Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 04:31 PM EDT

PDB ID	:	4TQV
Title	:	Crystal structure of a bacterial ABC transporter involved in the import of the acidic polysaccharide alginate
Authors	:	Maruyama, Y.; Itoh, T.; Kaneko, A.; Nishitani, Y.; Mikami, B.; Hashimoto, W.; Murata, K.
Deposited on	:	2014-06-12
Resolution	:	4.50 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:

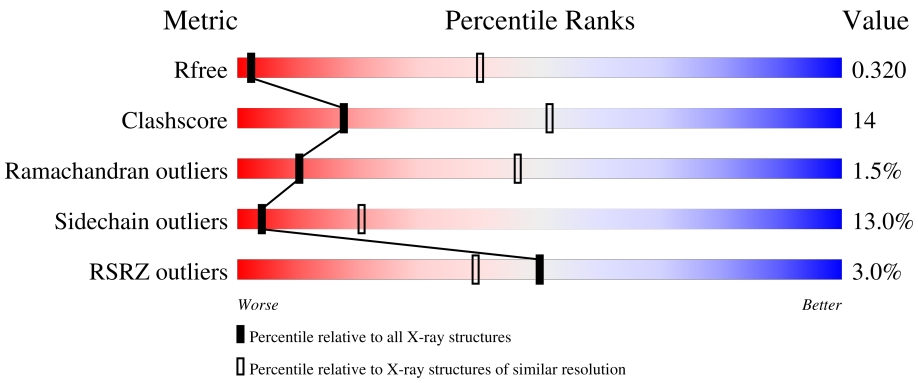
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 4.50 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	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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	301	54% 37% • • 5%
1	E	301	2% 53% 36% 5% • 5%
1	I	301	56% 34% • • 5%
1	M	301	% 55% 35% • • 5%
2	B	305	2% 64% 26% • 7%

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Mol	Chain	Length	Quality of chain
2	F	305	2% 62% 26% 8%
2	J	305	2% 64% 26% 7%
2	N	305	2% 63% 27% 7%
3	C	363	3% 61% 33% 6%
3	D	363	7% 62% 31% 7%
3	G	363	3% 59% 35% 6%
3	H	363	4% 58% 34% 7%
3	K	363	2% 64% 31% 6%
3	L	363	5% 62% 31% 8%
3	O	363	7% 63% 32% 5%
3	P	363	3% 60% 33% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 40472 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 AlgM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	286	2314	1550	368	386	10	0	0	0
1	E	286	2314	1550	368	386	10	0	0	0
1	I	286	2314	1550	368	386	10	0	0	0
1	M	286	2314	1550	368	386	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	expression tag	UNP Q9KWT8
E	24	MET	-	expression tag	UNP Q9KWT8
I	24	MET	-	expression tag	UNP Q9KWT8
M	24	MET	-	expression tag	UNP Q9KWT8

- Molecule 2 is a protein called AlgM2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	284	2257	1506	359	379	13	0	0	0
2	F	280	2229	1488	354	375	12	0	0	0
2	J	284	2257	1506	359	379	13	0	0	0
2	N	284	2257	1506	359	379	13	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	294	LEU	-	expression tag	UNP Q9KWT7
B	295	GLU	-	expression tag	UNP Q9KWT7
B	296	HIS	-	expression tag	UNP Q9KWT7
B	297	HIS	-	expression tag	UNP Q9KWT7
B	298	HIS	-	expression tag	UNP Q9KWT7
B	299	HIS	-	expression tag	UNP Q9KWT7
B	300	HIS	-	expression tag	UNP Q9KWT7
B	301	HIS	-	expression tag	UNP Q9KWT7
B	302	HIS	-	expression tag	UNP Q9KWT7
B	303	HIS	-	expression tag	UNP Q9KWT7
B	304	HIS	-	expression tag	UNP Q9KWT7
B	305	HIS	-	expression tag	UNP Q9KWT7
F	294	LEU	-	expression tag	UNP Q9KWT7
F	295	GLU	-	expression tag	UNP Q9KWT7
F	296	HIS	-	expression tag	UNP Q9KWT7
F	297	HIS	-	expression tag	UNP Q9KWT7
F	298	HIS	-	expression tag	UNP Q9KWT7
F	299	HIS	-	expression tag	UNP Q9KWT7
F	300	HIS	-	expression tag	UNP Q9KWT7
F	301	HIS	-	expression tag	UNP Q9KWT7
F	302	HIS	-	expression tag	UNP Q9KWT7
F	303	HIS	-	expression tag	UNP Q9KWT7
F	304	HIS	-	expression tag	UNP Q9KWT7
F	305	HIS	-	expression tag	UNP Q9KWT7
J	294	LEU	-	expression tag	UNP Q9KWT7
J	295	GLU	-	expression tag	UNP Q9KWT7
J	296	HIS	-	expression tag	UNP Q9KWT7
J	297	HIS	-	expression tag	UNP Q9KWT7
J	298	HIS	-	expression tag	UNP Q9KWT7
J	299	HIS	-	expression tag	UNP Q9KWT7
J	300	HIS	-	expression tag	UNP Q9KWT7
J	301	HIS	-	expression tag	UNP Q9KWT7
J	302	HIS	-	expression tag	UNP Q9KWT7
J	303	HIS	-	expression tag	UNP Q9KWT7
J	304	HIS	-	expression tag	UNP Q9KWT7
J	305	HIS	-	expression tag	UNP Q9KWT7
N	294	LEU	-	expression tag	UNP Q9KWT7
N	295	GLU	-	expression tag	UNP Q9KWT7
N	296	HIS	-	expression tag	UNP Q9KWT7
N	297	HIS	-	expression tag	UNP Q9KWT7
N	298	HIS	-	expression tag	UNP Q9KWT7
N	299	HIS	-	expression tag	UNP Q9KWT7
N	300	HIS	-	expression tag	UNP Q9KWT7

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Chain	Residue	Modelled	Actual	Comment	Reference
N	301	HIS	-	expression tag	UNP Q9KWT7
N	302	HIS	-	expression tag	UNP Q9KWT7
N	303	HIS	-	expression tag	UNP Q9KWT7
N	304	HIS	-	expression tag	UNP Q9KWT7
N	305	HIS	-	expression tag	UNP Q9KWT7

- Molecule 3 is a protein called AlgS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	363	2777	1745	503	518	11	0	0	0
3	D	363	2777	1745	503	518	11	0	0	0
3	G	363	2777	1745	503	518	11	0	0	0
3	H	363	2777	1745	503	518	11	0	0	0
3	K	363	2777	1745	503	518	11	0	0	0
3	L	363	2777	1745	503	518	11	0	0	0
3	O	363	2777	1745	503	518	11	0	0	0
3	P	363	2777	1745	503	518	11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

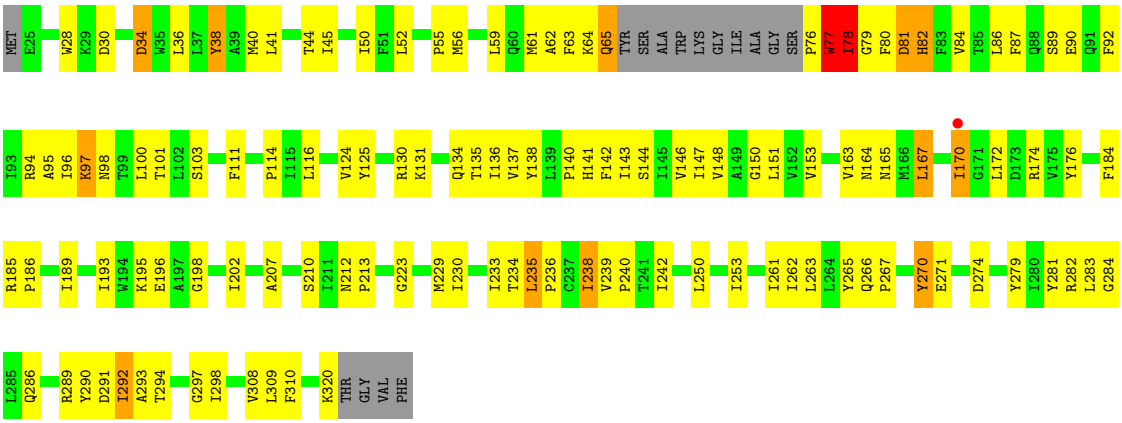
Chain	Residue	Modelled	Actual	Comment	Reference
C	160	GLN	GLU	engineered mutation	UNP Q9KWT9
D	160	GLN	GLU	engineered mutation	UNP Q9KWT9
G	160	GLN	GLU	engineered mutation	UNP Q9KWT9
H	160	GLN	GLU	engineered mutation	UNP Q9KWT9
K	160	GLN	GLU	engineered mutation	UNP Q9KWT9
L	160	GLN	GLU	engineered mutation	UNP Q9KWT9
O	160	GLN	GLU	engineered mutation	UNP Q9KWT9
P	160	GLN	GLU	engineered mutation	UNP Q9KWT9

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.

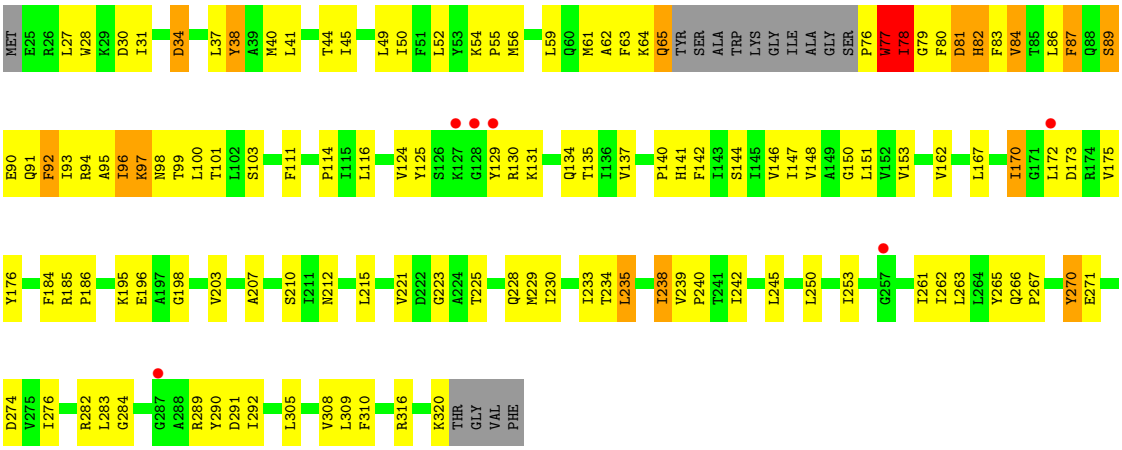
• Molecule 1: AlgM1

Chain A: 54% 37% • • 5%



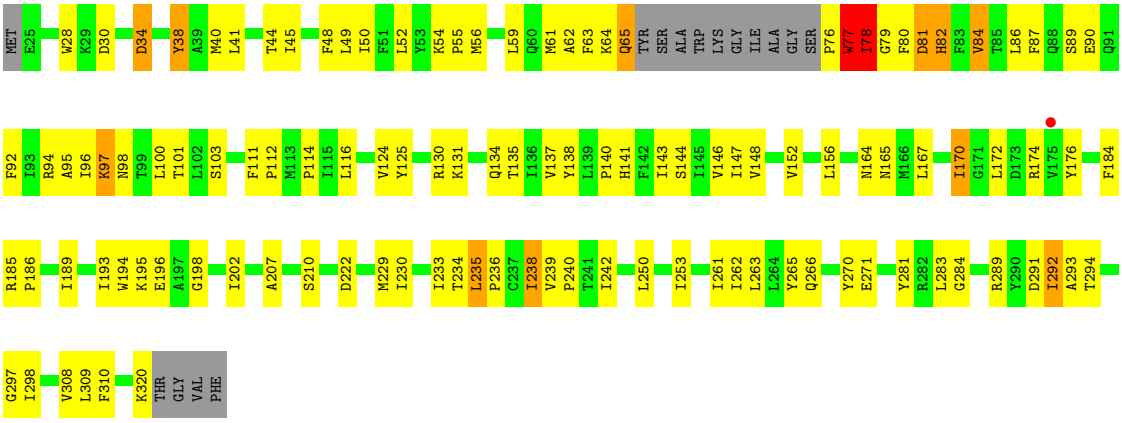
• Molecule 1: AlgM1

Chain E: 2% 53% 36% 5% • 5%



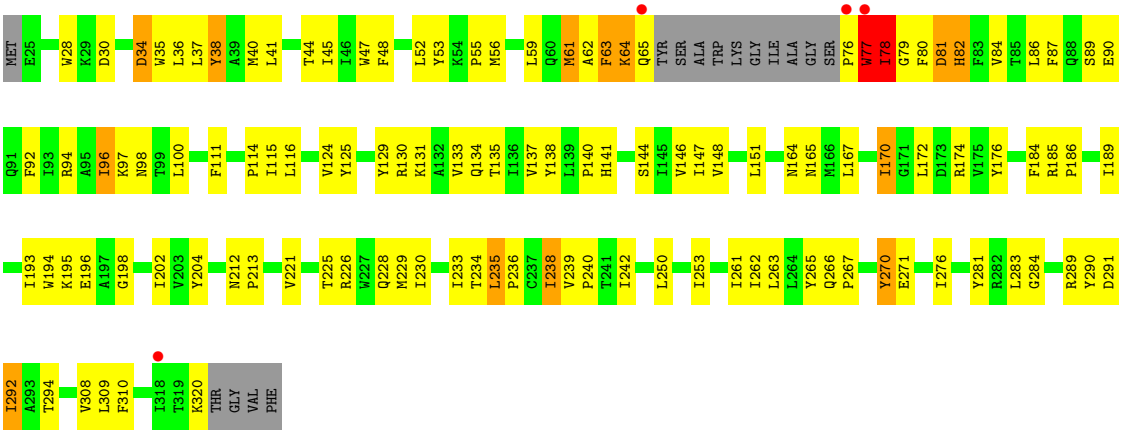
• Molecule 1: AlgM1

Chain I: 56% 34% • • 5%



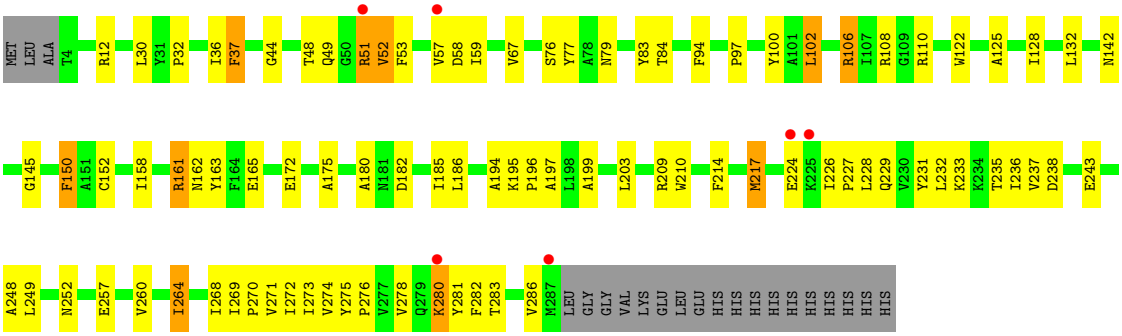
• Molecule 1: AlgM1

Chain M:



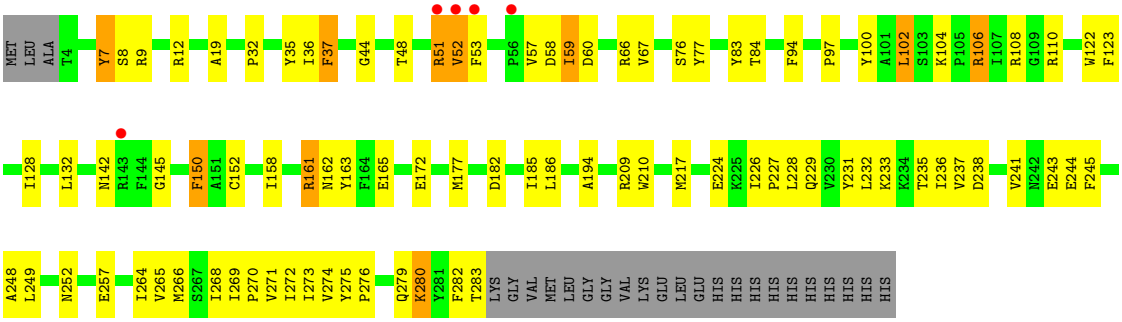
• Molecule 2: AlgM2

Chain B:



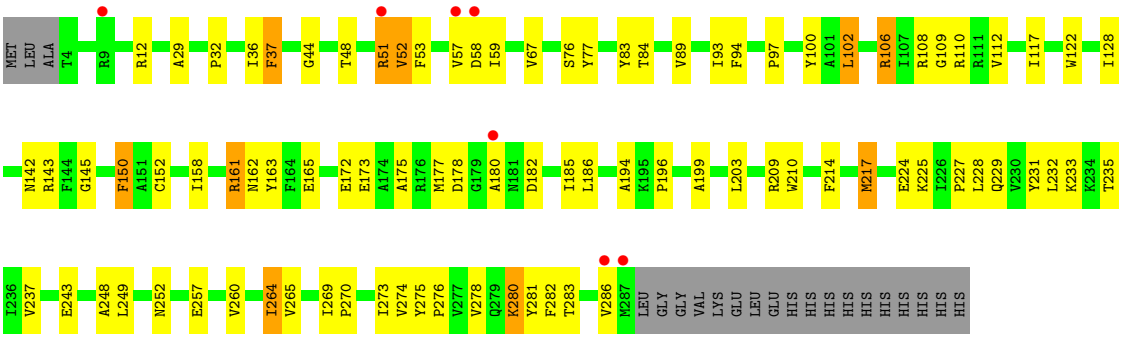
• Molecule 2: AlgM2

Chain F:



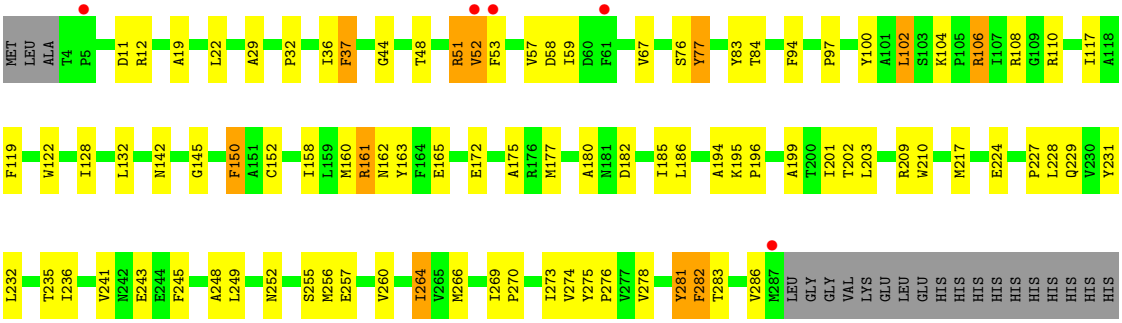
- Molecule 2: AlgM2

Chain J:



