



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:50 AM UTC

PDB ID : 3FOK / pdb_00003fok
Title : Crystal Structure of Cgl0159 From *Corynebacterium glutamicum* (*Brevibacterium flavum*). Northeast Structural Genomics Target CgR115
Authors : Seetharaman, J.; Neely, H.; Wang, H.; Janjua, H.; Foote, E.L.; Xiao, R.; Everett, J.K.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-12-30
Resolution : 2.50 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:

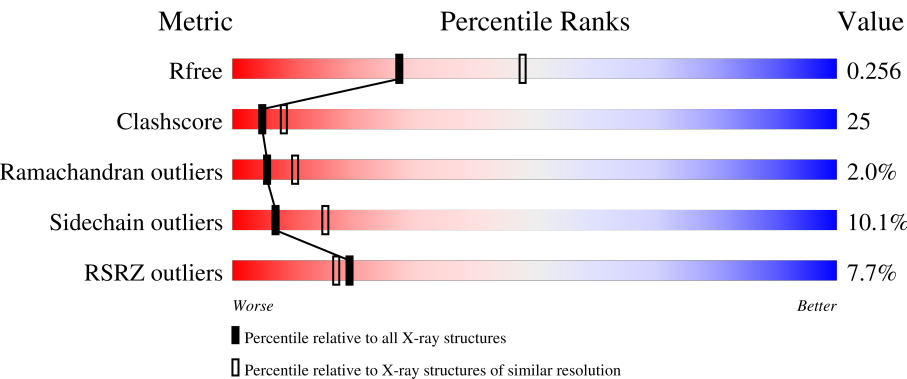
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	307	6% 61% 28% 7% .
1	B	307	7% 63% 26% 7% .
1	C	307	7% 59% 29% 7% .
1	D	307	9% 62% 26% 7% .

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Mol	Chain	Length	Quality of chain			
1	E	307	7% 63% 26% 7%			
1	F	307	6% 62% 27% 7%			
1	G	307	7% 62% 26% 7%			
1	H	307	9% 61% 29% 7%			
1	I	307	6% 61% 27% 8%			
1	J	307	7% 59% 30% 7%			

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22795 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 uncharacterized protein Cgl0159.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	Se	0	0	0
			2208	1379	387	429	13			
1	B	295	Total	C	N	O	Se	0	0	0
			2208	1379	387	429	13			
1	C	295	Total	C	N	O	Se	0	0	0
			2208	1379	387	429	13			
1	D	295	Total	C	N	O	Se	0	0	0
			2208	1379	387	429	13			
1	E	295	Total	C	N	O	Se	0	0	0
			2208	1379	387	429	13			
1	F	295	Total	C	N	O	Se	0	0	0
			2208	1379	387	429	13			
1	G	295	Total	C	N	O	Se	0	0	0
			2208	1379	387	429	13			
1	H	295	Total	C	N	O	Se	0	0	0
			2208	1379	387	429	13			
1	I	295	Total	C	N	O	Se	0	0	0
			2208	1379	387	429	13			
1	J	295	Total	C	N	O	Se	0	0	0
			2208	1379	387	429	13			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	72	Total	O	0	0
			72	72		
2	B	90	Total	O	0	0
			90	90		
2	C	77	Total	O	0	0
			77	77		
2	D	95	Total	O	0	0
			95	95		

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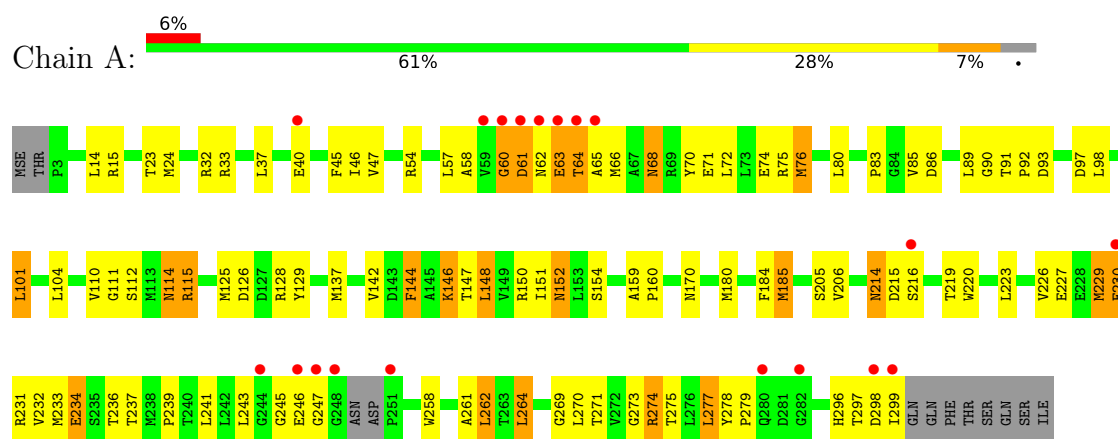
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	79	Total 79	O 79	0	0
2	F	62	Total 62	O 62	0	0
2	G	66	Total 66	O 66	0	0
2	H	74	Total 74	O 74	0	0
2	I	47	Total 47	O 47	0	0
2	J	53	Total 53	O 53	0	0

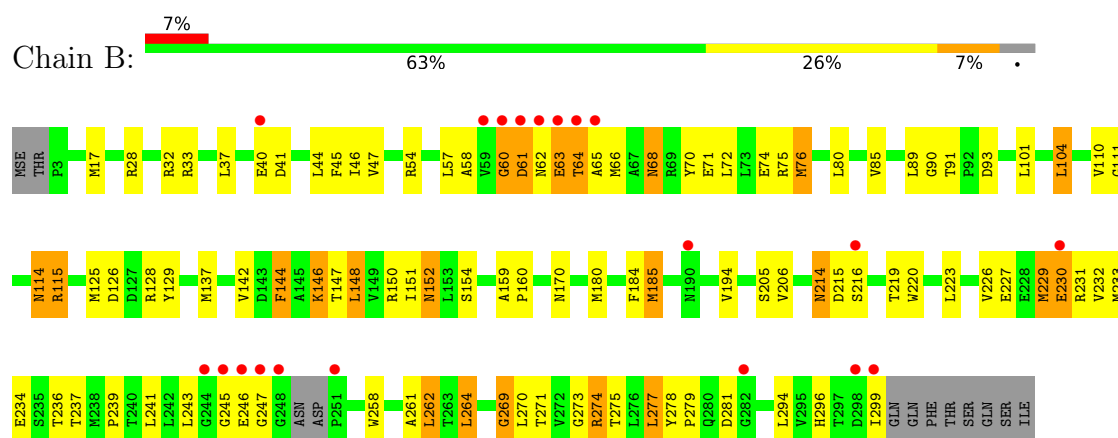
3 Residue-property plots [i](#)

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

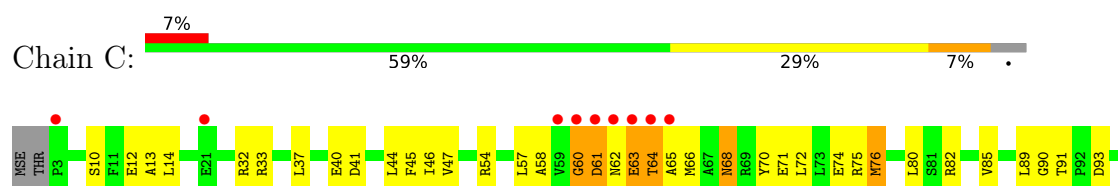
• Molecule 1: uncharacterized protein Cgl0159

