:LYS:O	2:B:291:LYS:HG2	2.07	0.54
1:C:1071:TYR:HE2	1:C:1141:PHE:HB2	1.71	0.54
1:C:1181:ILE:HD12	1:C:1181:ILE:N	2.22	0.54
1:E:952:THR:HA	2:F:249:THR:HG21	1.89	0.54
1:E:1035:HIS:O	1:E:1039:GLU:HG2	2.08	0.54
1:A:981:LEU:HB3	1:A:982:PRO:HD2	1.90	0.54
2:B:30:ASP:CB	2:B:33:LEU:HD12	2.38	0.54
1:C:1094:PHE:C	1:C:1096:HIS:H	2.10	0.54
2:F:69:THR:CB	2:F:71:ASN:OD1	2.56	0.54
2:F:149:THR:C	2:F:151:ALA:N	2.60	0.54
1:C:1035:HIS:O	1:C:1039:GLU:HG2	2.08	0.54
2:D:30:ASP:CB	2:D:33:LEU:HD12	2.37	0.54
2:D:37:LYS:HE2	2:D:50:GLN:HE22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:166:LEU:O	2:D:169:SER:HB3	2.08	0.54
1:E:961:LEU:HD23	1:E:962:PRO:N	2.23	0.54
1:A:1025:VAL:CG1	1:A:1030:ASP:HB2	2.31	0.53
1:A:1071:TYR:HE2	1:A:1141:PHE:HB2	1.73	0.53
1:C:1066:LEU:HB3	1:C:1093:HIS:CE1	2.43	0.53
1:C:1113:ILE:HD11	2:F:227:TYR:CD1	2.43	0.53
1:E:981:LEU:HB3	1:E:982:PRO:HD2	1.90	0.53
2:F:35:PHE:CG	2:F:87:TYR:HD2	2.24	0.53
1:A:1094:PHE:C	1:A:1096:HIS:H	2.10	0.53
2:B:162:MSE:HE3	2:B:163:ILE:HD13	1.90	0.53
1:C:1006:PRO:HG2	1:C:1007:ASP:H	1.73	0.53
1:E:975:VAL:O	1:E:976:SER:C	2.45	0.53
1:E:1025:VAL:HG23	1:E:1199:ILE:CG2	2.39	0.53
1:E:1189:LYS:CE	1:E:1192:ALA:HB2	2.36	0.53
2:F:166:LEU:O	2:F:169:SER:HB3	2.08	0.53
1:A:966:GLY:HA3	2:B:173:PHE:CZ	2.43	0.53
1:A:1035:HIS:O	1:A:1039:GLU:HG2	2.08	0.53
2:D:162:MSE:HE3	2:D:163:ILE:HD13	1.90	0.53
2:D:222:LEU:CD2	2:D:228:TYR:CE1	2.92	0.53
2:B:222:LEU:CD2	2:B:228:TYR:CE1	2.92	0.53
2:D:4:PHE:HD1	2:D:159:ASP:HB2	1.73	0.53
2:D:44:LEU:O	2:D:45:GLY:C	2.46	0.53
2:D:102:LEU:HD13	2:D:135:ASN:HB2	1.91	0.53
1:E:974:THR:O	1:E:975:VAL:HG23	2.08	0.53
1:E:994:MSE:HE2	1:E:1013:PHE:HD2	1.73	0.53
1:E:1018:TYR:HE2	1:E:1187:ILE:HG12	1.73	0.53
1:E:1065:MSE:SE	1:E:1066:LEU:HD23	2.58	0.53
1:A:962:PRO:HG2	2:B:134:LEU:CD1	2.38	0.53
1:A:974:THR:O	1:A:975:VAL:HG23	2.08	0.53
1:C:974:THR:O	1:C:975:VAL:HG23	2.08	0.53
1:C:998:TYR:HD1	1:C:998:TYR:N	2.07	0.53
1:C:1123:ARG:HG2	1:C:1123:ARG:NH1	2.24	0.53
1:E:1099:PHE:HB3	1:E:1129:ALA:HB1	1.91	0.53
1:A:962:PRO:HG2	2:B:134:LEU:HD11	1.89	0.53
1:A:971:TYR:HA	2:B:211:ARG:HH21	1.71	0.53
1:A:1189:LYS:CE	1:A:1192:ALA:HB2	2.36	0.53
2:B:149:THR:C	2:B:151:ALA:N	2.60	0.53
1:C:961:LEU:HD23	1:C:962:PRO:N	2.23	0.53
2:F:14:ASN:O	2:F:14:ASN:ND2	2.37	0.53
2:F:291:LYS:O	2:F:291:LYS:HG2	2.08	0.53
2:B:227:TYR:HA	2:B:231:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1099:PHE:HB3	1:C:1129:ALA:HB1	1.91	0.53
2:D:157:SER:C	2:D:159:ASP:H	2.13	0.53
1:E:998:TYR:N	1:E:998:TYR:HD1	2.07	0.53
1:E:1045:ILE:CD1	1:E:1184:ILE:HG23	2.37	0.53
1:A:904:TRP:CH2	1:A:982:PRO:HB3	2.44	0.53
1:A:975:VAL:O	1:A:976:SER:C	2.45	0.53
2:F:227:TYR:HA	2:F:231:GLU:HG3	1.91	0.53
1:A:1025:VAL:HG12	1:A:1026:ASP:N	2.24	0.53
1:A:1090:MSE:CE	1:A:1106:ALA:HA	2.21	0.53
1:C:1147:PHE:CD1	1:C:1147:PHE:C	2.82	0.53
1:A:931:VAL:HG12	1:A:933:VAL:HG23	1.91	0.52
1:A:998:TYR:N	1:A:998:TYR:CD1	2.77	0.52
1:A:1181:ILE:HD12	1:A:1181:ILE:N	2.22	0.52
1:C:1136:ALA:C	1:C:1137:ILE:HG13	2.28	0.52
1:E:1002:LYS:HZ1	1:E:1080:ILE:HD11	1.73	0.52
1:E:1132:MSE:O	1:E:1134:SER:N	2.42	0.52
2:F:135:ASN:O	2:F:136:ASN:HB2	2.09	0.52
2:B:35:PHE:CG	2:B:87:TYR:CD2	2.97	0.52
1:C:1065:MSE:SE	1:C:1066:LEU:HD23	2.59	0.52
2:D:231:GLU:HB3	1:E:1113:ILE:CD1	2.38	0.52
1:E:1075:ALA:O	1:E:1077:LEU:HG	2.09	0.52
1:A:998:TYR:N	1:A:998:TYR:HD1	2.07	0.52
1:A:1101:GLN:O	1:A:1104:TYR:HB3	2.09	0.52
1:C:1025:VAL:HG12	1:C:1026:ASP:N	2.24	0.52
1:C:1101:GLN:O	1:C:1104:TYR:HB3	2.10	0.52
2:D:178:GLU:OE1	2:D:182:SER:HB3	2.10	0.52
1:E:961:LEU:CD2	1:E:962:PRO:HD2	2.39	0.52
1:A:961:LEU:CD2	1:A:962:PRO:HD2	2.39	0.52
1:C:1042:ARG:HD3	1:C:1169:THR:HG22	1.90	0.52
2:D:157:SER:C	2:D:159:ASP:N	2.63	0.52
1:E:1029:GLU:O	1:E:1032:LYS:HB3	2.10	0.52
1:E:1136:ALA:C	1:E:1137:ILE:HG13	2.28	0.52
1:A:1075:ALA:O	1:A:1077:LEU:HG	2.10	0.52
1:C:961:LEU:CD2	1:C:962:PRO:HD2	2.39	0.52
1:C:998:TYR:N	1:C:998:TYR:CD1	2.77	0.52
1:C:1147:PHE:HD1	1:C:1147:PHE:C	2.13	0.52
2:D:222:LEU:CD2	2:D:228:TYR:HE1	2.22	0.52
1:E:1008:ILE:HD12	1:E:1008:ILE:N	2.25	0.52
2:F:222:LEU:CD2	2:F:228:TYR:HE1	2.23	0.52
1:A:1073:THR:HG23	1:A:1086:LEU:CD2	2.40	0.52
1:C:1073:THR:HG23	1:C:1086:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1147:PHE:CD1	1:E:1147:PHE:C	2.83	0.52
2:F:178:GLU:OE1	2:F:182:SER:HB3	2.10	0.52
1:A:938:PRO:HG2	1:A:1187:ILE:HD11	1.92	0.52
2:B:166:LEU:O	2:B:169:SER:HB3	2.08	0.52
2:B:181:THR:CG2	2:B:182:SER:H	2.07	0.52
2:B:260:ASP:O	2:B:262:THR:N	2.43	0.52
1:C:974:THR:O	1:C:975:VAL:CG2	2.58	0.52
1:C:1075:ALA:O	1:C:1077:LEU:HG	2.09	0.52
2:D:87:TYR:CE1	2:D:120:GLY:CA	2.92	0.52
2:D:112:GLY:HA2	2:D:115:ASN:OD1	2.09	0.52
2:D:135:ASN:O	2:D:136:ASN:HB2	2.10	0.52
2:D:158:GLY:O	2:D:159:ASP:HB3	2.10	0.52
1:E:920:PHE:CD2	2:F:285:PHE:HD1	2.28	0.52
2:F:222:LEU:CD2	2:F:228:TYR:CE1	2.92	0.52
1:A:994:MSE:HE2	1:A:1013:PHE:HD2	1.73	0.52
1:A:1118:ARG:NH2	2:D:143:THR:HA	2.25	0.52
1:A:1123:ARG:HG2	1:A:1123:ARG:NH1	2.24	0.52
1:A:1147:PHE:CD1	1:A:1147:PHE:C	2.82	0.52
2:D:227:TYR:CE2	1:E:1080:ILE:HB	2.45	0.52
1:E:1094:PHE:HE1	1:E:1129:ALA:HB2	1.75	0.52
2:F:158:GLY:O	2:F:159:ASP:HB3	2.10	0.52
1:A:974:THR:O	1:A:975:VAL:CG2	2.58	0.52
1:C:1132:MSE:O	1:C:1134:SER:N	2.43	0.52
2:D:227:TYR:HA	2:D:231:GLU:HG3	1.91	0.52
1:E:974:THR:O	1:E:975:VAL:CG2	2.58	0.52
1:E:1109:PHE:HZ	1:E:1118:ARG:HD3	1.75	0.52
2:F:56:LEU:O	2:F:59:VAL:HB	2.10	0.52
1:A:989:VAL:O	1:A:990:VAL:C	2.48	0.52
2:B:135:ASN:O	2:B:136:ASN:HB2	2.09	0.52
1:C:981:LEU:HB3	1:C:982:PRO:HD2	1.90	0.52