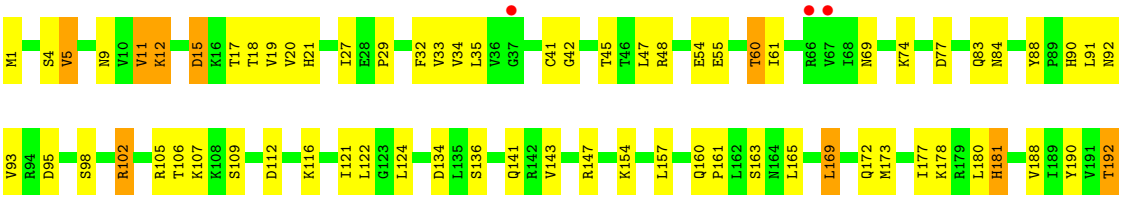
- Molecule 2: AlgM2

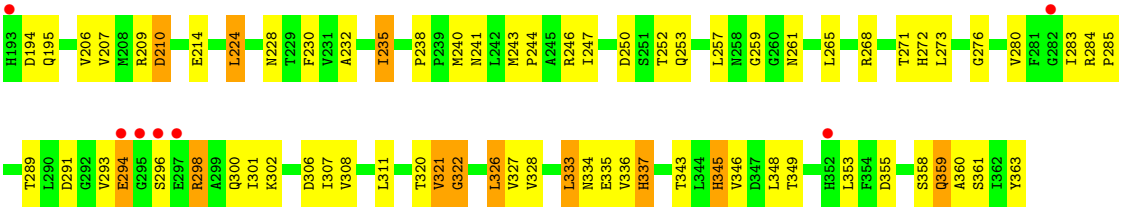
Chain N:



- Molecule 3: AlgS

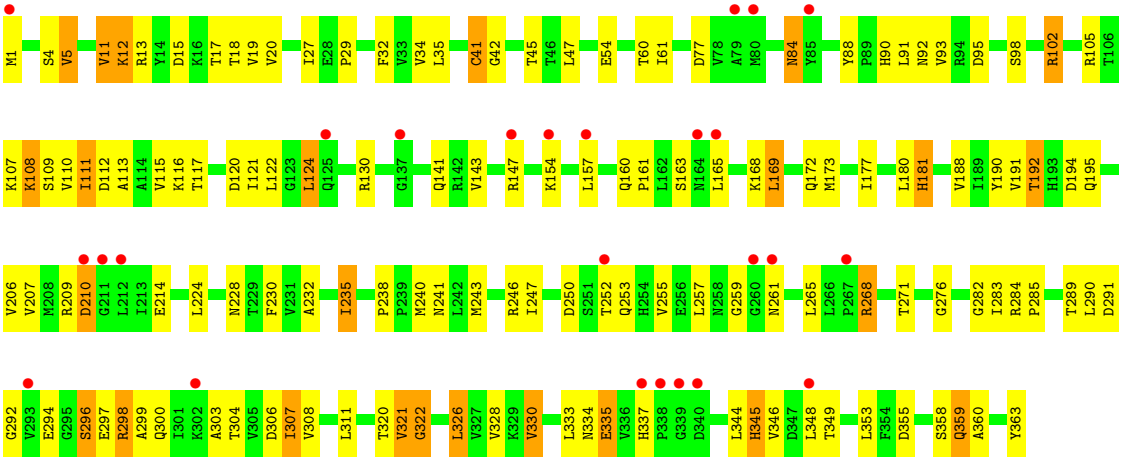
Chain C:





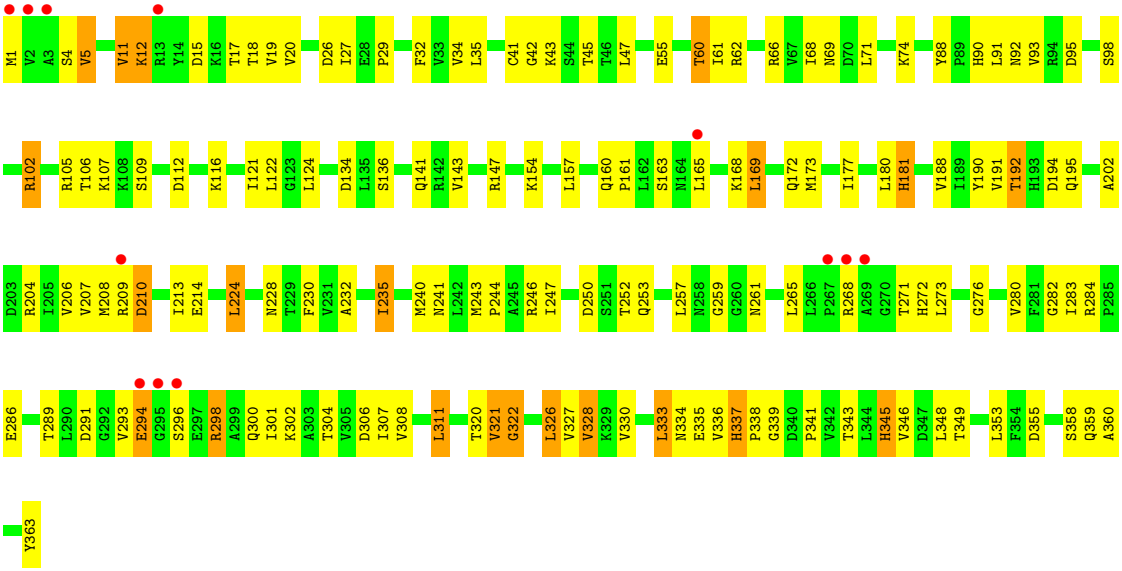
- Molecule 3: AlgS

Chain D:



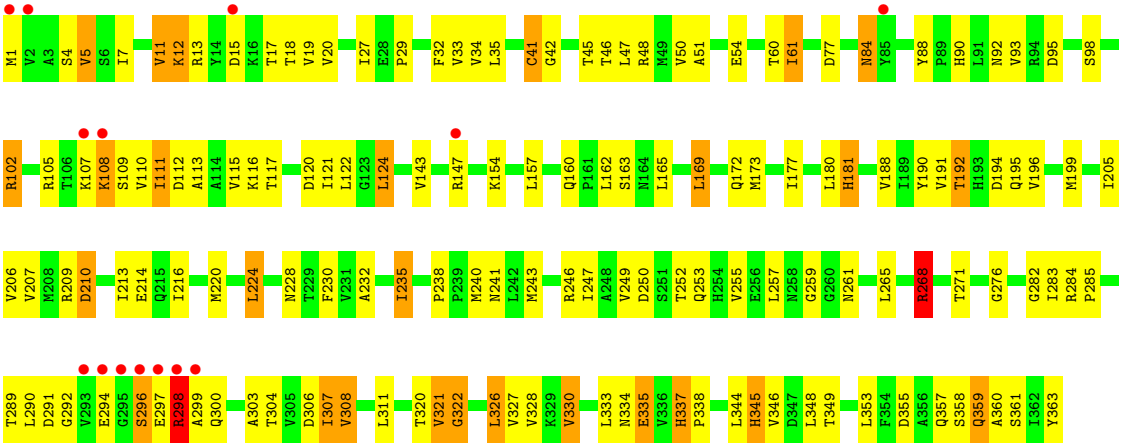
- Molecule 3: AlgS

Chain G:



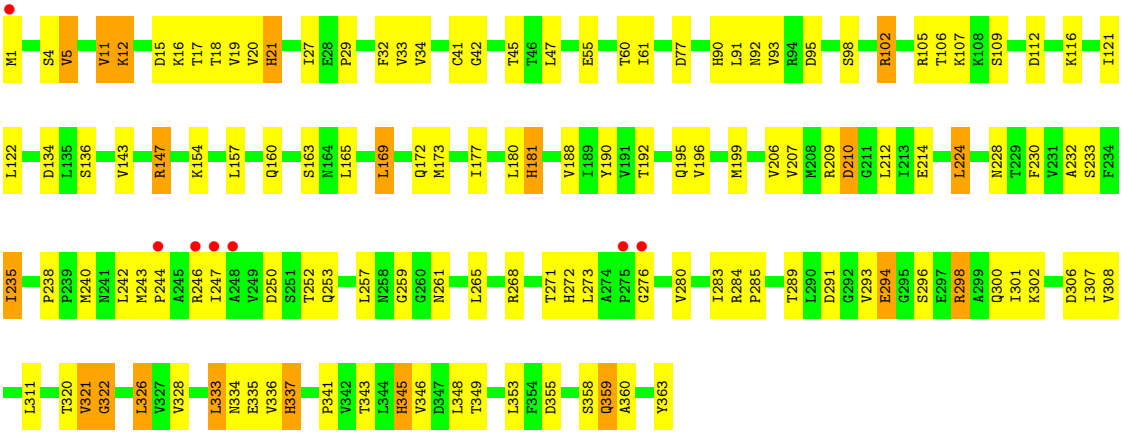
- Molecule 3: AlgS

Chain H:



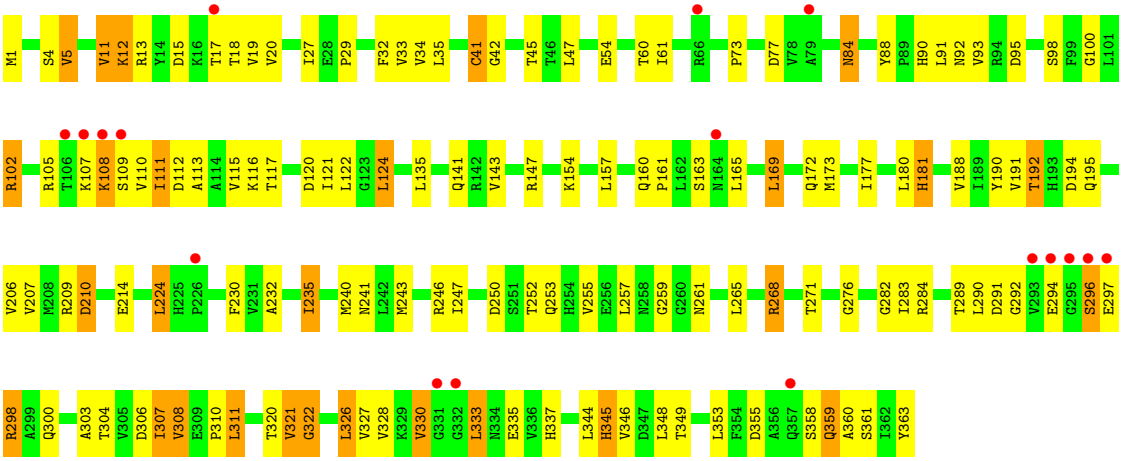
- Molecule 3: AlgS

Chain K:



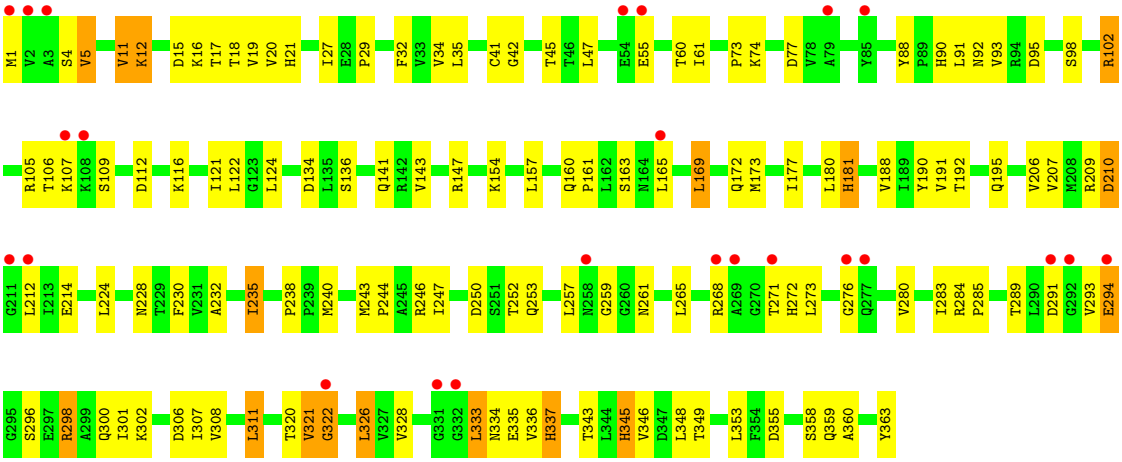
- Molecule 3: AlgS

Chain L:



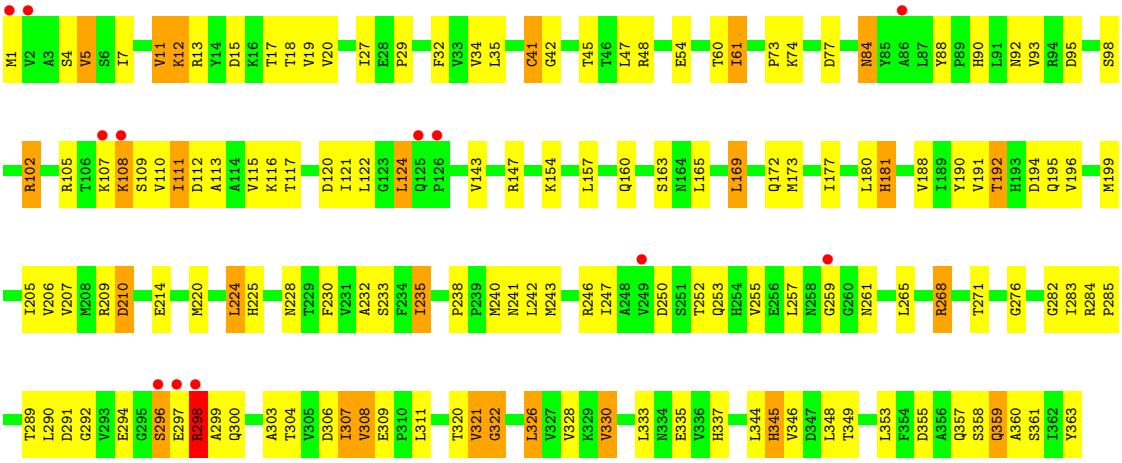
- Molecule 3: AlgS

Chain O:



- Molecule 3: AlgS

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	115.25Å 151.19Å 162.41Å 68.66° 81.76° 90.10°	Depositor
Resolution (Å)	29.82 – 4.50 29.82 – 4.50	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.82-4.50) 80.3 (29.82-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 4.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.279 , 0.320 0.281 , 0.320	Depositor DCC
R_{free} test set	2000 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å^2)	169.5	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	40472	wwPDB-VP
Average B, all atoms (Å^2)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 (i)

5.1 Standard geometry (i)

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	0.24	0/2377	0.48	1/3241 (0.0%)
1	E	0.25	0/2377	0.52	1/3241 (0.0%)
1	I	0.24	0/2377	0.47	1/3241 (0.0%)
1	M	0.24	0/2377	0.49	2/3241 (0.1%)
2	B	0.26	0/2316	0.50	1/3149 (0.0%)
2	F	0.26	0/2288	0.52	1/3113 (0.0%)
2	J	0.26	0/2316	0.50	1/3149 (0.0%)
2	N	0.28	0/2316	0.53	2/3149 (0.1%)
3	C	0.25	0/2822	0.56	0/3826
3	D	0.26	0/2822	0.60	0/3826
3	G	0.26	0/2822	0.59	0/3826
3	H	0.25	0/2822	0.61	2/3826 (0.1%)
3	K	0.26	0/2822	0.57	0/3826
3	L	0.25	0/2822	0.60	0/3826
3	O	0.26	0/2822	0.56	0/3826
3	P	0.26	0/2822	0.62	2/3826 (0.1%)
All	All	0.26	0/41320	0.55	14/56132 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	I	0	1
1	M	0	1
3	C	0	1
3	K	0	1
All	All	0	6

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	298	ARG	NE-CZ-NH1	-7.79	116.41	120.30
2	N	282	PHE	CB-CA-C	-6.60	97.20	110.40
2	J	282	PHE	CB-CA-C	-5.93	98.55	110.40
3	H	298	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	P	298	ARG	CA-CB-CG	5.56	125.64	113.40
1	M	64	LYS	C-N-CA	5.55	135.57	121.70
2	B	282	PHE	CB-CA-C	-5.48	99.43	110.40
3	H	298	ARG	CA-CB-CG	5.44	125.37	113.40
1	A	34	ASP	CB-CG-OD2	5.22	123.00	118.30
1	I	34	ASP	CB-CG-OD2	5.21	122.99	118.30
1	M	34	ASP	CB-CG-OD2	5.21	122.99	118.30
1	E	34	ASP	CB-CG-OD2	5.20	122.98	118.30
2	N	281	TYR	CB-CG-CD2	-5.10	117.94	121.00
2	F	282	PHE	CB-CA-C	-5.02	100.36	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	77	TRP	Peptide
3	C	21	HIS	Mainchain
1	E	77	TRP	Peptide
1	I	77	TRP	Peptide
3	K	21	HIS	Mainchain
1	M	77	TRP	Peptide

5.2 Too-close contacts (i)

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	2314	0	2402	81	1
1	E	2314	0	2402	82	0
1	I	2314	0	2402	72	1
1	M	2314	0	2402	79	0
2	B	2257	0	2320	63	0
2	F	2229	0	2286	60	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	2257	0	2320	62	0
2	N	2257	0	2320	71	1
3	C	2777	0	2854	76	0
3	D	2777	0	2854	77	0
3	G	2777	0	2854	90	0
3	H	2777	0	2854	90	0
3	K	2777	0	2854	71	0
3	L	2777	0	2854	84	0
3	O	2777	0	2854	70	0
3	P	2777	0	2854	86	0
All	All	40472	0	41686	1126	2

