



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 10:53 AM EDT

PDB ID : 4TQV / pdb_00004tqv
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

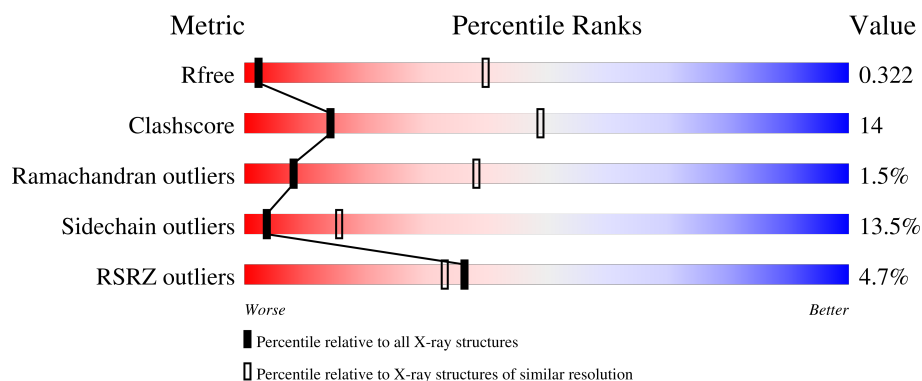
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

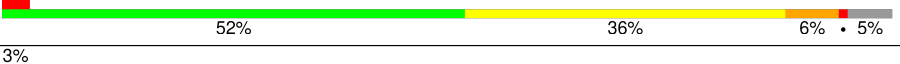
The reported resolution of this entry is 4.50 Å.

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.



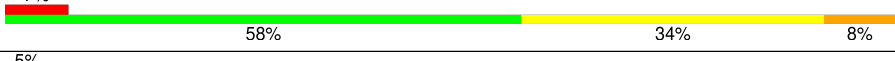
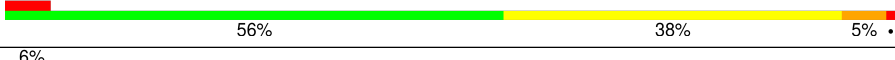
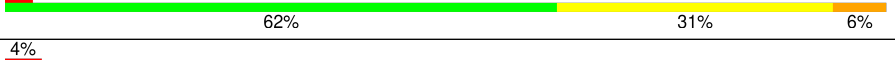
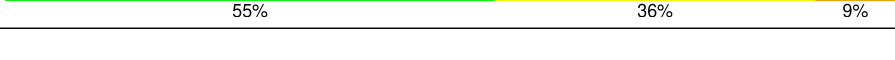
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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 $\leq 5\%$. 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	
1	E	301	
1	I	301	
1	M	301	
2	B	305	

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Mol	Chain	Length	Quality of chain
2	F	305	
2	J	305	
2	N	305	
3	C	363	
3	D	363	
3	G	363	
3	H	363	
3	K	363	
3	L	363	
3	O	363	
3	P	363	

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
1	A	286	Total	C	N	O	S	0	0	0
			2314	1550	368	386	10			
1	E	286	Total	C	N	O	S	0	0	0
			2314	1550	368	386	10			
1	I	286	Total	C	N	O	S	0	0	0
			2314	1550	368	386	10			
1	M	286	Total	C	N	O	S	0	0	0
			2314	1550	368	386	10			

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
2	B	284	Total	C	N	O	S	0	0	0
			2257	1506	359	379	13			
2	F	280	Total	C	N	O	S	0	0	0
			2229	1488	354	375	12			
2	J	284	Total	C	N	O	S	0	0	0
			2257	1506	359	379	13			
2	N	284	Total	C	N	O	S	0	0	0
			2257	1506	359	379	13			

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
3	C	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	D	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	G	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	H	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	K	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	L	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	O	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			
3	P	363	Total	C	N	O	S	0	0	0
			2777	1745	503	518	11			

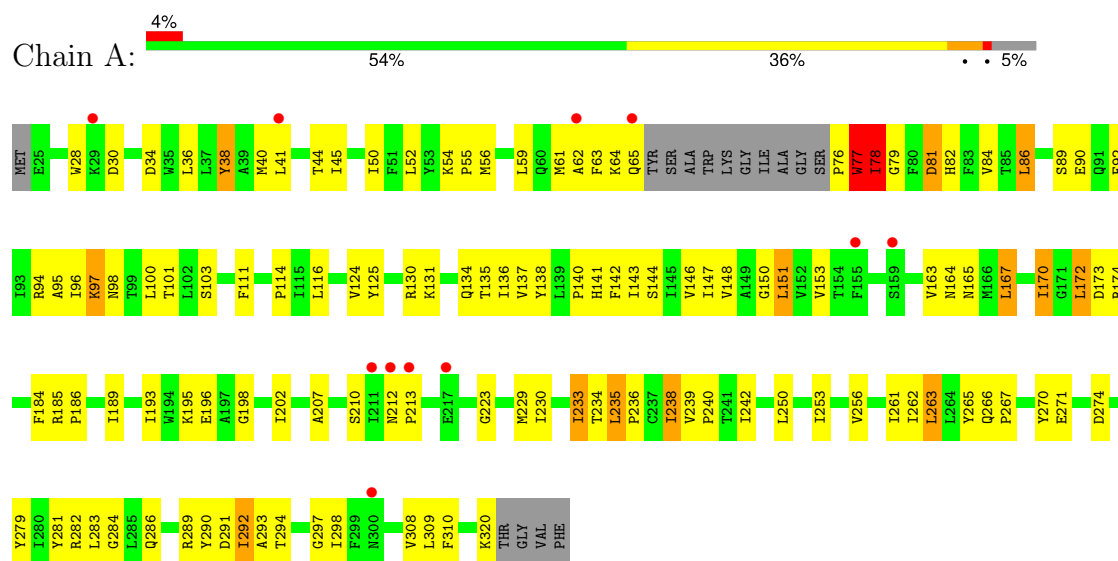
There are 8 discrepancies between the modelled and reference sequences:

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

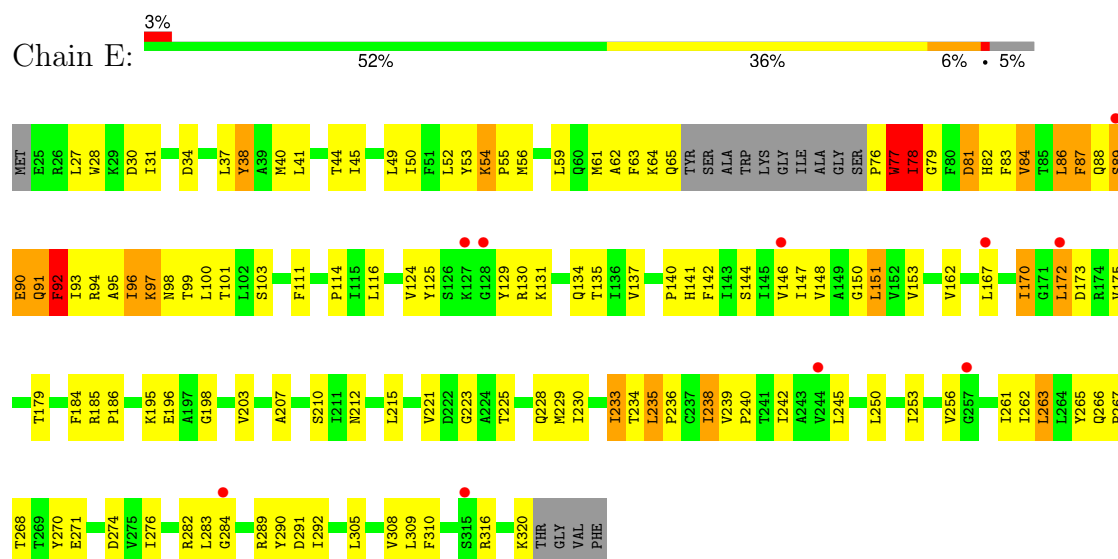
3 Residue-property plots [i](#)

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.