2:F:30:ASP:CB	2:F:33:LEU:HD12	2.38	0.52
1:A:1094:PHE:HE1	1:A:1129:ALA:HB2	1.75	0.51
1:A:1099:PHE:HB3	1:A:1129:ALA:HB1	1.91	0.51
1:C:987:LEU:HD23	1:C:1033:LEU:HD22	1.92	0.51
1:C:1094:PHE:HE1	1:C:1129:ALA:HB2	1.75	0.51
2:D:260:ASP:O	2:D:262:THR:N	2.43	0.51
1:A:1018:TYR:HE2	1:A:1187:ILE:HG12	1.74	0.51
1:A:1029:GLU:O	1:A:1032:LYS:HB3	2.10	0.51
2:B:222:LEU:CD2	2:B:228:TYR:HE1	2.23	0.51
2:B:241:PRO:HG2	2:B:242:THR:H	1.75	0.51
1:C:931:VAL:HG12	1:C:933:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:LEU:O	2:D:59:VAL:HB	2.10	0.51
1:E:904:TRP:CZ2	1:E:982:PRO:HB3	2.45	0.51
1:E:1073:THR:HG23	1:E:1086:LEU:CD2	2.39	0.51
2:D:54:SER:O	2:D:56:LEU:N	2.37	0.51
1:A:987:LEU:HD23	1:A:1033:LEU:HD22	1.92	0.51
1:A:994:MSE:HE1	1:A:1013:PHE:CD2	2.45	0.51
1:A:1097:LYS:O	1:A:1097:LYS:HG2	2.10	0.51
2:B:96:GLN:O	2:B:99:LEU:HB2	2.10	0.51
2:B:178:GLU:OE1	2:B:182:SER:HB3	2.10	0.51
1:C:994:MSE:HE2	1:C:1013:PHE:HD2	1.74	0.51
1:C:1097:LYS:O	1:C:1097:LYS:HG2	2.10	0.51
1:E:998:TYR:N	1:E:998:TYR:CD1	2.77	0.51
1:E:1097:LYS:O	1:E:1097:LYS:HG2	2.10	0.51
2:F:241:PRO:HG2	2:F:242:THR:H	1.75	0.51
1:A:1008:ILE:HD12	1:A:1008:ILE:N	2.25	0.51
1:A:1045:ILE:CD1	1:A:1184:ILE:HG23	2.36	0.51
1:A:1109:PHE:HZ	1:A:1118:ARG:HD3	1.75	0.51
2:D:96:GLN:O	2:D:99:LEU:HB2	2.11	0.51
1:E:1020:ILE:O	1:E:1023:LEU:HB2	2.11	0.51
1:E:1025:VAL:HG12	1:E:1026:ASP:N	2.25	0.51
2:F:1:MSE:CG	2:F:2:ASP:H	2.10	0.51
2:F:260:ASP:O	2:F:262:THR:N	2.43	0.51
2:B:222:LEU:HD23	2:B:222:LEU:C	2.30	0.51
2:B:291:LYS:HD2	2:B:292:TYR:CE1	2.46	0.51
2:D:86:PRO:HG2	2:D:119:GLU:O	2.10	0.51
2:D:222:LEU:HD23	2:D:222:LEU:C	2.31	0.51
1:E:1101:GLN:O	1:E:1104:TYR:HB3	2.09	0.51
1:E:1147:PHE:HD1	1:E:1147:PHE:C	2.13	0.51
1:A:983:TYR:HE2	2:B:253:MSE:HG2	1.72	0.51
2:B:54:SER:C	2:B:56:LEU:N	2.64	0.51
1:C:928:SER:O	1:C:932:GLY:HA2	2.11	0.51
1:C:950:CYS:O	1:C:968:VAL:HG23	2.11	0.51
1:C:994:MSE:HE1	1:C:1013:PHE:CD2	2.45	0.51
2:D:231:GLU:OE2	1:E:1118:ARG:NH1	2.44	0.51
2:F:222:LEU:HD23	2:F:222:LEU:C	2.31	0.51
1:A:1020:ILE:HD13	1:A:1023:LEU:HD12	1.93	0.51
1:A:1113:ILE:CD1	2:D:150:ASN:ND2	2.73	0.51
2:B:56:LEU:O	2:B:59:VAL:HB	2.10	0.51
2:D:25:PHE:O	2:D:26:SER:C	2.50	0.51
1:E:928:SER:O	1:E:932:GLY:HA2	2.11	0.51
1:E:931:VAL:HG12	1:E:933:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:987:LEU:HD23	1:E:1033:LEU:HD22	1.92	0.51
1:E:989:VAL:O	1:E:990:VAL:C	2.48	0.51
1:E:993:LYS:HG2	1:E:1015:GLU:HG2	1.93	0.51
1:A:947:TYR:CE1	1:A:951:ARG:NH2	2.79	0.50
1:A:993:LYS:HG2	1:A:1015:GLU:HG2	1.93	0.50
1:C:987:LEU:O	1:C:988:ASP:C	2.49	0.50
1:C:1020:ILE:HD13	1:C:1023:LEU:HD12	1.94	0.50
1:C:1020:ILE:O	1:C:1023:LEU:HB2	2.12	0.50
1:E:1123:ARG:HG2	1:E:1123:ARG:NH1	2.24	0.50
2:F:197:TRP:O	2:F:201:LEU:HB2	2.10	0.50
1:A:928:SER:O	1:A:932:GLY:HA2	2.11	0.50
2:B:197:TRP:O	2:B:201:LEU:HB2	2.10	0.50
2:D:97:ALA:HB2	2:D:105:SER:OG	2.11	0.50
2:D:241:PRO:HG2	2:D:242:THR:H	1.75	0.50
2:F:41:LEU:HD13	2:F:46:GLN:O	2.11	0.50
1:A:0:MSE:CE	2:B:138:VAL:HG21	2.41	0.50
1:A:950:CYS:O	1:A:968:VAL:HG23	2.11	0.50
1:A:952:THR:HA	2:B:249:THR:HG21	1.94	0.50
1:A:971:TYR:HA	2:B:211:ARG:NH2	2.25	0.50
1:C:932:GLY:O	1:C:1188:SER:HB2	2.10	0.50
1:C:989:VAL:O	1:C:990:VAL:C	2.48	0.50
1:E:950:CYS:O	1:E:968:VAL:HG23	2.11	0.50
1:E:994:MSE:HE1	1:E:1013:PHE:CD2	2.45	0.50
2:F:42:LEU:HD21	2:F:64:VAL:HG13	1.94	0.50
1:C:1180:LYS:O	1:C:1190:ILE:HG13	2.11	0.50
1:E:983:TYR:HE2	2:F:253:MSE:HG2	1.70	0.50
2:F:159:ASP:OD1	2:F:160:ASN:N	2.45	0.50
1:A:1147:PHE:HD1	1:A:1147:PHE:C	2.13	0.50
1:C:1029:GLU:O	1:C:1032:LYS:HB3	2.10	0.50
1:C:1079:PRO:O	1:C:1082:ARG:N	2.45	0.50
2:D:197:TRP:O	2:D:201:LEU:HB2	2.11	0.50
1:E:961:LEU:HD23	1:E:962:PRO:HD2	1.94	0.50
1:A:987:LEU:O	1:A:988:ASP:C	2.49	0.50
1:A:1003:LEU:HD21	2:D:106:LEU:HD22	1.94	0.50
2:B:158:GLY:O	2:B:159:ASP:HB3	2.10	0.50
1:C:931:VAL:HG11	1:C:1168:LEU:HD13	1.94	0.50
2:F:96:GLN:O	2:F:99:LEU:HB2	2.11	0.50
2:F:157:SER:O	2:F:159:ASP:N	2.45	0.50
1:A:961:LEU:HD23	1:A:962:PRO:HD2	1.94	0.50
2:B:72:ILE:H	2:B:72:ILE:CD1	2.03	0.50
1:C:993:LYS:HG2	1:C:1015:GLU:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:227:TYR:CD1	1:E:1113:ILE:HD11	2.47	0.50
1:E:987:LEU:O	1:E:988:ASP:C	2.49	0.50
1:A:1079:PRO:O	1:A:1082:ARG:N	2.45	0.50
1:A:1126:LYS:O	1:A:1130:ASP:HB2	2.12	0.50
1:C:1008:ILE:HD12	1:C:1008:ILE:N	2.25	0.50
1:C:1083:THR:CG2	1:C:1118:ARG:NH1	2.67	0.50
1:C:1109:PHE:HZ	1:C:1118:ARG:HD3	1.75	0.50
2:D:184:PHE:CE2	2:D:188:GLU:HG3	2.47	0.50
2:D:213:ILE:HG13	2:D:214:ALA:N	2.26	0.50
2:F:213:ILE:HG13	2:F:214:ALA:N	2.27	0.50
2:B:97:ALA:HB2	2:B:105:SER:OG	2.11	0.49
2:B:263:ASN:C	2:B:263:ASN:OD1	2.50	0.49
1:C:939:LEU:HD13	1:C:1187:ILE:CD1	2.41	0.49
1:C:1090:MSE:CE	1:C:1106:ALA:HA	2.21	0.49
1:E:1126:LYS:O	1:E:1130:ASP:HB2	2.12	0.49
2:F:97:ALA:HB2	2:F:105:SER:OG	2.11	0.49
2:F:258:THR:O	2:F:259:GLU:C	2.50	0.49
1:A:1045:ILE:HB	1:A:1184:ILE:CD1	2.41	0.49
2:B:25:PHE:O	2:B:26:SER:C	2.50	0.49
2:D:159:ASP:OD1	2:D:160:ASN:N	2.45	0.49
2:D:277:HIS:O	2:D:281:ILE:HG22	2.13	0.49
2:F:54:SER:C	2:F:56:LEU:N	2.64	0.49
1:A:1020:ILE:O	1:A:1023:LEU:HB2	2.11	0.49
1:A:1180:LYS:O	1:A:1190:ILE:HG13	2.12	0.49
2:B:156:VAL:HG12	2:B:156:VAL:O	2.13	0.49
1:C:938:PRO:HG2	1:C:1187:ILE:HD11	1.93	0.49
1:C:1126:LYS:O	1:C:1130:ASP:HB2	2.12	0.49
1:E:1079:PRO:O	1:E:1082:ARG:N	2.45	0.49
2:F:184:PHE:CE2	2:F:188:GLU:HG3	2.47	0.49
2:F:242:THR:O	2:F:245:ALA:HB3	2.12	0.49
2:B:102:LEU:HD13	2:B:135:ASN:HB2	1.95	0.49
1:C:947:TYR:CE1	1:C:951:ARG:CZ	2.96	0.49
1:C:1002:LYS:HZ3	1:C:1080:ILE:HD11	1.76	0.49
1:C:1093:HIS:O	1:C:1102:ALA:HB2	2.13	0.49