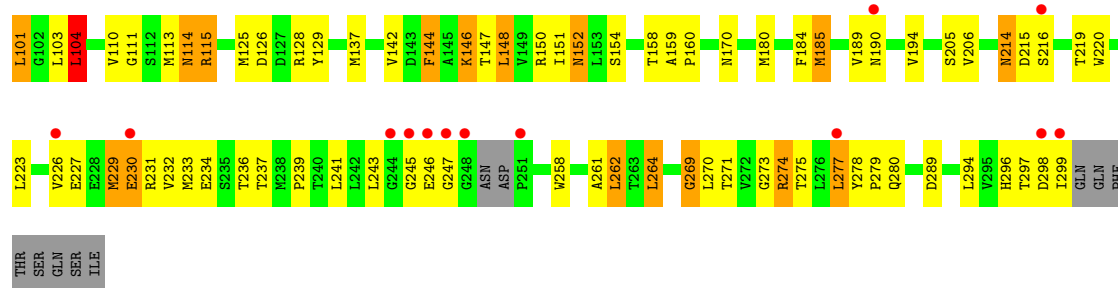


• Molecule 1: uncharacterized protein Cgl0159

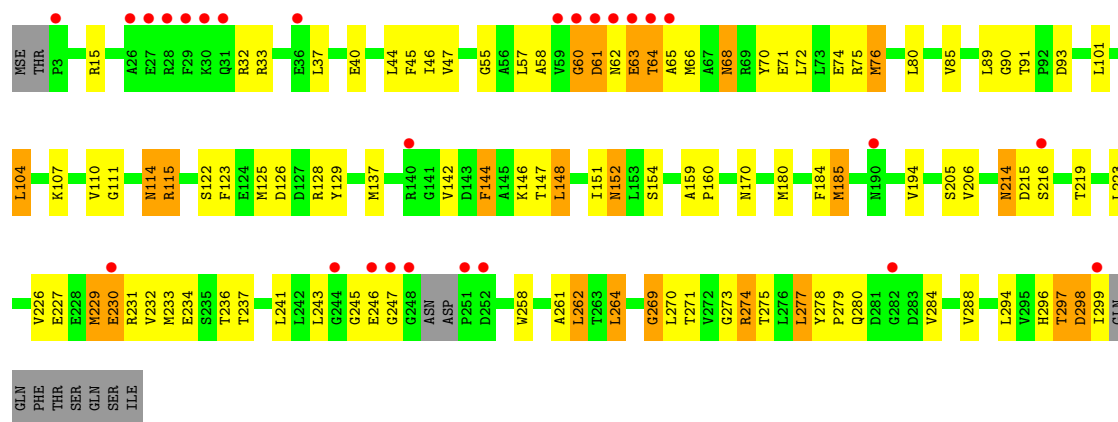


• Molecule 1: uncharacterized protein Cgl0159

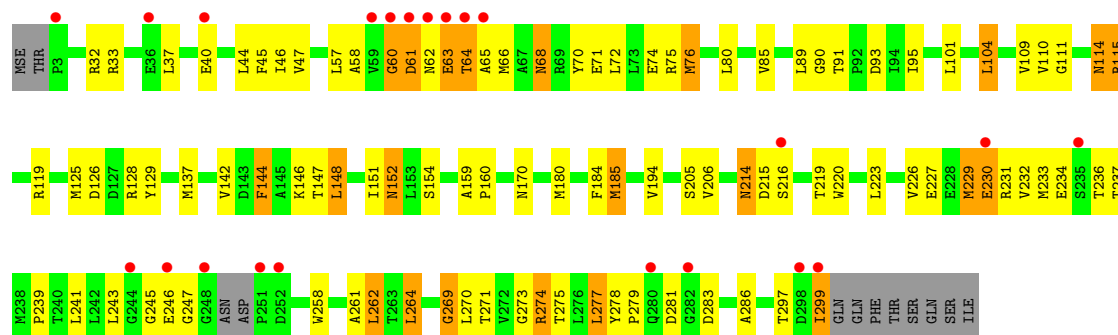




• Molecule 1: uncharacterized protein Cgl0159

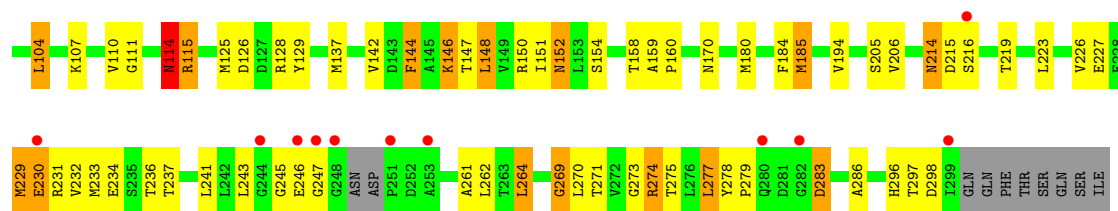


• Molecule 1: uncharacterized protein Cgl0159

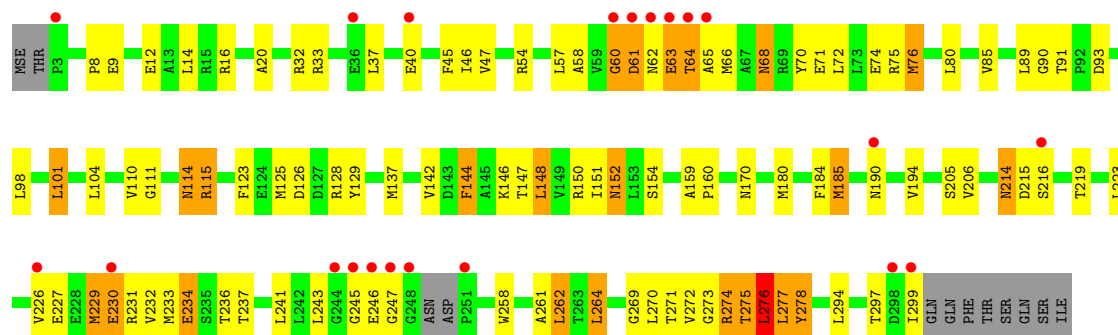


• Molecule 1: uncharacterized protein Cgl0159

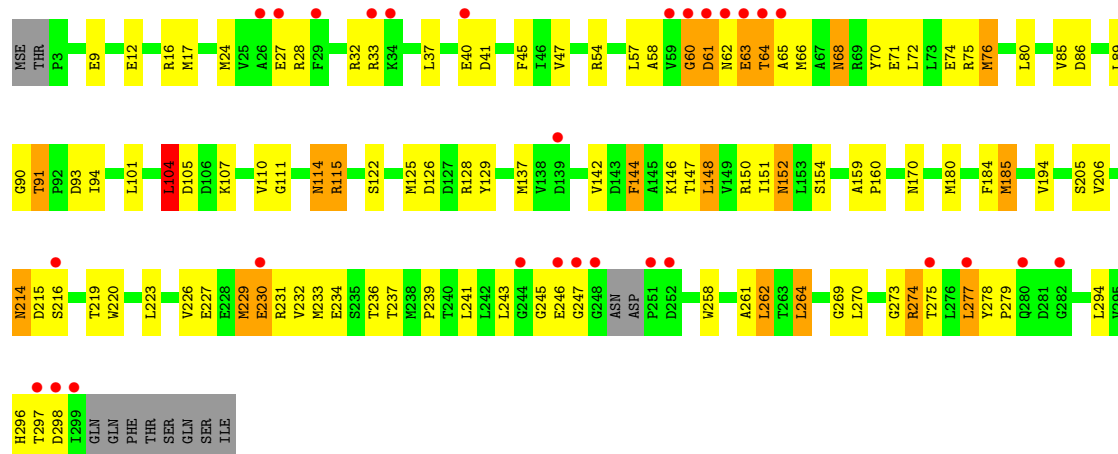




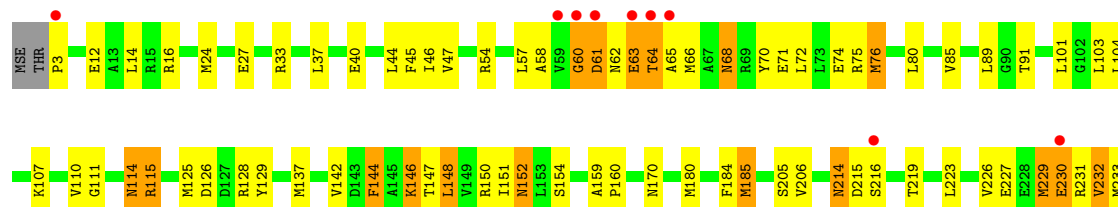
• Molecule 1: uncharacterized protein Cgl0159

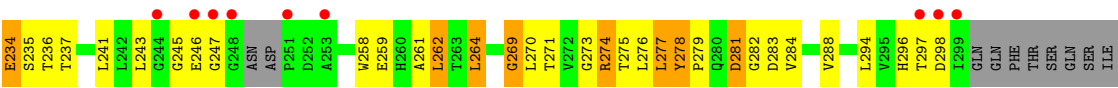


• Molecule 1: uncharacterized protein Cgl0159

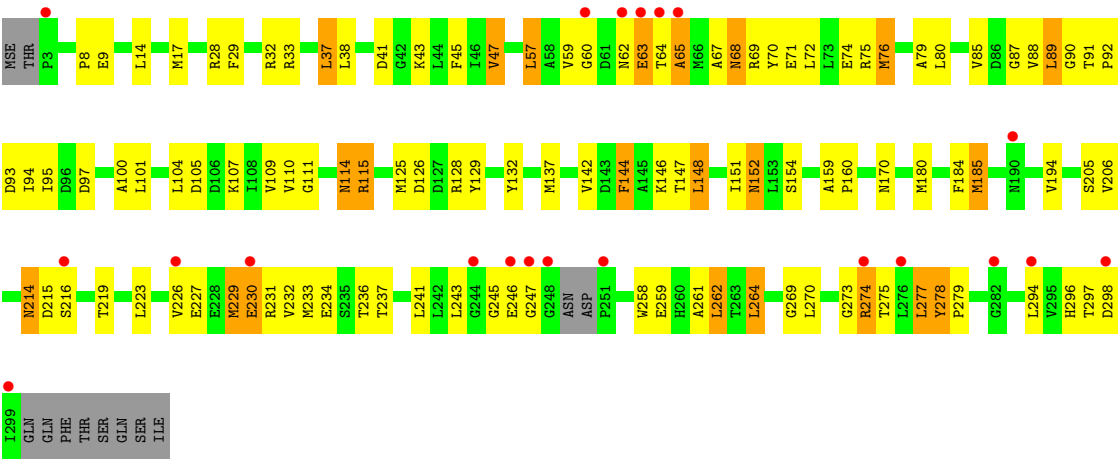


• Molecule 1: uncharacterized protein Cgl0159





● Molecule 1: uncharacterized protein Cgl0159



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.00Å 176.21Å 104.24Å 90.00° 101.94° 90.00°	Depositor
Resolution (Å)	39.00 – 2.50 39.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.9 (39.00-2.50) 95.2 (39.00-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.225 , 0.254 0.228 , 0.256	Depositor DCC
R_{free} test set	9931 reflections (3.88%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22795	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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	0.38	0/2230	1.01	12/3005 (0.4%)
1	B	0.39	0/2230	1.01	11/3005 (0.4%)
1	C	0.39	0/2230	1.02	12/3005 (0.4%)
1	D	0.39	0/2230	1.01	11/3005 (0.4%)
1	E	0.38	0/2230	1.01	11/3005 (0.4%)
1	F	0.37	0/2230	1.01	13/3005 (0.4%)
1	G	0.70	11/2230 (0.5%)	1.03	14/3005 (0.5%)
1	H	0.39	0/2230	1.01	12/3005 (0.4%)
1	I	0.54	3/2230 (0.1%)	1.03	12/3005 (0.4%)
1	J	0.61	8/2230 (0.4%)	1.02	11/3005 (0.4%)
All	All	0.47	22/22300 (0.1%)	1.01	119/30050 (0.4%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	276	LEU	C-O	-9.29	1.11	1.24
1	G	277	LEU	CA-C	-9.20	1.41	1.52
1	G	277	LEU	CG-CD2	-8.93	1.23	1.52
1	J	278	TYR	CD1-CE1	-8.48	1.13	1.38
1	J	278	TYR	C-O	-8.38	1.13	1.24
1	G	277	LEU	N-CA	-7.99	1.36	1.46
1	J	278	TYR	CD2-CE2	-7.96	1.14	1.38
1	I	277	LEU	N-CA	-7.37	1.36	1.46
1	J	277	LEU	CG-CD1	-7.35	1.28	1.52
1	J	278	TYR	CG-CD1	-7.21	1.24	1.39
1	G	277	LEU	CG-CD1	-6.91	1.29	1.52
1	G	278	TYR	CD1-CE1	-6.90	1.18	1.38
1	G	276	LEU	N-CA	-6.42	1.37	1.46
1	G	276	LEU	CG-CD2	-6.30	1.31	1.52
1	G	278	TYR	CD2-CE2	-6.25	1.20	1.38
1	J	277	LEU	CG-CD2	-6.04	1.32	1.52
1	I	276	LEU	C-N	-5.87	1.25	1.33
1	G	278	TYR	C-O	-5.77	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	278	TYR	CG-CD1	-5.72	1.27	1.39
1	G	278	TYR	CB-CG	-5.20	1.40	1.51
1	J	278	TYR	CE2-CZ	-5.14	1.25	1.38
1	J	278	TYR	CE1-CZ	-5.01	1.26	1.38