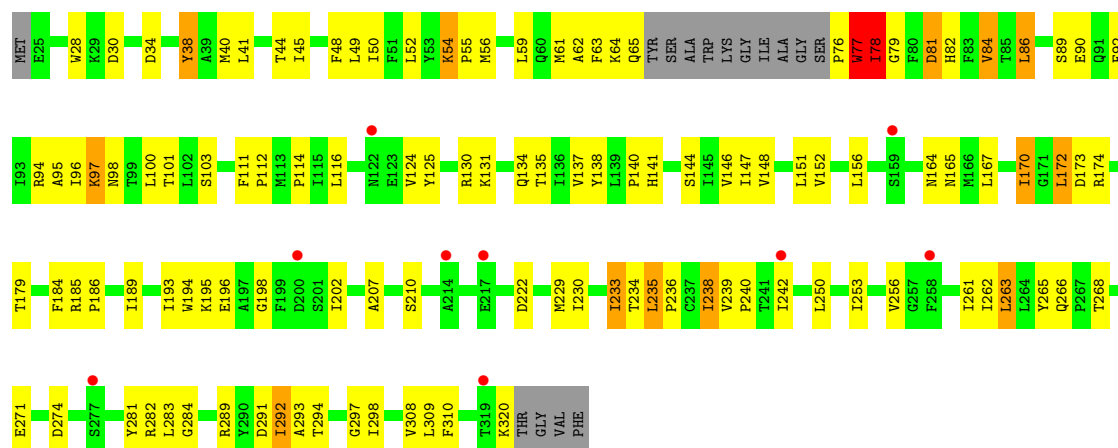
• Molecule 1: AlgM1



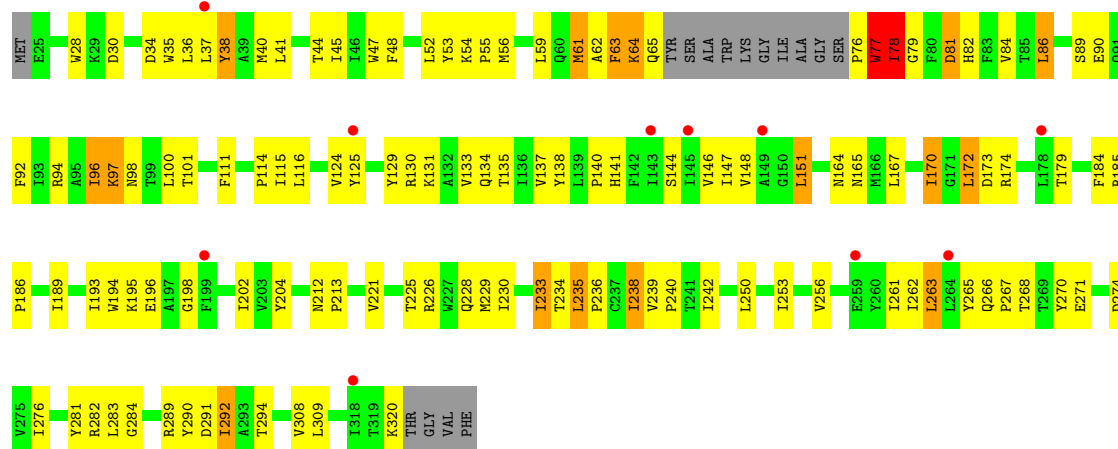
• Molecule 1: AlgM1



• Molecule 1: AlgM1



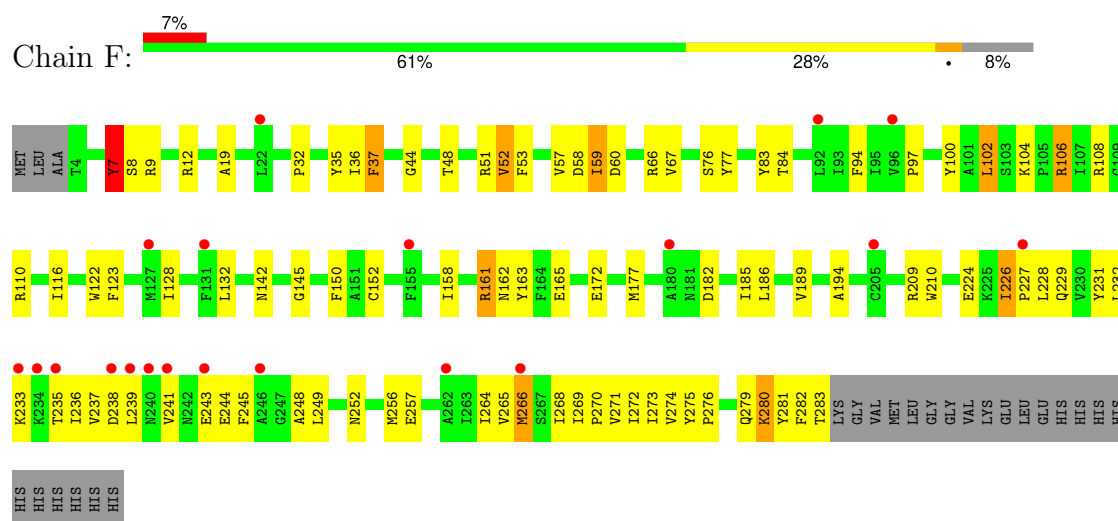
• Molecule 1: AlgM1



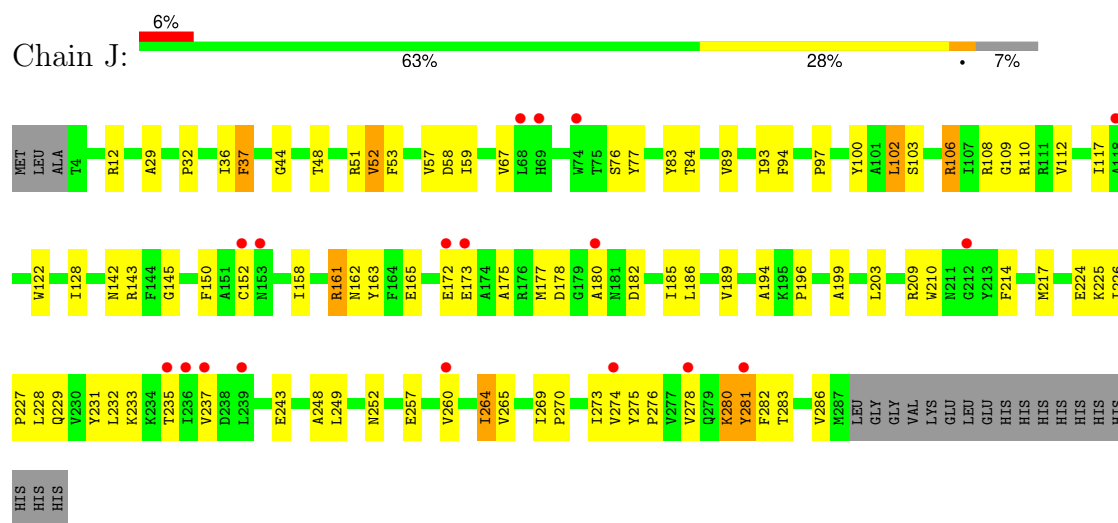
• Molecule 2: AlgM2



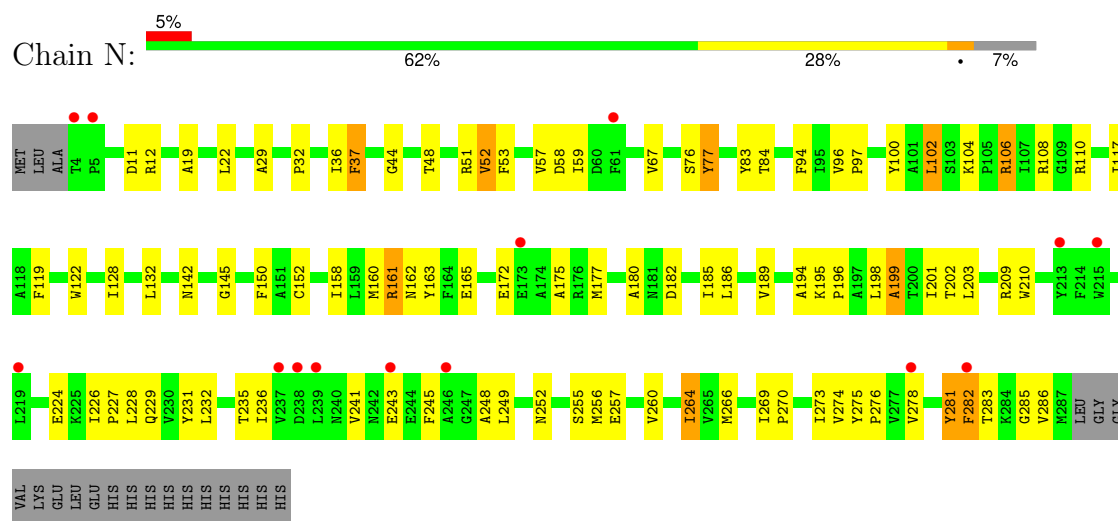
• Molecule 2: AlgM2



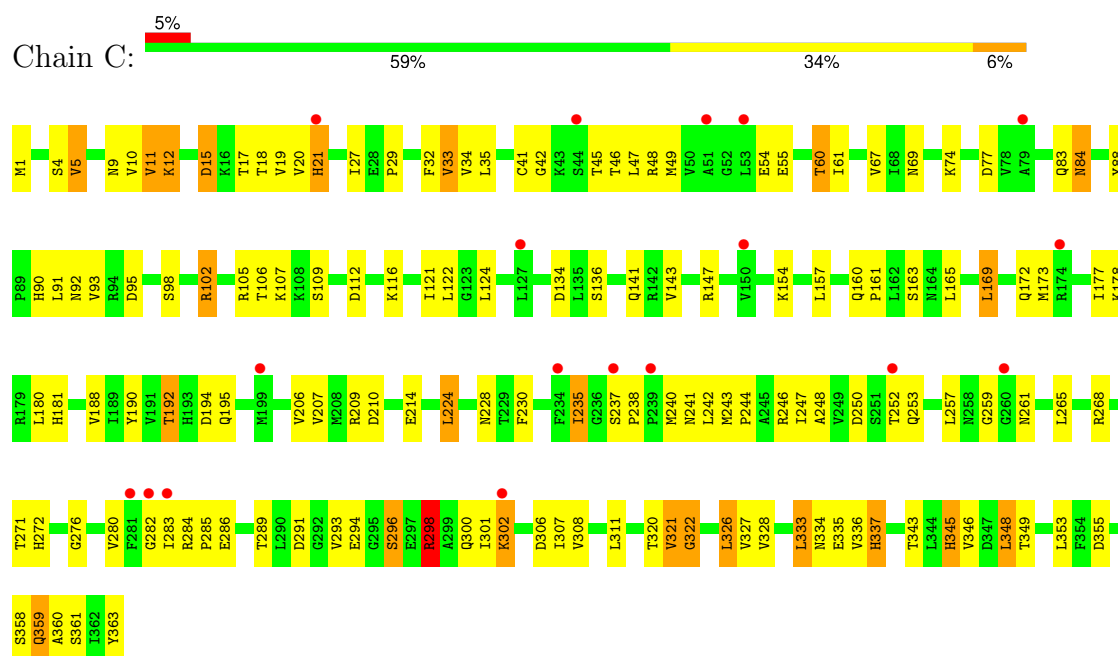
- Molecule 2: AlgM2



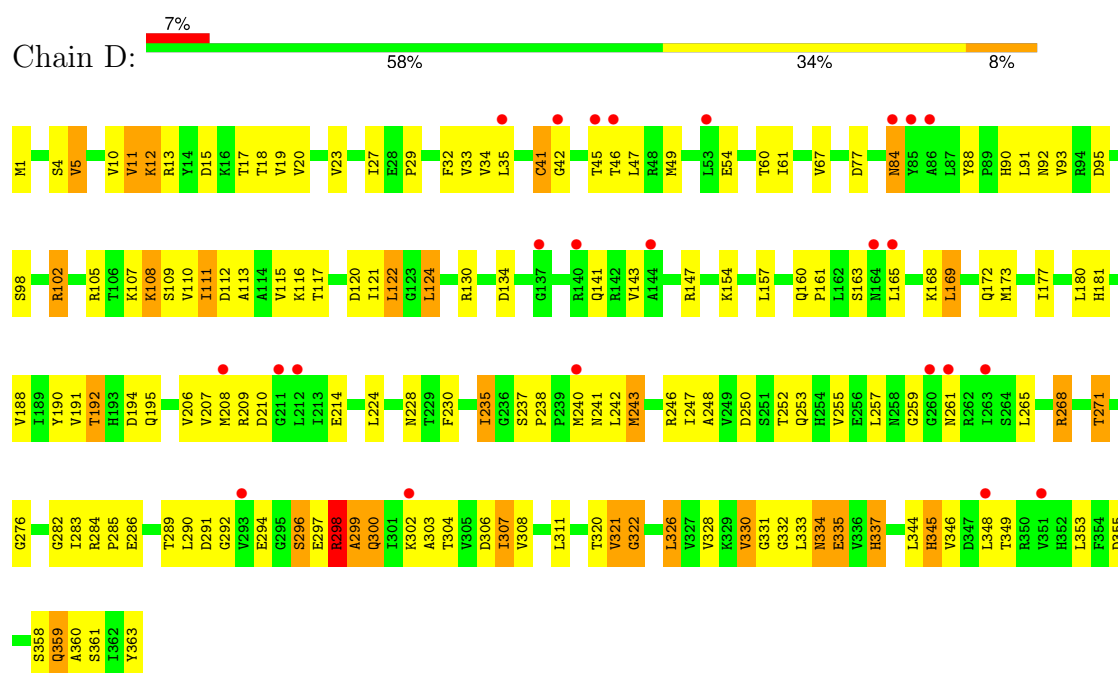
- Molecule 2: AlgM2



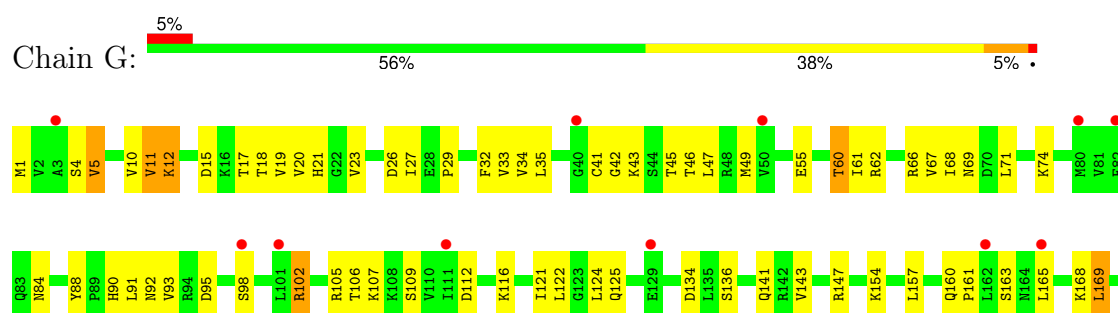
- Molecule 3: AlgS

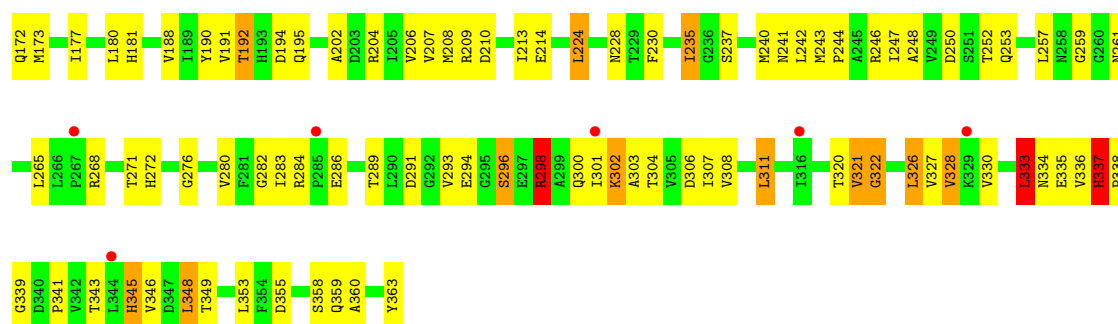


• Molecule 3: Algs

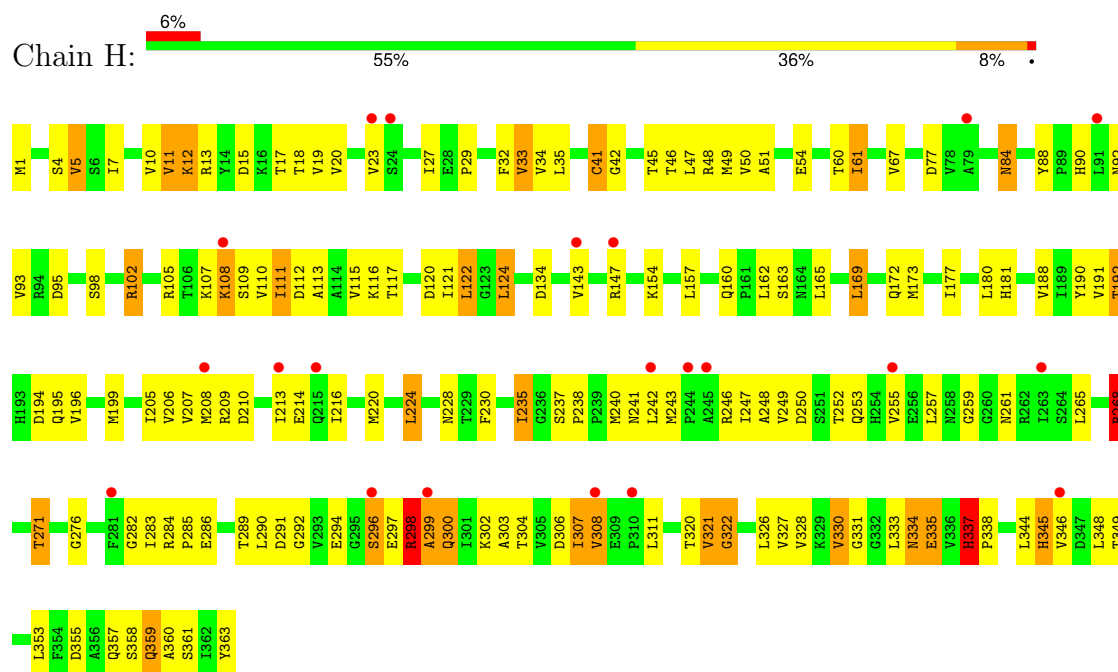


• Molecule 3: Algs





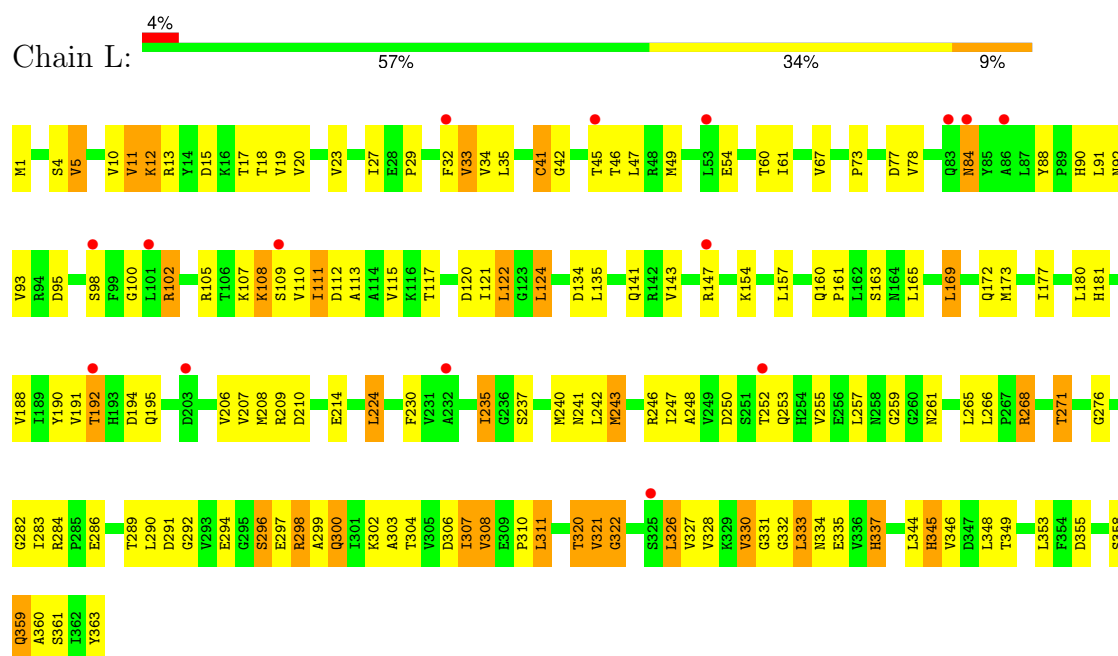
- Molecule 3: AlgS



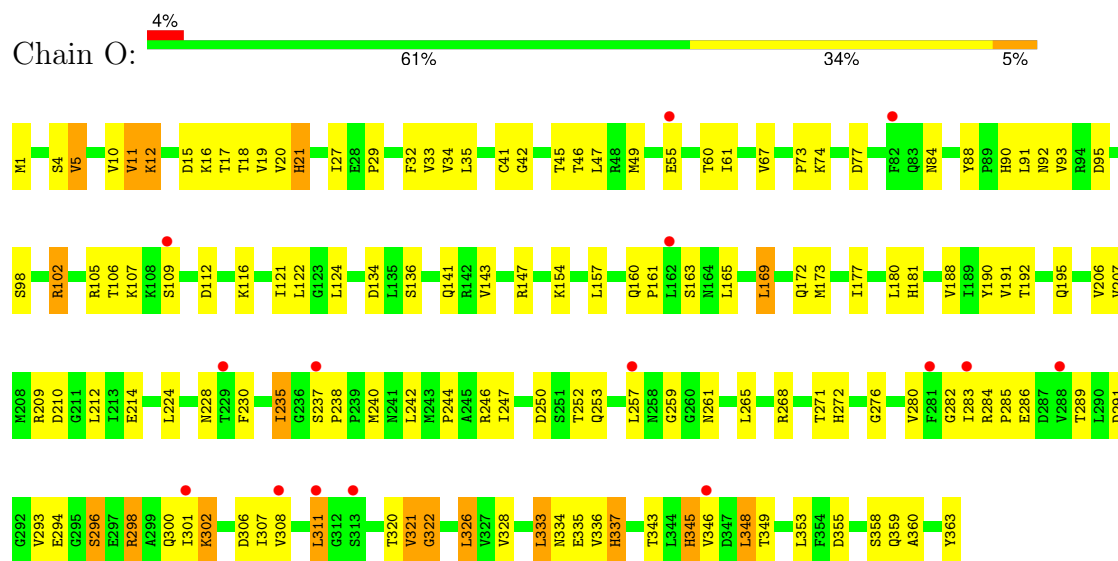
- Molecule 3: AlgS



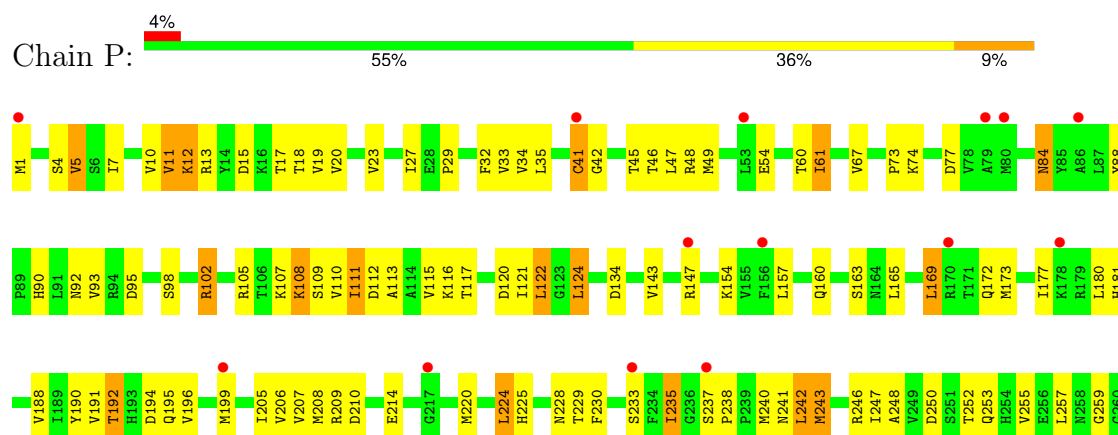
- Molecule 3: AlgS

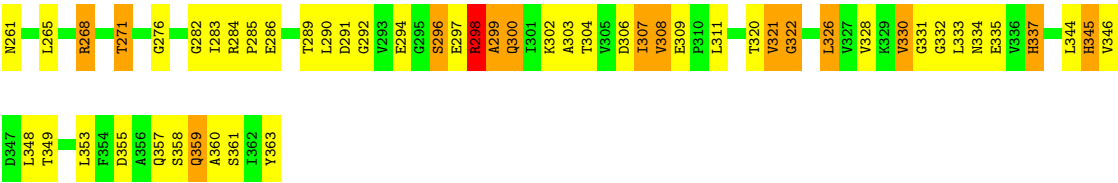


- Molecule 3: AlgS



- Molecule 3: AlgS





4 Data and refinement statistics

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) 80.1 (29.82-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 4.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.279 , 0.320 0.282 , 0.322	Depositor DCC
R_{free} test set	2000 reflections (3.35%)	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)	0.21 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.35	0/2377	0.80	1/3241 (0.0%)
1	E	0.37	0/2377	0.88	6/3241 (0.2%)
1	I	0.34	0/2377	0.80	1/3241 (0.0%)
1	M	0.35	0/2377	0.83	3/3241 (0.1%)
2	B	0.38	0/2316	0.91	5/3149 (0.2%)
2	F	0.38	0/2288	0.93	6/3113 (0.2%)
2	J	0.37	0/2316	0.91	5/3149 (0.2%)
2	N	0.40	1/2316 (0.0%)	0.93	8/3149 (0.3%)
3	C	0.36	0/2822	0.96	7/3826 (0.2%)
3	D	0.38	0/2822	1.00	15/3826 (0.4%)
3	G	0.38	0/2822	1.00	13/3826 (0.3%)
3	H	0.36	0/2822	1.00	14/3826 (0.4%)
3	K	0.37	0/2822	0.95	8/3826 (0.2%)