2:D:263:ASN:C	2:D:263:ASN:OD1	2.51	0.49
1:E:1060:GLY:C	1:E:1062:THR:H	2.16	0.49
1:E:1180:LYS:O	1:E:1190:ILE:HG13	2.12	0.49
2:F:263:ASN:OD1	2:F:263:ASN:C	2.51	0.49
1:A:1060:GLY:C	1:A:1062:THR:H	2.16	0.49
2:D:54:SER:C	2:D:56:LEU:N	2.65	0.49
1:E:1051:GLU:O	1:E:1055:ARG:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:LYS:HE3	1:A:1147:PHE:CD1	2.48	0.49
2:B:37:LYS:HE2	2:B:50:GLN:HE22	1.77	0.49
2:B:184:PHE:CE2	2:B:188:GLU:HG3	2.47	0.49
2:B:184:PHE:HD2	2:B:184:PHE:O	1.95	0.49
2:B:277:HIS:O	2:B:281:ILE:HG22	2.13	0.49
2:D:72:ILE:CG1	2:D:99:LEU:HD11	2.43	0.49
2:D:156:VAL:O	2:D:156:VAL:HG12	2.13	0.49
1:E:1020:ILE:HD13	1:E:1023:LEU:HD12	1.93	0.49
1:E:1025:VAL:O	1:E:1201:VAL:HG23	2.12	0.49
1:A:947:TYR:CE1	1:A:951:ARG:CZ	2.96	0.49
2:B:159:ASP:OD1	2:B:160:ASN:N	2.46	0.49
2:B:213:ILE:HG13	2:B:214:ALA:N	2.26	0.49
2:B:258:THR:O	2:B:259:GLU:C	2.50	0.49
1:E:1071:TYR:CE2	1:E:1141:PHE:HB2	2.47	0.49
1:E:1083:THR:HG22	1:E:1084:ASN:N	2.28	0.49
1:A:954:ILE:HA	2:B:205:ASN:HD21	1.78	0.49
1:A:1051:GLU:O	1:A:1055:ARG:HG3	2.13	0.49
1:A:1109:PHE:HZ	1:A:1118:ARG:CD	2.26	0.49
1:C:954:ILE:HA	2:D:205:ASN:HD21	1.76	0.49
1:C:1189:LYS:CE	1:C:1192:ALA:HB2	2.36	0.49
1:E:1028:ALA:HB2	1:E:1200:ARG:NH1	2.26	0.49
1:A:1161:THR:HG23	1:A:1162:PRO:HD2	1.95	0.48
1:C:1161:THR:HG23	1:C:1162:PRO:HD2	1.95	0.48
2:F:54:SER:O	2:F:56:LEU:N	2.37	0.48
2:F:184:PHE:HD2	2:F:184:PHE:O	1.95	0.48
1:A:1083:THR:HG22	1:A:1084:ASN:N	2.28	0.48
2:B:117:GLU:O	2:B:119:GLU:N	2.33	0.48
2:B:242:THR:O	2:B:245:ALA:HB3	2.13	0.48
1:C:904:TRP:CH2	1:C:982:PRO:HB3	2.48	0.48
2:D:184:PHE:HD2	2:D:184:PHE:O	1.95	0.48
1:E:1074:LYS:HE3	1:E:1147:PHE:CD1	2.48	0.48
1:E:1093:HIS:O	1:E:1102:ALA:HB2	2.12	0.48
2:F:15:PHE:HB3	2:F:40:THR:CG2	2.43	0.48
2:F:102:LEU:HD13	2:F:135:ASN:HB2	1.94	0.48
2:B:15:PHE:HB3	2:B:40:THR:CG2	2.43	0.48
2:B:18:CYS:O	2:B:22:ILE:HG13	2.13	0.48
2:B:272:HIS:O	2:B:273:ALA:C	2.52	0.48
2:D:242:THR:O	2:D:245:ALA:HB3	2.12	0.48
1:E:920:PHE:HB3	2:F:288:LEU:HD12	1.95	0.48
2:F:156:VAL:C	2:F:158:GLY:N	2.66	0.48
1:A:940:LYS:CB	2:B:285:PHE:CE2	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1028:ALA:CB	1:C:1200:ARG:NH1	2.65	0.48
2:F:277:HIS:O	2:F:281:ILE:HG22	2.13	0.48
2:B:284:LYS:O	2:B:287:GLU:HB3	2.14	0.48
1:C:947:TYR:CE1	1:C:951:ARG:NH2	2.81	0.48
2:D:258:THR:O	2:D:259:GLU:C	2.50	0.48
1:E:1073:THR:HG23	1:E:1086:LEU:HD23	1.95	0.48
1:E:1109:PHE:HZ	1:E:1118:ARG:CD	2.26	0.48
1:E:1164:VAL:HG22	1:E:1175:ILE:HD13	1.96	0.48
2:F:269:ASP:OD1	2:F:269:ASP:C	2.52	0.48
2:F:272:HIS:O	2:F:273:ALA:C	2.52	0.48
1:C:1004:ASN:CG	1:C:1004:ASN:O	2.52	0.48
1:C:1083:THR:HG22	1:C:1084:ASN:N	2.28	0.48
2:D:15:PHE:HB3	2:D:40:THR:CG2	2.43	0.48
2:D:269:ASP:OD1	2:D:269:ASP:C	2.52	0.48
1:E:1109:PHE:C	1:E:1109:PHE:CD2	2.87	0.48
2:F:25:PHE:O	2:F:26:SER:C	2.50	0.48
1:A:1109:PHE:C	1:A:1109:PHE:CD2	2.87	0.48
2:B:72:ILE:HG13	2:B:99:LEU:HD11	1.94	0.48
2:D:14:ASN:O	2:D:14:ASN:ND2	2.37	0.48
2:D:85:SER:HB3	2:D:88:GLU:OE2	2.14	0.48
2:D:156:VAL:C	2:D:158:GLY:N	2.64	0.48
1:A:1093:HIS:O	1:A:1102:ALA:HB2	2.13	0.48
2:B:73:GLU:HB2	2:B:74:GLU:H	1.56	0.48
1:C:952:THR:HA	2:D:249:THR:HG21	1.96	0.48
1:C:1109:PHE:C	1:C:1109:PHE:CD2	2.87	0.48
1:C:1109:PHE:HZ	1:C:1118:ARG:CD	2.26	0.48
2:F:72:ILE:HG13	2:F:99:LEU:HD11	1.96	0.48
1:A:1164:VAL:HG22	1:A:1175:ILE:HD13	1.96	0.47
1:C:1104:TYR:CZ	1:C:1143:PRO:HB3	2.48	0.47
2:D:272:HIS:O	2:D:273:ALA:C	2.52	0.47
1:E:1004:ASN:O	1:E:1004:ASN:CG	2.52	0.47
2:F:18:CYS:O	2:F:22:ILE:HG13	2.13	0.47
1:A:1070:ALA:O	1:A:1073:THR:HB	2.14	0.47
2:B:232:GLN:O	2:B:234:GLU:N	2.47	0.47
1:C:1067:GLU:HG2	1:C:1071:TYR:CE1	2.50	0.47
1:C:1073:THR:HG23	1:C:1086:LEU:HD23	1.95	0.47
1:C:1164:VAL:HG22	1:C:1175:ILE:HD13	1.96	0.47
1:E:970:ALA:HB2	1:E:982:PRO:O	2.14	0.47
2:F:232:GLN:O	2:F:234:GLU:N	2.47	0.47
1:A:1067:GLU:HG2	1:A:1071:TYR:CE1	2.49	0.47
1:C:1051:GLU:O	1:C:1055:ARG:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:904:TRP:CD2	1:E:982:PRO:HD3	2.50	0.47
1:E:946:ILE:CD1	1:E:1022:LEU:HB3	2.44	0.47
2:F:206:LEU:HD13	2:F:206:LEU:HA	1.67	0.47
1:A:1004:ASN:CG	1:A:1004:ASN:O	2.51	0.47
1:A:1083:THR:CG2	1:A:1118:ARG:NH1	2.68	0.47
2:F:187:TYR:O	2:F:188:GLU:C	2.53	0.47
2:F:284:LYS:O	2:F:287:GLU:HB3	2.14	0.47
1:A:1018:TYR:CE2	1:A:1187:ILE:CG1	2.95	0.47
2:B:54:SER:O	2:B:56:LEU:N	2.36	0.47
2:F:288:LEU:O	2:F:292:TYR:HD1	1.98	0.47
1:A:969:ARG:O	2:B:211:ARG:NE	2.42	0.47
1:A:1113:ILE:CG2	1:A:1119:ALA:HB2	2.45	0.47
1:C:1087:GLN:OE1	1:C:1118:ARG:HG3	2.15	0.47
1:C:1109:PHE:CE1	1:C:1118:ARG:HD3	2.49	0.47
1:E:1070:ALA:O	1:E:1073:THR:HB	2.14	0.47
1:E:1087:GLN:OE1	1:E:1118:ARG:HG3	2.15	0.47
2:F:156:VAL:O	2:F:156:VAL:HG12	2.13	0.47
2:F:267:LYS:O	2:F:269:ASP:N	2.45	0.47
1:A:954:ILE:HG22	1:A:964:GLN:HB2	1.97	0.47
1:A:970:ALA:HB2	1:A:982:PRO:O	2.14	0.47
1:A:1025:VAL:O	1:A:1201:VAL:HG23	2.15	0.47
2:B:66:PHE:CE1	2:B:72:ILE:HG23	2.50	0.47
1:C:910:LEU:HB2	1:C:911:PRO:CD	2.45	0.47
1:C:970:ALA:HB2	1:C:982:PRO:O	2.14	0.47
1:C:994:MSE:CE	1:C:1013:PHE:HA	2.45	0.47
1:C:1070:ALA:O	1:C:1073:THR:HB	2.14	0.47
2:D:87:TYR:CE1	2:D:120:GLY:HA3	2.50	0.47
2:D:267:LYS:O	2:D:269:ASP:N	2.45	0.47
1:E:1161:THR:HG23	1:E:1162:PRO:HD2	1.95	0.47
2:F:159:ASP:O	2:F:162:MSE:CE	2.62	0.47
1:A:1109:PHE:CE1	1:A:1118:ARG:HD3	2.50	0.47
1:C:1060:GLY:C	1:C:1062:THR:H	2.16	0.47
2:B:269:ASP:C	2:B:269:ASP:OD1	2.52	0.47
1:C:954:ILE:HG22	1:C:964:GLN:HB2	1.96	0.47
2:D:232:GLN:O	2:D:234:GLU:N	2.47	0.47
2:D:284:LYS:O	2:D:287:GLU:HB3	2.14	0.47
1:E:1067:GLU:HG2	1:E:1071:TYR:CE1	2.49	0.47