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 (1126) 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:M:34:ASP:OD1	2:N:106:ARG:NH1	1.72	1.23
1:E:34:ASP:OD1	2:F:106:ARG:NH1	2.02	0.92
2:N:102:LEU:HD12	2:N:161:ARG:HE	1.40	0.87
3:L:195:GLN:HG3	3:L:235:ILE:HA	1.59	0.84
2:N:76:SER:HB3	2:N:228:LEU:H	1.42	0.84
2:F:102:LEU:HD12	2:F:161:ARG:HE	1.42	0.84
3:D:195:GLN:HG3	3:D:235:ILE:HA	1.60	0.84
3:G:300:GLN:OE1	3:G:300:GLN:N	2.10	0.83
2:J:102:LEU:HD12	2:J:161:ARG:HE	1.42	0.83
3:K:195:GLN:HG3	3:K:235:ILE:HA	1.61	0.83
2:B:102:LEU:HD12	2:B:161:ARG:HE	1.41	0.82
3:K:300:GLN:N	3:K:300:GLN:OE1	2.11	0.82
3:O:300:GLN:N	3:O:300:GLN:OE1	2.11	0.82
3:G:195:GLN:HG3	3:G:235:ILE:HA	1.61	0.82
3:C:300:GLN:N	3:C:300:GLN:OE1	2.11	0.82
3:H:195:GLN:HG3	3:H:235:ILE:HA	1.61	0.82
3:O:195:GLN:HG3	3:O:235:ILE:HA	1.59	0.81
3:C:195:GLN:HG3	3:C:235:ILE:HA	1.61	0.81
3:H:247:ILE:HB	3:H:276:GLY:H	1.48	0.79
2:F:76:SER:HB3	2:F:228:LEU:H	1.45	0.79
3:P:195:GLN:HG3	3:P:235:ILE:HA	1.63	0.78
3:G:247:ILE:HB	3:G:276:GLY:H	1.49	0.78
3:L:247:ILE:HB	3:L:276:GLY:H	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:SER:HB3	2:B:228:LEU:H	1.47	0.78
2:J:76:SER:HB3	2:J:228:LEU:H	1.47	0.78
3:G:66:ARG:HH11	3:K:341:PRO:HD3	1.49	0.77
3:C:15:ASP:OD2	3:H:268:ARG:NH2	2.17	0.77
3:D:247:ILE:HB	3:D:276:GLY:H	1.50	0.77
3:O:247:ILE:HB	3:O:276:GLY:H	1.49	0.76
3:C:247:ILE:HB	3:C:276:GLY:H	1.49	0.76
3:C:335:GLU:O	3:C:337:HIS:N	2.19	0.76
3:K:247:ILE:HB	3:K:276:GLY:H	1.50	0.75
3:P:247:ILE:HB	3:P:276:GLY:H	1.51	0.75
3:O:335:GLU:O	3:O:337:HIS:N	2.19	0.74
3:G:208:MET:HG2	3:G:213:ILE:HA	1.70	0.74
3:G:335:GLU:O	3:G:337:HIS:N	2.20	0.74
3:H:32:PHE:HD2	3:H:181:HIS:HD2	1.36	0.73
3:K:335:GLU:O	3:K:337:HIS:N	2.20	0.73
3:O:333:LEU:HD13	3:P:220:MET:HG3	1.70	0.73
1:E:92:PHE:O	1:E:95:ALA:N	2.21	0.73
3:K:224:LEU:HD21	3:L:333:LEU:HD13	1.68	0.73
3:D:130:ARG:HH22	3:H:249:VAL:HA	1.54	0.73
1:M:98:ASN:ND2	1:M:271:GLU:O	2.22	0.72
3:D:32:PHE:HD2	3:D:181:HIS:HD2	1.38	0.72
3:L:296:SER:O	3:L:298:ARG:NH1	2.21	0.72
1:M:65:GLN:HG3	1:M:76:PRO:HB2	1.71	0.72
1:I:34:ASP:OD1	2:J:106:ARG:NH1	2.23	0.71
3:P:32:PHE:HD2	3:P:181:HIS:HD2	1.37	0.71
3:G:333:LEU:HD13	3:H:220:MET:HG3	1.72	0.70
3:H:290:LEU:O	3:H:292:GLY:N	2.25	0.70
3:L:32:PHE:HD2	3:L:181:HIS:HD2	1.38	0.69
1:A:98:ASN:ND2	1:A:271:GLU:O	2.24	0.69
3:L:290:LEU:O	3:L:292:GLY:N	2.26	0.69
3:D:290:LEU:HG	3:D:330:VAL:HG11	1.75	0.69
1:E:98:ASN:ND2	1:E:271:GLU:O	2.25	0.69
3:C:32:PHE:HD2	3:C:181:HIS:HD2	1.39	0.69
3:P:290:LEU:O	3:P:292:GLY:N	2.25	0.69
3:K:32:PHE:HD2	3:K:181:HIS:HD2	1.38	0.69
3:D:290:LEU:O	3:D:292:GLY:N	2.25	0.69
1:E:62:ALA:O	1:E:82:HIS:NE2	2.26	0.69
2:B:44:GLY:O	2:B:48:THR:OG1	2.11	0.68
1:A:65:GLN:HB2	1:A:76:PRO:HB2	1.76	0.68
2:J:248:ALA:O	2:J:252:ASN:ND2	2.24	0.68
2:F:248:ALA:O	2:F:252:ASN:ND2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:40:MET:HB3	2:J:97:PRO:HB2	1.76	0.68
1:A:62:ALA:O	1:A:82:HIS:NE2	2.27	0.68
2:N:44:GLY:O	2:N:48:THR:OG1	2.13	0.67
3:C:359:GLN:OE1	3:H:357:GLN:NE2	2.24	0.67
3:L:290:LEU:HG	3:L:330:VAL:HG11	1.75	0.67
1:I:98:ASN:ND2	1:I:271:GLU:O	2.28	0.67
1:I:62:ALA:O	1:I:82:HIS:NE2	2.27	0.67
1:M:62:ALA:O	1:M:82:HIS:NE2	2.28	0.67
3:O:207:VAL:HG13	3:O:214:GLU:HB3	1.76	0.67
3:O:32:PHE:HD2	3:O:181:HIS:HD2	1.42	0.67
3:H:290:LEU:HG	3:H:330:VAL:HG11	1.76	0.67
3:K:34:VAL:HG22	3:K:190:TYR:HB3	1.77	0.67
3:O:34:VAL:HG22	3:O:190:TYR:HB3	1.76	0.67
3:L:207:VAL:HG13	3:L:214:GLU:HB3	1.77	0.66
3:H:296:SER:OG	3:H:297:GLU:N	2.28	0.66
3:O:358:SER:O	3:O:360:ALA:N	2.28	0.66
3:P:34:VAL:HG22	3:P:190:TYR:HB3	1.77	0.66
3:G:32:PHE:HD2	3:G:181:HIS:HD2	1.42	0.66
1:A:40:MET:HB3	2:B:97:PRO:HB2	1.78	0.66
3:D:34:VAL:HG22	3:D:190:TYR:HB3	1.77	0.66
3:G:358:SER:O	3:G:360:ALA:N	2.27	0.66
3:P:290:LEU:HG	3:P:330:VAL:HG11	1.77	0.66
2:B:248:ALA:O	2:B:252:ASN:ND2	2.26	0.66
3:D:296:SER:OG	3:D:297:GLU:N	2.29	0.66
1:E:90:GLU:O	1:E:92:PHE:N	2.28	0.66
3:K:253:GLN:O	3:K:265:LEU:N	2.28	0.66
2:N:248:ALA:O	2:N:252:ASN:ND2	2.25	0.66
2:F:44:GLY:O	2:F:48:THR:OG1	2.12	0.65
1:I:65:GLN:HB2	1:I:76:PRO:HB2	1.77	0.65
2:J:44:GLY:O	2:J:48:THR:OG1	2.12	0.65
3:L:34:VAL:HG22	3:L:190:TYR:HB3	1.77	0.65
3:H:34:VAL:HG22	3:H:190:TYR:HB3	1.79	0.65
1:E:223:GLY:HA3	3:G:74:LYS:HD3	1.76	0.65
1:M:34:ASP:OD2	2:N:106:ARG:HD2	1.95	0.65
3:D:207:VAL:HG13	3:D:214:GLU:HB3	1.77	0.65
3:K:207:VAL:HG13	3:K:214:GLU:HB3	1.79	0.65
3:O:306:ASP:HB2	3:O:320:THR:HG23	1.78	0.65
3:P:296:SER:OG	3:P:297:GLU:N	2.28	0.65
3:G:34:VAL:HG22	3:G:190:TYR:HB3	1.78	0.65
3:C:253:GLN:O	3:C:265:LEU:N	2.27	0.65
2:N:196:PRO:HB3	2:N:286:VAL:HB	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:296:SER:O	3:D:298:ARG:NH1	2.28	0.65
2:B:273:ILE:O	2:B:276:PRO:HD2	1.97	0.65
3:D:306:ASP:HB2	3:D:320:THR:HG23	1.79	0.64
3:H:358:SER:O	3:H:360:ALA:N	2.29	0.64
2:N:273:ILE:O	2:N:276:PRO:HD2	1.98	0.64
3:C:207:VAL:HG13	3:C:214:GLU:HB3	1.78	0.64
1:M:284:GLY:HA3	2:N:128:ILE:HD11	1.79	0.64
3:P:253:GLN:O	3:P:265:LEU:N	2.29	0.64
3:P:358:SER:O	3:P:360:ALA:N	2.27	0.64
3:P:353:LEU:HB2	3:P:363:TYR:HB2	1.80	0.64
3:C:34:VAL:HG22	3:C:190:TYR:HB3	1.78	0.64
3:C:358:SER:O	3:C:360:ALA:N	2.28	0.64
3:P:207:VAL:HG13	3:P:214:GLU:HB3	1.78	0.64
2:N:199:ALA:HA	2:N:202:THR:HG22	1.80	0.64
3:P:306:ASP:HB2	3:P:320:THR:HG23	1.80	0.64
2:F:273:ILE:O	2:F:276:PRO:HD2	1.97	0.64
2:J:273:ILE:O	2:J:276:PRO:HD2	1.97	0.64
3:H:207:VAL:HG13	3:H:214:GLU:HB3	1.79	0.63
2:F:228:LEU:O	2:F:231:TYR:N	2.31	0.63
3:K:196:VAL:HG13	3:L:311:LEU:HD21	1.80	0.63
2:F:51:ARG:HB3	2:F:57:VAL:HG21	1.81	0.63
3:H:353:LEU:HB2	3:H:363:TYR:HB2	1.81	0.63
3:G:253:GLN:O	3:G:265:LEU:N	2.28	0.63
1:E:144:SER:HB3	1:E:147:ILE:HG13	1.79	0.63
3:D:259:GLY:O	3:D:261:ASN:ND2	2.32	0.63
1:A:148:VAL:HG21	1:A:195:LYS:HD2	1.81	0.62
2:B:228:LEU:O	2:B:231:TYR:N	2.32	0.62
3:D:353:LEU:HB2	3:D:363:TYR:HB2	1.81	0.62
3:H:253:GLN:O	3:H:265:LEU:N	2.28	0.62
3:H:296:SER:O	3:H:298:ARG:NH1	2.32	0.62
2:N:106:ARG:NH2	2:N:172:GLU:OE2	2.33	0.62
3:H:306:ASP:HB2	3:H:320:THR:HG23	1.82	0.62
2:J:228:LEU:O	2:J:231:TYR:N	2.32	0.62
3:C:165:LEU:HD13	3:C:169:LEU:HD22	1.82	0.62
3:L:296:SER:OG	3:L:297:GLU:N	2.32	0.62
3:P:259:GLY:O	3:P:261:ASN:ND2	2.32	0.62
3:L:353:LEU:HB2	3:L:363:TYR:HB2	1.81	0.62
3:H:259:GLY:O	3:H:261:ASN:ND2	2.32	0.62
1:I:184:PHE:HZ	1:I:261:ILE:HG12	1.65	0.62
3:L:98:SER:O	3:L:102:ARG:HG2	2.00	0.62
2:N:228:LEU:O	2:N:231:TYR:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:306:ASP:HB2	3:K:320:THR:HG23	1.81	0.62
3:O:253:GLN:O	3:O:265:LEU:N	2.28	0.62
3:K:259:GLY:O	3:K:261:ASN:ND2	2.33	0.61
3:G:98:SER:O	3:G:102:ARG:HG2	1.99	0.61
1:I:284:GLY:HA3	2:J:128:ILE:HD11	1.82	0.61
3:L:259:GLY:O	3:L:261:ASN:ND2	2.32	0.61
3:O:259:GLY:O	3:O:261:ASN:ND2	2.33	0.61
1:E:56:MET:HA	1:E:59:LEU:HD23	1.82	0.61
1:E:284:GLY:HA3	2:F:128:ILE:HD11	1.81	0.61
3:C:4:SER:HB3	3:C:29:PRO:HG3	1.83	0.61
1:E:82:HIS:O	1:E:86:LEU:N	2.25	0.61
3:C:259:GLY:O	3:C:261:ASN:ND2	2.33	0.61
3:C:306:ASP:HB2	3:C:320:THR:HG23	1.81	0.61
1:E:65:GLN:HB2	1:E:76:PRO:HB2	1.82	0.61
3:G:353:LEU:HB2	3:G:363:TYR:HB2	1.82	0.61
1:I:148:VAL:HG21	1:I:195:LYS:HD2	1.83	0.61
3:P:98:SER:O	3:P:102:ARG:HG2	2.01	0.61
3:G:259:GLY:O	3:G:261:ASN:ND2	2.33	0.61
1:M:40:MET:HB3	2:N:97:PRO:HB2	1.81	0.61
3:O:98:SER:O	3:O:102:ARG:HG2	2.00	0.61
3:G:306:ASP:HB2	3:G:320:THR:HG23	1.82	0.61
2:N:51:ARG:HB3	2:N:57:VAL:HG21	1.82	0.61
3:P:4:SER:HB3	3:P:29:PRO:HG3	1.83	0.61
3:D:253:GLN:O	3:D:265:LEU:N	2.28	0.61
3:K:98:SER:O	3:K:102:ARG:HG2	2.01	0.61
3:K:353:LEU:HB2	3:K:363:TYR:HB2	1.83	0.61
1:A:56:MET:HA	1:A:59:LEU:HD23	1.84	0.60
2:F:110:ARG:NH1	2:F:165:GLU:OE1	2.34	0.60
3:D:297:GLU:O	3:D:300:GLN:NE2	2.34	0.60
3:P:296:SER:O	3:P:298:ARG:NH1	2.34	0.60
1:A:34:ASP:OD1	2:B:106:ARG:NH1	2.34	0.60
3:D:358:SER:O	3:D:360:ALA:N	2.32	0.60
2:N:51:ARG:HG2	2:N:57:VAL:HG11	1.83	0.60
3:C:98:SER:O	3:C:102:ARG:HG2	2.01	0.60
2:F:51:ARG:HG2	2:F:57:VAL:HG11	1.82	0.60
2:J:51:ARG:HB3	2:J:57:VAL:HG21	1.82	0.60
3:D:98:SER:O	3:D:102:ARG:HG2	2.02	0.60
3:G:293:VAL:HB	3:G:345:HIS:ND1	2.17	0.60
1:M:78:ILE:HG23	1:M:79:GLY:O	2.02	0.60
3:O:4:SER:HB3	3:O:29:PRO:HG3	1.83	0.60
1:E:78:ILE:HG23	1:E:79:GLY:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:47:LEU:HD11	3:G:157:LEU:HB3	1.84	0.60
3:H:11:VAL:HA	3:H:20:VAL:HG23	1.84	0.60
3:K:358:SER:O	3:K:360:ALA:N	2.29	0.60
3:O:353:LEU:HB2	3:O:363:TYR:HB2	1.82	0.60
2:J:51:ARG:HG2	2:J:57:VAL:HG11	1.84	0.59
1:M:44:THR:OG1	2:N:94:PHE:O	2.18	0.59
1:A:78:ILE:HG23	1:A:79:GLY:O	2.02	0.59
1:A:184:PHE:HZ	1:A:261:ILE:HG12	1.67	0.59
3:C:293:VAL:HB	3:C:345:HIS:ND1	2.18	0.59
3:D:11:VAL:HA	3:D:20:VAL:HG23	1.84	0.59
3:G:4:SER:HB3	3:G:29:PRO:HG3	1.85	0.59
2:J:196:PRO:HB3	2:J:286:VAL:HB	1.83	0.59
3:O:293:VAL:HB	3:O:345:HIS:ND1	2.17	0.59
1:I:78:ILE:HG23	1:I:79:GLY:O	2.02	0.59
3:L:253:GLN:O	3:L:265:LEU:N	2.31	0.59
2:N:110:ARG:NH1	2:N:165:GLU:OE1	2.35	0.59
2:B:51:ARG:HG2	2:B:57:VAL:HG11	1.84	0.59
3:H:4:SER:HB3	3:H:29:PRO:HG3	1.83	0.59
3:H:98:SER:O	3:H:102:ARG:HG2	2.03	0.59
1:I:56:MET:HA	1:I:59:LEU:HD23	1.85	0.59
3:P:11:VAL:HA	3:P:20:VAL:HG23	1.84	0.58
3:K:4:SER:HB3	3:K:29:PRO:HG3	1.84	0.58
1:M:82:HIS:O	1:M:86:LEU:N	2.29	0.58
3:D:4:SER:HB3	3:D:29:PRO:HG3	1.85	0.58
3:P:297:GLU:O	3:P:300:GLN:NE2	2.34	0.58
3:L:358:SER:O	3:L:360:ALA:N	2.32	0.58
1:M:230:ILE:HA	1:M:234:THR:HB	1.86	0.58
1:E:230:ILE:HA	1:E:234:THR:HB	1.84	0.58
3:G:12:LYS:NZ	3:G:55:GLU:O	2.36	0.58
3:K:165:LEU:HD13	3:K:169:LEU:HD22	1.84	0.58
3:L:297:GLU:O	3:L:300:GLN:NE2	2.34	0.58
1:M:221:VAL:HA	3:O:73:PRO:HB2	1.84	0.58
3:K:12:LYS:NZ	3:K:55:GLU:O	2.37	0.58
3:K:240:MET:HG3	3:K:284:ARG:HG2	1.86	0.58
3:L:11:VAL:HA	3:L:20:VAL:HG23	1.86	0.58
1:M:56:MET:HA	1:M:59:LEU:HD23	1.84	0.58
3:O:165:LEU:HD13	3:O:169:LEU:HD22	1.86	0.58
1:E:95:ALA:O	1:E:99:THR:N	2.36	0.57
3:L:4:SER:HB3	3:L:29:PRO:HG3	1.85	0.57
2:B:158:ILE:HA	2:B:161:ARG:HG2	1.86	0.57
3:O:12:LYS:NZ	3:O:55:GLU:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:PRO:HB3	2:B:286:VAL:HB	1.85	0.57
1:E:89:SER:OG	1:E:90:GLU:N	2.34	0.57
3:K:293:VAL:HB	3:K:345:HIS:ND1	2.18	0.57
2:N:196:PRO:HA	2:N:281:TYR:OH	2.04	0.57
2:B:51:ARG:HB3	2:B:57:VAL:HG21	1.85	0.57
2:B:106:ARG:NH2	2:B:172:GLU:OE2	2.37	0.57
3:L:41:CYS:SG	3:L:42:GLY:N	2.77	0.57
1:E:148:VAL:HG21	1:E:195:LYS:HD2	1.85	0.57
1:A:165:ASN:ND2	2:B:49:GLN:O	2.38	0.57
3:C:12:LYS:NZ	3:C:55:GLU:O	2.37	0.57
1:E:316:ARG:O	1:E:320:LYS:HB3	2.05	0.57
1:M:148:VAL:HG21	1:M:195:LYS:HD2	1.87	0.57
3:P:165:LEU:HD13	3:P:169:LEU:HD22	1.86	0.57
1:A:284:GLY:HA3	2:B:128:ILE:HD11	1.87	0.57
2:F:106:ARG:NH2	2:F:172:GLU:OE2	2.38	0.57
1:I:165:ASN:OD1	1:I:174:ARG:NH1	2.36	0.57
1:I:82:HIS:O	1:I:86:LEU:N	2.29	0.57
3:L:306:ASP:HB2	3:L:320:THR:HG23	1.86	0.56
1:M:184:PHE:HZ	1:M:261:ILE:HG12	1.70	0.56
1:A:230:ILE:HA	1:A:234:THR:HB	1.86	0.56
1:M:129:TYR:OH	2:N:19:ALA:O	2.22	0.56
3:H:165:LEU:HD13	3:H:169:LEU:HD22	1.87	0.56
1:I:144:SER:HB3	1:I:147:ILE:HG13	1.87	0.56
1:I:229:MET:O	1:I:233:ILE:HG12	2.05	0.56
3:P:124:LEU:HD23	3:P:124:LEU:H	1.70	0.56
1:A:56:MET:HG2	2:B:125:ALA:HB2	1.88	0.56
3:C:353:LEU:HB2	3:C:363:TYR:HB2	1.87	0.56
2:J:158:ILE:HA	2:J:161:ARG:HG2	1.87	0.56
3:C:293:VAL:O	3:C:294:GLU:HG3	2.06	0.56
3:H:297:GLU:O	3:H:300:GLN:NE2	2.34	0.56
2:N:76:SER:HB3	2:N:228:LEU:N	2.18	0.56
3:L:124:LEU:H	3:L:124:LEU:HD23	1.70	0.56
1:M:37:LEU:HD11	2:N:104:LYS:HG3	1.88	0.56
1:I:140:PRO:HB2	1:I:195:LYS:HA	1.88	0.56
2:J:178:ASP:OD2	3:L:100:GLY:HA3	2.06	0.56
3:O:293:VAL:O	3:O:294:GLU:HG3	2.06	0.56
3:D:41:CYS:SG	3:D:42:GLY:N	2.78	0.56
3:K:293:VAL:O	3:K:294:GLU:HG3	2.06	0.56
3:G:105:ARG:O	3:G:106:THR:OG1	2.24	0.56
3:H:88:TYR:HB3	3:H:90:HIS:CE1	2.41	0.56
3:D:124:LEU:HD23	3:D:124:LEU:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:158:ILE:HA	2:F:161:ARG:HG2	1.88	0.55
1:E:184:PHE:HZ	1:E:261:ILE:HG12	1.70	0.55
3:L:165:LEU:HD13	3:L:169:LEU:HD22	1.88	0.55
1:M:144:SER:HB3	1:M:147:ILE:HG13	1.87	0.55
2:B:110:ARG:NH1	2:B:165:GLU:OE1	2.40	0.55
3:G:43:LYS:NZ	3:G:208:MET:SD	2.64	0.55
1:A:82:HIS:O	1:A:86:LEU:N	2.30	0.55
2:B:76:SER:HB3	2:B:228:LEU:N	2.21	0.55
3:G:165:LEU:HD13	3:G:169:LEU:HD22	1.87	0.55
1:A:144:SER:HB3	1:A:147:ILE:HG13	1.89	0.55
3:D:165:LEU:HD13	3:D:169:LEU:HD22	1.89	0.55
3:H:209:ARG:HG2	3:H:210:ASP:OD2	2.07	0.55
1:A:44:THR:OG1	2:B:94:PHE:O	2.23	0.55
3:K:32:PHE:CD2	3:K:181:HIS:HD2	2.23	0.55
3:L:92:ASN:ND2	3:L:95:ASP:OD2	2.40	0.55
1:E:215:LEU:HG	3:G:88:TYR:CD1	2.42	0.55
2:F:84:THR:HG21	2:F:210:TRP:HE3	1.72	0.55
3:H:12:LYS:H	3:H:20:VAL:HG22	1.72	0.55
3:O:47:LEU:HD11	3:O:157:LEU:HB3	1.89	0.55
3:P:47:LEU:HD11	3:P:157:LEU:HB3	1.89	0.55
3:G:293:VAL:O	3:G:294:GLU:HG3	2.06	0.54
3:K:300:GLN:HE21	3:K:343:THR:CG2	2.19	0.54
3:O:240:MET:HG3	3:O:284:ARG:HG2	1.89	0.54
3:P:32:PHE:CD2	3:P:181:HIS:HD2	2.24	0.54
3:G:88:TYR:HB3	3:G:90:HIS:CE1	2.42	0.54
3:H:124:LEU:HD23	3:H:124:LEU:H	1.71	0.54
3:H:240:MET:HG3	3:H:284:ARG:HG2	1.89	0.54
1:I:230:ILE:HA	1:I:234:THR:HB	1.90	0.54
3:G:43:LYS:HE3	3:G:208:MET:HB2	1.88	0.54
3:L:240:MET:HG3	3:L:284:ARG:HG2	1.90	0.54
3:P:12:LYS:H	3:P:20:VAL:HG22	1.73	0.54
3:P:300:GLN:HB2	3:P:344:LEU:O	2.07	0.54
3:D:92:ASN:ND2	3:D:95:ASP:OD2	2.41	0.54
3:H:41:CYS:SG	3:H:42:GLY:N	2.80	0.54
1:M:89:SER:HB2	1:M:92:PHE:HB3	1.90	0.54
1:M:146:VAL:HG12	1:M:263:LEU:HD21	1.88	0.54
1:A:140:PRO:HB2	1:A:195:LYS:HA	1.88	0.54
3:C:209:ARG:HG2	3:C:210:ASP:OD2	2.07	0.54
1:E:135:THR:HA	2:F:275:TYR:OH	2.07	0.54
3:C:300:GLN:HE21	3:C:343:THR:CG2	2.21	0.54
1:E:135:THR:HG22	2:F:279:GLN:HE22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:110:ARG:NH1	2:J:165:GLU:OE1	2.41	0.54
3:P:240:MET:HG3	3:P:284:ARG:HG2	1.90	0.54
2:J:203:LEU:HD13	2:J:278:VAL:HG22	1.89	0.54
3:O:300:GLN:HE21	3:O:343:THR:CG2	2.21	0.54
3:K:359:GLN:OE1	3:P:357:GLN:NE2	2.29	0.54
2:N:278:VAL:HG12	2:N:282:PHE:HE1	1.73	0.54
1:E:40:MET:HB3	2:F:97:PRO:HB2	1.89	0.53
1:E:90:GLU:C	1:E:92:PHE:H	2.10	0.53
3:G:35:LEU:HB3	3:G:43:LYS:HD3	1.90	0.53
3:O:11:VAL:HA	3:O:20:VAL:HG23	1.89	0.53
3:P:41:CYS:SG	3:P:42:GLY:N	2.81	0.53
1:E:150:GLY:HA3	2:F:236:ILE:HG22	1.89	0.53
3:G:121:ILE:HB	3:G:122:LEU:HD12	1.91	0.53
3:K:105:ARG:O	3:K:106:THR:OG1	2.24	0.53
3:O:121:ILE:HB	3:O:122:LEU:HD12	1.90	0.53
3:D:12:LYS:H	3:D:20:VAL:HG22	1.74	0.53
3:G:311:LEU:HD21	3:H:196:VAL:HG13	1.89	0.53
3:L:209:ARG:HG2	3:L:210:ASP:OD2	2.07	0.53
1:M:194:TRP:HE1	2:N:29:ALA:HA	1.74	0.53
3:P:209:ARG:HG2	3:P:210:ASP:OD2	2.08	0.53
3:K:11:VAL:HA	3:K:20:VAL:HG23	1.91	0.53
3:K:41:CYS:SG	3:K:42:GLY:N	2.81	0.53
1:E:64:LYS:HD3	1:E:291:ASP:OD2	2.09	0.53
3:H:47:LEU:HD11	3:H:157:LEU:HB3	1.91	0.53
3:O:209:ARG:HG2	3:O:210:ASP:OD2	2.08	0.53
3:C:298:ARG:HG2	3:C:348:LEU:HD21	1.91	0.53
3:D:209:ARG:HG2	3:D:210:ASP:OD2	2.07	0.53
3:C:41:CYS:SG	3:C:42:GLY:N	2.82	0.53
1:E:140:PRO:HB2	1:E:195:LYS:HA	1.90	0.53
2:F:76:SER:HB3	2:F:228:LEU:N	2.20	0.53
2:J:177:MET:SD	3:L:73:PRO:HB3	2.48	0.53
3:O:92:ASN:ND2	3:O:95:ASP:OD2	2.41	0.53
1:E:79:GLY:C	1:E:81:ASP:H	2.12	0.53
3:G:207:VAL:HG13	3:G:214:GLU:HB3	1.90	0.53
1:I:164:ASN:HB3	1:I:174:ARG:HG2	1.91	0.53
3:L:247:ILE:HB	3:L:276:GLY:N	2.22	0.53
1:M:47:TRP:CE3	2:N:152:CYS:HB2	2.44	0.53
2:N:195:LYS:O	2:N:281:TYR:OH	2.27	0.53
3:H:92:ASN:ND2	3:H:95:ASP:OD2	2.42	0.53
3:D:300:GLN:HB3	3:D:345:HIS:CD2	2.44	0.52
3:G:11:VAL:HA	3:G:20:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:76:SER:HB3	2:J:228:LEU:N	2.22	0.52
3:O:41:CYS:SG	3:O:42:GLY:N	2.81	0.52
2:N:94:PHE:HB3	2:N:152:CYS:SG	2.49	0.52
1:A:89:SER:HB2	1:A:92:PHE:HB3	1.89	0.52
3:D:300:GLN:HB2	3:D:344:LEU:O	2.08	0.52
1:E:131:LYS:O	1:E:135:THR:HG23	2.09	0.52
1:M:64:LYS:HD3	1:M:291:ASP:OD2	2.08	0.52
2:N:161:ARG:HG3	2:N:162:ASN:N	2.25	0.52
2:B:203:LEU:HD13	2:B:278:VAL:HG22	1.91	0.52
2:J:163:TYR:CE1	2:J:194:ALA:HA	2.45	0.52
3:L:12:LYS:H	3:L:20:VAL:HG22	1.74	0.52
3:L:300:GLN:HB2	3:L:344:LEU:O	2.08	0.52
1:A:150:GLY:HA3	2:B:236:ILE:HG22	1.92	0.52
3:P:92:ASN:ND2	3:P:95:ASP:OD2	2.42	0.52
3:P:300:GLN:HB3	3:P:345:HIS:CD2	2.44	0.52
1:E:221:VAL:O	3:G:74:LYS:HA	2.10	0.52
3:C:9:ASN:ND2	3:H:216:ILE:HD12	2.25	0.52
3:D:240:MET:HG3	3:D:284:ARG:HG2	1.92	0.52
3:H:12:LYS:NZ	3:H:54:GLU:HB3	2.25	0.52
2:N:199:ALA:O	2:N:203:LEU:N	2.36	0.52
1:E:83:PHE:O	1:E:87:PHE:N	2.39	0.52
3:L:300:GLN:HB3	3:L:345:HIS:CD2	2.44	0.52
3:G:300:GLN:HE21	3:G:343:THR:CG2	2.22	0.51
3:K:121:ILE:HB	3:K:122:LEU:HD12	1.90	0.51