3	L	0.36	0/2822	1.00	17/3826 (0.4%)
3	O	0.37	0/2822	0.95	5/3826 (0.1%)
3	P	0.36	0/2822	1.00	16/3826 (0.4%)
All	All	0.37	1/41320 (0.0%)	0.94	130/56132 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	199	ALA	CA-CB	-5.14	1.45	1.53

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	282	PHE	N-CA-C	9.84	123.23	111.82
2	B	282	PHE	N-CA-C	9.44	122.77	111.82
2	N	282	PHE	N-CA-C	9.22	122.51	111.82
2	F	281	TYR	N-CA-C	8.16	120.98	111.02
1	E	91	GLN	CA-C-N	8.06	131.40	120.44
1	E	91	GLN	C-N-CA	8.06	131.40	120.44
2	N	281	TYR	N-CA-C	7.84	120.59	111.02
1	M	64	LYS	CA-C-N	7.71	135.57	121.70
1	M	64	LYS	C-N-CA	7.71	135.57	121.70
2	B	281	TYR	N-CA-C	7.54	120.22	111.02
3	G	296	SER	N-CA-C	7.47	120.36	111.02
3	C	237	SER	CA-C-N	-7.30	112.86	120.38
3	C	237	SER	C-N-CA	-7.30	112.86	120.38
2	J	281	TYR	N-CA-C	7.25	119.87	111.02
3	O	296	SER	N-CA-C	7.22	120.04	111.02
3	L	237	SER	CA-C-N	-7.16	113.01	120.38
3	L	237	SER	C-N-CA	-7.16	113.01	120.38
3	K	296	SER	N-CA-C	7.16	119.96	111.02
3	C	296	SER	N-CA-C	7.15	119.96	111.02
3	K	237	SER	CA-C-N	-7.09	113.08	120.38
3	K	237	SER	C-N-CA	-7.09	113.08	120.38
3	P	237	SER	CA-C-N	-7.05	113.11	120.38
3	P	237	SER	C-N-CA	-7.05	113.11	120.38
3	H	237	SER	CA-C-N	-7.03	113.14	120.38
3	H	237	SER	C-N-CA	-7.03	113.14	120.38
2	F	282	PHE	N-CA-C	7.02	119.97	111.82
2	N	282	PHE	CB-CA-C	-7.02	97.20	110.67
3	O	237	SER	CA-C-N	-6.95	113.22	120.38
3	O	237	SER	C-N-CA	-6.95	113.22	120.38
3	D	237	SER	CA-C-N	-6.94	113.23	120.38
3	D	237	SER	C-N-CA	-6.94	113.23	120.38
3	G	237	SER	CA-C-N	-6.88	113.29	120.38
3	G	237	SER	C-N-CA	-6.88	113.29	120.38
3	D	271	THR	N-CA-C	6.82	118.50	111.14
3	P	300	GLN	N-CA-C	6.58	118.14	108.86
3	H	300	GLN	N-CA-C	6.56	118.11	108.86
3	D	300	GLN	N-CA-C	6.51	118.03	108.86
3	L	300	GLN	N-CA-C	6.46	117.96	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	92	PHE	N-CA-C	-6.45	104.18	111.14