1:E:1109:PHE:CE1	1:E:1118:ARG:HD3	2.50	0.47
1:A:994:MSE:CE	1:A:1013:PHE:HA	2.45	0.47
1:E:994:MSE:CE	1:E:1013:PHE:HA	2.45	0.47
1:E:1018:TYR:CE2	1:E:1187:ILE:CG1	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:LEU:HD11	1:A:1133:ALA:HB1	1.97	0.46
2:B:187:TYR:O	2:B:188:GLU:C	2.53	0.46
2:D:18:CYS:O	2:D:22:ILE:HG13	2.13	0.46
2:D:187:TYR:O	2:D:188:GLU:C	2.53	0.46
1:A:1073:THR:HG23	1:A:1086:LEU:HD23	1.95	0.46
1:C:911:PRO:O	1:C:915:VAL:HG23	2.15	0.46
1:C:1128:LYS:O	1:C:1132:MSE:HE3	2.16	0.46
1:E:921:ASP:HA	2:F:288:LEU:HD13	1.97	0.46
2:F:157:SER:C	2:F:159:ASP:H	2.19	0.46
1:A:1087:GLN:OE1	1:A:1118:ARG:HG3	2.15	0.46
2:B:14:ASN:O	2:B:14:ASN:ND2	2.37	0.46
2:D:76:GLU:CD	2:D:104:LYS:NZ	2.68	0.46
1:E:1121:GLN:O	1:E:1125:ILE:HG12	2.15	0.46
1:A:904:TRP:CZ3	1:A:982:PRO:HB3	2.50	0.46
2:B:117:GLU:C	2:B:119:GLU:H	2.17	0.46
1:C:1113:ILE:HD11	2:F:227:TYR:HD1	1.81	0.46
1:C:1113:ILE:CG2	1:C:1119:ALA:HB2	2.45	0.46
2:D:49:SER:HB2	2:D:61:ASP:OD2	2.15	0.46
1:E:1042:ARG:HB3	1:E:1169:THR:HG23	1.98	0.46
1:A:911:PRO:O	1:A:912:ALA:C	2.54	0.46
1:A:911:PRO:O	1:A:915:VAL:HG23	2.15	0.46
2:B:156:VAL:C	2:B:158:GLY:H	2.19	0.46
1:C:911:PRO:O	1:C:912:ALA:C	2.54	0.46
1:E:987:LEU:HA	1:E:990:VAL:HG23	1.98	0.46
1:E:1113:ILE:CG2	1:E:1119:ALA:HB2	2.45	0.46
1:E:1128:LYS:O	1:E:1132:MSE:HE3	2.16	0.46
2:B:211:ARG:HH11	2:B:211:ARG:CG	2.29	0.46
2:B:267:LYS:O	2:B:269:ASP:N	2.45	0.46
1:C:981:LEU:HD13	1:C:1024:MSE:HE2	1.98	0.46
1:E:911:PRO:O	1:E:915:VAL:HG23	2.15	0.46
1:E:1045:ILE:HB	1:E:1184:ILE:CD1	2.42	0.46
1:A:930:GLN:C	1:A:1194:ALA:HB1	2.36	0.46
1:A:1050:ILE:HD11	1:A:1149:ILE:HG21	1.97	0.46
2:B:48:GLN:O	2:B:49:SER:C	2.54	0.46
2:D:69:THR:HB	2:D:71:ASN:OD1	2.15	0.46
1:E:1083:THR:CG2	1:E:1118:ARG:NH1	2.67	0.46
1:A:1128:LYS:O	1:A:1132:MSE:HE3	2.16	0.46
1:C:1121:GLN:O	1:C:1125:ILE:HG12	2.16	0.46
1:E:1033:LEU:CD2	1:E:1037:ILE:HG13	2.44	0.46
1:E:1100:LEU:HD11	1:E:1133:ALA:HB1	1.97	0.46
1:A:987:LEU:HA	1:A:990:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:VAL:HG23	1:A:1199:ILE:CG2	2.45	0.46
1:A:1162:PRO:HB2	1:A:1175:ILE:CG1	2.45	0.46
2:B:49:SER:HB2	2:B:61:ASP:OD2	2.16	0.46
1:C:903:ILE:O	1:C:907:ASN:HB2	2.16	0.46
1:C:1042:ARG:HB3	1:C:1169:THR:HG23	1.98	0.46
1:C:1142:ASP:OD1	1:C:1145:ALA:HB3	2.16	0.46
1:C:1162:PRO:HB2	1:C:1175:ILE:CG1	2.45	0.46
2:D:124:LEU:HA	2:D:124:LEU:HD23	1.77	0.46
1:E:903:ILE:O	1:E:907:ASN:HB2	2.16	0.46
2:F:48:GLN:O	2:F:49:SER:C	2.54	0.46
1:A:1084:ASN:HD21	2:D:143:THR:CG2	2.28	0.46
2:B:260:ASP:C	2:B:262:THR:N	2.70	0.46
1:C:1033:LEU:CD2	1:C:1037:ILE:HG13	2.44	0.46
1:A:903:ILE:O	1:A:907:ASN:HB2	2.16	0.45
1:A:1142:ASP:OD1	1:A:1145:ALA:HB3	2.16	0.45
2:D:260:ASP:C	2:D:262:THR:N	2.70	0.45
1:E:954:ILE:HG22	1:E:964:GLN:HB2	1.97	0.45
2:D:197:TRP:CH2	2:D:223:LEU:HD22	2.52	0.45
1:E:1166:ASP:HA	1:E:1167:PRO:HD2	1.78	0.45
2:F:197:TRP:CH2	2:F:223:LEU:HD22	2.51	0.45
1:C:1113:ILE:CD1	2:F:231:GLU:HB3	2.47	0.45
2:D:1:MSE:O	2:D:2:ASP:HB2	2.17	0.45
1:E:910:LEU:HB2	1:E:911:PRO:CD	2.45	0.45
1:E:1142:ASP:OD1	1:E:1145:ALA:HB3	2.16	0.45
1:E:1191:GLY:O	1:E:1192:ALA:C	2.55	0.45
2:F:109:CYS:O	2:F:124:LEU:HD13	2.17	0.45
1:A:1042:ARG:HB3	1:A:1169:THR:HG23	1.97	0.45
1:A:1121:GLN:O	1:A:1125:ILE:HG12	2.15	0.45
1:A:1191:GLY:O	1:A:1192:ALA:C	2.55	0.45
2:F:62:LEU:HB3	2:F:75:LEU:HG	1.98	0.45
2:F:129:ILE:HD12	2:F:129:ILE:N	2.32	0.45
2:F:260:ASP:O	2:F:264:GLN:HG2	2.17	0.45
1:A:974:THR:C	1:A:975:VAL:HG23	2.37	0.45
2:B:117:GLU:OE2	2:B:152:ILE:CD1	2.65	0.45
2:B:129:ILE:HD12	2:B:129:ILE:N	2.31	0.45
1:C:961:LEU:HD23	1:C:962:PRO:HD2	1.94	0.45
2:D:1:MSE:CG	2:D:2:ASP:H	2.11	0.45
1:E:1075:ALA:O	1:E:1077:LEU:N	2.50	0.45
2:F:62:LEU:HD13	2:F:75:LEU:HA	1.99	0.45
1:A:910:LEU:HB2	1:A:911:PRO:CD	2.45	0.45
1:A:1002:LYS:NZ	2:D:147:ASN:CB	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:ALA:HB2	1:A:1200:ARG:NH1	2.31	0.45
2:B:159:ASP:O	2:B:162:MSE:CE	2.62	0.45
1:C:1100:LEU:HD11	1:C:1133:ALA:HB1	1.98	0.45
2:D:244:LEU:O	2:D:245:ALA:C	2.55	0.45
2:F:1:MSE:O	2:F:2:ASP:HB2	2.16	0.45
1:A:1028:ALA:HB2	1:A:1200:ARG:NH2	2.28	0.45
2:B:44:LEU:O	2:B:45:GLY:C	2.55	0.45
1:C:972:ASP:O	1:C:974:THR:N	2.50	0.45
1:C:1075:ALA:O	1:C:1077:LEU:N	2.50	0.45
1:C:1184:ILE:HG22	1:C:1185:ALA:N	2.32	0.45
2:D:211:ARG:HH11	2:D:211:ARG:CG	2.29	0.45
2:B:44:LEU:O	2:B:46:GLN:N	2.50	0.45
2:D:129:ILE:HD12	2:D:129:ILE:N	2.31	0.45
1:E:954:ILE:HA	2:F:205:ASN:ND2	2.31	0.45
1:E:1162:PRO:HB2	1:E:1175:ILE:CG1	2.45	0.45
2:F:11:TYR:CZ	2:F:163:ILE:HD11	2.48	0.45
2:F:49:SER:HB2	2:F:61:ASP:OD2	2.16	0.45
1:A:1184:ILE:HG22	1:A:1185:ALA:N	2.32	0.45
2:B:1:MSE:O	2:B:2:ASP:HB2	2.16	0.45
2:B:54:SER:HB2	2:B:57:GLY:H	1.82	0.45
2:D:48:GLN:O	2:D:49:SER:C	2.54	0.45
1:E:979:GLN:O	1:E:979:GLN:HG2	2.17	0.45
2:F:157:SER:C	2:F:159:ASP:N	2.70	0.45
1:A:0:MSE:SE	2:B:138:VAL:HB	2.67	0.45
1:C:1016:ALA:O	1:C:1020:ILE:HG12	2.17	0.45
1:C:1161:THR:CG2	1:C:1162:PRO:HD2	2.47	0.45
2:D:56:LEU:HG	2:D:57:GLY:N	2.32	0.45
2:F:184:PHE:C	2:F:184:PHE:CD2	2.90	0.45
1:A:972:ASP:O	1:A:974:THR:N	2.50	0.44
2:B:66:PHE:HE2	2:B:98:ILE:HD12	1.83	0.44
2:D:244:LEU:HB2	2:D:266:VAL:HG23	1.99	0.44
2:F:120:GLY:HA2	2:F:123:GLU:OE1	2.17	0.44
2:F:244:LEU:HB2	2:F:266:VAL:HG23	2.00	0.44
1:A:1161:THR:CG2	1:A:1162:PRO:HD2	2.47	0.44
1:C:954:ILE:HB	2:D:173:PHE:CE2	2.52	0.44
1:E:911:PRO:O	1:E:912:ALA:C	2.54	0.44
1:E:1050:ILE:HD11	1:E:1149:ILE:HG21	1.99	0.44
2:F:211:ARG:HH11	2:F:211:ARG:CG	2.30	0.44
1:A:913:VAL:CG2	1:A:1024:MSE:HE3	2.48	0.44
1:A:1018:TYR:CE2	1:A:1187:ILE:HG13	2.53	0.44