2:N:150:PHE:O	2:N:209:ARG:NH2	2.43	0.51
3:C:47:LEU:HD11	3:C:157:LEU:HB3	1.91	0.51
1:I:89:SER:HB2	1:I:92:PHE:HB3	1.92	0.51
2:J:106:ARG:NH2	2:J:172:GLU:OE2	2.43	0.51
2:F:66:ARG:HH12	2:F:244:GLU:CD	2.13	0.51
2:N:84:THR:HG21	2:N:210:TRP:HE3	1.75	0.51
3:L:122:LEU:HB2	3:L:124:LEU:HD22	1.92	0.51
3:L:141:GLN:NE2	3:L:161:PRO:O	2.43	0.51
2:B:84:THR:HG21	2:B:210:TRP:HE3	1.76	0.51
3:D:122:LEU:HB2	3:D:124:LEU:HD22	1.92	0.51
1:A:165:ASN:OD1	1:A:174:ARG:NH1	2.41	0.51
3:C:121:ILE:HB	3:C:122:LEU:HD12	1.91	0.51
3:G:240:MET:HG3	3:G:284:ARG:HG2	1.90	0.51
3:H:300:GLN:HB2	3:H:344:LEU:O	2.10	0.51
3:K:47:LEU:HD11	3:K:157:LEU:HB3	1.93	0.51
3:L:47:LEU:HD11	3:L:157:LEU:HB3	1.93	0.51
3:C:240:MET:HG3	3:C:284:ARG:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:240:MET:HE3	3:D:282:GLY:HA3	1.93	0.51
3:H:361:SER:O	3:H:361:SER:OG	2.29	0.51
3:L:12:LYS:NZ	3:L:54:GLU:HB3	2.26	0.51
3:O:298:ARG:HG2	3:O:348:LEU:HD21	1.93	0.51
3:G:301:ILE:HD11	3:G:321:VAL:HG11	1.93	0.51
2:J:84:THR:HG21	2:J:210:TRP:HE3	1.76	0.51
3:K:298:ARG:HG2	3:K:348:LEU:HD21	1.92	0.51
3:H:117:THR:O	3:H:121:ILE:HG12	2.11	0.51
1:I:131:LYS:O	1:I:135:THR:HG23	2.11	0.51
2:J:175:ALA:HB1	2:J:180:ALA:HB3	1.92	0.51
1:M:64:LYS:O	1:M:65:GLN:OE1	2.29	0.51
3:P:12:LYS:NZ	3:P:54:GLU:HB3	2.26	0.51
1:A:79:GLY:C	1:A:81:ASP:H	2.14	0.50
2:B:275:TYR:O	2:B:278:VAL:HB	2.11	0.50
3:C:181:HIS:O	3:C:181:HIS:ND1	2.38	0.50
3:H:32:PHE:CD2	3:H:181:HIS:HD2	2.23	0.50
3:H:300:GLN:HB3	3:H:345:HIS:CD2	2.46	0.50
2:J:199:ALA:HB1	2:J:281:TYR:HD2	1.76	0.50
3:L:361:SER:O	3:L:361:SER:OG	2.29	0.50
3:O:232:ALA:HB1	3:O:240:MET:HE2	1.93	0.50
2:J:275:TYR:O	2:J:278:VAL:HB	2.11	0.50
1:M:140:PRO:HB2	1:M:195:LYS:HA	1.92	0.50
2:B:150:PHE:O	2:B:209:ARG:NH2	2.44	0.50
2:B:270:PRO:HA	2:B:273:ILE:HD12	1.93	0.50
3:D:12:LYS:NZ	3:D:54:GLU:HB3	2.27	0.50
3:G:283:ILE:HG12	3:G:346:VAL:HG23	1.92	0.50
1:I:79:GLY:C	1:I:81:ASP:H	2.14	0.50
3:D:32:PHE:CD2	3:D:181:HIS:HD2	2.24	0.50
1:E:229:MET:O	1:E:233:ILE:HG12	2.12	0.50
3:G:209:ARG:HG2	3:G:210:ASP:OD2	2.11	0.50
1:M:229:MET:O	1:M:233:ILE:HG12	2.11	0.50
1:A:34:ASP:O	1:A:38:TYR:N	2.37	0.50
2:B:163:TYR:CE1	2:B:194:ALA:HA	2.46	0.50
3:C:32:PHE:CD2	3:C:181:HIS:HD2	2.24	0.50
3:D:117:THR:O	3:D:121:ILE:HG12	2.12	0.50
3:K:160:GLN:HB3	3:K:163:SER:OG	2.12	0.50
3:D:110:VAL:O	3:D:112:ASP:N	2.44	0.50
1:I:111:PHE:O	1:I:114:PRO:HD2	2.12	0.50
3:K:214:GLU:OE2	3:K:228:ASN:ND2	2.44	0.50
2:B:94:PHE:HB3	2:B:152:CYS:SG	2.51	0.50
3:H:232:ALA:HB1	3:H:240:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:275:TYR:O	2:N:278:VAL:HB	2.12	0.50
3:K:243:MET:HE1	3:K:326:LEU:HB3	1.92	0.50
3:C:11:VAL:HA	3:C:20:VAL:HG23	1.94	0.50
3:D:47:LEU:HD11	3:D:157:LEU:HB3	1.94	0.50
3:L:283:ILE:HG12	3:L:346:VAL:HG23	1.92	0.50
3:O:333:LEU:HG	3:O:334:ASN:H	1.77	0.50
3:P:240:MET:HE3	3:P:282:GLY:HA3	1.94	0.50
2:B:83:TYR:CD2	2:B:227:PRO:HB3	2.47	0.49
3:C:160:GLN:HB3	3:C:163:SER:OG	2.12	0.49
1:E:96:ILE:HB	1:E:276:ILE:HD11	1.94	0.49
3:H:214:GLU:OE2	3:H:228:ASN:ND2	2.45	0.49
3:L:32:PHE:CD2	3:L:181:HIS:HD2	2.24	0.49
3:P:283:ILE:HG12	3:P:346:VAL:HG23	1.93	0.49
2:B:280:LYS:HE3	2:B:280:LYS:HA	1.94	0.49
2:F:161:ARG:HG3	2:F:162:ASN:N	2.27	0.49
3:G:32:PHE:CD2	3:G:181:HIS:HD2	2.26	0.49
3:C:232:ALA:HB1	3:C:240:MET:HE2	1.94	0.49
2:F:150:PHE:O	2:F:209:ARG:NH2	2.45	0.49
3:G:43:LYS:HE2	3:G:43:LYS:HA	1.95	0.49
2:N:77:TYR:OH	2:N:266:MET:O	2.18	0.49
3:O:32:PHE:CD2	3:O:181:HIS:HD2	2.26	0.49
3:D:110:VAL:C	3:D:112:ASP:H	2.15	0.49
3:O:88:TYR:HB3	3:O:90:HIS:CE1	2.47	0.49
3:O:160:GLN:HB3	3:O:163:SER:OG	2.12	0.49
3:D:141:GLN:NE2	3:D:161:PRO:O	2.46	0.49
3:P:110:VAL:C	3:P:112:ASP:H	2.15	0.49
1:A:131:LYS:O	1:A:135:THR:HG23	2.12	0.49
2:J:94:PHE:HB3	2:J:152:CYS:SG	2.52	0.49
3:K:32:PHE:HD2	3:K:181:HIS:CD2	2.26	0.49
3:K:283:ILE:HG12	3:K:346:VAL:HG23	1.94	0.49
3:L:117:THR:O	3:L:121:ILE:HG12	2.13	0.49
3:P:110:VAL:O	3:P:112:ASP:N	2.43	0.49
1:A:164:ASN:HB3	1:A:174:ARG:HG2	1.94	0.49
3:H:110:VAL:O	3:H:112:ASP:N	2.43	0.49
3:H:307:ILE:HG13	3:H:308:VAL:N	2.25	0.49
3:K:209:ARG:HG2	3:K:210:ASP:OD2	2.12	0.49
3:P:105:ARG:HB3	3:P:109:SER:HB2	1.95	0.49
3:L:84:ASN:OD1	3:L:84:ASN:N	2.46	0.49
3:P:117:THR:O	3:P:121:ILE:HG12	2.12	0.49
3:P:122:LEU:HB2	3:P:124:LEU:HD22	1.93	0.49
3:D:283:ILE:HG12	3:D:346:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:61:MET:HB3	1:M:294:THR:HG21	1.95	0.49
2:B:199:ALA:HB1	2:B:281:TYR:HD2	1.77	0.49
3:D:247:ILE:HB	3:D:276:GLY:N	2.25	0.49
3:G:41:CYS:SG	3:G:42:GLY:N	2.86	0.49
1:A:229:MET:O	1:A:233:ILE:HG12	2.13	0.48
3:D:84:ASN:OD1	3:D:84:ASN:N	2.46	0.48
3:K:92:ASN:ND2	3:K:95:ASP:OD2	2.43	0.48
3:O:106:THR:O	3:O:107:LYS:HB2	2.13	0.48
3:C:88:TYR:HB3	3:C:90:HIS:CE1	2.49	0.48
3:C:106:THR:O	3:C:107:LYS:HB2	2.13	0.48
2:J:150:PHE:O	2:J:209:ARG:NH2	2.46	0.48
3:K:181:HIS:O	3:K:181:HIS:ND1	2.38	0.48
1:M:111:PHE:O	1:M:114:PRO:HD2	2.12	0.48
3:O:301:ILE:HD11	3:O:321:VAL:HG11	1.94	0.48
3:P:84:ASN:OD1	3:P:84:ASN:N	2.46	0.48
1:A:308:VAL:HG21	2:B:122:TRP:CE3	2.48	0.48
2:B:161:ARG:HG3	2:B:162:ASN:N	2.28	0.48
3:C:355:ASP:OD2	3:C:358:SER:N	2.46	0.48
2:F:94:PHE:HB3	2:F:152:CYS:SG	2.52	0.48
3:G:92:ASN:ND2	3:G:95:ASP:OD2	2.43	0.48
3:K:232:ALA:HB1	3:K:240:MET:HE2	1.95	0.48
3:O:355:ASP:OD2	3:O:358:SER:N	2.47	0.48
3:G:160:GLN:HB3	3:G:163:SER:OG	2.13	0.48
3:G:243:MET:HE1	3:G:326:LEU:HB3	1.96	0.48
3:H:84:ASN:N	3:H:84:ASN:OD1	2.46	0.48
1:A:207:ALA:O	1:A:210:SER:OG	2.26	0.48
3:K:106:THR:O	3:K:107:LYS:HB2	2.13	0.48
3:L:110:VAL:C	3:L:112:ASP:H	2.16	0.48
1:A:293:ALA:O	1:A:297:GLY:N	2.44	0.48
1:E:290:TYR:CE2	2:F:132:LEU:HD21	2.49	0.48
3:G:181:HIS:O	3:G:181:HIS:ND1	2.38	0.48
1:I:194:TRP:HE1	2:J:29:ALA:HA	1.77	0.48
3:L:105:ARG:HB3	3:L:109:SER:HB2	1.94	0.48
3:O:12:LYS:H	3:O:20:VAL:HG22	1.78	0.48
3:H:110:VAL:C	3:H:112:ASP:H	2.15	0.48
3:H:247:ILE:HB	3:H:276:GLY:N	2.22	0.48
2:J:161:ARG:HG3	2:J:162:ASN:N	2.27	0.48
3:L:232:ALA:HB1	3:L:240:MET:HE2	1.95	0.48
3:P:160:GLN:HB3	3:P:163:SER:OG	2.13	0.48
1:A:141:HIS:ND1	1:A:196:GLU:OE2	2.37	0.48
3:H:93:VAL:HG13	3:H:143:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:44:THR:OG1	2:J:94:PHE:O	2.27	0.48
2:J:280:LYS:HE3	2:J:280:LYS:HA	1.95	0.48
2:N:158:ILE:HA	2:N:161:ARG:HG2	1.96	0.48
2:N:182:ASP:O	2:N:185:ILE:N	2.43	0.48
3:O:209:ARG:HD3	3:O:230:PHE:CE1	2.49	0.48
3:O:283:ILE:HG12	3:O:346:VAL:HG23	1.95	0.48
1:A:111:PHE:O	1:A:114:PRO:HD2	2.12	0.48
1:E:111:PHE:O	1:E:114:PRO:HD2	2.13	0.48
1:E:146:VAL:HG12	1:E:263:LEU:HD21	1.95	0.48
3:K:12:LYS:H	3:K:20:VAL:HG22	1.79	0.48
1:M:131:LYS:O	1:M:135:THR:HG23	2.14	0.48
3:H:122:LEU:HB2	3:H:124:LEU:HD22	1.95	0.48
3:L:160:GLN:HB3	3:L:163:SER:OG	2.14	0.48
3:P:307:ILE:HG13	3:P:308:VAL:N	2.27	0.48
3:G:60:THR:HA	3:G:69:ASN:HD21	1.80	0.47
3:G:106:THR:O	3:G:107:LYS:HB2	2.13	0.47
3:G:209:ARG:HD3	3:G:230:PHE:CE1	2.48	0.47
3:H:160:GLN:HB3	3:H:163:SER:OG	2.13	0.47
3:K:16:LYS:HD2	3:P:225:HIS:CE1	2.49	0.47
3:K:301:ILE:HD11	3:K:321:VAL:HG11	1.95	0.47
1:M:235:LEU:O	1:M:239:VAL:HG23	2.14	0.47
2:N:274:VAL:O	2:N:278:VAL:HG23	2.14	0.47
3:D:93:VAL:HG13	3:D:143:VAL:HG21	1.96	0.47
1:E:86:LEU:O	1:E:92:PHE:CE2	2.66	0.47
3:G:232:ALA:HB1	3:G:240:MET:HE2	1.95	0.47
3:H:240:MET:HE3	3:H:282:GLY:HA3	1.96	0.47
1:M:137:VAL:HG12	1:M:198:GLY:HA3	1.95	0.47
3:O:105:ARG:O	3:O:106:THR:OG1	2.24	0.47
3:D:181:HIS:O	3:D:181:HIS:ND1	2.39	0.47
1:E:124:VAL:HG12	1:E:125:TYR:O	2.14	0.47
1:E:212:ASN:OD1	1:E:215:LEU:HD13	2.14	0.47
2:F:66:ARG:NH2	2:F:245:PHE:HB2	2.29	0.47
3:G:304:THR:HA	3:G:341:PRO:HA	1.95	0.47
1:M:48:PHE:CZ	2:N:117:ILE:HG23	2.50	0.47
1:M:124:VAL:HG12	1:M:125:TYR:O	2.15	0.47
1:A:143:ILE:O	1:A:195:LYS:NZ	2.45	0.47
2:B:175:ALA:HB1	2:B:180:ALA:HB3	1.96	0.47
1:E:97:LYS:O	1:E:101:THR:OG1	2.22	0.47
1:E:129:TYR:OH	2:F:19:ALA:O	2.31	0.47
1:E:141:HIS:ND1	1:E:196:GLU:OE2	2.38	0.47
2:J:100:TYR:CD1	2:J:186:LEU:HD13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:333:LEU:HG	3:K:334:ASN:H	1.79	0.47
1:I:124:VAL:HG12	1:I:125:TYR:O	2.15	0.47
1:I:137:VAL:HG12	1:I:198:GLY:HA3	1.97	0.47
2:B:142:ASN:OD1	2:B:145:GLY:N	2.47	0.47
2:B:229:GLN:HA	2:B:232:LEU:HB2	1.96	0.47
3:C:301:ILE:HD11	3:C:321:VAL:HG11	1.95	0.47
2:F:270:PRO:HA	2:F:273:ILE:HD12	1.96	0.47
1:I:235:LEU:O	1:I:239:VAL:HG23	2.15	0.47
1:M:77:TRP:O	1:M:78:ILE:HB	2.15	0.47
3:P:93:VAL:HG13	3:P:143:VAL:HG21	1.95	0.47
1:A:137:VAL:HG12	1:A:198:GLY:HA3	1.95	0.47
2:F:37:PHE:HA	2:F:265:VAL:HG21	1.96	0.47
3:G:338:PRO:HA	3:G:339:GLY:HA2	1.55	0.47
2:J:270:PRO:HA	2:J:273:ILE:HD12	1.96	0.47
3:L:93:VAL:HG13	3:L:143:VAL:HG21	1.96	0.47
3:O:181:HIS:O	3:O:181:HIS:ND1	2.39	0.47
3:C:35:LEU:N	3:C:190:TYR:O	2.44	0.47
3:C:333:LEU:HG	3:C:334:ASN:H	1.80	0.47
3:D:1:MET:N	3:D:154:LYS:HG2	2.30	0.47
2:F:32:PRO:O	2:F:36:ILE:HG13	2.15	0.47
2:F:83:TYR:CD2	2:F:227:PRO:HB3	2.50	0.47
3:G:298:ARG:HG2	3:G:348:LEU:HD21	1.96	0.47
3:H:105:ARG:HB3	3:H:109:SER:HB2	1.97	0.47
2:N:241:VAL:HG21	2:N:245:PHE:HD2	1.80	0.47
3:D:35:LEU:N	3:D:190:TYR:O	2.44	0.47
3:D:209:ARG:HD3	3:D:230:PHE:CE1	2.50	0.47
1:E:170:ILE:HG23	1:E:172:LEU:HD13	1.96	0.47
2:J:229:GLN:HA	2:J:232:LEU:HB2	1.97	0.47
3:L:110:VAL:O	3:L:112:ASP:N	2.45	0.47
1:A:294:THR:O	1:A:298:ILE:HG13	2.15	0.46
1:E:151:LEU:HD13	1:E:151:LEU:HA	1.84	0.46
2:F:229:GLN:HA	2:F:232:LEU:HB2	1.97	0.46
3:C:283:ILE:HG12	3:C:346:VAL:HG23	1.97	0.46
3:C:298:ARG:HD2	3:C:298:ARG:N	2.30	0.46
3:G:5:VAL:HG13	3:G:27:ILE:HB	1.97	0.46
1:M:34:ASP:O	1:M:38:TYR:N	2.43	0.46
1:M:133:VAL:HG11	2:N:22:LEU:HG	1.96	0.46
1:A:52:LEU:C	1:A:55:PRO:HD2	2.36	0.46
3:D:5:VAL:HG13	3:D:27:ILE:HB	1.97	0.46
3:D:105:ARG:HB3	3:D:109:SER:HB2	1.96	0.46
2:J:182:ASP:O	2:J:185:ILE:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:182:ASP:O	2:F:185:ILE:N	2.45	0.46
2:J:36:ILE:HD12	2:J:37:PHE:N	2.30	0.46
3:K:5:VAL:HG13	3:K:27:ILE:HB	1.97	0.46
2:N:163:TYR:CE1	2:N:194:ALA:HA	2.50	0.46
3:C:209:ARG:HD3	3:C:230:PHE:CE1	2.50	0.46
2:F:66:ARG:NH1	2:F:244:GLU:OE2	2.41	0.46
2:N:100:TYR:CD1	2:N:186:LEU:HD13	2.50	0.46
2:N:177:MET:SD	3:P:73:PRO:HB3	2.56	0.46
2:N:269:ILE:O	2:N:273:ILE:HG13	2.16	0.46
1:A:124:VAL:HG12	1:A:125:TYR:O	2.15	0.46
1:A:279:TYR:O	1:A:283:LEU:HG	2.15	0.46
1:M:226:ARG:NH2	2:N:11:ASP:OD2	2.49	0.46
1:A:184:PHE:CZ	1:A:261:ILE:HG12	2.50	0.46
3:C:5:VAL:HG13	3:C:27:ILE:HB	1.98	0.46
1:E:235:LEU:O	1:E:239:VAL:HG23	2.15	0.46
2:F:163:TYR:CE1	2:F:194:ALA:HA	2.50	0.46
2:J:83:TYR:CD2	2:J:227:PRO:HB3	2.50	0.46
3:L:5:VAL:HG13	3:L:27:ILE:HB	1.96	0.46
3:L:240:MET:HE3	3:L:282:GLY:HA3	1.97	0.46
3:P:5:VAL:HG13	3:P:27:ILE:HB	1.98	0.46
3:D:160:GLN:HB3	3:D:163:SER:OG	2.14	0.46
3:D:214:GLU:OE2	3:D:228:ASN:ND2	2.47	0.46
1:I:308:VAL:HG21	2:J:122:TRP:CE3	2.51	0.46
2:N:36:ILE:HD12	2:N:37:PHE:N	2.30	0.46
3:O:272:HIS:O	3:O:272:HIS:ND1	2.49	0.46
1:A:151:LEU:HD21	2:B:264:ILE:HD13	1.98	0.46
3:C:90:HIS:CD2	3:C:91:LEU:HG	2.51	0.46
3:D:355:ASP:OD2	3:D:358:SER:N	2.48	0.46
2:F:270:PRO:O	2:F:274:VAL:HG23	2.16	0.46
3:H:283:ILE:HG12	3:H:346:VAL:HG23	1.97	0.46
3:H:296:SER:HA	3:H:345:HIS:CE1	2.51	0.46
3:L:355:ASP:OD2	3:L:358:SER:N	2.49	0.46
2:N:229:GLN:HA	2:N:232:LEU:HB2	1.98	0.46
1:A:94:ARG:O	1:A:98:ASN:N	2.49	0.46
3:C:92:ASN:ND2	3:C:95:ASP:OD2	2.47	0.46
3:H:213:ILE:HD11	3:H:216:ILE:HD11	1.96	0.46
2:J:173:GLU:O	2:J:177:MET:HG2	2.16	0.46
3:P:243:MET:HE1	3:P:326:LEU:HB3	1.97	0.46
2:B:36:ILE:HD12	2:B:37:PHE:N	2.31	0.45
3:C:107:LYS:HG3	3:C:109:SER:H	1.81	0.45
1:E:308:VAL:HG21	2:F:122:TRP:CE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:241:ASN:OD1	3:H:327:VAL:N	2.45	0.45
1:I:165:ASN:HB3	2:J:53:PHE:CZ	2.51	0.45
1:I:165:ASN:HB3	2:J:53:PHE:HZ	1.81	0.45
3:K:17:THR:O	3:K:19:VAL:N	2.49	0.45
3:K:261:ASN:OD1	3:K:302:LYS:N	2.49	0.45
1:M:308:VAL:HG21	2:N:122:TRP:CE3	2.51	0.45
1:E:52:LEU:O	1:E:56:MET:HG3	2.17	0.45
2:N:203:LEU:HD13	2:N:278:VAL:HG22	1.97	0.45
3:O:5:VAL:HG13	3:O:27:ILE:HB	1.99	0.45
3:P:232:ALA:HB1	3:P:240:MET:HE2	1.98	0.45
2:B:100:TYR:CD1	2:B:186:LEU:HD13	2.51	0.45
3:C:272:HIS:O	3:C:272:HIS:ND1	2.49	0.45
3:G:12:LYS:H	3:G:20:VAL:HG22	1.81	0.45
3:G:298:ARG:HD2	3:G:298:ARG:N	2.31	0.45
3:H:355:ASP:OD2	3:H:358:SER:N	2.49	0.45
3:L:1:MET:N	3:L:154:LYS:HG2	2.31	0.45
2:N:32:PRO:O	2:N:36:ILE:HG13	2.16	0.45
2:N:270:PRO:HA	2:N:273:ILE:HD12	1.99	0.45
3:P:209:ARG:HD3	3:P:230:PHE:CE1	2.51	0.45
1:E:137:VAL:HG12	1:E:198:GLY:HA3	1.98	0.45
3:G:272:HIS:O	3:G:272:HIS:ND1	2.49	0.45
2:F:100:TYR:CD1	2:F:186:LEU:HD13	2.51	0.45
3:G:32:PHE:HB2	3:G:181:HIS:CD2	2.52	0.45
3:G:68:ILE:HA	3:G:71:LEU:HB2	1.99	0.45
3:G:173:MET:O	3:G:177:ILE:HG13	2.15	0.45
3:G:328:VAL:HG22	3:G:330:VAL:HG13	1.99	0.45
3:K:199:MET:O	3:L:310:PRO:HG2	2.16	0.45
3:K:355:ASP:OD2	3:K:358:SER:N	2.49	0.45
3:P:88:TYR:HB3	3:P:90:HIS:CE1	2.52	0.45
2:F:269:ILE:O	2:F:273:ILE:HG13	2.16	0.45
3:K:272:HIS:O	3:K:272:HIS:ND1	2.50	0.45
2:N:175:ALA:HB1	2:N:180:ALA:HB3	1.99	0.45
3:O:90:HIS:CD2	3:O:91:LEU:HG	2.52	0.45
3:P:199:MET:HA	3:P:205:ILE:HD11	1.99	0.45
3:P:247:ILE:HB	3:P:276:GLY:N	2.25	0.45
3:D:243:MET:HE1	3:D:326:LEU:HB3	1.99	0.45
3:G:355:ASP:OD2	3:G:358:SER:N	2.49	0.45
2:J:142:ASN:OD1	2:J:145:GLY:N	2.45	0.45
1:M:194:TRP:NE1	2:N:29:ALA:HA	2.31	0.45
1:A:130:ARG:O	1:A:134:GLN:HG3	2.16	0.45
3:D:296:SER:HA	3:D:345:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:207:ALA:O	1:I:210:SER:OG	2.26	0.45
2:B:83:TYR:HD2	2:B:227:PRO:HB3	1.81	0.45
1:E:283:LEU:O	1:E:289:ARG:N	2.42	0.45
3:G:1:MET:N	3:G:154:LYS:HG2	2.32	0.45
2:J:228:LEU:HD12	2:J:228:LEU:HA	1.83	0.45
3:K:298:ARG:N	3:K:298:ARG:HD2	2.31	0.45
1:M:189:ILE:O	1:M:193:ILE:HG23	2.17	0.45
2:N:160:MET:HB2	2:N:201:ILE:HD11	1.99	0.45
3:O:243:MET:HE1	3:O:326:LEU:HB3	1.98	0.45
3:C:361:SER:O	3:C:361:SER:OG	2.33	0.45
1:E:78:ILE:HA	1:E:79:GLY:HA3	1.84	0.45
1:E:94:ARG:O	1:E:98:ASN:N	2.46	0.45
1:I:130:ARG:O	1:I:134:GLN:HG3	2.17	0.45
1:I:138:TYR:CZ	1:I:202:ILE:HG12	2.52	0.45
3:K:293:VAL:C	3:K:294:GLU:HG3	2.38	0.45
3:L:243:MET:HE1	3:L:326:LEU:HB3	1.98	0.45
1:A:235:LEU:O	1:A:239:VAL:HG23	2.17	0.44
3:C:60:THR:HA	3:C:69:ASN:HD21	1.82	0.44
3:C:244:PRO:HA	3:C:280:VAL:HA	1.99	0.44
3:C:293:VAL:C	3:C:294:GLU:HG3	2.38	0.44
3:H:48:ARG:NE	3:H:54:GLU:OE1	2.34	0.44
3:K:196:VAL:HG22	3:L:311:LEU:HD11	1.98	0.44
3:L:32:PHE:HD2	3:L:181:HIS:CD2	2.28	0.44
3:O:93:VAL:HG13	3:O:143:VAL:HG21	1.98	0.44
3:O:298:ARG:HD2	3:O:298:ARG:N	2.31	0.44
3:C:32:PHE:HD2	3:C:181:HIS:CD2	2.28	0.44
3:D:107:LYS:O	3:D:108:LYS:HB2	2.18	0.44
3:H:113:ALA:O	3:H:117:THR:HG23	2.17	0.44
1:I:233:ILE:C	1:I:236:PRO:HD2	2.38	0.44
1:I:283:LEU:O	1:I:289:ARG:N	2.42	0.44
3:L:303:ALA:HB2	3:L:321:VAL:HG13	2.00	0.44
1:A:135:THR:HA	2:B:275:TYR:OH	2.16	0.44
3:D:232:ALA:HB1	3:D:240:MET:HE2	1.99	0.44
1:E:130:ARG:O	1:E:134:GLN:HG3	2.17	0.44
3:L:107:LYS:O	3:L:108:LYS:HB2	2.17	0.44
3:O:17:THR:O	3:O:19:VAL:N	2.50	0.44
3:O:35:LEU:N	3:O:190:TYR:O	2.44	0.44
3:O:107:LYS:HG3	3:O:109:SER:H	1.82	0.44
1:A:230:ILE:O	1:A:235:LEU:HB2	2.18	0.44
2:B:79:ASN:ND2	2:B:226:ILE:O	2.40	0.44
1:E:49:LEU:O	1:E:54:LYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:268:ILE:O	2:F:272:ILE:HG13	2.18	0.44
3:H:1:MET:N	3:H:154:LYS:HG2	2.33	0.44
3:K:107:LYS:HG3	3:K:109:SER:H	1.82	0.44
3:L:88:TYR:HB3	3:L:90:HIS:CE1	2.53	0.44
3:O:293:VAL:C	3:O:294:GLU:HG3	2.37	0.44
1:A:64:LYS:HG3	1:A:65:GLN:N	2.32	0.44
1:A:86:LEU:HD23	1:A:292:ILE:HD11	1.99	0.44
1:A:274:ASP:CG	1:A:282:ARG:HH22	2.21	0.44
1:E:225:THR:H	1:E:228:GLN:HB2	1.82	0.44
2:F:37:PHE:CZ	2:F:265:VAL:HG13	2.53	0.44
3:G:293:VAL:C	3:G:294:GLU:HG3	2.38	0.44
3:H:12:LYS:HZ3	3:H:54:GLU:HB3	1.81	0.44
1:I:78:ILE:HA	1:I:79:GLY:HA3	1.81	0.44
3:O:141:GLN:NE2	3:O:161:PRO:O	2.50	0.44
3:P:181:HIS:O	3:P:181:HIS:ND1	2.39	0.44
3:P:303:ALA:HB2	3:P:321:VAL:HG13	1.99	0.44
1:A:138:TYR:CZ	1:A:202:ILE:HG12	2.52	0.44
2:B:32:PRO:O	2:B:36:ILE:HG13	2.18	0.44
1:E:81:ASP:O	1:E:84:VAL:N	2.51	0.44
3:G:122:LEU:HB2	3:G:124:LEU:HG	2.00	0.44
3:H:181:HIS:O	3:H:181:HIS:ND1	2.39	0.44
1:I:170:ILE:HG23	1:I:172:LEU:HD13	2.00	0.44
1:M:63:PHE:HD1	1:M:79:GLY:HA3	1.83	0.44
1:M:64:LYS:HG3	1:M:65:GLN:N	2.33	0.44
1:A:150:GLY:HA2	1:A:153:VAL:HG12	2.00	0.44
2:B:260:VAL:O	2:B:264:ILE:HG23	2.17	0.44
2:B:269:ILE:O	2:B:273:ILE:HG13	2.18	0.44
3:C:173:MET:O	3:C:177:ILE:HG13	2.17	0.44
3:C:241:ASN:OD1	3:C:327:VAL:N	2.46	0.44
2:F:142:ASN:OD1	2:F:145:GLY:N	2.51	0.44
3:H:209:ARG:HD3	3:H:230:PHE:CE1	2.52	0.44