2	J	282	PHE	CB-CA-C	-6.32	98.55	110.67
3	H	331	GLY	N-CA-C	6.30	120.79	110.97
3	L	332	GLY	N-CA-C	6.28	119.43	110.46
2	N	226	ILE	CA-C-N	6.26	127.67	119.84
2	N	226	ILE	C-N-CA	6.26	127.67	119.84
3	D	331	GLY	N-CA-C	6.25	120.72	110.97
3	G	337	HIS	CA-C-N	6.23	127.63	119.84
3	G	337	HIS	C-N-CA	6.23	127.63	119.84
2	J	226	ILE	CA-C-N	6.22	127.61	119.84
2	J	226	ILE	C-N-CA	6.22	127.61	119.84
2	N	198	LEU	N-CA-C	6.21	118.05	111.28
3	K	21	HIS	N-CA-C	6.21	119.58	112.57
3	C	21	HIS	N-CA-C	6.17	119.54	112.57
2	F	226	ILE	CA-C-N	6.16	127.54	119.84
2	F	226	ILE	C-N-CA	6.16	127.54	119.84
2	B	226	ILE	CA-C-N	6.13	127.50	119.84
2	B	226	ILE	C-N-CA	6.13	127.50	119.84
1	E	87	PHE	N-CA-C	6.05	117.55	111.07
1	E	88	GLN	N-CA-C	6.02	118.49	108.20
3	L	271	THR	N-CA-C	5.97	117.58	111.14
3	P	331	GLY	N-CA-C	5.95	120.25	110.97
3	D	337	HIS	CA-C-N	5.90	125.92	119.90
3	D	337	HIS	C-N-CA	5.90	125.92	119.90
3	L	266	LEU	CA-C-N	5.88	125.09	118.97
3	L	266	LEU	C-N-CA	5.88	125.09	118.97
3	L	337	HIS	CA-C-N	5.86	125.88	119.90
3	L	337	HIS	C-N-CA	5.86	125.88	119.90
2	B	282	PHE	CB-CA-C	-5.85	99.43	110.67
3	P	337	HIS	CA-C-N	5.82	125.83	119.90
3	P	337	HIS	C-N-CA	5.82	125.83	119.90
3	P	271	THR	N-CA-C	5.79	117.40	111.14
3	H	299	ALA	N-CA-C	5.78	119.40	112.93
3	P	298	ARG	CA-CB-CG	5.77	125.64	114.10
3	P	299	ALA	N-CA-C	5.75	119.36	112.93
3	D	299	ALA	N-CA-C	5.70	119.32	112.93
3	H	242	LEU	N-CA-C	5.68	118.45	108.56
3	H	337	HIS	CA-C-N	5.67	125.68	119.90
3	H	337	HIS	C-N-CA	5.67	125.68	119.90
1	M	173	ASP	CB-CA-C	-5.65	110.07	116.63
3	H	298	ARG	CA-CB-CG	5.63	125.37	114.10
1	A	173	ASP	CB-CA-C	-5.62	110.11	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	7	TYR	CB-CA-C	-5.59	109.63	117.23
3	H	243	MET	CA-C-N	5.57	125.47	119.85
3	H	243	MET	C-N-CA	5.57	125.47	119.85
3	L	243	MET	CA-C-N	5.57	125.47	119.85