2:B:125:LEU:O	2:B:129:ILE:CD1	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:TRP:CH2	2:B:223:LEU:HD22	2.51	0.44
1:C:1191:GLY:O	1:C:1192:ALA:C	2.55	0.44
2:D:222:LEU:CD2	2:D:222:LEU:C	2.86	0.44
1:E:1016:ALA:O	1:E:1020:ILE:HG12	2.17	0.44
2:F:73:GLU:HB2	2:F:74:GLU:H	1.57	0.44
2:F:222:LEU:CD2	2:F:222:LEU:C	2.86	0.44
2:F:260:ASP:C	2:F:262:THR:N	2.70	0.44
1:A:946:ILE:HD11	1:A:1022:LEU:HB3	1.99	0.44
1:A:1033:LEU:CD2	1:A:1037:ILE:HG13	2.45	0.44
1:A:1074:LYS:HG3	1:A:1147:PHE:HE1	1.83	0.44
1:C:979:GLN:O	1:C:979:GLN:HG2	2.18	0.44
1:E:974:THR:C	1:E:975:VAL:HG23	2.37	0.44
2:F:54:SER:HB2	2:F:57:GLY:H	1.82	0.44
2:F:56:LEU:HG	2:F:57:GLY:N	2.32	0.44
1:C:974:THR:C	1:C:975:VAL:HG23	2.37	0.44
1:C:987:LEU:HA	1:C:990:VAL:HG23	1.99	0.44
1:C:1094:PHE:C	1:C:1096:HIS:N	2.70	0.44
2:D:260:ASP:O	2:D:264:GLN:HG2	2.16	0.44
1:E:956:SER:O	1:E:957:THR:C	2.56	0.44
1:E:972:ASP:O	1:E:974:THR:N	2.50	0.44
1:A:997:GLY:HA3	1:A:1013:PHE:CE2	2.53	0.44
2:F:6:ILE:CG2	2:F:22:ILE:HG12	2.48	0.44
2:F:41:LEU:HB3	2:F:47:TYR:HA	1.99	0.44
2:F:85:SER:HB3	2:F:88:GLU:OE2	2.18	0.44
1:A:907:ASN:ND2	1:A:978:ASP:O	2.50	0.44
2:B:96:GLN:OE1	2:B:105:SER:HA	2.18	0.44
2:B:184:PHE:O	2:B:188:GLU:HB2	2.18	0.44
2:B:260:ASP:O	2:B:264:GLN:HG2	2.17	0.44
1:E:1042:ARG:HD3	1:E:1169:THR:HG22	2.00	0.44
1:A:1002:LYS:HZ2	2:D:147:ASN:CB	2.31	0.44
1:A:1018:TYR:HE2	1:A:1187:ILE:HG13	1.81	0.44
1:C:933:VAL:HG13	1:C:1187:ILE:CG2	2.43	0.44
2:D:193:THR:HG22	2:D:193:THR:O	2.18	0.44
2:F:96:GLN:OE1	2:F:105:SER:HA	2.18	0.44
2:F:248:ILE:HD11	2:F:263:ASN:CB	2.46	0.44
1:E:997:GLY:HA3	1:E:1013:PHE:CE2	2.53	0.44
1:E:1074:LYS:HG3	1:E:1147:PHE:HE1	1.83	0.44
2:B:270:HIS:CG	2:B:271:GLU:N	2.86	0.43
2:D:35:PHE:CD1	2:D:87:TYR:CD2	2.91	0.43
2:D:184:PHE:C	2:D:184:PHE:CD2	2.90	0.43
1:A:1071:TYR:CE2	1:A:1141:PHE:HB2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:ALA:O	1:A:1077:LEU:N	2.50	0.43
1:C:939:LEU:HD13	1:C:1187:ILE:HD12	2.00	0.43
1:C:997:GLY:HA3	1:C:1013:PHE:CE2	2.54	0.43
1:E:1090:MSE:CE	1:E:1106:ALA:HA	2.21	0.43
1:E:1161:THR:CG2	1:E:1162:PRO:HD2	2.47	0.43
2:F:244:LEU:O	2:F:245:ALA:C	2.56	0.43
1:A:979:GLN:O	1:A:979:GLN:HG2	2.18	0.43
2:D:96:GLN:OE1	2:D:105:SER:HA	2.18	0.43
2:D:159:ASP:O	2:D:162:MSE:CE	2.62	0.43
2:D:184:PHE:O	2:D:188:GLU:HB2	2.18	0.43
2:D:248:ILE:HD11	2:D:263:ASN:CB	2.47	0.43
1:A:956:SER:O	1:A:957:THR:C	2.56	0.43
2:F:112:GLY:O	2:F:115:ASN:N	2.51	0.43
1:A:1097:LYS:O	1:A:1136:ALA:CB	2.67	0.43
2:B:6:ILE:CG2	2:B:22:ILE:HG12	2.48	0.43
2:B:222:LEU:CD2	2:B:222:LEU:C	2.85	0.43
2:B:248:ILE:HD11	2:B:263:ASN:CB	2.47	0.43
2:B:256:LEU:O	2:B:257:ASP:C	2.56	0.43
2:D:54:SER:HB2	2:D:57:GLY:H	1.82	0.43
1:E:1009:ALA:O	1:E:1012:CYS:HB2	2.18	0.43
1:E:1184:ILE:HG22	1:E:1185:ALA:N	2.32	0.43
2:F:184:PHE:O	2:F:188:GLU:HB2	2.18	0.43
2:F:187:TYR:CD1	2:F:206:LEU:HD21	2.54	0.43
1:A:1016:ALA:O	1:A:1020:ILE:HG12	2.18	0.43
1:A:1186:MSE:H	1:A:1186:MSE:HG3	1.64	0.43
2:B:117:GLU:HA	2:B:121:THR:HB	1.99	0.43
2:B:175:THR:O	2:B:176:ASN:CB	2.67	0.43
2:D:270:HIS:CG	2:D:271:GLU:N	2.86	0.43
2:F:193:THR:O	2:F:193:THR:HG22	2.18	0.43
2:F:244:LEU:O	2:F:247:GLN:HB2	2.19	0.43
2:B:66:PHE:CE2	2:B:95:ALA:HA	2.53	0.43
2:B:187:TYR:CD1	2:B:206:LEU:HD21	2.54	0.43
2:B:193:THR:O	2:B:193:THR:HG22	2.17	0.43
2:B:244:LEU:O	2:B:245:ALA:C	2.55	0.43
1:C:1009:ALA:O	1:C:1012:CYS:HB2	2.18	0.43
2:D:125:LEU:O	2:D:129:ILE:CD1	2.63	0.43
1:E:908:SER:OG	1:E:910:LEU:HD23	2.19	0.43
2:F:66:PHE:HE2	2:F:98:ILE:HD12	1.82	0.43
1:A:1094:PHE:C	1:A:1096:HIS:N	2.70	0.43
2:B:94:THR:HG22	2:B:98:ILE:HD11	2.01	0.43
2:B:156:VAL:O	2:B:158:GLY:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:908:SER:OG	1:C:910:LEU:HD23	2.18	0.43
1:C:981:LEU:HD22	1:C:1024:MSE:HE1	2.00	0.43
1:C:1008:ILE:H	1:C:1008:ILE:CD1	2.31	0.43
2:D:197:TRP:CE3	2:D:223:LEU:HD22	2.54	0.43
1:E:994:MSE:HE2	1:E:994:MSE:HA	2.01	0.43
1:A:931:VAL:O	1:A:931:VAL:CG1	2.67	0.43
1:C:1079:PRO:HG2	1:C:1080:ILE:H	1.84	0.43
2:D:244:LEU:O	2:D:247:GLN:HB2	2.19	0.43
1:E:1028:ALA:HB2	1:E:1200:ARG:NH2	2.31	0.43
1:A:908:SER:OG	1:A:910:LEU:HD23	2.18	0.43
2:D:94:THR:HG22	2:D:98:ILE:HD11	2.01	0.43
2:D:197:TRP:O	2:D:198:LYS:C	2.58	0.43
1:E:931:VAL:CG1	1:E:931:VAL:O	2.67	0.43
2:F:256:LEU:O	2:F:257:ASP:C	2.57	0.43
1:A:994:MSE:HE2	1:A:994:MSE:HA	2.01	0.42
2:B:106:LEU:HD23	2:B:106:LEU:C	2.39	0.42
1:E:921:ASP:N	2:F:288:LEU:HD11	2.34	0.42
1:E:987:LEU:HA	1:E:990:VAL:CG2	2.49	0.42
1:E:1157:ILE:HG23	1:E:1161:THR:HB	2.01	0.42
2:F:44:LEU:HA	2:F:234:GLU:OE1	2.19	0.42
2:F:71:ASN:HB2	2:F:73:GLU:OE1	2.19	0.42
2:F:106:LEU:HD23	2:F:106:LEU:C	2.39	0.42
1:A:1009:ALA:O	1:A:1012:CYS:HB2	2.18	0.42
1:A:1127:ASN:C	1:A:1129:ALA:N	2.73	0.42
2:B:244:LEU:HB2	2:B:266:VAL:HG23	2.00	0.42
1:C:994:MSE:CE	1:C:1013:PHE:CD2	2.96	0.42
2:D:49:SER:HB2	2:D:61:ASP:CG	2.40	0.42
2:D:106:LEU:HD23	2:D:106:LEU:C	2.39	0.42
2:D:187:TYR:CD1	2:D:206:LEU:HD21	2.54	0.42
1:A:1142:ASP:O	1:A:1142:ASP:CG	2.58	0.42
1:A:1157:ILE:HG23	1:A:1161:THR:HB	2.01	0.42
2:B:184:PHE:C	2:B:184:PHE:CD2	2.90	0.42
1:E:913:VAL:HG22	1:E:1024:MSE:HE3	2.00	0.42
1:E:1094:PHE:C	1:E:1096:HIS:N	2.70	0.42
2:F:197:TRP:CE3	2:F:223:LEU:HD22	2.54	0.42
2:F:270:HIS:CG	2:F:271:GLU:N	2.86	0.42
2:B:56:LEU:HG	2:B:57:GLY:N	2.32	0.42
2:B:244:LEU:O	2:B:247:GLN:HB2	2.19	0.42
2:B:245:ALA:O	2:B:248:ILE:HB	2.20	0.42
1:C:931:VAL:O	1:C:931:VAL:CG1	2.67	0.42
1:C:956:SER:O	1:C:957:THR:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:981:LEU:HD13	1:C:1024:MSE:HE1	2.00	0.42
2:D:134:LEU:HD23	2:D:134:LEU:HA	1.90	0.42