3:P:7:ILE:HG12	3:P:61:ILE:HD12	2.00	0.44
3:D:88:TYR:HB3	3:D:90:HIS:CE1	2.53	0.44
1:E:77:TRP:O	1:E:77:TRP:CD1	2.71	0.44
1:E:77:TRP:O	1:E:78:ILE:HB	2.18	0.44
3:H:5:VAL:HG13	3:H:27:ILE:HB	1.99	0.44
3:H:299:ALA:O	3:H:346:VAL:HG12	2.18	0.44
3:H:337:HIS:HA	3:H:338:PRO:HD2	1.83	0.44
2:J:229:GLN:H	2:J:229:GLN:HG2	1.63	0.44
2:J:275:TYR:HB3	2:J:276:PRO:HD3	1.99	0.44
3:K:173:MET:O	3:K:177:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:209:ARG:HD3	3:K:230:PHE:CE1	2.53	0.44
1:M:36:LEU:HB3	2:N:182:ASP:HB2	1.98	0.44
3:P:224:LEU:HD13	3:P:224:LEU:HA	1.85	0.44
1:A:146:VAL:HG12	1:A:263:LEU:HD21	1.99	0.44
3:C:122:LEU:HB2	3:C:124:LEU:HG	2.00	0.44
1:E:92:PHE:CG	1:E:93:ILE:N	2.86	0.44
3:G:62:ARG:HB2	3:G:66:ARG:O	2.18	0.44
3:G:296:SER:HA	3:G:345:HIS:CE1	2.53	0.44
3:H:17:THR:O	3:H:19:VAL:N	2.50	0.44
3:H:224:LEU:HD13	3:H:224:LEU:HA	1.86	0.44
3:L:12:LYS:HD3	3:L:13:ARG:N	2.33	0.44
3:L:35:LEU:N	3:L:190:TYR:O	2.43	0.44
3:L:243:MET:CE	3:L:326:LEU:HB3	2.48	0.44
1:M:226:ARG:HG2	2:N:11:ASP:OD1	2.18	0.44
2:N:260:VAL:O	2:N:264:ILE:HG23	2.18	0.44
3:C:141:GLN:NE2	3:C:161:PRO:O	2.51	0.43
3:C:214:GLU:OE2	3:C:228:ASN:ND2	2.48	0.43
1:I:90:GLU:O	1:I:94:ARG:HG2	2.18	0.43
1:I:235:LEU:O	1:I:238:ILE:HG22	2.18	0.43
3:K:244:PRO:HA	3:K:280:VAL:HA	2.00	0.43
3:L:17:THR:O	3:L:19:VAL:N	2.51	0.43
1:M:77:TRP:O	1:M:77:TRP:CD1	2.71	0.43
2:N:229:GLN:H	2:N:229:GLN:HG2	1.61	0.43
3:P:12:LYS:HZ3	3:P:54:GLU:HB3	1.83	0.43
1:A:77:TRP:CD1	1:A:77:TRP:O	2.71	0.43
3:D:334:ASN:HB2	3:D:335:GLU:H	1.53	0.43
3:G:43:LYS:HB3	3:G:191:VAL:HG13	2.00	0.43
3:G:141:GLN:NE2	3:G:161:PRO:O	2.51	0.43
3:H:12:LYS:HD3	3:H:13:ARG:N	2.32	0.43
3:H:107:LYS:O	3:H:108:LYS:HB2	2.18	0.43
1:I:49:LEU:O	1:I:54:LYS:N	2.50	0.43
1:M:225:THR:H	1:M:228:GLN:HB2	1.83	0.43
3:O:244:PRO:HA	3:O:280:VAL:HA	1.99	0.43
3:P:17:THR:O	3:P:19:VAL:N	2.51	0.43
1:A:235:LEU:O	1:A:238:ILE:HG22	2.18	0.43
2:B:233:LYS:O	2:B:237:VAL:HG22	2.18	0.43
1:E:146:VAL:HG21	2:F:229:GLN:HB3	1.99	0.43
3:G:107:LYS:HG3	3:G:109:SER:H	1.83	0.43
3:L:333:LEU:N	3:L:333:LEU:HD23	2.33	0.43
1:M:230:ILE:O	1:M:235:LEU:HB2	2.19	0.43
1:M:283:LEU:O	1:M:289:ARG:N	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:1:MET:N	3:O:154:LYS:HG2	2.34	0.43
1:A:77:TRP:O	1:A:78:ILE:HB	2.19	0.43
2:B:268:ILE:O	2:B:272:ILE:HG13	2.19	0.43
3:C:1:MET:N	3:C:154:LYS:HG2	2.34	0.43
1:E:103:SER:HB3	1:E:253:ILE:HG12	2.00	0.43
1:E:150:GLY:HA2	1:E:153:VAL:HG12	2.01	0.43
3:G:35:LEU:N	3:G:190:TYR:O	2.42	0.43
3:L:209:ARG:HD3	3:L:230:PHE:CE1	2.52	0.43
1:M:90:GLU:O	1:M:94:ARG:HG2	2.19	0.43
3:C:12:LYS:H	3:C:20:VAL:HG22	1.83	0.43
3:D:12:LYS:HZ3	3:D:54:GLU:HB3	1.84	0.43
3:D:303:ALA:HB2	3:D:321:VAL:HG13	2.00	0.43
3:G:244:PRO:HA	3:G:280:VAL:HA	1.99	0.43
1:I:77:TRP:O	1:I:77:TRP:CD1	2.72	0.43
1:A:151:LEU:HD13	1:A:151:LEU:HA	1.86	0.43
1:I:141:HIS:ND1	1:I:196:GLU:OE2	2.35	0.43
1:I:146:VAL:HG12	1:I:263:LEU:HD21	1.99	0.43
3:L:296:SER:HA	3:L:345:HIS:CE1	2.54	0.43
1:M:290:TYR:CE2	2:N:132:LEU:HD21	2.54	0.43
3:O:122:LEU:HB2	3:O:124:LEU:HG	2.00	0.43
3:O:173:MET:O	3:O:177:ILE:HG13	2.18	0.43
1:A:90:GLU:O	1:A:94:ARG:HG2	2.19	0.43
3:D:113:ALA:O	3:D:117:THR:HG23	2.19	0.43
1:E:44:THR:OG1	2:F:94:PHE:O	2.31	0.43
3:H:303:ALA:HB2	3:H:321:VAL:HG13	2.00	0.43
1:I:77:TRP:O	1:I:78:ILE:HB	2.18	0.43
3:K:1:MET:N	3:K:154:LYS:HG2	2.33	0.43
3:L:181:HIS:O	3:L:181:HIS:ND1	2.38	0.43
1:M:96:ILE:HB	1:M:276:ILE:HD11	2.01	0.43
2:N:142:ASN:OD1	2:N:145:GLY:N	2.49	0.43
3:O:35:LEU:HD12	3:O:191:VAL:HG22	2.01	0.43
3:D:306:ASP:HB2	3:D:320:THR:CG2	2.48	0.43
3:G:321:VAL:O	3:G:322:GLY:O	2.37	0.43
1:I:103:SER:HB3	1:I:253:ILE:HG12	2.01	0.43
1:I:294:THR:O	1:I:298:ILE:HG13	2.19	0.43
2:J:52:VAL:O	2:J:53:PHE:HB2	2.18	0.43
2:J:269:ILE:O	2:J:273:ILE:HG13	2.19	0.43
3:K:321:VAL:O	3:K:322:GLY:O	2.37	0.43
1:M:151:LEU:HD13	1:M:151:LEU:HA	1.84	0.43
1:A:170:ILE:HG23	1:A:172:LEU:HD13	2.00	0.43
3:D:238:PRO:HB2	3:D:285:PRO:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:LEU:O	1:E:238:ILE:HG22	2.18	0.43
2:F:275:TYR:HB3	2:F:276:PRO:HD3	1.99	0.43
3:G:90:HIS:CD2	3:G:91:LEU:HG	2.54	0.43
3:G:261:ASN:OD1	3:G:302:LYS:N	2.52	0.43
1:I:34:ASP:O	1:I:38:TYR:N	2.40	0.43
1:I:86:LEU:HD23	1:I:292:ILE:HD11	2.01	0.43
1:I:293:ALA:O	1:I:297:GLY:N	2.52	0.43
2:J:36:ILE:H	2:J:36:ILE:HG13	1.71	0.43
3:L:113:ALA:O	3:L:117:THR:HG23	2.19	0.43
1:M:52:LEU:O	1:M:56:MET:HG3	2.18	0.43
3:O:32:PHE:HB2	3:O:181:HIS:CD2	2.54	0.43
3:P:12:LYS:HD3	3:P:13:ARG:N	2.33	0.43
3:P:107:LYS:O	3:P:108:LYS:HB2	2.19	0.43
2:B:52:VAL:O	2:B:53:PHE:HB2	2.19	0.43
2:B:214:PHE:O	2:B:217:MET:HG3	2.19	0.43
1:E:50:ILE:O	1:E:55:PRO:HD3	2.19	0.43
3:P:214:GLU:OE2	3:P:228:ASN:ND2	2.50	0.43
3:P:241:ASN:O	3:P:282:GLY:HA2	2.19	0.43
3:P:296:SER:HA	3:P:345:HIS:CE1	2.54	0.43
1:A:36:LEU:HD23	2:B:182:ASP:HB2	2.01	0.42
1:A:212:ASN:HA	1:A:213:PRO:HD3	1.86	0.42
1:A:289:ARG:HE	1:A:292:ILE:HG21	1.84	0.42
3:C:238:PRO:HB2	3:C:285:PRO:HG2	1.99	0.42
1:I:64:LYS:HD3	1:I:291:ASP:OD2	2.19	0.42
3:K:32:PHE:HB2	3:K:181:HIS:CD2	2.54	0.42
3:O:16:LYS:HD3	3:O:16:LYS:HA	1.81	0.42
3:O:238:PRO:HB2	3:O:285:PRO:HG2	2.00	0.42
1:A:290:TYR:CD2	2:B:132:LEU:HD21	2.54	0.42
1:E:203:VAL:HG11	1:E:245:LEU:HD11	2.01	0.42
2:F:52:VAL:O	2:F:53:PHE:HB2	2.19	0.42
3:K:27:ILE:HD13	3:K:33:VAL:HG11	2.01	0.42
3:L:241:ASN:OD1	3:L:327:VAL:N	2.48	0.42
1:M:86:LEU:HD23	1:M:292:ILE:HD11	2.01	0.42
1:M:165:ASN:OD1	1:M:174:ARG:NH1	2.49	0.42
3:D:17:THR:O	3:D:19:VAL:N	2.52	0.42
1:E:37:LEU:HD11	2:F:104:LYS:HG3	2.02	0.42
1:E:92:PHE:CD2	1:E:93:ILE:N	2.87	0.42
1:E:239:VAL:N	1:E:240:PRO:HD2	2.34	0.42
2:F:84:THR:HG22	2:F:209:ARG:HB2	2.02	0.42
2:J:83:TYR:HD2	2:J:227:PRO:HB3	1.84	0.42
1:M:94:ARG:O	1:M:98:ASN:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:170:ILE:HG23	1:M:172:LEU:HD13	2.00	0.42
3:O:311:LEU:HD21	3:P:196:VAL:HG13	2.01	0.42
3:P:361:SER:O	3:P:361:SER:OG	2.28	0.42
2:B:182:ASP:O	2:B:185:ILE:N	2.46	0.42
3:D:12:LYS:HD3	3:D:13:ARG:N	2.34	0.42
1:E:142:PHE:HB3	2:F:271:VAL:CG1	2.50	0.42
1:I:184:PHE:CZ	1:I:261:ILE:HG12	2.50	0.42
1:I:194:TRP:NE1	2:J:29:ALA:HA	2.34	0.42
2:J:260:VAL:O	2:J:264:ILE:HG23	2.18	0.42
3:K:16:LYS:HD3	3:K:16:LYS:HA	1.82	0.42
1:M:141:HIS:ND1	1:M:196:GLU:OE2	2.40	0.42
1:M:291:ASP:OD1	1:M:292:ILE:N	2.53	0.42
3:C:105:ARG:O	3:C:106:THR:OG1	2.24	0.42
3:D:192:THR:HG22	3:D:194:ASP:H	1.83	0.42
2:F:226:ILE:HA	2:F:227:PRO:HD3	1.70	0.42
1:I:152:VAL:HG13	1:I:156:LEU:HD22	2.02	0.42
1:I:250:LEU:HA	1:I:253:ILE:HB	2.00	0.42
3:L:241:ASN:O	3:L:282:GLY:HA2	2.20	0.42
1:M:79:GLY:C	1:M:81:ASP:H	2.21	0.42
1:M:262:ILE:HG23	1:M:263:LEU:HD13	2.02	0.42
3:P:48:ARG:NE	3:P:54:GLU:OE1	2.32	0.42
3:P:192:THR:HG22	3:P:194:ASP:H	1.85	0.42
1:A:262:ILE:HD11	1:A:281:TYR:CE2	2.55	0.42
2:B:275:TYR:HB3	2:B:276:PRO:HD3	2.00	0.42
3:C:93:VAL:HG13	3:C:143:VAL:HG21	2.02	0.42
3:C:261:ASN:OD1	3:C:302:LYS:N	2.52	0.42
3:D:241:ASN:O	3:D:282:GLY:HA2	2.20	0.42
2:F:280:LYS:HA	2:F:280:LYS:HE3	2.01	0.42
3:G:17:THR:O	3:G:19:VAL:N	2.52	0.42
3:H:111:ILE:O	3:H:115:VAL:HG22	2.20	0.42
1:I:52:LEU:O	1:I:56:MET:HG3	2.19	0.42
1:I:52:LEU:C	1:I:55:PRO:HD2	2.40	0.42
1:I:137:VAL:O	1:I:140:PRO:HD2	2.20	0.42
2:J:270:PRO:O	2:J:274:VAL:HG23	2.19	0.42
1:M:235:LEU:O	1:M:238:ILE:HG22	2.20	0.42
3:O:321:VAL:O	3:O:322:GLY:O	2.37	0.42
3:P:243:MET:CE	3:P:326:LEU:HB3	2.49	0.42
3:D:299:ALA:O	3:D:346:VAL:HG12	2.20	0.42
1:E:52:LEU:C	1:E:55:PRO:HD2	2.40	0.42
1:E:162:VAL:HB	2:F:35:TYR:OH	2.20	0.42
2:F:83:TYR:HD2	2:F:227:PRO:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:32:PHE:HD2	3:G:181:HIS:CD2	2.29	0.42
1:M:64:LYS:HB2	1:M:291:ASP:CG	2.40	0.42
2:N:52:VAL:O	2:N:53:PHE:HB2	2.19	0.42
3:O:261:ASN:OD1	3:O:302:LYS:N	2.52	0.42
2:B:195:LYS:HB2	2:B:196:PRO:HD3	2.02	0.42
3:C:321:VAL:O	3:C:322:GLY:O	2.37	0.42
3:D:90:HIS:CD2	3:D:91:LEU:HG	2.55	0.42
3:D:173:MET:O	3:D:177:ILE:HG13	2.19	0.42
3:D:290:LEU:C	3:D:292:GLY:H	2.23	0.42
1:E:185:ARG:HB2	1:E:186:PRO:HD3	2.01	0.42
3:G:214:GLU:OE2	3:G:228:ASN:ND2	2.51	0.42
3:G:240:MET:HE3	3:G:282:GLY:HA3	2.01	0.42
1:I:92:PHE:O	1:I:95:ALA:N	2.53	0.42
1:I:262:ILE:HD11	1:I:281:TYR:CE2	2.55	0.42
1:M:212:ASN:HA	1:M:213:PRO:HD3	1.88	0.42
1:M:267:PRO:HA	1:M:270:TYR:CD1	2.55	0.42
3:P:1:MET:N	3:P:154:LYS:HG2	2.35	0.42
3:P:306:ASP:HB2	3:P:320:THR:CG2	2.48	0.42
1:A:223:GLY:HA3	3:C:74:LYS:HD3	2.01	0.42
2:B:270:PRO:O	2:B:274:VAL:HG23	2.20	0.42
3:C:48:ARG:NE	3:C:54:GLU:OE1	2.39	0.42
1:I:135:THR:HA	2:J:275:TYR:OH	2.20	0.42
3:K:224:LEU:HD13	3:K:224:LEU:HA	1.84	0.42
3:L:35:LEU:HD12	3:L:191:VAL:HG22	2.02	0.42
1:M:164:ASN:HB3	1:M:174:ARG:HG2	2.02	0.42
2:N:199:ALA:CB	2:N:281:TYR:CZ	3.03	0.42
3:P:321:VAL:O	3:P:322:GLY:O	2.38	0.42
1:A:92:PHE:O	1:A:95:ALA:N	2.53	0.42
1:E:34:ASP:OD2	2:F:106:ARG:HD2	2.20	0.42
3:G:243:MET:CE	3:G:326:LEU:HB3	2.50	0.42
3:H:173:MET:O	3:H:177:ILE:HG13	2.20	0.42
3:H:321:VAL:O	3:H:322:GLY:O	2.38	0.42
1:I:50:ILE:O	1:I:55:PRO:HD3	2.19	0.42
1:I:185:ARG:HB2	1:I:186:PRO:HD3	2.02	0.42
3:L:192:THR:HG22	3:L:194:ASP:H	1.84	0.42
1:M:239:VAL:N	1:M:240:PRO:HD2	2.34	0.42
2:N:275:TYR:HB3	2:N:276:PRO:HD3	2.02	0.42
1:A:52:LEU:O	1:A:56:MET:HG3	2.20	0.41
2:F:241:VAL:HG21	2:F:245:PHE:HD2	1.85	0.41
2:J:84:THR:HG22	2:J:209:ARG:HB2	2.02	0.41
3:K:93:VAL:HG13	3:K:143:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:173:MET:O	3:L:177:ILE:HG13	2.20	0.41
1:M:52:LEU:C	1:M:55:PRO:HD2	2.41	0.41
2:N:228:LEU:HD12	2:N:228:LEU:HA	1.80	0.41
3:O:74:LYS:HE2	3:O:74:LYS:HB3	1.84	0.41
2:B:84:THR:HG22	2:B:209:ARG:HB2	2.01	0.41
3:C:32:PHE:HB2	3:C:181:HIS:CD2	2.55	0.41
3:C:224:LEU:HD13	3:C:224:LEU:HA	1.82	0.41
3:G:26:ASP:O	3:G:204:ARG:NH2	2.52	0.41
1:I:230:ILE:O	1:I:235:LEU:HB2	2.20	0.41
3:L:90:HIS:CD2	3:L:91:LEU:HG	2.54	0.41
3:L:307:ILE:HG13	3:L:308:VAL:N	2.34	0.41
1:M:250:LEU:HA	1:M:253:ILE:HB	2.02	0.41
2:N:83:TYR:CD2	2:N:227:PRO:HB3	2.54	0.41
2:N:281:TYR:CD1	2:N:281:TYR:C	2.93	0.41
3:O:214:GLU:OE2	3:O:228:ASN:ND2	2.53	0.41
3:P:74:LYS:HB3	3:P:74:LYS:HE2	1.86	0.41
3:P:173:MET:O	3:P:177:ILE:HG13	2.19	0.41
1:A:78:ILE:HA	1:A:79:GLY:HA3	1.82	0.41
1:A:185:ARG:HB2	1:A:186:PRO:HD3	2.02	0.41
3:C:335:GLU:O	3:C:337:HIS:ND1	2.53	0.41
3:G:241:ASN:OD1	3:G:327:VAL:N	2.49	0.41
2:J:32:PRO:O	2:J:36:ILE:HG13	2.20	0.41
1:M:130:ARG:O	1:M:134:GLN:HG3	2.20	0.41
2:N:270:PRO:O	2:N:274:VAL:HG23	2.20	0.41
3:P:238:PRO:HB2	3:P:285:PRO:HG2	2.02	0.41
1:A:137:VAL:O	1:A:140:PRO:HD2	2.20	0.41
2:F:7:TYR:HB3	2:F:8:SER:H	1.65	0.41
2:F:233:LYS:O	2:F:237:VAL:HG22	2.20	0.41
1:I:64:LYS:HG3	1:I:65:GLN:N	2.34	0.41
1:I:189:ILE:O	1:I:193:ILE:HG23	2.20	0.41
2:J:36:ILE:HD13	2:J:264:ILE:HD11	2.01	0.41
3:L:224:LEU:HD13	3:L:224:LEU:HA	1.86	0.41
1:M:36:LEU:HB3	2:N:182:ASP:CB	2.51	0.41
1:M:115:ILE:HG12	1:M:204:TYR:CE1	2.55	0.41
1:M:233:ILE:C	1:M:236:PRO:HD2	2.41	0.41
1:A:64:LYS:HD3	1:A:291:ASP:OD2	2.21	0.41
1:A:136:ILE:HG23	2:B:30:LEU:HB2	2.02	0.41
1:A:163:VAL:O	1:A:167:LEU:HD22	2.19	0.41
1:A:239:VAL:N	1:A:240:PRO:HD2	2.34	0.41
2:B:36:ILE:HD13	2:B:264:ILE:HD11	2.02	0.41
1:E:305:LEU:HD13	2:F:123:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:236:ILE:HD12	2:N:260:VAL:HG13	2.02	0.41
3:O:321:VAL:HG22	3:O:326:LEU:HD12	2.01	0.41
1:A:189:ILE:O	1:A:193:ILE:HG23	2.20	0.41
2:B:203:LEU:CD1	2:B:278:VAL:HG22	2.51	0.41
1:E:207:ALA:O	1:E:210:SER:OG	2.31	0.41
3:G:224:LEU:HD13	3:G:224:LEU:HA	1.83	0.41
3:H:334:ASN:HB2	3:H:335:GLU:H	1.53	0.41
1:I:48:PHE:CZ	2:J:117:ILE:HG23	2.55	0.41
1:I:143:ILE:O	1:I:195:LYS:NZ	2.50	0.41
3:P:113:ALA:O	3:P:117:THR:HG23	2.20	0.41
1:A:233:ILE:C	1:A:236:PRO:HD2	2.41	0.41
3:D:290:LEU:C	3:D:292:GLY:N	2.74	0.41
3:D:321:VAL:O	3:D:322:GLY:O	2.39	0.41
1:E:230:ILE:O	1:E:235:LEU:HB2	2.20	0.41
3:G:93:VAL:HG13	3:G:143:VAL:HG21	2.02	0.41
3:G:333:LEU:HG	3:G:334:ASN:H	1.85	0.41
3:H:290:LEU:C	3:H:292:GLY:H	2.24	0.41
1:I:111:PHE:HB3	1:I:112:PRO:HD3	2.03	0.41
1:I:239:VAL:N	1:I:240:PRO:HD2	2.35	0.41
1:M:53:TYR:OH	2:N:119:PHE:HB3	2.20	0.41
3:P:290:LEU:C	3:P:292:GLY:H	2.24	0.41
1:A:235:LEU:HD12	1:A:235:LEU:HA	1.93	0.41
1:E:250:LEU:HA	1:E:253:ILE:HB	2.02	0.41
2:F:177:MET:SD	3:H:51:ALA:HB1	2.61	0.41
1:I:97:LYS:O	1:I:101:THR:OG1	2.25	0.41
2:J:109:GLY:HA2	2:J:112:VAL:HG12	2.02	0.41
3:L:290:LEU:C	3:L:292:GLY:H	2.23	0.41
1:M:35:TRP:CG	1:M:36:LEU:N	2.88	0.41
3:O:107:LYS:HD2	3:O:107:LYS:HA	1.94	0.41
3:O:296:SER:HA	3:O:345:HIS:CE1	2.56	0.41
3:P:35:LEU:HD12	3:P:191:VAL:HG22	2.03	0.41
3:P:299:ALA:O	3:P:346:VAL:HG12	2.19	0.41
1:A:103:SER:HB3	1:A:253:ILE:HG12	2.02	0.41
1:A:267:PRO:O	1:A:270:TYR:HB2	2.21	0.41
2:B:237:VAL:HG23	2:B:238:ASP:N	2.36	0.41
3:D:35:LEU:HD12	3:D:191:VAL:HG22	2.02	0.41
3:D:168:LYS:HD2	3:D:168:LYS:HA	1.95	0.41
1:E:235:LEU:HD12	1:E:235:LEU:HA	1.92	0.41
3:G:168:LYS:HD2	3:G:168:LYS:HA	1.93	0.41
3:H:27:ILE:HD13	3:H:33:VAL:HG11	2.03	0.41
3:H:199:MET:HA	3:H:205:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:143:ARG:HE	2:J:225:LYS:HG2	1.85	0.41
2:J:264:ILE:HG13	2:J:265:VAL:N	2.36	0.41
3:K:21:HIS:HB2	3:K:212:LEU:HD23	2.03	0.41
3:K:233:SER:HB3	3:K:242:LEU:HD11	2.03	0.41
1:M:138:TYR:CZ	1:M:202:ILE:HG12	2.56	0.41
3:O:21:HIS:HB2	3:O:212:LEU:HD23	2.02	0.41
3:P:111:ILE:O	3:P:115:VAL:HG22	2.21	0.41
3:P:290:LEU:C	3:P:292:GLY:N	2.74	0.41
3:P:355:ASP:OD2	3:P:358:SER:N	2.54	0.41
2:B:163:TYR:CG	2:B:197:ALA:HB2	2.56	0.41
3:C:296:SER:HA	3:C:345:HIS:CE1	2.56	0.41
3:D:111:ILE:O	3:D:115:VAL:HG22	2.20	0.41
1:E:262:ILE:HG23	1:E:263:LEU:HD13	2.03	0.41
3:G:74:LYS:HE2	3:G:74:LYS:HB3	1.86	0.41
3:G:321:VAL:HG22	3:G:326:LEU:HD12	2.02	0.41
3:H:7:ILE:HG12	3:H:61:ILE:HD12	2.03	0.41
3:H:243:MET:HE1	3:H:326:LEU:HB3	2.03	0.41
3:L:122:LEU:HB2	3:L:124:LEU:CD2	2.51	0.41
3:P:209:ARG:HD3	3:P:230:PHE:CZ	2.56	0.41
2:B:226:ILE:HA	2:B:227:PRO:HD3	1.70	0.40
3:C:83:GLN:HG2	3:C:84:ASN:OD1	2.21	0.40
3:C:243:MET:CE	3:C:326:LEU:HB3	2.51	0.40
3:D:243:MET:CE	3:D:326:LEU:HB3	2.51	0.40
1:E:27:LEU:O	1:E:31:ILE:HG13	2.21	0.40
1:E:267:PRO:O	1:E:270:TYR:HB2	2.21	0.40
2:F:59:ILE:O	2:F:60:ASP:HB3	2.21	0.40
3:G:34:VAL:CG2	3:G:202:ALA:HB2	2.51	0.40
1:I:222:ASP:OD2	3:K:147:ARG:NE	2.54	0.40
2:J:89:VAL:O	2:J:93:ILE:HG13	2.21	0.40
3:L:111:ILE:O	3:L:115:VAL:HG22	2.21	0.40
3:L:290:LEU:C	3:L:292:GLY:N	2.74	0.40
3:L:321:VAL:O	3:L:322:GLY:O	2.38	0.40
3:P:233:SER:HB3	3:P:242:LEU:HD11	2.02	0.40
3:P:307:ILE:HD11	3:P:309:GLU:CG	2.51	0.40
3:C:192:THR:HG22	3:C:194:ASP:H	1.86	0.40
1:E:274:ASP:CG	1:E:282:ARG:HH22	2.24	0.40
3:H:46:THR:O	3:H:50:VAL:HG23	2.21	0.40
3:H:290:LEU:C	3:H:292:GLY:N	2.75	0.40
3:H:306:ASP:HB2	3:H:320:THR:CG2	2.50	0.40
2:J:214:PHE:O	2:J:217:MET:HG3	2.22	0.40
3:L:12:LYS:HZ3	3:L:54:GLU:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:O	1:A:101:THR:OG1	2.24	0.40
1:A:142:PHE:HB3	2:B:271:VAL:CG1	2.51	0.40
1:A:282:ARG:O	1:A:286:GLN:HB2	2.21	0.40
3:C:178:LYS:HB3	3:D:307:ILE:HD12	2.03	0.40
3:G:192:THR:HG22	3:G:194:ASP:H	1.85	0.40
3:H:35:LEU:N	3:H:190:TYR:O	2.48	0.40
3:H:35:LEU:HD12	3:H:191:VAL:HG22	2.03	0.40
3:H:220:MET:O	3:H:224:LEU:HB2	2.22	0.40
1:I:262:ILE:HG23	1:I:263:LEU:HD13	2.04	0.40
1:M:134:GLN:HB3	1:M:138:TYR:CE2	2.57	0.40
1:M:262:ILE:HD11	1:M:281:TYR:CE2	2.56	0.40
2:N:36:ILE:HG13	2:N:36:ILE:H	1.72	0.40
3:P:32:PHE:HD2	3:P:181:HIS:CD2	2.27	0.40
1:A:50:ILE:O	1:A:55:PRO:HD3	2.21	0.40
1:A:250:LEU:HA	1:A:253:ILE:HB	2.03	0.40
1:A:290:TYR:CE2	2:B:132:LEU:HD21	2.57	0.40
3:C:27:ILE:HD13	3:C:33:VAL:HG11	2.02	0.40
3:D:130:ARG:NH2	3:H:249:VAL:HA	2.30	0.40
1:E:34:ASP:O	1:E:38:TYR:N	2.42	0.40
2:F:237:VAL:HG23	2:F:238:ASP:N	2.36	0.40
3:H:162:LEU:HG	3:H:165:LEU:HD12	2.04	0.40
3:H:192:THR:HG22	3:H:194:ASP:H	1.86	0.40
2:J:233:LYS:O	2:J:237:VAL:HG22	2.21	0.40
3:K:90:HIS:CD2	3:K:91:LEU:HG	2.57	0.40
3:K:238:PRO:HB2	3:K:285:PRO:HG2	2.03	0.40
3:L:12:LYS:H	3:L:20:VAL:CG2	2.34	0.40
3:L:27:ILE:HD13	3:L:33:VAL:HG11	2.02	0.40
1:M:185:ARG:HB2	1:M:186:PRO:HD3	2.03	0.40
3:C:17:THR:O	3:C:19:VAL:N	2.54	0.40
3:G:247:ILE:HB	3:G:276:GLY:N	2.27	0.40
3:H:238:PRO:HB2	3:H:285:PRO:HG2	2.03	0.40
1:I:81:ASP:O	1:I:84:VAL:N	2.55	0.40
3:K:296:SER:HA	3:K:345:HIS:CE1	2.56	0.40
3:L:135:LEU:HD23	3:L:135:LEU:HA	1.95	0.40
2:N:228:LEU:HB3	2:N:229:GLN:H	1.68	0.40
2:N:255:SER:OG	2:N:256:MET:N	2.55	0.40
3:P:307:ILE:HD11	3:P:309:GLU:HG2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:289:ARG:NH1	2:N:241:VAL:O[1_654]	2.08	0.12
1:A:289:ARG:NH1	2:F:241:VAL:O[1_654]	2.09	0.11