3	L	243	MET	C-N-CA	5.57	125.47	119.85
3	H	271	THR	N-CA-C	5.50	117.08	111.14
3	D	242	LEU	N-CA-C	5.48	118.09	108.56
1	E	90	GLU	N-CA-C	5.46	119.12	111.74
1	I	173	ASP	CB-CA-C	-5.46	110.30	116.63
3	C	248	ALA	CB-CA-C	-5.43	109.85	117.23
3	C	242	LEU	N-CA-C	5.43	118.00	108.56
3	K	242	LEU	N-CA-C	5.42	117.99	108.56
3	P	242	LEU	N-CA-C	5.41	117.97	108.56
3	P	243	MET	CA-C-N	5.39	125.30	119.85
3	P	243	MET	C-N-CA	5.39	125.30	119.85
3	G	248	ALA	CB-CA-C	-5.39	109.90	117.23
3	G	333	LEU	N-CA-C	5.38	122.25	110.80
3	P	332	GLY	N-CA-C	5.37	118.14	110.46
2	F	282	PHE	CB-CA-C	-5.37	100.36	110.67
3	O	242	LEU	N-CA-C	5.37	117.90	108.56
3	G	242	LEU	N-CA-C	5.35	117.87	108.56
3	L	331	GLY	N-CA-C	5.33	119.28	110.97
3	L	299	ALA	N-CA-C	5.30	118.87	112.93
3	L	242	LEU	N-CA-C	5.30	117.78	108.56
3	D	243	MET	CA-C-N	5.30	125.20	119.85
3	D	243	MET	C-N-CA	5.30	125.20	119.85
3	D	248	ALA	CB-CA-C	-5.28	110.05	117.23
3	G	303	ALA	N-CA-C	5.28	116.82	108.96
3	G	298	ARG	N-CA-C	5.25	119.32	113.02
3	L	248	ALA	CB-CA-C	-5.24	110.11	117.23
3	O	21	HIS	N-CA-C	5.22	118.78	112.93
3	P	248	ALA	CB-CA-C	-5.21	110.14	117.23
3	H	248	ALA	CB-CA-C	-5.19	110.17	117.23
3	P	334	ASN	N-CA-C	5.19	121.85	110.80
2	N	96	VAL	CB-CA-C	-5.17	108.78	113.70
3	D	298	ARG	CA-CB-CG	5.14	124.39	114.10
3	L	334	ASN	N-CA-C	5.14	121.75	110.80
2	N	285	GLY	N-CA-C	-5.13	107.98	115.63
3	L	320	THR	N-CA-C	5.10	116.84	108.52
3	P	298	ARG	NE-CZ-NH1	-5.09	116.41	121.50
3	C	298	ARG	N-CA-C	5.08	119.12	113.02
3	D	334	ASN	N-CA-C	5.08	121.61	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	334	ASN	N-CA-C	5.07	121.60	110.80
3	D	332	GLY	N-CA-C	5.05	117.69	110.46
3	K	19	VAL	N-CA-C	5.04	115.26	110.42
3	K	238	PRO	CA-C-N	-5.04	114.80	120.14
3	K	238	PRO	C-N-CA	-5.04	114.80	120.14
3	G	21	HIS	N-CA-C	5.03	118.45	111.55
3	G	125	GLN	CA-C-N	-5.02	114.49	119.56
3	G	125	GLN	C-N-CA	-5.02	114.49	119.56