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	277	LEU	N-CA-C	-8.91	94.99	109.96
1	E	277	LEU	N-CA-C	-8.37	98.13	110.52
1	D	277	LEU	N-CA-C	-8.33	95.96	109.96
1	C	277	LEU	N-CA-C	-7.99	97.62	110.32
1	C	185	MSE	N-CA-C	-7.69	96.71	109.24
1	A	185	MSE	N-CA-C	-7.67	96.73	109.24
1	G	185	MSE	N-CA-C	-7.64	96.78	109.24
1	J	185	MSE	N-CA-C	-7.63	96.80	109.24
1	H	185	MSE	N-CA-C	-7.62	96.82	109.24
1	I	185	MSE	N-CA-C	-7.62	96.83	109.24
1	D	185	MSE	N-CA-C	-7.60	96.85	109.24
1	F	185	MSE	N-CA-C	-7.58	96.89	109.24
1	E	185	MSE	N-CA-C	-7.57	96.90	109.24
1	B	185	MSE	N-CA-C	-7.55	96.93	109.24
1	G	230	GLU	N-CA-C	-7.43	104.06	113.72
1	I	230	GLU	N-CA-C	-7.40	104.10	113.72
1	A	229	MSE	N-CA-C	7.39	121.98	113.19
1	E	229	MSE	N-CA-C	7.38	121.97	113.19
1	J	229	MSE	N-CA-C	7.37	121.96	113.19
1	E	230	GLU	N-CA-C	-7.36	104.15	113.72
1	D	230	GLU	N-CA-C	-7.34	104.18	113.72
1	D	229	MSE	N-CA-C	7.34	121.92	113.19
1	F	230	GLU	N-CA-C	-7.32	104.20	113.72
1	C	229	MSE	N-CA-C	7.30	121.88	113.19
1	F	229	MSE	N-CA-C	7.30	121.88	113.19
1	C	230	GLU	N-CA-C	-7.29	104.24	113.72
1	B	230	GLU	N-CA-C	-7.29	104.24	113.72
1	H	230	GLU	N-CA-C	-7.29	104.25	113.72
1	J	230	GLU	N-CA-C	-7.28	104.26	113.72
1	G	277	LEU	N-CA-C	-7.26	97.84	109.76
1	B	229	MSE	N-CA-C	7.26	121.82	113.19
1	H	229	MSE	N-CA-C	7.24	121.80	113.19
1	G	229	MSE	N-CA-C	7.23	121.80	113.19
1	A	230	GLU	N-CA-C	-7.23	104.32	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	229	MSE	N-CA-C	7.20	121.76	113.19
1	C	275	THR	N-CA-C	7.19	119.20	111.36
1	J	277	LEU	N-CA-C	-7.03	99.14	110.32
1	B	277	LEU	N-CA-C	-6.86	98.08	109.46
1	F	275	THR	N-CA-C	6.81	118.79	111.36
1	G	275	THR	N-CA-C	6.68	118.65	111.36
1	D	275	THR	N-CA-C	6.58	118.53	111.36
1	F	277	LEU	N-CA-C	-6.51	99.97	110.32
1	I	275	THR	N-CA-C	6.49	118.44	111.36
1	A	277	LEU	N-CA-C	-6.34	99.37	109.76
1	J	87	GLY	N-CA-C	6.28	119.65	110.80
1	H	104	LEU	N-CA-C	6.27	120.63	112.92
1	E	58	ALA	N-CA-C	6.26	119.01	110.55
1	C	58	ALA	N-CA-C	6.24	118.97	110.55
1	D	58	ALA	N-CA-C	6.23	118.96	110.55
1	A	58	ALA	N-CA-C	6.18	118.90	110.55
1	B	58	ALA	N-CA-C	6.17	118.88	110.55
1	G	58	ALA	N-CA-C	6.14	118.84	110.55
1	C	104	LEU	N-CA-C	6.13	119.71	112.72
1	E	275	THR	N-CA-C	6.12	118.03	111.36
1	F	58	ALA	N-CA-C	6.12	118.81	110.55
1	J	275	THR	N-CA-C	6.08	117.98	111.36
1	H	58	ALA	N-CA-C	6.06	118.74	110.55
1	B	275	THR	N-CA-C	6.04	117.95	111.36
1	H	277	LEU	N-CA-C	-6.03	101.55	110.48
1	J	278	TYR	N-CA-C	6.01	123.10	109.81
1	I	58	ALA	N-CA-C	6.01	118.66	110.55
1	G	231	ARG	N-CA-C	-5.99	106.10	113.41
1	D	231	ARG	N-CA-C	-5.98	106.12	113.41
1	J	231	ARG	N-CA-C	-5.96	106.14	113.41
1	E	231	ARG	N-CA-C	-5.96	106.14	113.41
1	C	231	ARG	N-CA-C	-5.93	106.17	113.41
1	B	231	ARG	N-CA-C	-5.92	106.18	113.41
1	I	231	ARG	N-CA-C	-5.90	106.21	113.41
1	F	231	ARG	N-CA-C	-5.90	106.21	113.41
1	H	231	ARG	N-CA-C	-5.89	106.22	113.41
1	A	231	ARG	N-CA-C	-5.85	106.27	113.41
1	A	275	THR	N-CA-C	5.79	117.67	111.36
1	G	269	GLY	N-CA-C	5.64	117.50	110.29
1	H	275	THR	N-CA-C	5.62	117.49	111.36
1	F	269	GLY	N-CA-C	5.60	117.45	110.29
1	H	269	GLY	N-CA-C	5.58	117.42	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	269	GLY	N-CA-C	5.56	117.41	110.29
1	B	269	GLY	N-CA-C	5.53	117.37	110.29
1	G	20	ALA	N-CA-C	5.52	120.13	112.90
1	A	269	GLY	N-CA-C	5.51	117.35	110.29
1	E	237	THR	N-CA-C	-5.51	105.92	113.30
1	F	237	THR	N-CA-C	-5.50	105.92	113.30
1	J	237	THR	N-CA-C	-5.49	105.95	113.30
1	C	269	GLY	N-CA-C	5.48	117.31	110.29
1	I	269	GLY	N-CA-C	5.47	117.30	110.29
1	J	232	VAL	N-CA-C	-5.47	105.20	110.72
1	B	237	THR	N-CA-C	-5.45	105.99	113.30
1	C	232	VAL	N-CA-C	-5.44	105.22	110.72
1	E	232	VAL	N-CA-C	-5.42	105.25	110.72
1	I	237	THR	N-CA-C	-5.40	106.07	113.30
1	F	232	VAL	N-CA-C	-5.39	105.27	110.72
1	H	232	VAL	N-CA-C	-5.39	105.28	110.72
1	J	269	GLY	N-CA-C	5.37	117.17	110.29
1	D	232	VAL	N-CA-C	-5.37	105.30	110.72
1	H	237	THR	N-CA-C	-5.36	106.12	113.30
1	C	237	THR	N-CA-C	-5.36	106.12	113.30
1	E	269	GLY	N-CA-C	5.35	117.14	110.29
1	D	237	THR	N-CA-C	-5.34	106.15	113.30
1	A	237	THR	N-CA-C	-5.33	106.16	113.30
1	B	232	VAL	N-CA-C	-5.33	105.34	110.72
1	I	232	VAL	N-CA-C	-5.30	105.36	110.72
1	F	60	GLY	N-CA-C	-5.30	100.61	113.18
1	H	60	GLY	N-CA-C	-5.30	100.61	113.18
1	G	237	THR	N-CA-C	-5.30	106.19	113.30
1	A	232	VAL	N-CA-C	-5.30	105.37	110.72
1	F	114	ASN	N-CA-C	5.29	117.53	108.90
1	B	60	GLY	N-CA-C	-5.29	100.64	113.18
1	E	60	GLY	N-CA-C	-5.28	100.67	113.18
1	I	60	GLY	N-CA-C	-5.27	100.69	113.18
1	A	60	GLY	N-CA-C	-5.25	100.75	113.18
1	C	60	GLY	N-CA-C	-5.23	100.79	113.18
1	D	60	GLY	N-CA-C	-5.21	100.83	113.18
1	G	60	GLY	N-CA-C	-5.21	100.83	113.18
1	I	234	GLU	N-CA-C	-5.15	106.84	113.02
1	G	232	VAL	N-CA-C	-5.13	105.54	110.72
1	F	19	ALA	N-CA-C	5.10	117.62	111.40
1	G	278	TYR	N-CA-C	5.08	121.04	109.81
1	A	234	GLU	N-CA-C	-5.08	107.11	113.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	234	GLU	N-CA-C	-5.00	107.01	113.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2208	0	2202	111	0
1	B	2208	0	2202	110	0
1	C	2208	0	2202	121	0
1	D	2208	0	2202	115	0
1	E	2208	0	2202	106	0
1	F	2208	0	2202	110	0
1	G	2208	0	2202	116	0
1	H	2208	0	2202	108	0
1	I	2208	0	2202	111	0
1	J	2208	0	2202	114	0
2	A	72	0	0	4	0
2	B	90	0	0	1	0
2	C	77	0	0	4	0
2	D	95	0	0	3	0
2	E	79	0	0	2	0
2	F	62	0	0	4	0
2	G	66	0	0	6	0
2	H	74	0	0	2	0
2	I	47	0	0	2	0
2	J	53	0	0	1	0
All	All	22795	0	22020	1112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (1112) 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:J:76:MSE:CE	1:J:277:LEU:HD21	1.71	1.20
1:C:137:MSE:HE2	1:C:142:VAL:HG21	1.20	1.16
1:F:137:MSE:HE2	1:F:142:VAL:HG21	1.22	1.15
1:A:137:MSE:HE2	1:A:142:VAL:HG21	1.22	1.14
1:J:137:MSE:HE2	1:J:142:VAL:HG21	1.23	1.12
1:G:137:MSE:HE2	1:G:142:VAL:HG21	1.22	1.11
1:I:137:MSE:HE2	1:I:142:VAL:HG21	1.23	1.11
1:D:137:MSE:HE2	1:D:142:VAL:HG21	1.23	1.11
1:B:137:MSE:HE2	1:B:142:VAL:HG21	1.21	1.10
1:H:137:MSE:HE2	1:H:142:VAL:HG21	1.21	1.10
1:E:137:MSE:HE2	1:E:142:VAL:HG21	1.22	1.09
1:C:190:ASN:OD1	1:H:122:SER:HA	1.54	1.08
1:J:76:MSE:HE3	1:J:277:LEU:HD21	1.39	0.99
1:J:76:MSE:HE2	1:J:277:LEU:HD21	1.47	0.94
1:C:190:ASN:OD1	1:H:122:SER:CA	2.19	0.90
1:C:111:GLY:HA3	1:C:137:MSE:HE3	1.52	0.90
1:C:189:VAL:HG12	1:C:190:ASN:ND2	1.86	0.90
1:J:114:ASN:HD22	1:J:114:ASN:H	1.20	0.89
1:E:111:GLY:HA3	1:E:137:MSE:HE3	1.54	0.89
1:I:76:MSE:HE3	1:I:277:LEU:HD21	1.56	0.88
1:J:68:ASN:C	1:J:68:ASN:HD22	1.83	0.87
1:A:111:GLY:HA3	1:A:137:MSE:HE3	1.56	0.87
1:G:76:MSE:HE2	1:G:76:MSE:HA	1.57	0.86
1:E:76:MSE:HE2	1:E:76:MSE:HA	1.58	0.86
1:A:76:MSE:HA	1:A:76:MSE:HE2	1.58	0.86
1:F:76:MSE:HA	1:F:76:MSE:HE2	1.57	0.86
1:H:76:MSE:HE2	1:H:76:MSE:HA	1.58	0.86
1:C:137:MSE:HE2	1:C:142:VAL:CG2	2.06	0.85
1:I:76:MSE:HE2	1:I:76:MSE:HA	1.57	0.85
1:D:122:SER:HA	1:G:190:ASN:OD1	1.76	0.85
1:C:76:MSE:HE2	1:C:76:MSE:HA	1.58	0.85
1:I:12:GLU:HG3	1:I:16:ARG:HH12	1.40	0.84
1:C:189:VAL:HG12	1:C:190:ASN:HD22	1.41	0.84
1:A:137:MSE:CE	1:A:142:VAL:HG21	2.07	0.84
1:A:114:ASN:HD22	1:A:114:ASN:H	1.24	0.84
1:H:75:ARG:HH21	1:H:278:TYR:HA	1.43	0.83
1:D:76:MSE:HA	1:D:76:MSE:HE2	1.58	0.83
1:E:137:MSE:HE2	1:E:142:VAL:CG2	2.07	0.83
1:B:137:MSE:CE	1:B:142:VAL:HG21	2.07	0.83
1:A:223:LEU:HD12	1:A:233:MSE:HE1	1.61	0.83
1:F:137:MSE:HE2	1:F:142:VAL:CG2	2.08	0.83
1:G:137:MSE:HE2	1:G:142:VAL:CG2	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:MSE:HE2	1:B:142:VAL:CG2	2.07	0.83
1:B:76:MSE:HE2	1:B:76:MSE:HA	1.57	0.82
1:H:137:MSE:HE2	1:H:142:VAL:CG2	2.07	0.82
1:B:223:LEU:HD12	1:B:233:MSE:HE1	1.61	0.82
1:I:137:MSE:HE2	1:I:142:VAL:CG2	2.09	0.82
1:B:274:ARG:H	1:B:274:ARG:HE	1.28	0.82
1:F:223:LEU:HD12	1:F:233:MSE:HE1	1.62	0.82
1:E:223:LEU:HD12	1:E:233:MSE:HE1	1.62	0.82
1:A:151:ILE:HD12	1:A:185:MSE:HE1	1.61	0.82
1:F:274:ARG:H	1:F:274:ARG:HE	1.27	0.82