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	282/301 (94%)	257 (91%)	24 (8%)	1 (0%)	34	72
1	E	282/301 (94%)	252 (89%)	26 (9%)	4 (1%)	11	47
1	I	282/301 (94%)	257 (91%)	24 (8%)	1 (0%)	34	72
1	M	282/301 (94%)	257 (91%)	24 (8%)	1 (0%)	34	72
2	B	282/305 (92%)	249 (88%)	31 (11%)	2 (1%)	22	62
2	F	278/305 (91%)	243 (87%)	32 (12%)	3 (1%)	14	52
2	J	282/305 (92%)	249 (88%)	31 (11%)	2 (1%)	22	62
2	N	282/305 (92%)	249 (88%)	31 (11%)	2 (1%)	22	62
3	C	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	9	43
3	D	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	5	33
3	G	361/363 (99%)	321 (89%)	35 (10%)	5 (1%)	11	47
3	H	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	5	33
3	K	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	9	43
3	L	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	5	33
3	O	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	9	43
3	P	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	5	33
All	All	5140/5328 (96%)	4583 (89%)	478 (9%)	79 (2%)	10	46

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ILE
3	C	18	THR
3	C	322	GLY
3	C	336	VAL
3	C	359	GLN
3	D	18	THR
3	D	108	LYS
3	D	268	ARG
3	D	291	ASP
3	D	322	GLY
3	D	359	GLN
1	E	78	ILE
1	E	173	ASP
1	E	175	VAL
3	G	18	THR
3	G	322	GLY
3	G	336	VAL
3	G	359	GLN
3	H	18	THR
3	H	108	LYS
3	H	268	ARG
3	H	291	ASP
3	H	322	GLY
3	H	359	GLN
1	I	78	ILE
3	K	18	THR
3	K	322	GLY
3	K	336	VAL
3	K	359	GLN
3	L	18	THR
3	L	108	LYS
3	L	268	ARG
3	L	291	ASP
3	L	322	GLY
3	L	359	GLN
1	M	78	ILE
3	O	18	THR
3	O	322	GLY
3	O	336	VAL
3	O	359	GLN
3	P	18	THR
3	P	108	LYS
3	P	268	ARG