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

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	83	1
1	E	2314	0	2402	90	0
1	I	2314	0	2402	74	1
1	M	2314	0	2402	83	0
2	B	2257	0	2320	64	0
2	F	2229	0	2286	64	1
2	J	2257	0	2320	65	0
2	N	2257	0	2320	72	1
3	C	2777	0	2854	78	0
3	D	2777	0	2854	80	0
3	G	2777	0	2854	92	0
3	H	2777	0	2854	91	0
3	K	2777	0	2854	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	2777	0	2854	87	0
3	O	2777	0	2854	74	0
3	P	2777	0	2854	89	0
All	All	40472	0	41686	1170	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 (1170) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:240:MET:HE3	3:G:282:GLY:HA3	1.80	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:C:240:MET:HE3	3:C:282:GLY:HA3	1.81	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
3:L:240:MET:HE3	3:L:282:GLY:HA3	1.80	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:O:240:MET:HE3	3:O:282:GLY:HA3	1.81	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:D:240:MET:HE3	3:D:282:GLY:HA3	1.82	0.62
3:L:353:LEU:HB2	3:L:363:TYR:HB2	1.81	0.62
3:P:240:MET:HE3	3:P:282:GLY:HA3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:296:SER:OG	3:D:297:GLU:N	2.29	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:H:240:MET:HE3	3:H:282:GLY:HA3	1.81	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
3:K:240:MET:HE3	3:K:282:GLY:HA3	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ILE:HG23	1:E:79:GLY:O	2.02	0.60
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: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
1:E:90:GLU:C	1:E:92:PHE:H	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:12:LYS:NZ	3:O:55:GLU:O	2.37	0.57
2:B:196:PRO:HB3	2:B:286:VAL:HB	1.85	0.57
1:E:79:GLY:C	1:E:81:ASP:H	2.12	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:L:46:THR:HA	3:L:49:MET:HE3	1.87	0.56
3:C:293:VAL:O	3:C:294:GLU:HG3	2.06	0.56
2:F:66:ARG:HH12	2:F:244:GLU:CD	2.13	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
1:M:44:THR:OG1	2:N:94:PHE:O	2.18	0.56
3:O:293:VAL:O	3:O:294:GLU:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:I:79:GLY:C	1:I:81:ASP:H	2.14	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:79:GLY:C	1:A:81:ASP:H	2.14	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
3:O:46:THR:HA	3:O:49:MET:HE3	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:110:VAL:C	3:D:112:ASP:H	2.15	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
2:J:110:ARG:NH1	2:J:165:GLU:OE1	2.41	0.54
3:P:110:VAL:C	3:P:112:ASP:H	2.15	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:A:97:LYS:O	1:A:101:THR:OG1	2.24	0.54
1:M:179:THR:O	1:M:268:THR:OG1	2.23	0.54
1:E:40:MET:HB3	2:F:97:PRO:HB2	1.89	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:C:46:THR:HA	3:C:49:MET:HE3	1.90	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
3:L:110:VAL:C	3:L:112:ASP:H	2.16	0.53
1:E:140:PRO:HB2	1:E:195:LYS:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:207:VAL:HG13	3:G:214:GLU:HB3	1.90	0.53
3:H:110:VAL:C	3:H:112:ASP:H	2.15	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
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
3:D:46:THR:HA	3:D:49:MET:HE3	1.91	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:I:207:ALA:O	1:I:210:SER:OG	2.26	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:G:105:ARG:O	3:G:106:THR:OG1	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:ARG:O	3:C:106:THR:OG1	2.24	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
1:M:97:LYS:O	1:M:101:THR:OG1	2.24	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
3:H:46:THR:HA	3:H:49:MET:HE3	1.92	0.51
1:A:52:LEU:C	1:A:55:PRO:HD2	2.36	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
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:HZ3	3:P:54:GLU:HB3	1.76	0.51
3:P:12:LYS:NZ	3:P:54:GLU:HB3	2.26	0.51
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:46:THR:HA	3:K:49:MET:HE3	1.93	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
3:G:46:THR:HA	3:G:49:MET:HE3	1.92	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
3:P:46:THR:HA	3:P:49:MET:HE3	1.93	0.50
3:P:361:SER:O	3:P:361:SER:OG	2.28	0.50
2:B:94:PHE:HB3	2:B:152:CYS:SG	2.51	0.50
3:C:20:VAL:HG21	3:C:49:MET:HE1	1.92	0.50
2:N:275:TYR:O	2:N:278:VAL:HB	2.12	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
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
1:E:179:THR:O	1:E:268:THR:OG1	2.26	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
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: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:C:293:VAL:C	3:C:294:GLU:HG3	2.38	0.49
3:D:141:GLN:NE2	3:D:161:PRO:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:O	1:A:135:THR:HG23	2.12	0.49
1:I:233:ILE:C	1:I:236:PRO:HD2	2.38	0.49
2:J:94:PHE:HB3	2:J:152:CYS:SG	2.52	0.49
2:J:177:MET:HE1	3:L:78:VAL:HG23	1.95	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
1:I:179:THR:O	1:I:268:THR:OG1	2.29	0.49
3:O:293:VAL:C	3:O:294:GLU:HG3	2.37	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
1:A:274:ASP:CG	1:A:282:ARG:HH22	2.21	0.49
3:D:283:ILE:HG12	3:D:346:VAL:HG23	1.95	0.49
3:G:293:VAL:C	3:G:294:GLU:HG3	2.38	0.49
3:K:293:VAL:C	3:K:294:GLU:HG3	2.38	0.49
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
1:E:97:LYS:O	1:E:101:THR:OG1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:92:ASN:ND2	3:G:95:ASP:OD2	2.43	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:H:84:ASN:N	3:H:84:ASN:OD1	2.46	0.48
1:I:97:LYS:O	1:I:101:THR:OG1	2.25	0.48
1:A:207:ALA:O	1:A:210:SER:OG	2.26	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: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: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
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
3:K:20:VAL:HG21	3:K:49:MET:HE1	1.96	0.48
3:L:358:SER:C	3:L:360:ALA:H	2.22	0.48
1:M:131:LYS:O	1:M:135:THR:HG23	2.14	0.48
1:A:141:HIS:HD1	1:A:196:GLU:CD	2.21	0.48
3:H:122:LEU:HB2	3:H:124:LEU:HD22	1.95	0.48
3:K:106:THR:O	3:K:107:LYS:HB2	2.13	0.48
3:L:160:GLN:HB3	3:L:163:SER:OG	2.14	0.48
1:M:79:GLY:C	1:M:81:ASP:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:D:361:SER:O	3:D:361:SER:OG	2.29	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
2:B:175:ALA:HB1	2:B:180:ALA:HB3	1.96	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
3:K:333:LEU:HG	3:K:334:ASN:H	1.79	0.47
1:E:141:HIS:HD1	1:E:196:GLU:CD	2.22	0.47
3:H:23:VAL:HG21	3:H:208:MET:HE3	1.96	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:52:LEU:C	1:I:55:PRO:HD2	2.40	0.47
1:I:235:LEU:O	1:I:239:VAL:HG23	2.15	0.47
3:L:84:ASN:OD1	3:L:84:ASN:N	2.46	0.47
1:M:77:TRP:O	1:M:78:ILE:HB	2.15	0.47
3:O:20:VAL:HG21	3:O:49:MET:HE1	1.97	0.47
3:O:333:LEU:HB3	3:P:220:MET:HE3	1.96	0.47
3:O:358:SER:C	3:O:360:ALA:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:290:LEU:C	3:D:292:GLY:H	2.23	0.47
1:E:52:LEU:C	1:E:55:PRO:HD2	2.40	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
3:G:358:SER:C	3:G:360:ALA:H	2.22	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
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
1:M:52:LEU:C	1:M:55:PRO:HD2	2.41	0.46
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
1:M:64:LYS:HB2	1:M:291:ASP:CG	2.40	0.46
2:N:163:TYR:CE1	2:N:194:ALA:HA	2.50	0.46
2:N:281:TYR:CD1	2:N:281:TYR:C	2.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:226:ARG:NH2	2:N:11:ASP:OD2	2.49	0.46
1:M:233:ILE:C	1:M:236:PRO:HD2	2.41	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
3:G:20:VAL:HG21	3:G:49:MET:HE1	1.98	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: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
1:A:233:ILE:C	1:A:236:PRO:HD2	2.41	0.46
3:C:90:HIS:CD2	3:C:91:LEU:HG	2.51	0.46
3:D:290:LEU:C	3:D:292:GLY:N	2.74	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:G:23:VAL:HG21	3:G:208:MET:HE3	1.97	0.46
3:H:283:ILE:HG12	3:H:346:VAL:HG23	1.97	0.46
3:H:290:LEU:C	3:H:292:GLY:H	2.24	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
3:P:290:LEU:C	3:P:292:GLY:H	2.24	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:L:290:LEU:C	3:L:292:GLY:H	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:361:SER:O	3:K:361:SER:OG	2.32	0.45
3:L:12:LYS:HZ3	3:L:54:GLU:HB3	1.82	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:290:LEU:C	3:P:292:GLY:N	2.74	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
3:L:290:LEU:C	3:L:292:GLY:N	2.74	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
1:E:274:ASP:CG	1:E:282:ARG:HH22	2.24	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:H:290:LEU:C	3:H:292:GLY:N	2.75	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:23:VAL:HG21	3:P:208:MET:HE3	1.99	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: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)
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: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
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:H:12:LYS:HZ3	3:H:54:GLU:HB3	1.80	0.44
3:H:48:ARG:NE	3:H:54:GLU:OE1	2.34	0.44
3:H:358:SER:C	3:H:360:ALA:H	2.23	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
1:M:274:ASP:CG	1:M:282:ARG:HH22	2.24	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:I:78:ILE:HA	1:I:79:GLY:HA3	1.81	0.44
1:I:141:HIS:HD1	1:I:196:GLU:CD	2.21	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:233:ILE:C	1:E:236:PRO:HD2	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:12:LYS:HZ3	3:D:54:GLU:HB3	1.83	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
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
1:E:207:ALA:O	1:E:210:SER:OG	2.31	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:I:274:ASP:CG	1:I:282:ARG:HH22	2.26	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:87:PHE:CD1	1:E:87:PHE:C	2.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:358:SER:C	3:D:360:ALA:H	2.22	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:143:ILE:O	1:A:195:LYS:NZ	2.45	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: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
1:E:79:GLY:C	1:E:81:ASP:N	2.76	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
3:H:361:SER:O	3:H:361:SER:OG	2.29	0.42
1:I:52:LEU:O	1:I:56:MET:HG3	2.19	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:P:307:ILE:HG13	3:P:308:VAL:N	2.27	0.42
3:D:299:ALA:O	3:D:346:VAL:HG12	2.20	0.42
1:E:77:TRP:O	1:E:78:ILE:HB	2.18	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
3:G:32:PHE:HD2	3:G:181:HIS:CD2	2.29	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
1:A:79:GLY:C	1:A:81:ASP:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:23:VAL:HG21	3:D:208:MET:HE3	2.02	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
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
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
3:L:20:VAL:HG21	3:L:49:MET:HE1	2.02	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:K:243:MET:CE	3:K:326:LEU:HB3	2.50	0.42
3:L:23:VAL:HG21	3:L:208:MET:HE3	2.00	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
3:L:173:MET:O	3:L:177:ILE:HG13	2.20	0.41
2:N:228:LEU:HD12	2:N:228:LEU:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:20:VAL:HG21	3:D:49:MET:HE1	2.02	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
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
1:E:53:TYR:OH	2:F:116:ILE:O	2.32	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: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:87:PHE:C	1:E:87:PHE:HD1	2.29	0.41
1:E:305:LEU:HD13	2:F:123:PHE:HB2	2.02	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:358:SER:C	3:P:360:ALA:H	2.25	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
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
2:J:100:TYR:O	2:J:103:SER:OG	2.36	0.41
3:P:113:ALA:O	3:P:117:THR:HG23	2.20	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
2:F:108:ARG:HD3	2:F:108:ARG:C	2.46	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
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
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
2:F:239:LEU:O	2:F:256:MET:HE1	2.21	0.41
2:J:109:GLY:HA2	2:J:112:VAL:HG12	2.02	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:20:VAL:HG21	3:P:49:MET:HE1	2.02	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
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:61:MET:C	1:M:63:PHE:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:138:TYR:CZ	1:M:202:ILE:HG12	2.56	0.41
2:N:108:ARG:HD3	2:N:108:ARG:C	2.46	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: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
2:J:108:ARG:HD3	2:J:108:ARG:C	2.46	0.41
3:L:122:LEU:HB2	3:L:124:LEU:CD2	2.51	0.41
3:O:181:HIS:HD1	3:O:181:HIS:C	2.27	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
2:F:266:MET:HE2	2:F:266:MET:HB3	1.98	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: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
2:B:108:ARG:HD3	2:B:108:ARG:C	2.46	0.40
3:C:192:THR:HG22	3:C:194:ASP:H	1.86	0.40
3:H:46:THR:O	3:H:50:VAL:HG23	2.21	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
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
1:E:62:ALA:C	1:E:82:HIS:HE2	2.28	0.40
3:G:192:THR:HG22	3:G:194:ASP:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:K:358:SER:C	3:K:360:ALA:H	2.22	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

5.3.1 Protein backbone

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%)	30	67
1	E	282/301 (94%)	252 (89%)	26 (9%)	4 (1%)	9	39
1	I	282/301 (94%)	257 (91%)	24 (8%)	1 (0%)	30	67
1	M	282/301 (94%)	257 (91%)	24 (8%)	1 (0%)	30	67
2	B	282/305 (92%)	249 (88%)	31 (11%)	2 (1%)	18	55
2	F	278/305 (91%)	243 (87%)	32 (12%)	3 (1%)	11	45
2	J	282/305 (92%)	249 (88%)	31 (11%)	2 (1%)	18	55
2	N	282/305 (92%)	249 (88%)	31 (11%)	2 (1%)	18	55
3	C	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	7	35
3	D	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	4	24
3	G	361/363 (99%)	321 (89%)	35 (10%)	5 (1%)	9	39
3	H	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	4	24
3	K	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	7	35
3	L	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	4	24
3	O	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	7	35
3	P	361/363 (99%)	320 (89%)	31 (9%)	10 (3%)	4	24
All	All	5140/5328 (96%)	4583 (89%)	478 (9%)	79 (2%)	8	38

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

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Mol	Chain	Res	Type
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
3	P	291	ASP
3	P	322	GLY
3	P	359	GLN
3	C	337	HIS
3	D	111	ILE

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Mol	Chain	Res	Type
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 ⓘ

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	
1	A	250/260 (96%)	217 (87%)	33 (13%)	4	16
1	E	250/260 (96%)	216 (86%)	34 (14%)	3	15
1	I	250/260 (96%)	217 (87%)	33 (13%)	4	16
1	M	250/260 (96%)	218 (87%)	32 (13%)	4	17
2	B	240/258 (93%)	223 (93%)	17 (7%)	13	35
2	F	237/258 (92%)	218 (92%)	19 (8%)	11	32
2	J	240/258 (93%)	223 (93%)	17 (7%)	13	35
2	N	240/258 (93%)	224 (93%)	16 (7%)	15	37
3	C	307/307 (100%)	261 (85%)	46 (15%)	3	14
3	D	307/307 (100%)	254 (83%)	53 (17%)	2	11
3	G	307/307 (100%)	261 (85%)	46 (15%)	3	14
3	H	307/307 (100%)	254 (83%)	53 (17%)	2	11
3	K	307/307 (100%)	261 (85%)	46 (15%)	3	14
3	L	307/307 (100%)	255 (83%)	52 (17%)	2	11
3	O	307/307 (100%)	261 (85%)	46 (15%)	3	14
3	P	307/307 (100%)	253 (82%)	54 (18%)	2	11
All	All	4413/4528 (98%)	3816 (86%)	597 (14%)	4	16

All (597) 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	54	LYS
1	A	61	MET
1	A	63	PHE
1	A	77	TRP
1	A	78	ILE
1	A	81	ASP
1	A	84	VAL
1	A	86	LEU
1	A	96	ILE