2:D:235:ASN:O	2:D:235:ASN:ND2	2.46	0.42
1:E:1079:PRO:HG2	1:E:1080:ILE:H	1.84	0.42
1:E:1100:LEU:HD12	1:E:1100:LEU:HA	1.72	0.42
1:E:1186:MSE:H	1:E:1186:MSE:HG3	1.63	0.42
2:B:12:THR:C	2:B:198:LYS:HD3	2.39	0.42
2:B:116:ASP:O	2:B:117:GLU:HB2	2.19	0.42
2:B:258:THR:O	2:B:260:ASP:N	2.53	0.42
1:C:987:LEU:HA	1:C:990:VAL:CG2	2.49	0.42
1:C:1100:LEU:HD12	1:C:1100:LEU:HA	1.72	0.42
2:D:6:ILE:CG2	2:D:22:ILE:HG12	2.48	0.42
2:D:92:LEU:O	2:D:96:GLN:HG3	2.20	0.42
2:D:238:LEU:HD23	2:D:239:TYR:CE1	2.55	0.42
1:A:1166:ASP:HA	1:A:1167:PRO:HD2	1.78	0.42
2:B:49:SER:HB2	2:B:61:ASP:CG	2.40	0.42
2:B:124:LEU:HD23	2:B:124:LEU:HA	1.76	0.42
2:B:154:ASP:O	2:B:155:THR:C	2.58	0.42
2:B:197:TRP:CE3	2:B:223:LEU:HD22	2.54	0.42
1:C:1028:ALA:O	1:C:1031:GLU:HB3	2.19	0.42
2:D:109:CYS:HB3	2:D:128:ALA:HB2	2.01	0.42
2:D:175:THR:O	2:D:176:ASN:CB	2.67	0.42
2:D:245:ALA:O	2:D:248:ILE:HB	2.20	0.42
2:D:256:LEU:O	2:D:257:ASP:C	2.57	0.42
1:E:1127:ASN:C	1:E:1129:ALA:H	2.23	0.42
1:E:1142:ASP:CG	1:E:1142:ASP:O	2.57	0.42
2:F:175:THR:O	2:F:176:ASN:CB	2.67	0.42
1:A:987:LEU:HA	1:A:990:VAL:CG2	2.49	0.42
1:C:946:ILE:HD11	1:C:1022:LEU:HB3	2.02	0.42
1:C:1071:TYR:CE2	1:C:1141:PHE:HB2	2.53	0.42
1:C:1074:LYS:HG3	1:C:1147:PHE:HE1	1.83	0.42
2:D:62:LEU:HD23	2:D:62:LEU:HA	1.82	0.42
1:E:1028:ALA:O	1:E:1031:GLU:HB3	2.19	0.42
2:F:45:GLY:HA2	2:F:234:GLU:OE2	2.20	0.42
2:F:262:THR:C	2:F:264:GLN:H	2.23	0.42
2:B:238:LEU:HD23	2:B:239:TYR:CE1	2.55	0.42
1:C:1157:ILE:HG23	1:C:1161:THR:HB	2.01	0.42
2:D:44:LEU:HA	2:D:234:GLU:OE1	2.19	0.42
2:D:63:TYR:CD1	2:D:91:LEU:HB3	2.55	0.42
2:D:262:THR:C	2:D:264:GLN:H	2.23	0.42
2:F:154:ASP:O	2:F:155:THR:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:ARG:HD3	1:A:1169:THR:HG22	2.00	0.42
1:A:1131:SER:O	1:A:1132:MSE:CB	2.68	0.42
1:C:901:THR:HG22	1:C:902:ALA:N	2.35	0.42
1:C:1114:SER:HB3	2:F:232:GLN:HA	2.01	0.42
2:D:154:ASP:O	2:D:155:THR:C	2.58	0.42
2:F:94:THR:HG22	2:F:98:ILE:HD11	2.01	0.42
2:F:238:LEU:HD23	2:F:239:TYR:CE1	2.55	0.42
2:B:157:SER:O	2:B:159:ASP:N	2.53	0.42
2:B:275:ILE:HD13	2:B:275:ILE:HA	1.95	0.42
1:C:994:MSE:HE2	1:C:994:MSE:HA	2.01	0.42
1:C:1142:ASP:CG	1:C:1142:ASP:O	2.57	0.42
2:D:62:LEU:HB3	2:D:75:LEU:HG	2.02	0.42
1:A:1079:PRO:HG2	1:A:1080:ILE:H	1.84	0.41
1:A:1127:ASN:C	1:A:1129:ALA:H	2.23	0.41
1:C:921:ASP:O	1:C:925:GLN:HG3	2.20	0.41
1:C:1022:LEU:HD23	1:C:1022:LEU:HA	1.83	0.41
1:C:1113:ILE:HG22	1:C:1119:ALA:HB2	2.01	0.41
2:D:71:ASN:HB2	2:D:73:GLU:OE1	2.19	0.41
1:E:1113:ILE:HG22	1:E:1119:ALA:HB2	2.01	0.41
1:E:1158:TYR:N	1:E:1158:TYR:CD1	2.88	0.41
2:B:15:PHE:HB2	2:B:44:LEU:CD2	2.47	0.41
2:B:71:ASN:HB2	2:B:73:GLU:OE1	2.19	0.41
2:B:197:TRP:O	2:B:198:LYS:C	2.57	0.41
1:C:989:VAL:O	1:C:992:GLU:N	2.54	0.41
2:D:234:GLU:C	2:D:236:ALA:H	2.23	0.41
2:D:244:LEU:HD12	2:D:266:VAL:HG23	2.01	0.41
2:F:156:VAL:O	2:F:156:VAL:CG1	2.69	0.41
2:F:244:LEU:HD12	2:F:266:VAL:HG23	2.01	0.41
1:A:1028:ALA:O	1:A:1031:GLU:HB3	2.19	0.41
1:C:991:ASN:O	1:C:992:GLU:C	2.59	0.41
1:C:1127:ASN:C	1:C:1129:ALA:H	2.23	0.41
1:C:1127:ASN:C	1:C:1129:ALA:N	2.73	0.41
1:C:1158:TYR:CD1	1:C:1158:TYR:N	2.88	0.41
2:D:15:PHE:HB2	2:D:44:LEU:CD2	2.47	0.41
2:D:193:THR:CG2	2:D:194:PHE:CE1	3.03	0.41
2:D:258:THR:O	2:D:260:ASP:N	2.53	0.41
1:E:989:VAL:O	1:E:992:GLU:N	2.53	0.41
1:E:1071:TYR:O	1:E:1074:LYS:HB2	2.20	0.41
2:F:4:PHE:HD1	2:F:159:ASP:HB2	1.85	0.41
2:F:87:TYR:CE1	2:F:119:GLU:HG2	2.49	0.41
2:F:245:ALA:O	2:F:248:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:991:ASN:O	1:A:992:GLU:C	2.59	0.41
1:A:1071:TYR:O	1:A:1074:LYS:HB2	2.20	0.41
1:A:1158:TYR:CD1	1:A:1158:TYR:N	2.88	0.41
1:A:1178:LYS:HE3	1:A:1191:GLY:HA3	2.02	0.41
2:B:1:MSE:O	2:B:2:ASP:CB	2.68	0.41
2:B:166:LEU:HA	2:B:166:LEU:HD12	1.60	0.41
2:D:206:LEU:HA	2:D:206:LEU:HD13	1.67	0.41
1:E:1018:TYR:O	1:E:1021:THR:HB	2.20	0.41
2:F:49:SER:HB2	2:F:61:ASP:CG	2.40	0.41
1:A:1018:TYR:O	1:A:1021:THR:HB	2.21	0.41
1:A:1142:ASP:HA	1:A:1143:PRO:HD2	1.91	0.41
2:B:117:GLU:OE2	2:B:152:ILE:HD12	2.20	0.41
1:C:1131:SER:O	1:C:1132:MSE:CB	2.68	0.41
2:D:1:MSE:O	2:D:2:ASP:CB	2.68	0.41
2:D:156:VAL:O	2:D:156:VAL:CG1	2.68	0.41
2:D:260:ASP:O	2:D:261:LEU:C	2.59	0.41
2:F:41:LEU:CD1	2:F:46:GLN:O	2.67	0.41
2:B:41:LEU:HD13	2:B:46:GLN:O	2.21	0.41
2:D:7:LYS:HE2	2:D:123:GLU:OE2	2.20	0.41
1:E:991:ASN:O	1:E:992:GLU:C	2.58	0.41
1:E:1117:PRO:HG2	1:E:1118:ARG:H	1.86	0.41
1:E:1127:ASN:C	1:E:1129:ALA:N	2.73	0.41
2:F:1:MSE:O	2:F:2:ASP:CB	2.68	0.41
2:F:92:LEU:O	2:F:96:GLN:HG3	2.20	0.41
1:A:959:CYS:C	1:A:961:LEU:H	2.24	0.41
1:A:1182:ASP:HA	1:A:1190:ILE:HD11	2.02	0.41
2:B:244:LEU:HD12	2:B:266:VAL:HG23	2.01	0.41
1:E:987:LEU:N	1:E:987:LEU:HD12	2.35	0.41
1:E:1178:LYS:HE3	1:E:1191:GLY:HA3	2.02	0.41
2:F:11:TYR:CD1	2:F:163:ILE:HD11	2.55	0.41
1:A:921:ASP:O	1:A:925:GLN:HG3	2.20	0.41
1:A:987:LEU:N	1:A:987:LEU:HD12	2.36	0.41
1:C:1071:TYR:O	1:C:1074:LYS:HB2	2.20	0.41
1:C:1166:ASP:HA	1:C:1167:PRO:HD2	1.78	0.41
1:C:1182:ASP:HA	1:C:1190:ILE:HD11	2.02	0.41
2:D:12:THR:C	2:D:198:LYS:HD3	2.41	0.41
2:F:234:GLU:C	2:F:236:ALA:H	2.23	0.41
2:F:258:THR:O	2:F:260:ASP:N	2.53	0.41
2:F:260:ASP:O	2:F:261:LEU:C	2.59	0.41
1:A:989:VAL:O	1:A:992:GLU:N	2.53	0.41
1:A:1003:LEU:CD2	2:D:110:VAL:HG21	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1080:ILE:HB	2:F:227:TYR:CE2	2.56	0.41
1:C:1109:PHE:CZ	1:C:1118:ARG:CD	3.01	0.41
1:C:1178:LYS:HE3	1:C:1191:GLY:HA3	2.02	0.41
2:D:106:LEU:C	2:D:106:LEU:CD2	2.89	0.41
2:D:266:VAL:CG1	2:D:275:ILE:HG12	2.51	0.41
1:E:1100:LEU:CD1	1:E:1133:ALA:HB1	2.51	0.41
1:E:1131:SER:O	1:E:1132:MSE:CB	2.68	0.41