1:G:111:GLY:HA3	1:G:137:MSE:HE3	1.62	0.82
1:I:137:MSE:CE	1:I:142:VAL:HG21	2.08	0.81
1:I:274:ARG:H	1:I:274:ARG:HE	1.28	0.81
1:A:137:MSE:HE2	1:A:142:VAL:CG2	2.08	0.81
1:B:114:ASN:H	1:B:114:ASN:HD22	1.28	0.81
1:H:137:MSE:CE	1:H:142:VAL:HG21	2.07	0.81
1:C:151:ILE:HD12	1:C:185:MSE:HE1	1.62	0.81
1:D:223:LEU:HD12	1:D:233:MSE:HE1	1.62	0.81
1:E:151:ILE:HD12	1:E:185:MSE:HE1	1.61	0.81
1:B:151:ILE:HD12	1:B:185:MSE:HE1	1.61	0.81
1:J:63:GLU:HG3	1:J:64:THR:H	1.44	0.81
1:F:151:ILE:HD12	1:F:185:MSE:HE1	1.62	0.81
1:C:137:MSE:CE	1:C:142:VAL:HG21	2.06	0.81
1:D:151:ILE:HD12	1:D:185:MSE:HE1	1.61	0.81
1:G:223:LEU:HD12	1:G:233:MSE:HE1	1.62	0.81
1:H:274:ARG:H	1:H:274:ARG:HE	1.27	0.81
1:G:114:ASN:H	1:G:114:ASN:HD22	1.29	0.81
1:D:274:ARG:H	1:D:274:ARG:HE	1.27	0.81
1:J:137:MSE:HB3	1:J:142:VAL:HG22	1.63	0.81
1:D:137:MSE:CE	1:D:142:VAL:HG21	2.09	0.80
1:F:137:MSE:HB3	1:F:142:VAL:HG22	1.63	0.80
1:C:223:LEU:HD12	1:C:233:MSE:HE1	1.62	0.80
1:F:114:ASN:HD21	1:F:148:LEU:H	1.25	0.80
1:D:137:MSE:HE2	1:D:142:VAL:CG2	2.09	0.80
1:J:274:ARG:H	1:J:274:ARG:HE	1.29	0.80
1:H:223:LEU:HD12	1:H:233:MSE:HE1	1.62	0.80
1:I:114:ASN:H	1:I:114:ASN:HD22	1.29	0.80
1:A:274:ARG:H	1:A:274:ARG:HE	1.27	0.80
1:B:137:MSE:HB3	1:B:142:VAL:HG22	1.63	0.80
1:H:151:ILE:HD12	1:H:185:MSE:HE1	1.61	0.80
1:J:137:MSE:HE2	1:J:142:VAL:CG2	2.09	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:151:ILE:HD12	1:J:185:MSE:HE1	1.62	0.80
1:C:125:MSE:HE2	1:C:152:ASN:HB2	1.64	0.80
1:D:137:MSE:HB3	1:D:142:VAL:HG22	1.64	0.80
1:G:137:MSE:HB3	1:G:142:VAL:HG22	1.63	0.80
1:I:125:MSE:HE2	1:I:152:ASN:HB2	1.63	0.80
1:F:137:MSE:CE	1:F:142:VAL:HG21	2.08	0.79
1:I:151:ILE:HD12	1:I:185:MSE:HE1	1.62	0.79
1:C:114:ASN:HD22	1:C:114:ASN:H	1.29	0.79
1:C:137:MSE:HB3	1:C:142:VAL:HG22	1.65	0.79
1:G:151:ILE:HD12	1:G:185:MSE:HE1	1.62	0.79
1:J:223:LEU:HD12	1:J:233:MSE:HE1	1.62	0.79
1:E:137:MSE:HB3	1:E:142:VAL:HG22	1.63	0.79
1:A:125:MSE:HE2	1:A:152:ASN:HB2	1.63	0.79
1:C:274:ARG:H	1:C:274:ARG:HE	1.27	0.79
1:G:125:MSE:HE2	1:G:152:ASN:HB2	1.64	0.79
1:H:137:MSE:HB3	1:H:142:VAL:HG22	1.63	0.79
1:I:137:MSE:HB3	1:I:142:VAL:HG22	1.64	0.79
1:G:137:MSE:CE	1:G:142:VAL:HG21	2.08	0.79
1:I:223:LEU:HD12	1:I:233:MSE:HE1	1.63	0.79
1:C:14:LEU:HD13	1:C:101:LEU:HD13	1.63	0.79
1:B:111:GLY:HA3	1:B:137:MSE:HE3	1.64	0.79
1:D:125:MSE:HE2	1:D:152:ASN:HB2	1.65	0.79
1:J:137:MSE:CE	1:J:142:VAL:HG21	2.09	0.79
1:F:125:MSE:HE2	1:F:152:ASN:HB2	1.64	0.78
1:J:125:MSE:HE2	1:J:152:ASN:HB2	1.64	0.78
1:H:111:GLY:HA3	1:H:137:MSE:HE3	1.64	0.78
1:H:125:MSE:HE2	1:H:152:ASN:HB2	1.63	0.78
1:J:71:GLU:O	1:J:75:ARG:HG3	1.83	0.78
1:A:137:MSE:HB3	1:A:142:VAL:HG22	1.63	0.78
1:G:274:ARG:H	1:G:274:ARG:HE	1.28	0.78
1:E:274:ARG:H	1:E:274:ARG:HE	1.28	0.77
1:E:137:MSE:CE	1:E:142:VAL:HG21	2.08	0.77
2:I:312:HOH:O	1:J:93:ASP:HA	1.84	0.77
1:A:185:MSE:HE3	1:A:205:SER:CB	2.14	0.77
1:D:114:ASN:H	1:D:114:ASN:HD22	1.32	0.77
1:I:76:MSE:CE	1:I:277:LEU:HD21	2.14	0.77
1:D:110:VAL:HG22	1:D:144:PHE:HB3	1.67	0.76
1:E:111:GLY:HA3	1:E:137:MSE:CE	2.15	0.76
1:E:185:MSE:HE3	1:E:205:SER:CB	2.15	0.76
1:F:111:GLY:HA3	1:F:137:MSE:HE3	1.66	0.76
1:G:114:ASN:HD21	1:G:148:LEU:H	1.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:185:MSE:HE3	1:H:205:SER:CB	2.15	0.76
1:B:125:MSE:HE2	1:B:152:ASN:HB2	1.65	0.76
1:D:32:ARG:HD2	1:D:104:LEU:HB3	1.67	0.76
1:D:114:ASN:HD21	1:D:148:LEU:H	1.32	0.76
1:E:125:MSE:HE2	1:E:152:ASN:HB2	1.65	0.76
1:E:63:GLU:HG3	1:E:64:THR:H	1.51	0.76
1:D:122:SER:CB	1:G:190:ASN:OD1	2.33	0.76
1:J:185:MSE:HE3	1:J:205:SER:CB	2.15	0.76
1:C:185:MSE:HE3	1:C:205:SER:CB	2.15	0.76
1:B:63:GLU:HG3	1:B:64:THR:H	1.51	0.75
1:B:114:ASN:HD21	1:B:148:LEU:H	1.31	0.75
1:H:68:ASN:HD22	1:H:68:ASN:C	1.95	0.75
1:C:68:ASN:HD22	1:C:68:ASN:C	1.94	0.75
1:G:185:MSE:HE3	1:G:205:SER:CB	2.15	0.75
1:F:63:GLU:HG3	1:F:64:THR:H	1.51	0.75
1:B:185:MSE:HE3	1:B:205:SER:CB	2.16	0.75
1:D:185:MSE:HE3	1:D:205:SER:CB	2.15	0.75
1:A:68:ASN:C	1:A:68:ASN:HD22	1.95	0.75
1:I:185:MSE:HE3	1:I:205:SER:CB	2.16	0.75
1:B:76:MSE:HE3	1:B:277:LEU:HD11	1.67	0.75
1:F:68:ASN:C	1:F:68:ASN:HD22	1.94	0.75
1:F:185:MSE:HE3	1:F:205:SER:CB	2.15	0.75
1:I:68:ASN:C	1:I:68:ASN:HD22	1.94	0.75
1:A:111:GLY:HA3	1:A:137:MSE:CE	2.17	0.75
1:D:63:GLU:HG3	1:D:64:THR:H	1.51	0.75
1:D:76:MSE:CE	1:D:277:LEU:HD21	2.17	0.74
1:A:63:GLU:HG3	1:A:64:THR:H	1.51	0.74
1:J:14:LEU:HD22	1:J:101:LEU:HD11	1.70	0.74
1:C:63:GLU:HG3	1:C:64:THR:H	1.52	0.74
1:C:111:GLY:HA3	1:C:137:MSE:CE	2.16	0.74
1:B:68:ASN:C	1:B:68:ASN:HD22	1.96	0.74
1:D:68:ASN:C	1:D:68:ASN:HD22	1.95	0.74
1:E:68:ASN:C	1:E:68:ASN:HD22	1.95	0.74
1:G:68:ASN:C	1:G:68:ASN:HD22	1.95	0.74
1:G:63:GLU:HG3	1:G:64:THR:H	1.52	0.73
1:F:41:ASP:OD2	1:F:296:HIS:HD2	1.71	0.73
1:G:272:VAL:HG13	2:G:549:HOH:O	1.87	0.73
1:H:63:GLU:HG3	1:H:64:THR:H	1.51	0.73
1:A:93:ASP:HA	2:A:308:HOH:O	1.87	0.73
1:I:63:GLU:HG3	1:I:64:THR:H	1.52	0.73
1:C:114:ASN:HD21	1:C:148:LEU:H	1.34	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:VAL:HG12	1:F:227:GLU:N	2.04	0.72
1:H:33:ARG:HG3	1:H:33:ARG:HH11	1.54	0.72
1:D:226:VAL:HG12	1:D:227:GLU:N	2.04	0.72
1:I:33:ARG:HH11	1:I:33:ARG:HG3	1.55	0.72
1:I:226:VAL:HG12	1:I:227:GLU:N	2.05	0.72
1:H:226:VAL:HG12	1:H:227:GLU:N	2.04	0.72
1:A:226:VAL:HG12	1:A:227:GLU:N	2.04	0.72
1:I:259:GLU:HB2	1:I:294:LEU:HD11	1.71	0.72
1:I:14:LEU:HD22	1:I:101:LEU:HD11	1.70	0.71
1:H:114:ASN:HD21	1:H:148:LEU:H	1.35	0.71
1:J:226:VAL:HG12	1:J:227:GLU:N	2.04	0.71
1:G:226:VAL:HG12	1:G:227:GLU:N	2.05	0.71
1:D:75:ARG:HH21	1:D:278:TYR:HA	1.55	0.71
1:C:226:VAL:HG12	1:C:227:GLU:N	2.04	0.71
1:J:111:GLY:HA3	1:J:137:MSE:HE3	1.73	0.71
1:I:71:GLU:O	1:I:75:ARG:HG3	1.91	0.71
1:F:33:ARG:HG3	1:F:33:ARG:HH11	1.56	0.71
1:E:33:ARG:HG3	1:E:33:ARG:HH11	1.56	0.70
1:E:226:VAL:HG12	1:E:227:GLU:N	2.04	0.70
1:D:111:GLY:HA3	1:D:137:MSE:HE3	1.71	0.70
2:G:308:HOH:O	1:H:93:ASP:HA	1.91	0.70
1:J:45:PHE:CE2	1:J:85:VAL:HG12	2.26	0.70
1:C:33:ARG:HG3	1:C:33:ARG:HH11	1.56	0.70
1:A:33:ARG:HG3	1:A:33:ARG:HH11	1.55	0.70
1:D:122:SER:CA	1:G:190:ASN:OD1	2.39	0.70
1:B:226:VAL:HG12	1:B:227:GLU:N	2.05	0.70
1:G:71:GLU:O	1:G:75:ARG:HG3	1.92	0.70
1:A:71:GLU:O	1:A:75:ARG:HG3	1.91	0.70
1:F:230:GLU:O	1:F:234:GLU:HG3	1.92	0.70
1:G:33:ARG:HG3	1:G:33:ARG:HH11	1.57	0.70
1:D:71:GLU:O	1:D:75:ARG:HG3	1.91	0.70
1:C:230:GLU:O	1:C:234:GLU:HG3	1.92	0.70
1:A:114:ASN:HD21	1:A:148:LEU:H	1.39	0.70
1:B:33:ARG:HH11	1:B:33:ARG:HG3	1.56	0.70
1:I:230:GLU:O	1:I:234:GLU:HG3	1.92	0.70
1:J:230:GLU:O	1:J:234:GLU:HG3	1.92	0.70
2:A:317:HOH:O	1:B:93:ASP:HA	1.91	0.69
1:H:71:GLU:O	1:H:75:ARG:HG3	1.92	0.69
1:H:230:GLU:O	1:H:234:GLU:HG3	1.92	0.69
1:A:230:GLU:O	1:A:234:GLU:HG3	1.92	0.69
1:B:230:GLU:O	1:B:234:GLU:HG3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:GLU:O	1:E:234:GLU:HG3	1.92	0.69
1:G:230:GLU:O	1:G:234:GLU:HG3	1.92	0.69
1:D:33:ARG:HG3	1:D:33:ARG:HH11	1.56	0.69
1:J:114:ASN:HD22	1:J:114:ASN:N	1.91	0.69
1:D:230:GLU:O	1:D:234:GLU:HG3	1.92	0.69
1:F:114:ASN:HD22	1:F:114:ASN:H	1.40	0.69
1:A:76:MSE:HE3	1:A:277:LEU:HD21	1.75	0.69
1:E:71:GLU:O	1:E:75:ARG:HG3	1.93	0.69
1:D:76:MSE:HE3	1:D:277:LEU:HD21	1.75	0.68
1:F:71:GLU:O	1:F:75:ARG:HG3	1.92	0.68
1:C:80:LEU:HA	1:C:85:VAL:HG21	1.76	0.68
1:B:80:LEU:HA	1:B:85:VAL:HG21	1.76	0.68
1:C:71:GLU:O	1:C:75:ARG:HG3	1.93	0.68
1:F:93:ASP:HA	2:F:309:HOH:O	1.92	0.68
1:B:71:GLU:O	1:B:75:ARG:HG3	1.93	0.68
1:D:80:LEU:HA	1:D:85:VAL:HG21	1.76	0.68
1:J:76:MSE:HE3	1:J:277:LEU:HD11	1.76	0.68
1:I:80:LEU:HA	1:I:85:VAL:HG21	1.76	0.68
1:I:111:GLY:HA3	1:I:137:MSE:HE3	1.75	0.68
1:C:111:GLY:H	1:C:137:MSE:HE1	1.60	0.67
1:A:137:MSE:HB3	1:A:142:VAL:CG2	2.25	0.67
1:J:151:ILE:HB	1:J:185:MSE:CE	2.25	0.67
1:E:151:ILE:HB	1:E:185:MSE:CE	2.25	0.66
1:F:226:VAL:CG1	1:F:227:GLU:N	2.59	0.66
1:E:226:VAL:CG1	1:E:227:GLU:N	2.59	0.66
1:H:137:MSE:HB3	1:H:142:VAL:CG2	2.26	0.66