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Mol	Chain	Res	Type
1	A	97	LYS
1	A	100	LEU
1	A	116	LEU
1	A	151	LEU
1	A	167	LEU
1	A	170	ILE
1	A	172	LEU
1	A	233	ILE
1	A	235	LEU
1	A	238	ILE
1	A	242	ILE
1	A	256	VAL
1	A	263	LEU
1	A	265	TYR
1	A	266	GLN
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	58	ASP
2	B	67	VAL
2	B	77	TYR
2	B	102	LEU
2	B	106	ARG
2	B	161	ARG
2	B	189	VAL
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	10	VAL
3	C	11	VAL
3	C	12	LYS
3	C	33	VAL
3	C	45	THR

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Mol	Chain	Res	Type
3	C	60	THR
3	C	61	ILE
3	C	67	VAL
3	C	77	ASP
3	C	84	ASN
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	188	VAL
3	C	192	THR
3	C	206	VAL
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	286	GLU
3	C	289	THR
3	C	291	ASP
3	C	298	ARG
3	C	302	LYS
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	348	LEU
3	C	349	THR
3	D	5	VAL
3	D	10	VAL

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Mol	Chain	Res	Type
3	D	11	VAL
3	D	12	LYS
3	D	33	VAL
3	D	41	CYS
3	D	45	THR
3	D	60	THR
3	D	61	ILE
3	D	67	VAL
3	D	77	ASP
3	D	84	ASN
3	D	102	ARG
3	D	116	LYS
3	D	120	ASP
3	D	122	LEU
3	D	124	LEU
3	D	134	ASP
3	D	147	ARG
3	D	169	LEU
3	D	172	GLN
3	D	180	LEU
3	D	188	VAL
3	D	192	THR
3	D	206	VAL
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	286	GLU
3	D	289	THR
3	D	294	GLU
3	D	298	ARG
3	D	302	LYS
3	D	304	THR
3	D	307	ILE
3	D	308	VAL
3	D	311	LEU
3	D	321	VAL

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Mol	Chain	Res	Type
3	D	326	LEU
3	D	328	VAL
3	D	330	VAL
3	D	333	LEU
3	D	335	GLU
3	D	345	HIS
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	54	LYS
1	E	61	MET
1	E	63	PHE
1	E	77	TRP
1	E	78	ILE
1	E	81	ASP
1	E	84	VAL
1	E	86	LEU
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	151	LEU
1	E	167	LEU
1	E	170	ILE
1	E	172	LEU
1	E	233	ILE
1	E	235	LEU
1	E	238	ILE
1	E	242	ILE
1	E	256	VAL
1	E	263	LEU
1	E	265	TYR
1	E	266	GLN
1	E	292	ILE
1	E	309	LEU

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Mol	Chain	Res	Type
1	E	310	PHE
2	F	7	TYR
2	F	9	ARG
2	F	12	ARG
2	F	37	PHE
2	F	58	ASP
2	F	67	VAL
2	F	77	TYR
2	F	102	LEU
2	F	106	ARG
2	F	161	ARG
2	F	189	VAL
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	10	VAL
3	G	11	VAL
3	G	12	LYS
3	G	33	VAL
3	G	45	THR
3	G	60	THR
3	G	61	ILE
3	G	67	VAL
3	G	84	ASN
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	188	VAL
3	G	192	THR
3	G	206	VAL

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Mol	Chain	Res	Type
3	G	224	LEU
3	G	235	ILE
3	G	246	ARG
3	G	250	ASP
3	G	252	THR
3	G	257	LEU
3	G	268	ARG
3	G	271	THR
3	G	286	GLU
3	G	289	THR
3	G	291	ASP
3	G	298	ARG
3	G	302	LYS
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	348	LEU
3	G	349	THR
3	H	5	VAL
3	H	10	VAL
3	H	11	VAL
3	H	12	LYS
3	H	33	VAL
3	H	41	CYS
3	H	45	THR
3	H	60	THR
3	H	61	ILE
3	H	67	VAL
3	H	77	ASP
3	H	84	ASN
3	H	102	ARG
3	H	116	LYS
3	H	120	ASP
3	H	122	LEU
3	H	124	LEU
3	H	134	ASP

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Mol	Chain	Res	Type
3	H	147	ARG
3	H	169	LEU
3	H	172	GLN
3	H	180	LEU
3	H	188	VAL
3	H	192	THR
3	H	206	VAL
3	H	224	LEU
3	H	235	ILE
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	286	GLU
3	H	289	THR
3	H	294	GLU
3	H	298	ARG
3	H	302	LYS
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	54	LYS
1	I	61	MET

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Mol	Chain	Res	Type
1	I	63	PHE
1	I	77	TRP
1	I	78	ILE
1	I	81	ASP
1	I	84	VAL
1	I	86	LEU
1	I	96	ILE
1	I	97	LYS
1	I	100	LEU
1	I	116	LEU
1	I	151	LEU
1	I	167	LEU
1	I	170	ILE
1	I	172	LEU
1	I	233	ILE
1	I	235	LEU
1	I	238	ILE
1	I	242	ILE
1	I	256	VAL
1	I	263	LEU
1	I	265	TYR
1	I	266	GLN
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	58	ASP
2	J	67	VAL
2	J	77	TYR
2	J	102	LEU
2	J	106	ARG
2	J	161	ARG
2	J	189	VAL
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

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Mol	Chain	Res	Type
2	J	283	THR
3	K	5	VAL
3	K	10	VAL
3	K	11	VAL
3	K	12	LYS
3	K	33	VAL
3	K	45	THR
3	K	60	THR
3	K	61	ILE
3	K	67	VAL
3	K	77	ASP
3	K	84	ASN
3	K	102	ARG
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	188	VAL
3	K	192	THR
3	K	206	VAL
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	286	GLU
3	K	289	THR
3	K	291	ASP
3	K	298	ARG
3	K	302	LYS
3	K	307	ILE
3	K	308	VAL
3	K	311	LEU
3	K	321	VAL
3	K	326	LEU

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Mol	Chain	Res	Type
3	K	328	VAL
3	K	333	LEU
3	K	345	HIS
3	K	348	LEU
3	K	349	THR
3	L	5	VAL
3	L	10	VAL
3	L	11	VAL
3	L	12	LYS
3	L	33	VAL
3	L	41	CYS
3	L	45	THR
3	L	60	THR
3	L	61	ILE
3	L	67	VAL
3	L	77	ASP
3	L	84	ASN
3	L	102	ARG
3	L	120	ASP
3	L	122	LEU
3	L	124	LEU
3	L	134	ASP
3	L	147	ARG
3	L	169	LEU
3	L	172	GLN
3	L	180	LEU
3	L	188	VAL
3	L	192	THR
3	L	206	VAL
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	286	GLU
3	L	289	THR
3	L	294	GLU
3	L	298	ARG

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Mol	Chain	Res	Type
3	L	302	LYS
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
1	M	30	ASP
1	M	38	TYR
1	M	41	LEU
1	M	45	ILE
1	M	54	LYS
1	M	61	MET
1	M	63	PHE
1	M	77	TRP
1	M	78	ILE
1	M	81	ASP
1	M	84	VAL
1	M	86	LEU
1	M	96	ILE
1	M	97	LYS
1	M	100	LEU
1	M	116	LEU
1	M	151	LEU
1	M	167	LEU
1	M	170	ILE
1	M	172	LEU
1	M	233	ILE
1	M	235	LEU
1	M	238	ILE
1	M	242	ILE
1	M	256	VAL
1	M	263	LEU

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Mol	Chain	Res	Type
1	M	265	TYR
1	M	266	GLN
1	M	292	ILE
1	M	309	LEU
1	M	320	LYS
2	N	12	ARG
2	N	37	PHE
2	N	58	ASP
2	N	67	VAL
2	N	77	TYR
2	N	102	LEU
2	N	106	ARG
2	N	161	ARG
2	N	189	VAL
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	10	VAL
3	O	11	VAL
3	O	12	LYS
3	O	33	VAL
3	O	45	THR
3	O	60	THR
3	O	61	ILE
3	O	67	VAL
3	O	77	ASP
3	O	84	ASN
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	188	VAL

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Mol	Chain	Res	Type
3	O	192	THR
3	O	206	VAL
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	286	GLU
3	O	289	THR
3	O	291	ASP
3	O	298	ARG
3	O	302	LYS
3	O	307	ILE
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	348	LEU
3	O	349	THR
3	P	5	VAL
3	P	10	VAL
3	P	11	VAL
3	P	12	LYS
3	P	33	VAL
3	P	41	CYS
3	P	45	THR
3	P	60	THR
3	P	61	ILE
3	P	67	VAL
3	P	77	ASP
3	P	84	ASN
3	P	102	ARG
3	P	116	LYS
3	P	120	ASP
3	P	122	LEU
3	P	124	LEU

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Mol	Chain	Res	Type
3	P	134	ASP
3	P	147	ARG
3	P	169	LEU
3	P	172	GLN
3	P	180	LEU
3	P	188	VAL
3	P	192	THR
3	P	206	VAL
3	P	224	LEU
3	P	229	THR
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	286	GLU
3	P	289	THR
3	P	294	GLU
3	P	298	ARG
3	P	302	LYS
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 (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN

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Mol	Chain	Res	Type
2	B	181	ASN
2	B	279	GLN
3	C	8	GLN
3	C	9	ASN
3	C	182	GLN
3	C	357	GLN
3	D	21	HIS
3	D	182	GLN
3	D	345	HIS
3	D	357	GLN
3	D	359	GLN
1	E	65	GLN
2	F	181	ASN
2	F	279	GLN
3	G	21	HIS
3	G	90	HIS
3	G	182	GLN
3	G	357	GLN
3	H	21	HIS
3	H	182	GLN
3	H	272	HIS
3	H	345	HIS
3	H	359	GLN
1	I	65	GLN
2	J	279	GLN
3	K	182	GLN
3	K	357	GLN
3	L	21	HIS
3	L	90	HIS
3	L	182	GLN
3	L	345	HIS
3	L	357	GLN
3	L	359	GLN
1	M	65	GLN
1	M	220	GLN
2	N	181	ASN
2	N	279	GLN
3	O	21	HIS
3	O	90	HIS
3	O	160	GLN
3	O	182	GLN
3	O	193	HIS