2:F:106:LEU:C	2:F:106:LEU:CD2	2.90	0.41
1:A:904:TRP:CD2	1:A:982:PRO:HD3	2.56	0.41
1:A:1100:LEU:HB3	1:A:1101:GLN:NE2	2.36	0.41
2:B:266:VAL:CG1	2:B:275:ILE:HG12	2.51	0.41
1:C:0:MSE:O	1:C:900:GLU:C	2.59	0.41
1:C:1100:LEU:CD1	1:C:1133:ALA:HB1	2.51	0.41
1:C:1117:PRO:HG2	1:C:1118:ARG:H	1.86	0.41
1:E:904:TRP:CG	1:E:982:PRO:HD3	2.56	0.41
1:E:921:ASP:O	1:E:925:GLN:HG3	2.20	0.41
1:E:931:VAL:HG11	1:E:1168:LEU:HD13	2.02	0.41
1:E:959:CYS:C	1:E:961:LEU:H	2.24	0.41
2:F:266:VAL:CG1	2:F:275:ILE:HG12	2.51	0.41
1:A:901:THR:HG22	1:A:902:ALA:N	2.35	0.40
1:A:940:LYS:HA	2:B:285:PHE:CE2	2.55	0.40
1:A:1113:ILE:HG22	1:A:1119:ALA:HB2	2.01	0.40
2:B:92:LEU:O	2:B:96:GLN:HG3	2.21	0.40
2:B:106:LEU:C	2:B:106:LEU:CD2	2.89	0.40
2:B:134:LEU:HD23	2:B:134:LEU:HA	1.90	0.40
2:B:193:THR:CG2	2:B:194:PHE:CE1	3.04	0.40
2:B:234:GLU:C	2:B:236:ALA:H	2.23	0.40
2:B:260:ASP:O	2:B:261:LEU:C	2.59	0.40
1:C:901:THR:O	1:C:904:TRP:HB2	2.21	0.40
1:E:954:ILE:HD12	2:F:170:TYR:HE2	1.87	0.40
1:E:1045:ILE:HD12	1:E:1184:ILE:CG2	2.43	0.40
1:E:1100:LEU:HD13	1:E:1133:ALA:CA	2.52	0.40
2:F:193:THR:CG2	2:F:194:PHE:CE1	3.04	0.40
1:A:904:TRP:CG	1:A:982:PRO:HD3	2.56	0.40
2:B:87:TYR:CE1	2:B:120:GLY:CA	3.04	0.40
1:C:957:THR:CB	1:C:958:PRO:HD3	2.48	0.40
1:C:959:CYS:C	1:C:961:LEU:H	2.24	0.40
1:C:983:TYR:HE2	2:D:253:MSE:HG2	1.86	0.40
1:C:1018:TYR:O	1:C:1021:THR:HB	2.20	0.40
2:D:140:THR:O	2:D:141:ALA:C	2.59	0.40
1:A:901:THR:O	1:A:904:TRP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:ILE:CG2	1:A:964:GLN:HB2	2.51	0.40
1:C:941:LYS:HE2	1:C:942:TYR:CZ	2.56	0.40
1:C:954:ILE:CG2	1:C:964:GLN:HB2	2.51	0.40
2:D:35:PHE:CG	2:D:87:TYR:CE2	3.09	0.40
1:E:941:LYS:HE2	1:E:942:TYR:CZ	2.56	0.40
2:F:15:PHE:HB2	2:F:44:LEU:CD2	2.47	0.40
1:A:1080:ILE:CG1	2:D:147:ASN:OD1	2.55	0.40
1:A:1097:LYS:O	1:A:1136:ALA:HB3	2.21	0.40
1:A:1117:PRO:HG2	1:A:1118:ARG:H	1.86	0.40
2:B:15:PHE:HA	2:B:18:CYS:HB3	2.03	0.40
2:B:125:LEU:HD22	2:B:148:TYR:CE2	2.56	0.40
2:B:140:THR:O	2:B:141:ALA:C	2.59	0.40
2:B:156:VAL:O	2:B:156:VAL:CG1	2.68	0.40
1:C:904:TRP:CG	1:C:982:PRO:HD3	2.57	0.40
2:D:63:TYR:CD2	2:D:63:TYR:C	2.95	0.40
1:E:954:ILE:HA	2:F:205:ASN:HD21	1.86	0.40
2:F:15:PHE:HA	2:F:18:CYS:HB3	2.04	0.40
2:F:201:LEU:O	2:F:204:LEU:HB3	2.22	0.40
2:B:147:ASN:O	2:B:151:ALA:HB2	2.22	0.40
1:E:901:THR:HG22	1:E:902:ALA:N	2.35	0.40
1:E:1131:SER:C	1:E:1132:MSE:HG2	2.42	0.40
1:E:1182:ASP:HA	1:E:1190:ILE:HD11	2.02	0.40
2:F:147:ASN:O	2:F:151:ALA:HB2	2.22	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	301/325 (93%)	233 (77%)	53 (18%)	15 (5%)	2 13
1	C	301/325 (93%)	232 (77%)	53 (18%)	16 (5%)	2 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	301/325 (93%)	233 (77%)	53 (18%)	15 (5%)	2 13
2	B	291/310 (94%)	211 (72%)	59 (20%)	21 (7%)	1 7
2	D	291/310 (94%)	215 (74%)	56 (19%)	20 (7%)	1 8
2	F	291/310 (94%)	212 (73%)	61 (21%)	18 (6%)	1 10
All	All	1776/1905 (93%)	1336 (75%)	335 (19%)	105 (6%)	1 10

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	957	THR
1	A	973	ASP
1	A	977	GLU
1	A	979	GLN
1	A	985	PRO
1	A	1132	MSE
1	A	1133	ALA
1	A	1186	MSE
2	B	2	ASP
2	B	73	GLU
2	B	159	ASP
2	B	181	THR
2	B	258	THR
2	B	273	ALA
1	C	957	THR
1	C	973	ASP
1	C	977	GLU
1	C	979	GLN
1	C	985	PRO
1	C	1132	MSE
1	C	1133	ALA
1	C	1186	MSE
2	D	2	ASP
2	D	73	GLU
2	D	159	ASP
2	D	181	THR
2	D	258	THR
2	D	273	ALA
1	E	957	THR
1	E	973	ASP
1	E	977	GLU
1	E	979	GLN

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Mol	Chain	Res	Type
1	E	985	PRO
1	E	1132	MSE
1	E	1133	ALA
1	E	1186	MSE
2	F	2	ASP
2	F	73	GLU
2	F	159	ASP
2	F	181	THR
2	F	258	THR
2	F	273	ALA
1	A	1076	LYS
1	A	1154	TYR
2	B	119	GLU
2	B	157	SER
2	B	233	LYS
2	B	234	GLU
2	B	261	LEU
1	C	900	GLU
1	C	1076	LYS
1	C	1154	TYR
2	D	157	SER
2	D	158	GLY
2	D	233	LYS
2	D	234	GLU
2	D	261	LEU
1	E	1076	LYS
1	E	1154	TYR
2	F	157	SER
2	F	158	GLY
2	F	233	LYS
2	F	234	GLU
2	F	261	LEU
1	A	901	THR
1	A	959	CYS
1	A	1062	THR
2	B	26	SER
2	B	27	LYS
2	B	45	GLY
2	B	116	ASP
2	B	118	ALA
2	B	149	THR
2	B	150	ASN

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Mol	Chain	Res	Type
2	B	269	ASP
1	C	901	THR
1	C	959	CYS
1	C	1062	THR
2	D	26	SER
2	D	27	LYS
2	D	149	THR
2	D	150	ASN
2	D	269	ASP
1	E	901	THR
1	E	959	CYS
1	E	1062	THR
2	F	26	SER
2	F	27	LYS
2	F	149	THR
2	F	150	ASN
2	F	269	ASP
1	A	1039	GLU
2	B	241	PRO
2	B	259	GLU
1	C	1039	GLU
2	D	69	THR
2	D	241	PRO
1	E	1039	GLU
2	F	241	PRO
1	A	911	PRO
1	C	911	PRO
2	D	259	GLU
1	E	911	PRO
2	F	259	GLU
2	D	45	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	257/268 (96%)	226 (88%)	31 (12%)	5 20
1	C	257/268 (96%)	226 (88%)	31 (12%)	5 20
1	E	257/268 (96%)	226 (88%)	31 (12%)	5 20
2	B	263/275 (96%)	221 (84%)	42 (16%)	2 10
2	D	263/275 (96%)	218 (83%)	45 (17%)	2 9
2	F	263/275 (96%)	220 (84%)	43 (16%)	2 10
All	All	1560/1629 (96%)	1337 (86%)	223 (14%)	3 14

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	901	THR
1	A	909	LYS
1	A	952	THR
1	A	954	ILE
1	A	956	SER
1	A	960	GLU
1	A	969	ARG
1	A	985	PRO
1	A	993	LYS
1	A	1046	LEU
1	A	1052	LEU
1	A	1062	THR
1	A	1063	VAL
1	A	1065	MSE
1	A	1080	ILE
1	A	1083	THR
1	A	1091	SER
1	A	1098	ASN
1	A	1099	PHE
1	A	1130	ASP
1	A	1132	MSE
1	A	1134	SER
1	A	1142	ASP
1	A	1147	PHE
1	A	1153	THR
1	A	1160	ASP
1	A	1164	VAL

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Mol	Chain	Res	Type
1	A	1166	ASP
1	A	1171	SER
1	A	1181	ILE
1	A	1182	ASP
2	B	2	ASP
2	B	3	TYR
2	B	6	ILE
2	B	14	ASN
2	B	16	VAL
2	B	34	LEU
2	B	39	LYS
2	B	41	LEU
2	B	68	ASP
2	B	69	THR
2	B	72	ILE
2	B	73	GLU
2	B	75	LEU