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Mol	Chain	Res	Type
3	P	291	ASP
3	P	322	GLY
3	P	359	GLN
3	C	337	HIS
3	D	111	ILE
1	E	89	SER
3	H	111	ILE
3	K	337	HIS
3	L	111	ILE
3	O	337	HIS
3	P	111	ILE
3	D	296	SER
2	F	266	MET
3	H	296	SER
3	L	296	SER
3	P	296	SER
2	B	52	VAL
2	B	59	ILE
3	D	15	ASP
2	F	52	VAL
2	F	59	ILE
2	J	52	VAL
2	J	59	ILE
3	K	15	ASP
2	N	52	VAL
2	N	59	ILE
3	C	15	ASP
3	D	337	HIS
3	G	15	ASP
3	H	15	ASP
3	H	337	HIS
3	L	15	ASP
3	L	337	HIS
3	O	15	ASP
3	P	15	ASP
3	P	337	HIS

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	250/260 (96%)	218 (87%)	32 (13%)	4	21
1	E	250/260 (96%)	217 (87%)	33 (13%)	4	20
1	I	250/260 (96%)	218 (87%)	32 (13%)	4	21
1	M	250/260 (96%)	219 (88%)	31 (12%)	4	22
2	B	240/258 (93%)	220 (92%)	20 (8%)	11	36
2	F	237/258 (92%)	215 (91%)	22 (9%)	9	30
2	J	240/258 (93%)	220 (92%)	20 (8%)	11	36
2	N	240/258 (93%)	221 (92%)	19 (8%)	12	38
3	C	307/307 (100%)	264 (86%)	43 (14%)	3	19
3	D	307/307 (100%)	259 (84%)	48 (16%)	2	16
3	G	307/307 (100%)	263 (86%)	44 (14%)	3	18
3	H	307/307 (100%)	259 (84%)	48 (16%)	2	16
3	K	307/307 (100%)	264 (86%)	43 (14%)	3	19
3	L	307/307 (100%)	259 (84%)	48 (16%)	2	16
3	O	307/307 (100%)	264 (86%)	43 (14%)	3	19
3	P	307/307 (100%)	259 (84%)	48 (16%)	2	16
All	All	4413/4528 (98%)	3839 (87%)	574 (13%)	4	20

All (574) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	TRP
1	A	30	ASP
1	A	38	TYR
1	A	41	LEU
1	A	45	ILE
1	A	61	MET
1	A	63	PHE
1	A	65	GLN
1	A	77	TRP
1	A	78	ILE
1	A	80	PHE
1	A	81	ASP
1	A	82	HIS
1	A	84	VAL

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Mol	Chain	Res	Type
1	A	87	PHE
1	A	96	ILE
1	A	97	LYS
1	A	100	LEU
1	A	116	LEU
1	A	167	LEU
1	A	170	ILE
1	A	176	TYR
1	A	235	LEU
1	A	238	ILE
1	A	242	ILE
1	A	265	TYR
1	A	266	GLN
1	A	270	TYR
1	A	292	ILE
1	A	309	LEU
1	A	310	PHE
1	A	320	LYS
2	B	12	ARG
2	B	37	PHE
2	B	51	ARG
2	B	58	ASP
2	B	67	VAL
2	B	77	TYR
2	B	102	LEU
2	B	106	ARG
2	B	108	ARG
2	B	150	PHE
2	B	161	ARG
2	B	217	MET
2	B	224	GLU
2	B	235	THR
2	B	243	GLU
2	B	249	LEU
2	B	257	GLU
2	B	264	ILE
2	B	280	LYS
2	B	283	THR
3	C	5	VAL
3	C	11	VAL
3	C	12	LYS
3	C	45	THR

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Mol	Chain	Res	Type
3	C	60	THR
3	C	61	ILE
3	C	77	ASP
3	C	102	ARG
3	C	112	ASP
3	C	116	LYS
3	C	134	ASP
3	C	136	SER
3	C	147	ARG
3	C	169	LEU
3	C	172	GLN
3	C	180	LEU
3	C	181	HIS
3	C	188	VAL
3	C	192	THR
3	C	206	VAL
3	C	210	ASP
3	C	224	LEU
3	C	235	ILE
3	C	246	ARG
3	C	250	ASP
3	C	252	THR
3	C	257	LEU
3	C	268	ARG
3	C	271	THR
3	C	273	LEU
3	C	289	THR
3	C	291	ASP
3	C	294	GLU
3	C	298	ARG
3	C	307	ILE
3	C	308	VAL
3	C	311	LEU
3	C	321	VAL
3	C	326	LEU
3	C	328	VAL
3	C	333	LEU
3	C	345	HIS
3	C	349	THR
3	D	5	VAL
3	D	11	VAL
3	D	12	LYS