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Mol	Chain	Res	Type
3	O	357	GLN
3	P	21	HIS
3	P	90	HIS
3	P	345	HIS
3	P	359	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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%)	0.00	11 (3%)	44	37	45, 123, 232, 396	0
1	E	286/301 (95%)	-0.04	10 (3%)	47	38	72, 144, 245, 389	0
1	I	286/301 (95%)	0.07	9 (3%)	51	40	63, 110, 236, 381	0
1	M	286/301 (95%)	0.01	10 (3%)	47	38	63, 137, 231, 308	0
2	B	284/305 (93%)	0.11	15 (5%)	32	30	40, 135, 260, 432	0
2	F	280/305 (91%)	0.21	20 (7%)	22	24	74, 138, 252, 482	0
2	J	284/305 (93%)	0.11	18 (6%)	26	27	64, 129, 253, 401	0
2	N	284/305 (93%)	0.08	14 (4%)	35	32	50, 112, 244, 387	0
3	C	363/363 (100%)	0.17	18 (4%)	34	31	44, 179, 275, 344	0
3	D	363/363 (100%)	0.27	24 (6%)	24	26	72, 187, 302, 373	0
3	G	363/363 (100%)	0.21	17 (4%)	36	33	70, 160, 285, 349	0
3	H	363/363 (100%)	0.21	21 (5%)	29	29	46, 146, 267, 367	0
3	K	363/363 (100%)	0.09	10 (2%)	55	43	47, 156, 263, 338	0
3	L	363/363 (100%)	0.08	15 (4%)	41	36	69, 154, 276, 340	0
3	O	363/363 (100%)	0.23	15 (4%)	41	36	65, 198, 291, 376	0
3	P	363/363 (100%)	0.13	14 (3%)	43	37	57, 162, 279, 355	0
All	All	5180/5328 (97%)	0.13	241 (4%)	36	33	40, 151, 275, 482	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	4	THR	8.0
2	B	278	VAL	7.2
3	O	237	SER	7.0
2	J	239	LEU	7.0
3	K	86	ALA	6.9

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Mol	Chain	Res	Type	RSRZ
3	L	203	ASP	6.2
1	I	214	ALA	5.8
2	J	180	ALA	5.8
1	A	213	PRO	5.6
2	J	278	VAL	5.5
3	D	53	LEU	5.4
2	F	243	GLU	5.3
2	J	236	ILE	5.2
3	D	208	MET	4.9
3	C	283	ILE	4.8
2	J	68	LEU	4.7
3	O	288	VAL	4.7
3	D	212	LEU	4.7
3	H	242	LEU	4.6
2	J	152	CYS	4.5
3	D	137	GLY	4.5
3	G	267	PRO	4.4
3	O	311	LEU	4.4
3	C	239	PRO	4.2
2	F	235	THR	4.2
3	P	86	ALA	4.2
3	O	281	PHE	4.1
1	M	199	PHE	4.1
3	C	282	GLY	4.1
3	P	53	LEU	4.0
2	B	274	VAL	3.9
2	N	278	VAL	3.9
3	G	329	LYS	3.9
2	B	176	ARG	3.8
2	J	237	VAL	3.8
2	J	274	VAL	3.7
1	I	159	SER	3.7
3	H	23	VAL	3.6
1	E	128	GLY	3.6
2	F	234	LYS	3.6
3	P	156	PHE	3.6
3	G	165	LEU	3.5
2	F	22	LEU	3.5
3	D	211	GLY	3.5
3	D	261	ASN	3.5
3	K	82	PHE	3.4
1	M	264	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	259	GLU	3.4
2	N	237	VAL	3.4
3	C	51	ALA	3.3
1	A	211	ILE	3.3
2	F	155	PHE	3.3
1	I	200	ASP	3.3
3	O	283	ILE	3.3
3	H	215	GLN	3.3
3	L	32	PHE	3.3
2	F	240	ASN	3.2
3	G	344	LEU	3.2
3	D	351	VAL	3.2
1	M	318	ILE	3.2
2	F	233	LYS	3.2
3	G	80	MET	3.2
2	B	280	LYS	3.1
1	A	41	LEU	3.1
2	N	213	TYR	3.1
1	A	65	GLN	3.1
3	L	53	LEU	3.1
3	L	86	ALA	3.0
1	I	258	PHE	3.0
3	L	101	LEU	3.0
3	D	85	TYR	3.0
2	B	102	LEU	3.0
2	N	239	LEU	2.9
3	D	260	GLY	2.9
2	N	243	GLU	2.9
3	C	237	SER	2.9
3	L	98	SER	2.9
2	N	5	PRO	2.9
3	G	82	PHE	2.9
3	K	53	LEU	2.9
2	J	69	HIS	2.8
3	H	108	LYS	2.8
3	L	232	ALA	2.8
3	L	45	THR	2.8
3	O	55	GLU	2.8
2	F	241	VAL	2.8
1	I	217	GLU	2.8
2	B	180	ALA	2.8
2	F	239	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	G	162	LEU	2.8
1	I	122	ASN	2.8
3	D	348	LEU	2.8
3	H	147	ARG	2.7
3	O	308	VAL	2.7
1	E	127	LYS	2.7
1	A	217	GLU	2.7
3	O	257	LEU	2.7
3	O	82	PHE	2.7
3	K	80	MET	2.7
3	G	40	GLY	2.7
2	N	282	PHE	2.7
3	P	80	MET	2.7
1	E	172	LEU	2.7
3	K	201	LEU	2.7
2	J	235	THR	2.7
2	N	61	PHE	2.7
3	H	281	PHE	2.7
1	E	284	GLY	2.7
3	C	79	ALA	2.7
3	K	39	SER	2.7
3	H	79	ALA	2.7
3	P	199	MET	2.6
3	P	178	LYS	2.6
2	J	153	ASN	2.6
2	J	173	GLU	2.6
1	I	277	SER	2.6
3	L	109	SER	2.6
3	H	308	VAL	2.6
3	O	162	LEU	2.6
3	G	98	SER	2.6
1	E	257	GLY	2.5
2	N	219	LEU	2.5
3	G	50	VAL	2.5
3	H	91	LEU	2.5
3	P	147	ARG	2.5
2	F	92	LEU	2.5
1	A	300	ASN	2.5
1	E	244	VAL	2.5
2	B	253	SER	2.5
3	C	44	SER	2.5
3	D	86	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	K	333	LEU	2.4
2	N	173	GLU	2.4
3	P	237	SER	2.4
3	D	164	ASN	2.4
3	D	46	THR	2.4
3	D	165	LEU	2.4
3	H	255	VAL	2.4
3	D	144	ALA	2.4
3	O	346	VAL	2.4
3	G	301	ILE	2.4
3	H	346	VAL	2.4
3	D	140	ARG	2.3
3	D	84	ASN	2.3
3	D	45	THR	2.3
2	J	260	VAL	2.3
2	B	256	MET	2.3
2	F	205	CYS	2.3
3	C	21	HIS	2.3
1	M	143	ILE	2.3
3	L	192	THR	2.3
3	H	263	ILE	2.3
1	A	212	ASN	2.3
2	F	96	VAL	2.3
3	D	293	VAL	2.3
1	I	319	THR	2.3
3	C	234	PHE	2.3
3	C	281	PHE	2.3
1	M	145	ILE	2.3
3	H	244	PRO	2.3
2	B	277	VAL	2.3
2	B	121	MET	2.3
3	C	174	ARG	2.3
2	F	180	ALA	2.3
2	F	238	ASP	2.3
2	N	246	ALA	2.3
3	H	245	ALA	2.3
3	H	296	SER	2.3
1	A	29	LYS	2.3
3	D	42	GLY	2.3
3	P	217	GLY	2.3
3	H	143	VAL	2.3
2	F	266	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	146	VAL	2.2
3	L	83	GLN	2.2
3	D	263	ILE	2.2
3	H	24	SER	2.2
2	F	227	PRO	2.2
3	H	299	ALA	2.2
3	P	1	MET	2.2
1	E	89	SER	2.2
3	D	302	LYS	2.2
3	K	40	GLY	2.2
2	B	158	ILE	2.2
1	E	167	LEU	2.2
2	B	147	LEU	2.2
2	F	127	MET	2.2
1	A	155	PHE	2.2
3	O	229	THR	2.2
2	J	281	TYR	2.2
2	B	172	GLU	2.2
3	G	129	GLU	2.2
2	J	74	TRP	2.2
3	P	79	ALA	2.1
2	B	82	PHE	2.1
3	G	111	ILE	2.1
3	L	252	THR	2.1
3	C	199	MET	2.1
2	N	215	TRP	2.1
1	A	159	SER	2.1
3	H	208	MET	2.1
2	J	118	ALA	2.1
3	C	260	GLY	2.1
3	G	101	LEU	2.1
3	H	213	ILE	2.1
3	L	147	ARG	2.1
3	O	313	SER	2.1
1	M	149	ALA	2.1
2	F	246	ALA	2.1
2	J	172	GLU	2.1
3	G	3	ALA	2.1
1	I	242	ILE	2.1
1	M	37	LEU	2.1
3	G	285	PRO	2.1
3	O	301	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	238	ASP	2.1
3	P	41	CYS	2.1
2	F	262	ALA	2.1
3	C	302	LYS	2.1
3	G	316	ILE	2.1
3	H	310	PRO	2.1
3	C	150	VAL	2.1
1	M	125	TYR	2.1
3	D	35	LEU	2.1
3	K	88	TYR	2.1
2	J	212	GLY	2.1
1	E	315	SER	2.1
2	B	260	VAL	2.1
3	C	127	LEU	2.0
1	A	62	ALA	2.0
3	C	252	THR	2.0
3	L	84	ASN	2.0
3	D	240	MET	2.0
3	C	53	LEU	2.0
3	K	46	THR	2.0
3	O	109	SER	2.0
3	P	170	ARG	2.0
1	M	178	LEU	2.0
3	L	325	SER	2.0
3	P	233	SER	2.0
2	F	131	PHE	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 oligosaccharides 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.