2	B	79	LEU
2	B	84	ASN
2	B	92	LEU
2	B	106	LEU
2	B	122	THR
2	B	124	LEU
2	B	131	VAL
2	B	138	VAL
2	B	139	SER
2	B	153	GLU
2	B	154	ASP
2	B	162	MSE
2	B	163	ILE
2	B	176	ASN
2	B	184	PHE
2	B	188	GLU
2	B	196	THR
2	B	201	LEU
2	B	211	ARG
2	B	235	ASN
2	B	237	VAL
2	B	249	THR
2	B	257	ASP
2	B	259	GLU
2	B	260	ASP

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Mol	Chain	Res	Type
2	B	266	VAL
2	B	271	GLU
2	B	272	HIS
2	B	281	ILE
1	C	901	THR
1	C	909	LYS
1	C	952	THR
1	C	954	ILE
1	C	956	SER
1	C	960	GLU
1	C	969	ARG
1	C	985	PRO
1	C	993	LYS
1	C	1046	LEU
1	C	1052	LEU
1	C	1062	THR
1	C	1063	VAL
1	C	1065	MSE
1	C	1080	ILE
1	C	1083	THR
1	C	1091	SER
1	C	1098	ASN
1	C	1099	PHE
1	C	1130	ASP
1	C	1132	MSE
1	C	1134	SER
1	C	1142	ASP
1	C	1147	PHE
1	C	1153	THR
1	C	1160	ASP
1	C	1164	VAL
1	C	1166	ASP
1	C	1171	SER
1	C	1181	ILE
1	C	1182	ASP
2	D	2	ASP
2	D	3	TYR
2	D	6	ILE
2	D	14	ASN
2	D	16	VAL
2	D	34	LEU
2	D	39	LYS

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Mol	Chain	Res	Type
2	D	41	LEU
2	D	68	ASP
2	D	69	THR
2	D	72	ILE
2	D	73	GLU
2	D	75	LEU
2	D	79	LEU
2	D	84	ASN
2	D	92	LEU
2	D	106	LEU
2	D	114	ASP
2	D	115	ASN
2	D	122	THR
2	D	124	LEU
2	D	131	VAL
2	D	138	VAL
2	D	139	SER
2	D	153	GLU
2	D	154	ASP
2	D	162	MSE
2	D	163	ILE
2	D	176	ASN
2	D	184	PHE
2	D	188	GLU
2	D	196	THR
2	D	201	LEU
2	D	211	ARG
2	D	235	ASN
2	D	237	VAL
2	D	249	THR
2	D	257	ASP
2	D	259	GLU
2	D	260	ASP
2	D	266	VAL
2	D	271	GLU
2	D	272	HIS
2	D	281	ILE
2	D	293	ASP
1	E	901	THR
1	E	909	LYS
1	E	952	THR
1	E	954	ILE

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Mol	Chain	Res	Type
1	E	956	SER
1	E	960	GLU
1	E	969	ARG
1	E	985	PRO
1	E	993	LYS
1	E	1046	LEU
1	E	1052	LEU
1	E	1062	THR
1	E	1063	VAL
1	E	1065	MSE
1	E	1080	ILE
1	E	1083	THR
1	E	1091	SER
1	E	1098	ASN
1	E	1099	PHE
1	E	1130	ASP
1	E	1132	MSE
1	E	1134	SER
1	E	1142	ASP
1	E	1147	PHE
1	E	1153	THR
1	E	1160	ASP
1	E	1164	VAL
1	E	1166	ASP
1	E	1171	SER
1	E	1181	ILE
1	E	1182	ASP
2	F	2	ASP
2	F	3	TYR
2	F	6	ILE
2	F	14	ASN
2	F	16	VAL
2	F	34	LEU
2	F	39	LYS
2	F	41	LEU
2	F	68	ASP
2	F	69	THR
2	F	72	ILE
2	F	73	GLU
2	F	75	LEU
2	F	79	LEU
2	F	84	ASN

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Mol	Chain	Res	Type
2	F	92	LEU
2	F	106	LEU
2	F	115	ASN
2	F	122	THR
2	F	124	LEU
2	F	131	VAL
2	F	138	VAL
2	F	139	SER
2	F	153	GLU
2	F	154	ASP
2	F	162	MSE
2	F	163	ILE
2	F	176	ASN
2	F	184	PHE
2	F	188	GLU
2	F	196	THR
2	F	201	LEU
2	F	211	ARG
2	F	235	ASN
2	F	237	VAL
2	F	249	THR
2	F	257	ASP
2	F	259	GLU
2	F	260	ASP
2	F	266	VAL
2	F	271	GLU
2	F	272	HIS
2	F	281	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	50	GLN
1	C	1093	HIS
1	C	1101	GLN
2	D	50	GLN
2	F	50	GLN

5.3.3 RNA

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	296/325 (91%)	-0.03	2 (0%) 87 88	47, 89, 147, 193	0
1	C	296/325 (91%)	0.08	3 (1%) 82 82	56, 111, 179, 201	0
1	E	296/325 (91%)	1.15	68 (22%) 0 1	113, 171, 201, 201	0
2	B	290/310 (93%)	-0.03	1 (0%) 94 94	44, 96, 169, 188	0
2	D	290/310 (93%)	0.05	5 (1%) 70 67	59, 110, 173, 201	0
2	F	290/310 (93%)	0.86	49 (16%) 1 1	92, 177, 201, 201	0
All	All	1758/1905 (92%)	0.35	128 (7%) 15 14	44, 127, 196, 201	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1141	PHE	10.0
1	E	1197	LEU	8.5
1	C	1135	ASP	7.5
1	E	1129	ALA	7.0
1	E	1149	ILE	6.5
2	F	160	ASN	6.4
1	E	1139	ILE	6.3
1	E	1133	ALA	5.2
2	F	55	LYS	5.1
1	E	909	LYS	5.0
2	F	227	TYR	5.0
1	E	1140	ASP	4.9
2	F	83	GLN	4.8
1	E	1138	PRO	4.8
2	F	285	PHE	4.8
1	E	1147	PHE	4.7
2	F	89	LEU	4.6
1	E	927	LEU	4.4
1	E	1146	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	911	PRO	4.3
2	F	154	ASP	4.3
1	E	1099	PHE	4.3
1	C	1059	GLU	4.2
1	E	1199	ILE	4.2
1	E	920	PHE	4.2
2	F	187	TYR	4.2
1	E	1154	TYR	4.1
2	F	29	THR	4.0
1	E	1160	ASP	4.0
2	F	179	THR	3.9
2	F	113	ILE	3.9
1	E	1127	ASN	3.9
1	E	1171	SER	3.9
1	E	1142	ASP	3.8
1	E	1155	LYS	3.8
1	E	1044	TYR	3.8
2	F	70	LYS	3.7
2	F	26	SER	3.6
1	E	1135	ASP	3.6
2	F	281	ILE	3.6
2	F	33	LEU	3.5
2	F	32	THR	3.5
1	E	1021	THR	3.5
1	E	1068	LEU	3.5
2	F	25	PHE	3.4
2	D	150	ASN	3.4
1	E	1071	TYR	3.3
2	F	164	LEU	3.3
2	F	75	LEU	3.3
2	F	116	ASP	3.2
1	E	1080	ILE	3.2
2	F	258	THR	3.2
2	F	35	PHE	3.2
1	E	1025	VAL	3.2
1	E	1156	PRO	3.2
1	E	1137	ILE	3.2
1	E	1190	ILE	3.1
1	E	979	GLN	3.1
2	F	84	ASN	3.1
2	F	81	ASP	3.1
1	E	1175	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	11	TYR	3.0
2	F	131	VAL	3.0
1	E	978	ASP	2.9
1	E	981	LEU	2.9
1	A	1144	TYR	2.9
2	D	268	LEU	2.9
1	E	1134	SER	2.8
2	F	24	LYS	2.8
1	E	936	LEU	2.8
1	E	1072	PHE	2.8
1	E	1096	HIS	2.8
1	E	1168	LEU	2.8
2	F	118	ALA	2.8
1	E	1128	LYS	2.7
2	D	81	ASP	2.7
1	E	912	ALA	2.7
2	F	22	ILE	2.7
1	E	1059	GLU	2.7
1	E	938	PRO	2.7
1	E	1174	VAL	2.7
2	F	30	ASP	2.7
1	E	967	TYR	2.7
2	F	34	LEU	2.7
1	E	1048	LEU	2.6
2	F	130	GLU	2.6
2	F	147	ASN	2.6
2	F	178	GLU	2.6
1	E	1195	SER	2.6
2	D	258	THR	2.6
2	F	67	LEU	2.6
2	D	227	TYR	2.6
1	E	1063	VAL	2.5
1	E	1124	LYS	2.5
2	F	7	LYS	2.5
1	E	1031	GLU	2.5
2	F	163	ILE	2.5
1	E	1153	THR	2.4
1	E	923	ALA	2.4
1	E	1187	ILE	2.4
1	E	1161	THR	2.4
2	F	60	LEU	2.4
2	F	3	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	28	VAL	2.4
1	E	1066	LEU	2.4
1	E	1176	THR	2.3
1	E	1067	GLU	2.3
2	F	8	GLN	2.3
2	F	90	TYR	2.3
1	E	1047	GLY	2.3
2	B	55	LYS	2.3
2	F	124	LEU	2.3
1	E	1159	GLU	2.3
1	E	1077	LEU	2.3
2	F	235	ASN	2.2
2	F	144	ILE	2.2
2	F	121	THR	2.2
1	E	1196	GLY	2.2
1	E	1150	CYS	2.1
2	F	274	PHE	2.1
2	F	183	ASN	2.1
1	E	1125	ILE	2.1
2	F	58	LYS	2.1
1	E	1009	ALA	2.1
1	A	1128	LYS	2.0
1	C	935	LYS	2.0
1	E	1094	PHE	2.0
1	E	1070	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.