1:J:114:ASN:HD21	1:J:148:LEU:H	1.43	0.66
1:A:151:ILE:HB	1:A:185:MSE:CE	2.25	0.66
1:C:190:ASN:OD1	1:H:122:SER:CB	2.42	0.66
1:E:114:ASN:H	1:E:114:ASN:HD22	1.42	0.66
1:G:274:ARG:NH2	2:G:549:HOH:O	2.27	0.66
1:B:137:MSE:HB3	1:B:142:VAL:CG2	2.26	0.66
1:D:122:SER:HB2	1:G:190:ASN:OD1	1.95	0.66
1:F:137:MSE:HB3	1:F:142:VAL:CG2	2.25	0.66
1:G:137:MSE:HB3	1:G:142:VAL:CG2	2.26	0.66
1:A:80:LEU:HA	1:A:85:VAL:HG21	1.76	0.66
1:F:80:LEU:HA	1:F:85:VAL:HG21	1.77	0.66
1:G:80:LEU:HA	1:G:85:VAL:HG21	1.76	0.66
1:H:32:ARG:HD2	1:H:104:LEU:HB3	1.77	0.66
1:H:151:ILE:HB	1:H:185:MSE:CE	2.26	0.66
1:D:226:VAL:CG1	1:D:227:GLU:N	2.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:ILE:HB	1:G:185:MSE:CE	2.25	0.66
1:H:226:VAL:CG1	1:H:227:GLU:N	2.58	0.66
1:I:226:VAL:CG1	1:I:227:GLU:N	2.59	0.66
1:J:68:ASN:HD21	1:J:70:TYR:HB2	1.61	0.66
1:B:226:VAL:CG1	1:B:227:GLU:N	2.59	0.66
1:C:226:VAL:CG1	1:C:227:GLU:N	2.59	0.66
1:D:111:GLY:H	1:D:137:MSE:HE1	1.60	0.66
1:E:80:LEU:HA	1:E:85:VAL:HG21	1.76	0.66
1:C:151:ILE:HB	1:C:185:MSE:CE	2.26	0.65
1:F:151:ILE:HB	1:F:185:MSE:CE	2.26	0.65
1:D:110:VAL:HG22	1:D:144:PHE:CB	2.26	0.65
1:E:226:VAL:O	1:E:229:MSE:HG2	1.97	0.65
1:J:226:VAL:CG1	1:J:227:GLU:N	2.58	0.65
1:A:226:VAL:CG1	1:A:227:GLU:N	2.59	0.65
1:G:226:VAL:CG1	1:G:227:GLU:N	2.59	0.65
1:H:75:ARG:NH2	1:H:278:TYR:HA	2.11	0.65
1:E:137:MSE:HB3	1:E:142:VAL:CG2	2.25	0.65
1:F:32:ARG:HD2	1:F:104:LEU:HB3	1.76	0.65
1:B:151:ILE:HB	1:B:185:MSE:CE	2.26	0.65
1:G:111:GLY:H	1:G:137:MSE:HE1	1.61	0.65
1:I:151:ILE:HB	1:I:185:MSE:CE	2.26	0.65
1:J:137:MSE:HB3	1:J:142:VAL:CG2	2.26	0.65
1:H:80:LEU:HA	1:H:85:VAL:HG21	1.76	0.65
1:B:111:GLY:H	1:B:137:MSE:HE1	1.62	0.65
1:B:151:ILE:CD1	1:B:185:MSE:HE1	2.27	0.65
1:D:151:ILE:HB	1:D:185:MSE:CE	2.26	0.65
1:F:226:VAL:O	1:F:229:MSE:HG2	1.97	0.65
2:F:310:HOH:O	1:G:93:ASP:HA	1.96	0.65
1:I:125:MSE:HE2	1:I:152:ASN:CB	2.27	0.65
1:I:226:VAL:O	1:I:229:MSE:HG2	1.97	0.65
1:H:151:ILE:CD1	1:H:185:MSE:HE1	2.27	0.65
1:A:76:MSE:CE	1:A:277:LEU:HD21	2.27	0.65
1:H:76:MSE:CE	1:H:277:LEU:HD21	2.27	0.64
1:D:151:ILE:CD1	1:D:185:MSE:HE1	2.28	0.64
1:E:151:ILE:CD1	1:E:185:MSE:HE1	2.27	0.64
1:A:151:ILE:CD1	1:A:185:MSE:HE1	2.28	0.64
1:F:151:ILE:CD1	1:F:185:MSE:HE1	2.28	0.64
1:D:226:VAL:O	1:D:229:MSE:HG2	1.96	0.64
1:G:151:ILE:CD1	1:G:185:MSE:HE1	2.27	0.64
1:I:151:ILE:CD1	1:I:185:MSE:HE1	2.28	0.64
1:J:125:MSE:HE2	1:J:152:ASN:CB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:VAL:O	1:B:229:MSE:HG2	1.97	0.64
1:D:137:MSE:HB3	1:D:142:VAL:CG2	2.26	0.64
1:F:125:MSE:HE2	1:F:152:ASN:CB	2.27	0.64
1:J:226:VAL:O	1:J:229:MSE:HG2	1.98	0.64
1:C:76:MSE:HE3	1:C:277:LEU:HD11	1.80	0.64
1:G:125:MSE:HE2	1:G:152:ASN:CB	2.27	0.64
1:A:114:ASN:HD22	1:A:114:ASN:N	1.94	0.64
1:C:151:ILE:CD1	1:C:185:MSE:HE1	2.28	0.64
1:D:125:MSE:HE2	1:D:152:ASN:CB	2.28	0.64
1:E:93:ASP:HA	2:J:308:HOH:O	1.97	0.64
1:C:137:MSE:HB3	1:C:142:VAL:CG2	2.26	0.64
1:D:278:TYR:N	1:D:279:PRO:HD3	2.12	0.64
1:I:137:MSE:HB3	1:I:142:VAL:CG2	2.26	0.64
1:C:226:VAL:O	1:C:229:MSE:HG2	1.98	0.64
1:A:125:MSE:HE2	1:A:152:ASN:CB	2.28	0.63
1:H:226:VAL:O	1:H:229:MSE:HG2	1.98	0.63
1:B:125:MSE:HE2	1:B:152:ASN:CB	2.28	0.63
1:J:151:ILE:CD1	1:J:185:MSE:HE1	2.28	0.63
1:H:125:MSE:HE2	1:H:152:ASN:CB	2.27	0.63
1:A:226:VAL:O	1:A:229:MSE:HG2	1.98	0.63
1:G:111:GLY:HA3	1:G:137:MSE:CE	2.28	0.63
1:I:278:TYR:N	1:I:279:PRO:HD3	2.13	0.63
1:C:125:MSE:HE2	1:C:152:ASN:CB	2.28	0.63
1:E:125:MSE:HE2	1:E:152:ASN:CB	2.28	0.63
1:E:152:ASN:C	1:E:152:ASN:HD22	2.06	0.63
1:F:111:GLY:H	1:F:137:MSE:HE1	1.64	0.62
1:A:185:MSE:HE3	1:A:205:SER:HB3	1.81	0.62
1:G:226:VAL:O	1:G:229:MSE:HG2	1.98	0.62
1:B:152:ASN:HD22	1:B:152:ASN:C	2.07	0.62
1:H:111:GLY:H	1:H:137:MSE:HE1	1.65	0.62
1:J:152:ASN:C	1:J:152:ASN:HD22	2.07	0.62
1:D:93:ASP:HA	2:D:310:HOH:O	1.97	0.62
1:J:68:ASN:C	1:J:68:ASN:ND2	2.55	0.62
1:G:152:ASN:HD22	1:G:152:ASN:C	2.06	0.62
1:I:152:ASN:C	1:I:152:ASN:HD22	2.07	0.62
1:G:54:ARG:HH21	1:G:150:ARG:HH12	1.46	0.62
1:H:111:GLY:HA3	1:H:137:MSE:CE	2.28	0.62
1:B:151:ILE:HD12	1:B:185:MSE:CE	2.30	0.62
1:C:152:ASN:C	1:C:152:ASN:HD22	2.07	0.62
1:D:277:LEU:O	1:D:278:TYR:HB2	1.98	0.62
1:H:114:ASN:HD22	1:H:114:ASN:H	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ASP:HA	2:E:308:HOH:O	1.99	0.62
1:E:278:TYR:N	1:E:279:PRO:HD3	2.14	0.62
1:F:152:ASN:C	1:F:152:ASN:HD22	2.06	0.62
1:G:151:ILE:HD12	1:G:185:MSE:CE	2.30	0.62
1:A:152:ASN:C	1:A:152:ASN:HD22	2.08	0.61
1:C:185:MSE:HE3	1:C:205:SER:HB3	1.81	0.61
1:D:151:ILE:HD12	1:D:185:MSE:CE	2.29	0.61
1:J:97:ASP:O	1:J:101:LEU:HD13	2.00	0.61
1:F:185:MSE:HE3	1:F:205:SER:HB3	1.82	0.61
1:B:185:MSE:HE3	1:B:205:SER:HB3	1.82	0.61
1:F:151:ILE:HD12	1:F:185:MSE:CE	2.30	0.61
1:G:185:MSE:HE3	1:G:205:SER:HB3	1.82	0.61
1:J:63:GLU:HG3	1:J:64:THR:N	2.13	0.61
1:B:111:GLY:HA3	1:B:137:MSE:CE	2.29	0.61
1:D:152:ASN:C	1:D:152:ASN:HD22	2.07	0.61
1:E:114:ASN:HD21	1:E:148:LEU:H	1.47	0.61
1:H:110:VAL:HG13	1:H:144:PHE:HB3	1.82	0.61
1:H:185:MSE:HE3	1:H:205:SER:HB3	1.81	0.61
1:I:111:GLY:H	1:I:137:MSE:HE1	1.65	0.61
1:E:151:ILE:HD12	1:E:185:MSE:CE	2.30	0.60
1:D:185:MSE:HE3	1:D:205:SER:HB3	1.81	0.60
1:E:76:MSE:HE3	1:E:277:LEU:HD21	1.82	0.60
1:H:76:MSE:HE3	1:H:277:LEU:HD21	1.82	0.60
1:C:114:ASN:HD22	1:C:114:ASN:N	1.98	0.60
1:G:246:GLU:HG2	1:G:247:GLY:H	1.67	0.60
1:J:151:ILE:HD12	1:J:185:MSE:CE	2.31	0.60
1:J:185:MSE:HE3	1:J:205:SER:HB3	1.82	0.60
1:C:76:MSE:CE	1:C:277:LEU:HD21	2.30	0.60
1:C:151:ILE:HD12	1:C:185:MSE:CE	2.31	0.60
1:E:76:MSE:CE	1:E:277:LEU:HD21	2.31	0.60
1:E:185:MSE:HE3	1:E:205:SER:HB3	1.82	0.60
1:E:246:GLU:HG2	1:E:247:GLY:H	1.67	0.60
1:F:75:ARG:HH21	1:F:278:TYR:HA	1.67	0.60
1:H:151:ILE:HD12	1:H:185:MSE:CE	2.29	0.60
1:H:152:ASN:C	1:H:152:ASN:HD22	2.07	0.60
1:J:151:ILE:HB	1:J:185:MSE:HE2	1.84	0.60
1:D:246:GLU:HG2	1:D:247:GLY:H	1.67	0.60
1:H:24:MSE:HE1	1:H:27:GLU:OE1	2.01	0.60
1:A:151:ILE:HB	1:A:185:MSE:HE2	1.82	0.60
1:F:110:VAL:HG22	1:F:144:PHE:HB3	1.84	0.60
1:F:246:GLU:HG2	1:F:247:GLY:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:MSE:CE	1:B:277:LEU:HD21	2.31	0.60
1:I:151:ILE:HD12	1:I:185:MSE:CE	2.30	0.60
1:A:151:ILE:HD12	1:A:185:MSE:CE	2.30	0.59
1:C:47:VAL:HG11	1:C:76:MSE:HE1	1.84	0.59
1:G:32:ARG:HD2	1:G:104:LEU:HB3	1.83	0.59
1:J:47:VAL:HB	1:J:76:MSE:HE1	1.84	0.59
1:B:273:GLY:N	1:B:274:ARG:HH21	2.00	0.59
1:E:75:ARG:HH21	1:E:278:TYR:HA	1.67	0.59
1:E:151:ILE:HB	1:E:185:MSE:HE2	1.83	0.59
1:F:111:GLY:HA3	1:F:137:MSE:CE	2.31	0.59
1:H:47:VAL:HG11	1:H:76:MSE:HE1	1.84	0.59
1:I:185:MSE:HE3	1:I:205:SER:HB3	1.83	0.59
1:H:246:GLU:HG2	1:H:247:GLY:H	1.67	0.59
1:I:246:GLU:HG2	1:I:247:GLY:H	1.67	0.59
1:C:273:GLY:H	1:C:274:ARG:HH21	1.51	0.59
1:D:226:VAL:CG1	1:D:227:GLU:H	2.16	0.59
1:I:85:VAL:HG23	1:I:85:VAL:O	2.03	0.59
1:B:274:ARG:O	1:B:277:LEU:O	2.21	0.59
1:C:85:VAL:O	1:C:85:VAL:HG23	2.03	0.59
1:H:273:GLY:H	1:H:274:ARG:HH21	1.51	0.59
1:C:151:ILE:HB	1:C:185:MSE:HE2	1.85	0.59
1:C:190:ASN:OD1	1:H:122:SER:HB2	2.03	0.59
1:C:273:GLY:N	1:C:274:ARG:HH21	2.01	0.59
1:E:261:ALA:HA	1:E:264:LEU:HD22	1.85	0.59
1:F:273:GLY:N	1:F:274:ARG:HH21	2.00	0.59
1:J:80:LEU:HA	1:J:85:VAL:HG21	1.85	0.59
1:J:226:VAL:CG1	1:J:227:GLU:H	2.16	0.59
1:A:111:GLY:H	1:A:137:MSE:HE1	1.67	0.59
1:A:246:GLU:HG2	1:A:247:GLY:H	1.67	0.59
1:D:151:ILE:HB	1:D:185:MSE:HE2	1.85	0.59
1:J:246:GLU:HG2	1:J:247:GLY:H	1.67	0.59
1:E:46:ILE:HD13	1:E:110:VAL:HG21	1.83	0.58
1:F:151:ILE:HB	1:F:185:MSE:HE2	1.84	0.58
1:E:226:VAL:CG1	1:E:227:GLU:H	2.16	0.58
1:I:151:ILE:HB	1:I:185:MSE:HE2	1.85	0.58
1:I:226:VAL:CG1	1:I:227:GLU:H	2.16	0.58
1:B:278:TYR:N	1:B:279:PRO:HD3	2.18	0.58
1:G:85:VAL:HG23	1:G:85:VAL:O	2.03	0.58
1:J:76:MSE:HE2	1:J:277:LEU:CD2	2.26	0.58
1:C:261:ALA:HA	1:C:264:LEU:HD22	1.86	0.58
1:F:226:VAL:CG1	1:F:227:GLU:H	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:VAL:CG1	1:A:227:GLU:H	2.16	0.58