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Mol	Chain	Res	Type
3	D	41	CYS
3	D	45	THR
3	D	60	THR
3	D	61	ILE
3	D	77	ASP
3	D	84	ASN
3	D	102	ARG
3	D	116	LYS
3	D	120	ASP
3	D	124	LEU
3	D	147	ARG
3	D	169	LEU
3	D	172	GLN
3	D	180	LEU
3	D	181	HIS
3	D	188	VAL
3	D	192	THR
3	D	206	VAL
3	D	210	ASP
3	D	224	LEU
3	D	235	ILE
3	D	246	ARG
3	D	250	ASP
3	D	252	THR
3	D	255	VAL
3	D	257	LEU
3	D	268	ARG
3	D	271	THR
3	D	289	THR
3	D	294	GLU
3	D	298	ARG
3	D	304	THR
3	D	307	ILE
3	D	308	VAL
3	D	311	LEU
3	D	321	VAL
3	D	326	LEU
3	D	328	VAL
3	D	330	VAL
3	D	333	LEU
3	D	335	GLU
3	D	345	HIS

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Mol	Chain	Res	Type
3	D	348	LEU
3	D	349	THR
3	D	359	GLN
1	E	28	TRP
1	E	30	ASP
1	E	38	TYR
1	E	41	LEU
1	E	45	ILE
1	E	61	MET
1	E	63	PHE
1	E	65	GLN
1	E	77	TRP
1	E	78	ILE
1	E	80	PHE
1	E	81	ASP
1	E	82	HIS
1	E	84	VAL
1	E	87	PHE
1	E	91	GLN
1	E	92	PHE
1	E	96	ILE
1	E	97	LYS
1	E	100	LEU
1	E	116	LEU
1	E	167	LEU
1	E	170	ILE
1	E	176	TYR
1	E	235	LEU
1	E	238	ILE
1	E	242	ILE
1	E	265	TYR
1	E	266	GLN
1	E	270	TYR
1	E	292	ILE
1	E	309	LEU
1	E	310	PHE
2	F	7	TYR
2	F	9	ARG
2	F	12	ARG
2	F	37	PHE
2	F	51	ARG
2	F	58	ASP

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Mol	Chain	Res	Type
2	F	67	VAL
2	F	77	TYR
2	F	102	LEU
2	F	106	ARG
2	F	108	ARG
2	F	150	PHE
2	F	161	ARG
2	F	217	MET
2	F	224	GLU
2	F	235	THR
2	F	243	GLU
2	F	249	LEU
2	F	257	GLU
2	F	264	ILE
2	F	280	LYS
2	F	283	THR
3	G	5	VAL
3	G	11	VAL
3	G	12	LYS
3	G	45	THR
3	G	60	THR
3	G	61	ILE
3	G	102	ARG
3	G	112	ASP
3	G	116	LYS
3	G	134	ASP
3	G	136	SER
3	G	147	ARG
3	G	169	LEU
3	G	172	GLN
3	G	180	LEU
3	G	181	HIS
3	G	188	VAL
3	G	192	THR
3	G	206	VAL
3	G	210	ASP
3	G	224	LEU
3	G	235	ILE
3	G	246	ARG
3	G	250	ASP
3	G	252	THR
3	G	257	LEU

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Mol	Chain	Res	Type
3	G	268	ARG
3	G	271	THR
3	G	273	LEU
3	G	286	GLU
3	G	289	THR
3	G	291	ASP
3	G	294	GLU
3	G	298	ARG
3	G	307	ILE
3	G	308	VAL
3	G	311	LEU
3	G	321	VAL
3	G	326	LEU
3	G	328	VAL
3	G	333	LEU
3	G	337	HIS
3	G	345	HIS
3	G	349	THR
3	H	5	VAL
3	H	11	VAL
3	H	12	LYS
3	H	41	CYS
3	H	45	THR
3	H	60	THR
3	H	61	ILE
3	H	77	ASP
3	H	84	ASN
3	H	102	ARG
3	H	116	LYS
3	H	120	ASP
3	H	124	LEU
3	H	147	ARG
3	H	169	LEU
3	H	172	GLN
3	H	180	LEU
3	H	181	HIS
3	H	188	VAL
3	H	192	THR
3	H	206	VAL
3	H	210	ASP
3	H	224	LEU
3	H	235	ILE

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Mol	Chain	Res	Type
3	H	246	ARG
3	H	250	ASP
3	H	252	THR
3	H	255	VAL
3	H	257	LEU
3	H	268	ARG
3	H	271	THR
3	H	289	THR
3	H	294	GLU
3	H	298	ARG
3	H	304	THR
3	H	307	ILE
3	H	308	VAL
3	H	311	LEU
3	H	321	VAL
3	H	326	LEU
3	H	328	VAL
3	H	330	VAL
3	H	333	LEU
3	H	335	GLU
3	H	345	HIS
3	H	348	LEU
3	H	349	THR
3	H	359	GLN
1	I	28	TRP
1	I	30	ASP
1	I	38	TYR
1	I	41	LEU
1	I	45	ILE
1	I	61	MET
1	I	63	PHE
1	I	65	GLN
1	I	77	TRP
1	I	78	ILE
1	I	80	PHE
1	I	81	ASP
1	I	82	HIS
1	I	84	VAL
1	I	87	PHE
1	I	96	ILE
1	I	97	LYS
1	I	100	LEU

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Mol	Chain	Res	Type
1	I	116	LEU
1	I	167	LEU
1	I	170	ILE
1	I	176	TYR
1	I	235	LEU
1	I	238	ILE
1	I	242	ILE
1	I	265	TYR
1	I	266	GLN
1	I	270	TYR
1	I	292	ILE
1	I	309	LEU
1	I	310	PHE
1	I	320	LYS
2	J	12	ARG
2	J	37	PHE
2	J	51	ARG
2	J	58	ASP
2	J	67	VAL
2	J	77	TYR
2	J	102	LEU
2	J	106	ARG
2	J	108	ARG
2	J	150	PHE
2	J	161	ARG
2	J	217	MET
2	J	224	GLU
2	J	235	THR
2	J	243	GLU
2	J	249	LEU
2	J	257	GLU
2	J	264	ILE
2	J	280	LYS
2	J	283	THR
3	K	5	VAL
3	K	11	VAL
3	K	12	LYS
3	K	45	THR
3	K	60	THR
3	K	61	ILE
3	K	77	ASP
3	K	102	ARG

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Mol	Chain	Res	Type
3	K	112	ASP
3	K	116	LYS
3	K	134	ASP
3	K	136	SER
3	K	147	ARG
3	K	169	LEU
3	K	172	GLN
3	K	180	LEU
3	K	181	HIS
3	K	188	VAL
3	K	192	THR
3	K	206	VAL
3	K	210	ASP
3	K	224	LEU
3	K	235	ILE
3	K	246	ARG
3	K	250	ASP
3	K	252	THR
3	K	257	LEU
3	K	268	ARG
3	K	271	THR
3	K	273	LEU
3	K	289	THR
3	K	291	ASP
3	K	294	GLU
3	K	298	ARG
3	K	307	ILE
3	K	308	VAL
3	K	311	LEU
3	K	321	VAL
3	K	326	LEU
3	K	328	VAL
3	K	333	LEU
3	K	345	HIS
3	K	349	THR
3	L	5	VAL
3	L	11	VAL
3	L	12	LYS
3	L	41	CYS
3	L	45	THR
3	L	60	THR
3	L	61	ILE

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Mol	Chain	Res	Type
3	L	77	ASP
3	L	84	ASN
3	L	102	ARG
3	L	116	LYS
3	L	120	ASP
3	L	124	LEU
3	L	147	ARG
3	L	169	LEU
3	L	172	GLN
3	L	180	LEU
3	L	181	HIS
3	L	188	VAL
3	L	192	THR
3	L	206	VAL
3	L	210	ASP
3	L	224	LEU
3	L	235	ILE
3	L	246	ARG
3	L	250	ASP
3	L	252	THR
3	L	255	VAL
3	L	257	LEU
3	L	268	ARG
3	L	271	THR
3	L	289	THR
3	L	294	GLU
3	L	298	ARG
3	L	304	THR
3	L	307	ILE
3	L	308	VAL
3	L	311	LEU
3	L	321	VAL
3	L	326	LEU
3	L	328	VAL
3	L	330	VAL
3	L	333	LEU
3	L	335	GLU
3	L	345	HIS
3	L	348	LEU
3	L	349	THR
3	L	359	GLN
1	M	28	TRP

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Mol	Chain	Res	Type
1	M	30	ASP
1	M	38	TYR
1	M	41	LEU
1	M	45	ILE
1	M	61	MET
1	M	63	PHE
1	M	77	TRP
1	M	78	ILE
1	M	80	PHE
1	M	81	ASP
1	M	82	HIS
1	M	84	VAL
1	M	87	PHE
1	M	96	ILE
1	M	97	LYS
1	M	100	LEU
1	M	116	LEU
1	M	167	LEU
1	M	170	ILE
1	M	176	TYR
1	M	235	LEU
1	M	238	ILE
1	M	242	ILE
1	M	265	TYR
1	M	266	GLN
1	M	270	TYR
1	M	292	ILE
1	M	309	LEU
1	M	310	PHE
1	M	320	LYS
2	N	12	ARG
2	N	37	PHE
2	N	51	ARG
2	N	58	ASP
2	N	67	VAL
2	N	77	TYR
2	N	102	LEU
2	N	106	ARG
2	N	108	ARG
2	N	150	PHE
2	N	161	ARG
2	N	217	MET

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Mol	Chain	Res	Type
2	N	224	GLU
2	N	235	THR
2	N	243	GLU
2	N	249	LEU
2	N	257	GLU
2	N	264	ILE
2	N	283	THR
3	O	5	VAL
3	O	11	VAL
3	O	12	LYS
3	O	45	THR
3	O	60	THR
3	O	61	ILE
3	O	77	ASP
3	O	102	ARG
3	O	112	ASP
3	O	116	LYS
3	O	134	ASP
3	O	136	SER
3	O	147	ARG
3	O	169	LEU
3	O	172	GLN
3	O	180	LEU
3	O	181	HIS
3	O	188	VAL
3	O	192	THR
3	O	206	VAL
3	O	210	ASP
3	O	224	LEU
3	O	235	ILE
3	O	246	ARG
3	O	250	ASP
3	O	252	THR
3	O	257	LEU
3	O	268	ARG
3	O	271	THR
3	O	273	LEU
3	O	289	THR
3	O	291	ASP
3	O	294	GLU
3	O	298	ARG
3	O	307	ILE

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Mol	Chain	Res	Type
3	O	308	VAL
3	O	311	LEU
3	O	321	VAL
3	O	326	LEU
3	O	328	VAL
3	O	333	LEU
3	O	345	HIS
3	O	349	THR
3	P	5	VAL
3	P	11	VAL
3	P	12	LYS
3	P	41	CYS
3	P	45	THR
3	P	60	THR
3	P	61	ILE
3	P	77	ASP
3	P	84	ASN
3	P	102	ARG
3	P	116	LYS
3	P	120	ASP
3	P	124	LEU
3	P	147	ARG
3	P	169	LEU
3	P	172	GLN
3	P	180	LEU
3	P	181	HIS
3	P	188	VAL
3	P	192	THR
3	P	206	VAL
3	P	210	ASP
3	P	224	LEU
3	P	235	ILE
3	P	246	ARG
3	P	250	ASP
3	P	252	THR
3	P	255	VAL
3	P	257	LEU
3	P	268	ARG
3	P	271	THR
3	P	289	THR
3	P	294	GLU
3	P	298	ARG

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Mol	Chain	Res	Type
3	P	304	THR
3	P	307	ILE
3	P	308	VAL
3	P	311	LEU
3	P	321	VAL
3	P	326	LEU
3	P	328	VAL
3	P	330	VAL
3	P	333	LEU
3	P	335	GLU
3	P	345	HIS
3	P	348	LEU
3	P	349	THR
3	P	359	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
2	B	279	GLN
3	C	9	ASN
3	C	160	GLN
3	C	182	GLN
3	C	193	HIS
3	C	357	GLN
3	D	160	GLN
3	D	182	GLN
3	D	193	HIS
3	D	345	HIS
3	D	357	GLN
1	E	65	GLN
2	F	279	GLN
3	G	160	GLN
3	G	182	GLN
3	G	193	HIS
3	G	357	GLN
3	H	160	GLN
3	H	182	GLN
3	H	193	HIS
3	H	345	HIS
1	I	65	GLN
2	J	279	GLN

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Mol	Chain	Res	Type
3	K	9	ASN
3	K	160	GLN
3	K	182	GLN
3	K	193	HIS
3	K	357	GLN
3	L	160	GLN
3	L	182	GLN
3	L	193	HIS
3	L	345	HIS
3	L	357	GLN
1	M	65	GLN
1	M	220	GLN
2	N	279	GLN
3	O	160	GLN
3	O	182	GLN
3	O	193	HIS
3	O	357	GLN
3	P	9	ASN
3	P	160	GLN
3	P	182	GLN
3	P	193	HIS
3	P	345	HIS

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)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	286/301 (95%)	-0.41	1 (0%)	94	90	45, 123, 232, 396	0
1	E	286/301 (95%)	-0.39	6 (2%)	63	54	72, 144, 245, 389	0
1	I	286/301 (95%)	-0.39	1 (0%)	94	90	63, 110, 236, 381	0
1	M	286/301 (95%)	-0.35	4 (1%)	75	66	63, 137, 231, 308	0
2	B	284/305 (93%)	-0.29	6 (2%)	63	54	40, 135, 260, 432	0
2	F	280/305 (91%)	-0.35	5 (1%)	68	59	74, 138, 252, 482	0
2	J	284/305 (93%)	-0.37	7 (2%)	57	48	64, 129, 253, 401	0
2	N	284/305 (93%)	-0.43	5 (1%)	68	59	50, 112, 244, 387	0
3	C	363/363 (100%)	-0.14	10 (2%)	53	43	44, 179, 275, 344	0
3	D	363/363 (100%)	0.11	25 (6%)	16	13	72, 187, 302, 373	0
3	G	363/363 (100%)	0.02	12 (3%)	46	37	70, 160, 285, 349	0
3	H	363/363 (100%)	-0.01	14 (3%)	39	31	46, 146, 267, 367	0
3	K	363/363 (100%)	-0.19	7 (1%)	66	58	47, 156, 263, 338	0
3	L	363/363 (100%)	-0.06	17 (4%)	31	26	69, 154, 276, 340	0
3	O	363/363 (100%)	0.12	24 (6%)	18	15	65, 198, 291, 376	0
3	P	363/363 (100%)	-0.04	12 (3%)	46	37	57, 162, 279, 355	0
All	All	5180/5328 (97%)	-0.18	156 (3%)	50	39	40, 151, 275, 482	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	1	MET	12.2
3	D	1	MET	8.8
3	O	1	MET	7.9
3	O	2	VAL	7.1
3	H	296	SER	6.6

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Mol	Chain	Res	Type	RSRZ
3	D	164	ASN	6.3
3	H	295	GLY	5.6
3	O	332	GLY	5.6
3	L	295	GLY	5.6
3	H	108	LYS	5.4
3	C	295	GLY	5.2
3	H	294	GLU	5.2
3	H	293	VAL	4.9
3	D	211	GLY	4.9
3	O	85	TYR	4.9
3	C	193	HIS	4.8
3	H	297	GLU	4.8
3	G	2	VAL	4.8
3	L	296	SER	4.6
3	C	296	SER	4.5
3	P	296	SER	4.5
3	O	79	ALA	4.5
3	H	1	MET	4.5
3	K	1	MET	4.5
2	F	51	ARG	4.5
3	O	54	GLU	4.4
3	O	292	GLY	4.3
3	L	109	SER	4.3
3	L	108	LYS	4.2
3	P	297	GLU	4.2
3	C	282	GLY	4.1
3	H	2	VAL	4.1
3	L	297	GLU	4.1
3	G	295	GLY	4.0
3	D	85	TYR	4.0
3	D	302	LYS	3.9
1	E	128	GLY	3.9
3	D	340	ASP	3.9
3	H	298	ARG	3.8
3	K	275	PRO	3.8
3	P	86	ALA	3.8
1	M	65	GLN	3.7
2	N	53	PHE	3.7
1	A	170	ILE	3.7
3	O	331	GLY	3.7
3	P	125	GLN	3.7
3	D	261	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
3	L	331	GLY	3.6
3	G	1	MET	3.6
3	G	267	PRO	3.6
3	G	3	ALA	3.6
3	P	2	VAL	3.5
3	O	55	GLU	3.5
3	D	210	ASP	3.5
3	O	322	GLY	3.5
3	D	137	GLY	3.4
3	D	252	THR	3.4
3	D	212	LEU	3.4
3	H	107	LYS	3.3
3	C	66	ARG	3.3
3	O	291	ASP	3.3
3	O	276	GLY	3.1
2	B	287	MET	3.1
3	D	337	HIS	3.1
3	L	357	GLN	3.1
3	D	267	PRO	3.1
2	J	57	VAL	3.1
3	L	294	GLU	3.0
3	P	298	ARG	3.0
3	L	293	VAL	3.0
3	D	293	VAL	3.0
2	N	287	MET	2.9
3	O	268	ARG	2.9
3	L	164	ASN	2.9
1	E	257	GLY	2.9
2	J	287	MET	2.8
3	K	276	GLY	2.8
3	L	79	ALA	2.8
3	D	339	GLY	2.8
1	E	172	LEU	2.8
2	J	180	ALA	2.8
3	C	297	GLU	2.8
3	G	269	ALA	2.7
3	K	248	ALA	2.7
2	F	53	PHE	2.7
3	G	209	ARG	2.7
3	L	107	LYS	2.7
2	J	9	ARG	2.7
3	D	79	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	N	5	PRO	2.6
3	L	17	THR	2.6
3	P	108	LYS	2.6
3	G	13	ARG	2.6
3	O	277	GLN	2.6
3	D	260	GLY	2.6
1	E	127	LYS	2.5
3	D	165	LEU	2.5
3	K	246	ARG	2.5
2	B	224	GLU	2.5
3	O	294	GLU	2.5
3	G	165	LEU	2.5
3	K	247	ILE	2.5
2	N	52	VAL	2.5
3	G	268	ARG	2.4
1	M	318	ILE	2.4
3	O	108	LYS	2.4
3	D	154	LYS	2.4
3	D	125	GLN	2.4
3	P	249	VAL	2.4
3	C	37	GLY	2.4
3	K	244	PRO	2.3
3	C	67	VAL	2.3
3	P	126	PRO	2.3
3	O	258	ASN	2.3
3	H	85	TYR	2.3
3	C	294	GLU	2.3
2	F	56	PRO	2.3
2	J	51	ARG	2.3
3	L	106	THR	2.3
3	O	3	ALA	2.3
1	M	76	PRO	2.3
1	M	77	TRP	2.2
2	B	51	ARG	2.2
3	P	259	GLY	2.2
3	G	294	GLU	2.2
2	B	57	VAL	2.2
1	E	287	GLY	2.2
2	J	58	ASP	2.2
3	H	299	ALA	2.2
3	O	269	ALA	2.2
2	F	52	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	P	107	LYS	2.2
3	D	338	PRO	2.2
3	D	80	MET	2.2
2	F	143	ARG	2.2
3	D	157	LEU	2.2
3	O	211	GLY	2.2
3	G	296	SER	2.2
3	L	226	PRO	2.2
3	H	147	ARG	2.2
3	L	66	ARG	2.1
3	C	352	HIS	2.1
2	B	280	LYS	2.1
2	J	286	VAL	2.1
3	O	165	LEU	2.1
3	O	271	THR	2.1
3	D	147	ARG	2.1
3	D	348	LEU	2.0
3	L	332	GLY	2.0
3	O	212	LEU	2.0
1	E	129	TYR	2.0
3	H	15	ASP	2.0
2	N	61	PHE	2.0
3	O	107	LYS	2.0
2	B	225	LYS	2.0
1	I	175	VAL	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.