1:F:47:VAL:HG11	1:F:76:MSE:HE1	1.85	0.58
1:I:273:GLY:N	1:I:274:ARG:HH21	2.02	0.58
1:C:246:GLU:HG2	1:C:247:GLY:H	1.67	0.58
1:G:151:ILE:HB	1:G:185:MSE:HE2	1.84	0.58
1:H:261:ALA:HA	1:H:264:LEU:HD22	1.86	0.58
1:C:226:VAL:CG1	1:C:227:GLU:H	2.16	0.58
1:D:261:ALA:HA	1:D:264:LEU:HD22	1.85	0.58
1:E:47:VAL:HG11	1:E:76:MSE:HE1	1.86	0.58
1:F:85:VAL:HG23	1:F:85:VAL:O	2.03	0.58
1:H:85:VAL:HG23	1:H:85:VAL:O	2.03	0.58
1:B:151:ILE:HB	1:B:185:MSE:HE2	1.85	0.58
1:B:246:GLU:HG2	1:B:247:GLY:H	1.67	0.58
1:B:274:ARG:H	1:B:274:ARG:NE	2.01	0.58
1:C:54:ARG:HH21	1:C:150:ARG:HH12	1.52	0.58
1:G:261:ALA:HA	1:G:264:LEU:HD22	1.85	0.58
1:B:261:ALA:HA	1:B:264:LEU:HD22	1.86	0.57
1:D:273:GLY:N	1:D:274:ARG:HH21	2.02	0.57
1:H:273:GLY:N	1:H:274:ARG:HH21	2.01	0.57
1:I:114:ASN:HD21	1:I:148:LEU:H	1.52	0.57
1:B:85:VAL:HG23	1:B:85:VAL:O	2.04	0.57
1:C:75:ARG:HH21	1:C:278:TYR:HA	1.69	0.57
1:C:111:GLY:CA	1:C:137:MSE:CE	2.82	0.57
1:E:85:VAL:HG23	1:E:85:VAL:O	2.03	0.57
1:F:273:GLY:H	1:F:274:ARG:HH21	1.51	0.57
1:H:226:VAL:CG1	1:H:227:GLU:H	2.16	0.57
1:H:274:ARG:H	1:H:274:ARG:NE	2.01	0.57
1:A:76:MSE:HA	1:A:76:MSE:CE	2.33	0.57
1:B:47:VAL:HG11	1:B:76:MSE:HE1	1.86	0.57
1:H:41:ASP:OD2	1:H:296:HIS:HD2	1.86	0.57
1:H:151:ILE:HB	1:H:185:MSE:HE2	1.85	0.57
1:J:76:MSE:HE2	1:J:76:MSE:HA	1.86	0.57
1:A:273:GLY:N	1:A:274:ARG:HH21	2.02	0.57
1:B:110:VAL:HG13	1:B:144:PHE:HB3	1.87	0.57
1:B:273:GLY:H	1:B:274:ARG:HH21	1.51	0.57
1:F:76:MSE:HA	1:F:76:MSE:CE	2.33	0.57
1:I:47:VAL:HG11	1:I:76:MSE:HE1	1.85	0.57
1:F:12:GLU:OE1	1:F:16:ARG:NH2	2.36	0.57
1:G:47:VAL:HG11	1:G:76:MSE:HE1	1.86	0.57
1:G:226:VAL:CG1	1:G:227:GLU:H	2.17	0.57
1:I:261:ALA:HA	1:I:264:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:VAL:HG23	1:D:85:VAL:O	2.04	0.57
1:G:114:ASN:HD22	1:G:114:ASN:N	1.98	0.57
1:D:47:VAL:HG11	1:D:76:MSE:HE1	1.86	0.57
1:F:261:ALA:HA	1:F:264:LEU:HD22	1.86	0.57
1:H:76:MSE:HA	1:H:76:MSE:CE	2.34	0.57
1:I:274:ARG:H	1:I:274:ARG:NE	2.01	0.57
1:A:47:VAL:HG11	1:A:76:MSE:HE1	1.86	0.57
1:D:68:ASN:CG	1:D:71:GLU:HG3	2.30	0.57
1:E:273:GLY:H	1:E:274:ARG:HH21	1.53	0.57
1:E:273:GLY:N	1:E:274:ARG:HH21	2.02	0.57
1:F:283:ASP:HB3	1:F:286:ALA:HB3	1.85	0.57
1:J:261:ALA:HA	1:J:264:LEU:HD22	1.86	0.57
1:A:296:HIS:C	1:A:298:ASP:H	2.13	0.56
1:B:226:VAL:CG1	1:B:227:GLU:H	2.17	0.56
1:I:274:ARG:O	1:I:277:LEU:O	2.23	0.56
1:A:85:VAL:HG23	1:A:85:VAL:O	2.04	0.56
1:A:261:ALA:HA	1:A:264:LEU:HD22	1.86	0.56
1:B:185:MSE:HE3	1:B:205:SER:HA	1.88	0.56
1:D:273:GLY:H	1:D:274:ARG:HH21	1.52	0.56
1:E:68:ASN:CG	1:E:71:GLU:HG3	2.30	0.56
1:F:86:ASP:OD2	1:F:296:HIS:HE1	1.88	0.56
1:J:273:GLY:N	1:J:274:ARG:HH21	2.02	0.56
1:C:110:VAL:HG22	1:C:144:PHE:HB3	1.87	0.56
1:D:297:THR:C	1:D:299:ILE:H	2.13	0.56
1:E:32:ARG:HD2	1:E:104:LEU:HB3	1.87	0.56
1:G:76:MSE:HA	1:G:76:MSE:CE	2.33	0.56
1:I:110:VAL:HG22	1:I:144:PHE:HB3	1.87	0.56
1:J:65:ALA:C	1:J:67:ALA:H	2.13	0.56
1:A:68:ASN:CG	1:A:71:GLU:HG3	2.31	0.56
1:G:68:ASN:CG	1:G:71:GLU:HG3	2.30	0.56
1:A:273:GLY:H	1:A:274:ARG:HH21	1.52	0.56
1:A:274:ARG:H	1:A:274:ARG:NE	2.01	0.56
1:C:68:ASN:CG	1:C:71:GLU:HG3	2.31	0.56
1:F:278:TYR:N	1:F:279:PRO:HD3	2.21	0.56
1:I:54:ARG:HH21	1:I:150:ARG:HH12	1.54	0.56
1:B:185:MSE:HE3	1:B:205:SER:CA	2.36	0.55
1:E:76:MSE:HA	1:E:76:MSE:CE	2.34	0.55
1:I:68:ASN:CG	1:I:71:GLU:HG3	2.31	0.55
1:J:111:GLY:H	1:J:137:MSE:HE1	1.71	0.55
1:A:97:ASP:O	1:A:101:LEU:HD22	2.06	0.55
1:D:76:MSE:HA	1:D:76:MSE:CE	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ASN:CG	1:B:71:GLU:HG3	2.31	0.55
1:D:76:MSE:HE2	1:D:277:LEU:HD21	1.88	0.55
1:G:274:ARG:H	1:G:274:ARG:NE	2.02	0.55
1:H:185:MSE:HE3	1:H:205:SER:HA	1.89	0.55
1:I:273:GLY:H	1:I:274:ARG:HH21	1.53	0.55
1:D:45:PHE:CE2	1:D:85:VAL:HG12	2.42	0.55
1:J:273:GLY:H	1:J:274:ARG:HH21	1.53	0.55
1:F:110:VAL:HG22	1:F:144:PHE:CB	2.37	0.55
1:G:185:MSE:HE3	1:G:205:SER:CA	2.37	0.55
1:G:273:GLY:N	1:G:274:ARG:HH21	2.05	0.55
1:C:113:MSE:HE3	2:C:704:HOH:O	2.07	0.55
1:H:105:ASP:O	1:H:107:LYS:HG2	2.07	0.55
1:J:75:ARG:HH21	1:J:278:TYR:HA	1.72	0.55
1:B:76:MSE:HA	1:B:76:MSE:CE	2.33	0.55
1:C:185:MSE:HE3	1:C:205:SER:CA	2.37	0.55
1:C:185:MSE:HE3	1:C:205:SER:HA	1.88	0.55
1:D:185:MSE:HE3	1:D:205:SER:CA	2.37	0.55
1:E:45:PHE:CE2	1:E:85:VAL:HG12	2.42	0.55
1:J:89:LEU:HD12	1:J:90:GLY:N	2.22	0.55
1:J:185:MSE:HE3	1:J:205:SER:HA	1.89	0.55
1:A:45:PHE:CE2	1:A:85:VAL:HG12	2.42	0.55
1:B:45:PHE:CE2	1:B:85:VAL:HG12	2.42	0.55
1:F:68:ASN:CG	1:F:71:GLU:HG3	2.32	0.55
1:J:9:GLU:OE1	1:J:9:GLU:N	2.39	0.55
1:B:41:ASP:OD2	1:B:296:HIS:HD2	1.90	0.54
1:C:45:PHE:CE2	1:C:85:VAL:HG12	2.42	0.54
1:F:185:MSE:HE3	1:F:205:SER:CA	2.38	0.54
1:G:185:MSE:HE3	1:G:205:SER:HA	1.89	0.54
1:J:185:MSE:HE3	1:J:205:SER:CA	2.37	0.54
1:A:278:TYR:N	1:A:279:PRO:HD3	2.23	0.54
1:E:185:MSE:HE3	1:E:205:SER:HA	1.90	0.54
1:H:45:PHE:CE2	1:H:85:VAL:HG12	2.42	0.54
1:I:76:MSE:HA	1:I:76:MSE:CE	2.33	0.54
1:I:185:MSE:HE3	1:I:205:SER:HA	1.88	0.54
1:C:76:MSE:HA	1:C:76:MSE:CE	2.34	0.54
1:I:14:LEU:HD22	1:I:101:LEU:CD1	2.37	0.54
1:I:185:MSE:HE3	1:I:205:SER:CA	2.37	0.54
1:I:259:GLU:CB	1:I:294:LEU:HD11	2.35	0.54
1:J:110:VAL:HG22	1:J:144:PHE:HB3	1.90	0.54
1:C:111:GLY:N	1:C:137:MSE:HE1	2.21	0.54
1:E:170:ASN:ND2	1:E:214:ASN:H	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:185:MSE:HE3	1:H:205:SER:CA	2.37	0.54
1:F:45:PHE:CE2	1:F:85:VAL:HG12	2.42	0.54
1:E:126:ASP:OD2	1:E:128:ARG:NH1	2.40	0.54
1:I:45:PHE:CE2	1:I:85:VAL:HG12	2.42	0.54
1:D:185:MSE:HE3	1:D:205:SER:HA	1.89	0.54
1:E:274:ARG:H	1:E:274:ARG:NE	2.02	0.54
1:F:185:MSE:HE3	1:F:205:SER:HA	1.89	0.54
1:G:45:PHE:CE2	1:G:85:VAL:HG12	2.43	0.53
1:J:29:PHE:O	1:J:32:ARG:HB3	2.07	0.53
2:C:569:HOH:O	1:D:55:GLY:HA2	2.07	0.53
1:D:297:THR:O	1:D:299:ILE:N	2.41	0.53
1:I:296:HIS:C	1:I:298:ASP:H	2.16	0.53
1:D:75:ARG:NH2	1:D:278:TYR:HA	2.23	0.53
1:G:273:GLY:H	1:G:274:ARG:HH21	1.56	0.53
1:H:33:ARG:HG3	1:H:33:ARG:NH1	2.23	0.53
1:H:68:ASN:CG	1:H:71:GLU:HG3	2.32	0.53
1:D:274:ARG:H	1:D:274:ARG:NE	2.00	0.53
1:A:214:ASN:HD22	1:A:214:ASN:C	2.17	0.53
1:B:54:ARG:HH21	1:B:150:ARG:HH12	1.54	0.53
1:D:214:ASN:C	1:D:214:ASN:HD22	2.17	0.53
1:F:114:ASN:O	1:F:115:ARG:HD2	2.08	0.53
1:J:170:ASN:ND2	1:J:214:ASN:H	2.07	0.53
1:A:110:VAL:HG13	1:A:144:PHE:HB3	1.91	0.53
1:F:170:ASN:ND2	1:F:214:ASN:H	2.07	0.53
1:E:185:MSE:HE3	1:E:205:SER:CA	2.38	0.53
1:H:126:ASP:OD2	1:H:128:ARG:NH1	2.41	0.53
1:H:274:ARG:O	1:H:277:LEU:O	2.27	0.53
1:I:229:MSE:O	1:I:264:LEU:HD23	2.09	0.53
1:B:46:ILE:HD13	1:B:110:VAL:HG21	1.91	0.53
1:B:277:LEU:O	1:B:278:TYR:HB2	2.09	0.53
1:G:170:ASN:ND2	1:G:214:ASN:H	2.07	0.53
1:H:278:TYR:N	1:H:279:PRO:HD3	2.24	0.53
1:G:214:ASN:C	1:G:214:ASN:HD22	2.16	0.52
1:J:47:VAL:CG1	1:J:76:MSE:HE1	2.39	0.52
1:F:12:GLU:OE2	1:F:15:ARG:NH2	2.42	0.52
1:F:229:MSE:O	1:F:264:LEU:HD23	2.09	0.52
1:G:64:THR:O	1:G:65:ALA:HB3	2.10	0.52
1:A:24:MSE:HG3	2:A:316:HOH:O	2.08	0.52
1:A:111:GLY:CA	1:A:137:MSE:CE	2.86	0.52
1:E:114:ASN:HD22	1:E:114:ASN:N	2.06	0.52
1:H:214:ASN:C	1:H:214:ASN:HD22	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ASN:C	1:C:214:ASN:HD22	2.16	0.52
1:E:111:GLY:CA	1:E:137:MSE:CE	2.86	0.52
1:I:170:ASN:ND2	1:I:214:ASN:H	2.07	0.52
1:I:214:ASN:C	1:I:214:ASN:HD22	2.17	0.52
1:J:274:ARG:H	1:J:274:ARG:NE	2.01	0.52
1:F:110:VAL:HG13	1:F:144:PHE:HB3	1.91	0.52
1:F:114:ASN:O	1:F:115:ARG:CD	2.58	0.52
1:H:64:THR:O	1:H:65:ALA:HB3	2.09	0.52
1:I:64:THR:O	1:I:65:ALA:HB3	2.09	0.52
1:J:64:THR:O	1:J:65:ALA:HB3	2.09	0.52
1:B:33:ARG:HG3	1:B:33:ARG:NH1	2.25	0.52
1:E:214:ASN:C	1:E:214:ASN:HD22	2.17	0.52
1:A:64:THR:O	1:A:65:ALA:HB3	2.09	0.52
1:H:47:VAL:HG11	1:H:76:MSE:CE	2.40	0.52
1:A:185:MSE:HE3	1:A:205:SER:CA	2.38	0.52
1:C:126:ASP:OD2	1:C:128:ARG:NH1	2.41	0.52
1:D:64:THR:O	1:D:65:ALA:HB3	2.10	0.52
1:F:64:THR:O	1:F:65:ALA:HB3	2.10	0.52
1:G:68:ASN:C	1:G:68:ASN:ND2	2.67	0.52
1:H:229:MSE:O	1:H:264:LEU:HD23	2.10	0.52
1:J:214:ASN:C	1:J:214:ASN:HD22	2.17	0.52
1:A:274:ARG:O	1:A:277:LEU:O	2.27	0.52
1:H:170:ASN:ND2	1:H:214:ASN:H	2.08	0.52
1:J:45:PHE:HE2	1:J:85:VAL:HG12	1.73	0.52
1:F:214:ASN:C	1:F:214:ASN:HD22	2.16	0.52
1:J:69:ARG:HH11	1:J:72:LEU:HD13	1.75	0.52
1:A:170:ASN:ND2	1:A:214:ASN:H	2.08	0.51
1:A:185:MSE:HE3	1:A:205:SER:HA	1.90	0.51
1:B:64:THR:O	1:B:65:ALA:HB3	2.10	0.51
1:B:76:MSE:HE2	1:B:277:LEU:HD21	1.92	0.51
1:C:64:THR:O	1:C:65:ALA:HB3	2.09	0.51
1:F:274:ARG:H	1:F:274:ARG:NE	2.00	0.51
1:H:47:VAL:CG1	1:H:76:MSE:HE1	2.40	0.51
1:B:170:ASN:ND2	1:B:214:ASN:H	2.08	0.51
1:B:180:MSE:HE2	1:B:241:LEU:HD12	1.92	0.51
1:C:229:MSE:O	1:C:264:LEU:HD23	2.11	0.51
1:D:111:GLY:HA3	1:D:137:MSE:CE	2.40	0.51
1:E:229:MSE:O	1:E:264:LEU:HD23	2.11	0.51
1:B:126:ASP:OD2	1:B:128:ARG:NH1	2.41	0.51
1:E:64:THR:O	1:E:65:ALA:HB3	2.09	0.51
1:G:229:MSE:O	1:G:264:LEU:HD23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:111:GLY:N	1:H:137:MSE:HE1	2.25	0.51
1:I:68:ASN:HD21	1:I:70:TYR:HB2	1.76	0.51
1:A:111:GLY:N	1:A:137:MSE:HE1	2.26	0.51
1:B:32:ARG:HD2	1:B:104:LEU:HB3	1.92	0.51
1:C:33:ARG:HG3	1:C:33:ARG:NH1	2.25	0.51
1:C:47:VAL:CG1	1:C:76:MSE:HE1	2.40	0.51
1:D:114:ASN:HD22	1:D:114:ASN:N	2.04	0.51
1:D:170:ASN:ND2	1:D:214:ASN:H	2.08	0.51
1:F:274:ARG:O	1:F:277:LEU:O	2.29	0.51
1:J:129:TYR:OH	1:J:147:THR:HG21	2.11	0.51
1:A:75:ARG:HH21	1:A:278:TYR:HA	1.74	0.51
1:E:68:ASN:C	1:E:68:ASN:ND2	2.67	0.51
1:F:47:VAL:HG11	1:F:76:MSE:CE	2.41	0.51
1:G:47:VAL:HG11	1:G:76:MSE:CE	2.41	0.51
1:B:75:ARG:HH21	1:B:278:TYR:HA	1.75	0.51
1:J:229:MSE:O	1:J:264:LEU:HD23	2.10	0.51
1:D:180:MSE:HE2	1:D:241:LEU:HD12	1.93	0.51
1:E:297:THR:OG1	1:E:299:ILE:HG12	2.11	0.51
1:C:47:VAL:HG11	1:C:76:MSE:CE	2.40	0.51
1:C:180:MSE:HE2	1:C:241:LEU:HD12	1.93	0.51
1:I:47:VAL:HG11	1:I:76:MSE:CE	2.41	0.51
1:A:46:ILE:HD13	1:A:110:VAL:HG21	1.93	0.51
1:D:33:ARG:HG3	1:D:33:ARG:NH1	2.25	0.51
1:D:229:MSE:O	1:D:264:LEU:HD23	2.10	0.51
1:E:129:TYR:OH	1:E:147:THR:HG21	2.11	0.51
1:G:275:THR:HG22	1:G:276:LEU:HD23	1.93	0.51
1:I:33:ARG:HG3	1:I:33:ARG:NH1	2.24	0.51
1:A:229:MSE:O	1:A:264:LEU:HD23	2.10	0.50
1:B:68:ASN:HD21	1:B:70:TYR:HB2	1.76	0.50
1:B:214:ASN:C	1:B:214:ASN:HD22	2.18	0.50
1:C:170:ASN:ND2	1:C:214:ASN:H	2.08	0.50
1:I:110:VAL:HG22	1:I:144:PHE:CB	2.42	0.50
1:A:47:VAL:HG11	1:A:76:MSE:CE	2.41	0.50
1:A:126:ASP:OD2	1:A:128:ARG:NH1	2.41	0.50
1:C:297:THR:O	1:C:298:ASP:HB2	2.11	0.50
1:D:47:VAL:HG11	1:D:76:MSE:CE	2.40	0.50
1:E:47:VAL:HG11	1:E:76:MSE:CE	2.41	0.50
1:G:129:TYR:OH	1:G:147:THR:HG21	2.11	0.50
1:G:274:ARG:O	1:G:277:LEU:O	2.29	0.50
1:H:57:LEU:O	1:H:65:ALA:O	2.30	0.50
1:F:68:ASN:HD21	1:F:70:TYR:HB2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:114:ASN:HD22	1:I:114:ASN:N	1.99	0.50
1:I:129:TYR:OH	1:I:147:THR:HG21	2.12	0.50
1:B:47:VAL:CG1	1:B:76:MSE:HE1	2.42	0.50
1:D:89:LEU:HD13	1:D:110:VAL:HG12	1.92	0.50
1:F:68:ASN:C	1:F:68:ASN:ND2	2.67	0.50
1:F:126:ASP:OD2	1:F:128:ARG:NH1	2.41	0.50
1:G:47:VAL:CG1	1:G:76:MSE:HE1	2.42	0.50
1:G:68:ASN:HD21	1:G:70:TYR:HB2	1.76	0.50
1:G:110:VAL:HG22	1:G:144:PHE:HB3	1.92	0.50
1:J:296:HIS:C	1:J:298:ASP:H	2.20	0.50
1:A:180:MSE:HE2	1:A:241:LEU:HD12	1.93	0.50
1:B:66:MSE:HG2	1:B:278:TYR:CE2	2.46	0.50
1:C:68:ASN:C	1:C:68:ASN:ND2	2.67	0.50
1:C:278:TYR:N	1:C:279:PRO:HD3	2.27	0.50
1:E:180:MSE:HE2	1:E:241:LEU:HD12	1.93	0.50
1:B:111:GLY:N	1:B:137:MSE:HE1	2.25	0.50
1:C:57:LEU:O	1:C:65:ALA:O	2.30	0.50
1:C:110:VAL:HG22	1:C:144:PHE:CB	2.42	0.50
1:G:126:ASP:OD2	1:G:128:ARG:NH1	2.41	0.50
1:H:12:GLU:OE1	1:H:16:ARG:NH2	2.42	0.50
1:J:17:MSE:HE1	1:J:28:ARG:HE	1.75	0.50
1:B:47:VAL:HG11	1:B:76:MSE:CE	2.41	0.50
1:C:68:ASN:HD21	1:C:70:TYR:HB2	1.77	0.50
1:F:180:MSE:HE2	1:F:241:LEU:HD12	1.92	0.50
1:J:111:GLY:HA3	1:J:137:MSE:CE	2.40	0.50
1:C:111:GLY:CA	1:C:137:MSE:HE1	2.42	0.50
1:D:126:ASP:OD2	1:D:128:ARG:NH1	2.41	0.50
1:G:12:GLU:OE1	1:G:16:ARG:NH2	2.45	0.50
1:H:68:ASN:HD21	1:H:70:TYR:HB2	1.76	0.50
1:H:296:HIS:C	1:H:298:ASP:H	2.19	0.50
1:A:47:VAL:CG1	1:A:76:MSE:HE1	2.41	0.49
1:B:229:MSE:O	1:B:264:LEU:HD23	2.10	0.49
1:D:68:ASN:HD21	1:D:70:TYR:HB2	1.76	0.49
1:E:33:ARG:HG3	1:E:33:ARG:NH1	2.25	0.49
1:E:68:ASN:HD21	1:E:70:TYR:HB2	1.76	0.49
1:F:76:MSE:CE	1:F:277:LEU:HD21	2.42	0.49
1:F:129:TYR:OH	1:F:147:THR:HG21	2.12	0.49
1:G:114:ASN:O	1:G:115:ARG:HD2	2.13	0.49
1:H:180:MSE:HE2	1:H:241:LEU:HD12	1.93	0.49
1:I:296:HIS:O	1:I:298:ASP:N	2.45	0.49
1:J:68:ASN:HD22	1:J:69:ARG:N	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:VAL:CG1	1:D:76:MSE:HE1	2.42	0.49
1:J:41:ASP:O	1:J:43:LYS:HD3	2.12	0.49
1:J:180:MSE:HE2	1:J:241:LEU:HD12	1.93	0.49
1:A:129:TYR:OH	1:A:147:THR:HG21	2.12	0.49
1:B:57:LEU:O	1:B:65:ALA:O	2.30	0.49
1:B:129:TYR:OH	1:B:147:THR:HG21	2.11	0.49
1:F:47:VAL:CG1	1:F:76:MSE:HE1	2.42	0.49
1:F:76:MSE:HE3	1:F:277:LEU:HD11	1.94	0.49
1:I:47:VAL:CG1	1:I:76:MSE:HE1	2.41	0.49
1:J:259:GLU:HB2	1:J:294:LEU:HD11	1.94	0.49
1:A:63:GLU:O	1:A:64:THR:O	2.31	0.49
1:C:274:ARG:H	1:C:274:ARG:NE	2.01	0.49
1:H:129:TYR:OH	1:H:147:THR:HG21	2.12	0.49
1:J:85:VAL:O	1:J:85:VAL:HG23	2.13	0.49
1:J:92:PRO:HG3	1:J:132:TYR:CD2	2.47	0.49
1:D:68:ASN:C	1:D:68:ASN:ND2	2.67	0.49
1:J:95:ILE:HD12	1:J:109:VAL:HG13	1.95	0.49
1:C:129:TYR:OH	1:C:147:THR:HG21	2.12	0.49
1:F:114:ASN:HD22	1:F:114:ASN:N	2.09	0.49
1:I:110:VAL:HG13	1:I:144:PHE:HB3	1.95	0.49
1:A:57:LEU:O	1:A:65:ALA:O	2.31	0.49
1:A:111:GLY:CA	1:A:137:MSE:HE1	2.43	0.49
1:C:32:ARG:HD2	1:C:104:LEU:HB3	1.94	0.49
1:E:46:ILE:HD13	1:E:110:VAL:CG2	2.43	0.49
1:G:76:MSE:HE3	1:G:277:LEU:HD21	1.94	0.49
1:I:57:LEU:O	1:I:65:ALA:O	2.31	0.49
1:B:17:MSE:HE1	1:B:28:ARG:NE	2.27	0.49
1:D:129:TYR:OH	1:D:147:THR:HG21	2.11	0.49
1:F:33:ARG:HG3	1:F:33:ARG:NH1	2.24	0.49
1:G:8:PRO:HG2	1:G:9:GLU:OE1	2.13	0.49
1:I:180:MSE:HE2	1:I:241:LEU:HD12	1.94	0.49
1:A:68:ASN:HD21	1:A:70:TYR:HB2	1.77	0.48
1:C:82:ARG:NH2	1:C:289:ASP:OD2	2.44	0.48
1:I:68:ASN:C	1:I:68:ASN:ND2	2.67	0.48
1:C:274:ARG:O	1:C:277:LEU:O	2.30	0.48
1:E:47:VAL:CG1	1:E:76:MSE:HE1	2.42	0.48
1:F:57:LEU:O	1:F:65:ALA:O	2.31	0.48
1:G:33:ARG:HG3	1:G:33:ARG:NH1	2.26	0.48
1:J:63:GLU:CG	1:J:64:THR:H	2.19	0.48
1:J:278:TYR:N	1:J:279:PRO:HD3	2.28	0.48
1:B:63:GLU:O	1:B:64:THR:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:MSE:HE2	1:C:277:LEU:HD21	1.95	0.48
1:A:61:ASP:OD1	1:A:61:ASP:C	2.56	0.48
1:I:152:ASN:HD22	1:I:154:SER:H	1.62	0.48
1:J:79:ALA:O	1:J:85:VAL:HG21	2.13	0.48
1:G:57:LEU:O	1:G:65:ALA:O	2.31	0.48
1:I:103:LEU:O	1:I:104:LEU:HD12	2.14	0.48
1:J:151:ILE:HB	1:J:185:MSE:HE1	1.96	0.48
1:D:63:GLU:O	1:D:64:THR:O	2.31	0.48
1:E:111:GLY:H	1:E:137:MSE:HE1	1.77	0.48
1:E:57:LEU:O	1:E:65:ALA:O	2.31	0.48
1:E:63:GLU:O	1:E:64:THR:O	2.32	0.48
1:G:180:MSE:HE2	1:G:241:LEU:HD12	1.94	0.48
1:H:151:ILE:HB	1:H:185:MSE:HE1	1.96	0.48
1:E:61:ASP:C	1:E:61:ASP:OD1	2.57	0.48
1:F:61:ASP:OD1	1:F:61:ASP:C	2.57	0.48
1:H:61:ASP:C	1:H:61:ASP:OD1	2.57	0.48
1:H:152:ASN:HD22	1:H:154:SER:H	1.62	0.48
1:D:111:GLY:N	1:D:137:MSE:HE1	2.29	0.47
1:F:115:ARG:HD2	1:F:115:ARG:HA	1.58	0.47
1:I:63:GLU:O	1:I:64:THR:O	2.32	0.47
1:E:110:VAL:HG13	1:E:144:PHE:HB3	1.96	0.47
1:G:14:LEU:HD13	1:G:101:LEU:HD13	1.95	0.47
1:A:15:ARG:HD3	1:A:70:TYR:OH	2.14	0.47
1:H:17:MSE:HE1	1:H:28:ARG:NE	2.30	0.47
1:I:111:GLY:HA3	1:I:137:MSE:CE	2.42	0.47
1:B:68:ASN:C	1:B:68:ASN:ND2	2.68	0.47
1:C:152:ASN:HD22	1:C:154:SER:H	1.63	0.47
1:F:151:ILE:HB	1:F:185:MSE:HE1	1.97	0.47
1:G:63:GLU:O	1:G:64:THR:O	2.31	0.47
1:H:63:GLU:O	1:H:64:THR:O	2.31	0.47
1:C:214:ASN:C	1:C:214:ASN:ND2	2.73	0.47
1:F:273:GLY:H	1:F:274:ARG:NH2	2.12	0.47
1:H:273:GLY:H	1:H:274:ARG:NH2	2.13	0.47
1:J:126:ASP:OD2	1:J:128:ARG:NH1	2.40	0.47
1:A:54:ARG:HH21	1:A:150:ARG:HH12	1.62	0.47
1:A:273:GLY:H	1:A:274:ARG:NH2	2.13	0.47
1:C:63:GLU:O	1:C:64:THR:O	2.32	0.47
1:D:61:ASP:OD1	1:D:61:ASP:C	2.57	0.47
1:D:151:ILE:HB	1:D:185:MSE:HE1	1.97	0.47
1:A:86:ASP:OD2	1:A:296:HIS:HE1	1.97	0.47
1:C:61:ASP:C	1:C:61:ASP:OD1	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:GLY:H	1:D:274:ARG:NH2	2.12	0.47
1:E:281:ASP:OD2	1:E:281:ASP:C	2.58	0.47
1:F:63:GLU:O	1:F:64:THR:O	2.31	0.47
1:F:85:VAL:HG23	1:F:107:LYS:HE3	1.96	0.47
1:I:61:ASP:OD1	1:I:61:ASP:C	2.57	0.47
1:E:214:ASN:C	1:E:214:ASN:ND2	2.73	0.47
1:G:152:ASN:HD22	1:G:154:SER:H	1.63	0.47
1:H:214:ASN:C	1:H:214:ASN:ND2	2.73	0.47
1:I:40:GLU:OE2	1:I:40:GLU:N	2.45	0.47
1:J:32:ARG:NH1	1:J:109:VAL:HG23	2.30	0.47
1:J:273:GLY:H	1:J:274:ARG:NH2	2.13	0.47
1:B:61:ASP:OD1	1:B:61:ASP:C	2.57	0.47
1:B:227:GLU:HB2	2:B:578:HOH:O	2.15	0.47
1:G:61:ASP:OD1	1:G:61:ASP:C	2.57	0.47
1:G:214:ASN:C	1:G:214:ASN:ND2	2.73	0.47
1:J:47:VAL:CB	1:J:76:MSE:HE1	2.44	0.47
1:D:284:VAL:O	1:D:288:VAL:HG23	2.14	0.47
1:F:296:HIS:C	1:F:298:ASP:H	2.23	0.47
1:A:14:LEU:HD22	1:A:101:LEU:HD11	1.97	0.46
1:A:23:THR:OG1	1:A:24:MSE:HE2	2.15	0.46
1:D:57:LEU:O	1:D:65:ALA:O	2.31	0.46
1:G:111:GLY:N	1:G:137:MSE:HE1	2.27	0.46
1:I:273:GLY:H	1:I:274:ARG:NH2	2.13	0.46
1:I:46:ILE:O	1:I:271:THR:HA	2.15	0.46
1:A:152:ASN:HD22	1:A:154:SER:H	1.62	0.46
1:D:296:HIS:C	1:D:298:ASP:H	2.21	0.46
1:J:214:ASN:C	1:J:214:ASN:ND2	2.73	0.46
1:B:152:ASN:HD22	1:B:154:SER:H	1.63	0.46
1:E:152:ASN:HD22	1:E:154:SER:H	1.62	0.46
1:G:54:ARG:NH2	1:G:150:ARG:HH12	2.12	0.46
1:I:115:ARG:HA	1:I:115:ARG:HD2	1.56	0.46
1:A:115:ARG:HD2	1:A:115:ARG:HA	1.58	0.46
1:C:273:GLY:H	1:C:274:ARG:NH2	2.13	0.46
1:H:54:ARG:HH21	1:H:150:ARG:HH12	1.62	0.46
1:D:15:ARG:HD3	1:D:70:TYR:OH	2.15	0.46
1:E:273:GLY:H	1:E:274:ARG:NH2	2.14	0.46
1:D:115:ARG:HA	1:D:115:ARG:HD2	1.57	0.46
1:E:111:GLY:CA	1:E:137:MSE:HE1	2.45	0.46
1:J:63:GLU:O	1:J:67:ALA:HB2	2.16	0.46
1:B:273:GLY:H	1:B:274:ARG:NH2	2.12	0.46
1:G:151:ILE:HB	1:G:185:MSE:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:152:ASN:HD22	1:J:154:SER:H	1.63	0.46
1:B:111:GLY:CA	1:B:137:MSE:CE	2.93	0.46
1:E:75:ARG:NH2	1:E:278:TYR:HA	2.29	0.46
1:E:89:LEU:HA	1:E:110:VAL:HB	1.97	0.46
1:H:111:GLY:CA	1:H:137:MSE:CE	2.93	0.46
1:I:126:ASP:OD2	1:I:128:ARG:NH1	2.41	0.46
1:D:152:ASN:HD22	1:D:154:SER:H	1.63	0.46
1:G:111:GLY:CA	1:G:137:MSE:CE	2.93	0.46
1:B:46:ILE:O	1:B:271:THR:HA	2.16	0.45
1:B:214:ASN:C	1:B:214:ASN:ND2	2.73	0.45
1:E:151:ILE:HB	1:E:185:MSE:HE1	1.97	0.45
1:F:111:GLY:CA	1:F:137:MSE:CE	2.93	0.45
1:F:146:LYS:HE3	2:F:308:HOH:O	2.16	0.45
1:G:297:THR:OG1	1:G:299:ILE:HG13	2.16	0.45
1:I:24:MSE:HE1	1:I:27:GLU:OE1	2.15	0.45
1:I:151:ILE:HB	1:I:185:MSE:HE1	1.96	0.45
1:F:111:GLY:N	1:F:137:MSE:HE1	2.30	0.45
1:F:152:ASN:HD22	1:F:154:SER:H	1.63	0.45
1:G:115:ARG:HD2	1:G:115:ARG:HA	1.58	0.45
1:G:273:GLY:H	1:G:274:ARG:NH2	2.15	0.45
1:I:214:ASN:C	1:I:214:ASN:ND2	2.74	0.45
1:C:151:ILE:HB	1:C:185:MSE:HE1	1.97	0.45
1:A:214:ASN:C	1:A:214:ASN:ND2	2.73	0.45
1:C:76:MSE:HE3	1:C:277:LEU:HD21	1.98	0.45
1:D:214:ASN:C	1:D:214:ASN:ND2	2.73	0.45
1:F:214:ASN:C	1:F:214:ASN:ND2	2.72	0.45
1:G:68:ASN:ND2	1:G:71:GLU:H	2.15	0.45
1:E:115:ARG:HD2	1:E:115:ARG:HA	1.56	0.45
1:I:284:VAL:O	1:I:288:VAL:HG23	2.17	0.45
1:E:283:ASP:HB3	1:E:286:ALA:HB3	1.99	0.45
1:H:115:ARG:HD2	1:H:115:ARG:HA	1.55	0.45
1:A:33:ARG:HG3	1:A:33:ARG:NH1	2.24	0.45
1:G:75:ARG:HH21	1:G:278:TYR:HA	1.81	0.45
1:H:68:ASN:ND2	1:H:71:GLU:H	2.15	0.45
1:C:41:ASP:OD2	1:C:296:HIS:HD2	2.00	0.45
1:I:68:ASN:ND2	1:I:71:GLU:H	2.15	0.45
1:F:41:ASP:OD2	1:F:296:HIS:CD2	2.61	0.44
1:G:16:ARG:HD2	2:G:489:HOH:O	2.16	0.44
1:G:76:MSE:CE	1:G:277:LEU:HD21	2.47	0.44
1:G:114:ASN:O	1:G:115:ARG:CD	2.65	0.44
1:H:76:MSE:HE2	1:H:277:LEU:HD21	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:HB3	1:A:104:LEU:HD11	1.99	0.44
1:B:151:ILE:HB	1:B:185:MSE:HE1	1.96	0.44
1:D:68:ASN:ND2	1:D:71:GLU:H	2.15	0.44
1:G:110:VAL:HG22	1:G:144:PHE:CB	2.48	0.44
1:J:8:PRO:HG2	1:J:9:GLU:OE1	2.18	0.44
1:C:46:ILE:O	1:C:271:THR:HA	2.17	0.44
1:D:85:VAL:HG23	1:D:107:LYS:NZ	2.32	0.44
1:I:103:LEU:C	1:I:104:LEU:HD12	2.42	0.44
1:A:68:ASN:ND2	1:A:71:GLU:H	2.16	0.44
1:I:111:GLY:N	1:I:137:MSE:HE1	2.33	0.44
1:I:281:ASP:C	1:I:283:ASP:H	2.25	0.44
1:B:40:GLU:OE2	1:B:40:GLU:N	2.46	0.44
1:C:103:LEU:HD22	2:C:522:HOH:O	2.16	0.44
1:J:85:VAL:HG23	1:J:107:LYS:NZ	2.33	0.44
1:D:247:GLY:HA3	2:D:361:HOH:O	2.18	0.44
1:A:63:GLU:HB3	2:H:637:HOH:O	2.16	0.44
1:A:246:GLU:HG2	1:A:247:GLY:N	2.33	0.44
1:B:114:ASN:HD22	1:B:114:ASN:N	1.97	0.44
1:B:159:ALA:HB3	1:B:160:PRO:CD	2.48	0.44
1:F:40:GLU:OE2	1:F:40:GLU:N	2.45	0.44
1:I:296:HIS:C	1:I:298:ASP:N	2.74	0.44
1:F:243:LEU:C	1:F:243:LEU:HD12	2.43	0.43
1:J:159:ALA:HB3	1:J:160:PRO:CD	2.48	0.43
1:A:159:ALA:HB3	1:A:160:PRO:CD	2.49	0.43
1:B:44:LEU:O	1:B:269:GLY:HA3	2.18	0.43
1:C:12:GLU:OE1	1:C:12:GLU:HA	2.18	0.43
1:C:44:LEU:O	1:C:269:GLY:HA3	2.17	0.43
1:C:115:ARG:HD2	1:C:115:ARG:HA	1.57	0.43
1:G:246:GLU:HG2	1:G:247:GLY:N	2.33	0.43
1:D:65:ALA:O	1:D:66:MSE:HB2	2.18	0.43
1:F:75:ARG:NH2	1:F:278:TYR:HA	2.33	0.43
1:G:98:LEU:HB3	1:G:104:LEU:CD1	2.49	0.43
1:J:110:VAL:HG22	1:J:144:PHE:CB	2.48	0.43
1:A:151:ILE:HB	1:A:185:MSE:HE1	1.97	0.43
1:B:68:ASN:ND2	1:B:71:GLU:H	2.15	0.43
1:B:114:ASN:O	1:B:115:ARG:HD2	2.18	0.43
1:B:243:LEU:C	1:B:243:LEU:HD12	2.43	0.43
1:C:89:LEU:HD11	1:C:146:LYS:HG2	2.00	0.43
1:D:114:ASN:O	1:D:115:ARG:HD2	2.17	0.43
1:E:274:ARG:O	1:E:277:LEU:O	2.37	0.43
1:F:68:ASN:ND2	1:F:71:GLU:H	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:ILE:O	1:G:271:THR:HA	2.19	0.43
1:I:85:VAL:HG23	1:I:107:LYS:NZ	2.34	0.43
1:C:65:ALA:O	1:C:66:MSE:HB2	2.19	0.43
1:C:243:LEU:HD12	1:C:243:LEU:C	2.44	0.43
1:G:40:GLU:OE2	1:G:40:GLU:N	2.46	0.43
1:G:243:LEU:HD12	1:G:243:LEU:C	2.44	0.43
1:I:243:LEU:C	1:I:243:LEU:HD12	2.43	0.43
1:J:68:ASN:ND2	1:J:70:TYR:N	2.67	0.43
1:C:158:THR:HB	1:D:123:PHE:CE2	2.54	0.43
1:C:214:ASN:HD22	1:C:215:ASP:N	2.17	0.43
1:F:63:GLU:C	1:F:64:THR:O	2.62	0.43
1:F:184:PHE:O	1:F:185:MSE:HE2	2.19	0.43
1:G:65:ALA:O	1:G:66:MSE:HB2	2.19	0.43
1:I:65:ALA:O	1:I:66:MSE:HB2	2.19	0.43
1:I:159:ALA:HB3	1:I:160:PRO:CD	2.49	0.43
1:I:277:LEU:O	1:I:278:TYR:HB2	2.17	0.43
1:A:46:ILE:HD13	1:A:110:VAL:CG2	2.49	0.43
1:A:63:GLU:C	1:A:64:THR:O	2.62	0.43
1:B:246:GLU:HG2	1:B:247:GLY:N	2.34	0.43
1:D:277:LEU:O	1:D:278:TYR:CB	2.62	0.43
1:H:40:GLU:OE2	1:H:40:GLU:N	2.46	0.43
1:C:125:MSE:CE	1:C:152:ASN:HB2	2.44	0.43
1:E:65:ALA:O	1:E:66:MSE:HB2	2.19	0.43
1:E:243:LEU:HD12	1:E:243:LEU:C	2.43	0.43
1:F:206:VAL:CG1	1:F:236:THR:HG23	2.49	0.43
1:F:236:THR:HG22	2:G:520:HOH:O	2.17	0.43
1:H:65:ALA:O	1:H:66:MSE:HB2	2.19	0.43
1:D:44:LEU:O	1:D:269:GLY:HA3	2.19	0.43
1:D:243:LEU:C	1:D:243:LEU:HD12	2.44	0.43
1:E:159:ALA:HB3	1:E:160:PRO:CD	2.49	0.43
1:E:214:ASN:HD22	1:E:215:ASP:N	2.17	0.43
1:F:159:ALA:HB3	1:F:160:PRO:CD	2.49	0.43
1:G:63:GLU:C	1:G:64:THR:O	2.62	0.43
1:H:243:LEU:HD12	1:H:243:LEU:C	2.43	0.43
1:J:184:PHE:O	1:J:185:MSE:HE2	2.19	0.43
1:J:223:LEU:CD1	1:J:233:MSE:HE1	2.43	0.43
1:A:40:GLU:OE2	1:A:40:GLU:N	2.45	0.43
1:C:68:ASN:ND2	1:C:71:GLU:H	2.16	0.43
1:C:246:GLU:HG2	1:C:247:GLY:N	2.33	0.43
1:E:68:ASN:ND2	1:E:71:GLU:H	2.16	0.43
1:J:243:LEU:HD12	1:J:243:LEU:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ARG:HB2	2:C:313:HOH:O	2.18	0.42
1:C:159:ALA:HB3	1:C:160:PRO:CD	2.49	0.42
1:H:86:ASP:OD2	1:H:296:HIS:HE1	2.02	0.42
1:J:274:ARG:O	1:J:277:LEU:O	2.37	0.42
1:A:65:ALA:O	1:A:66:MSE:HB2	2.19	0.42
1:E:111:GLY:N	1:E:137:MSE:HE1	2.34	0.42
1:H:184:PHE:O	1:H:185:MSE:HE2	2.19	0.42
1:I:214:ASN:HD22	1:I:215:ASP:N	2.17	0.42
1:J:214:ASN:HD22	1:J:215:ASP:N	2.17	0.42
1:F:214:ASN:HD22	1:F:215:ASP:N	2.16	0.42
1:G:194:VAL:O	1:G:194:VAL:HG23	2.20	0.42
1:I:44:LEU:O	1:I:269:GLY:HA3	2.19	0.42
1:J:65:ALA:C	1:J:67:ALA:N	2.74	0.42
1:A:243:LEU:C	1:A:243:LEU:HD12	2.44	0.42
1:C:40:GLU:OE2	1:C:40:GLU:N	2.46	0.42
1:C:184:PHE:O	1:C:185:MSE:HE2	2.19	0.42
1:F:54:ARG:HH21	1:F:150:ARG:HH12	1.66	0.42
1:G:272:VAL:HA	2:G:549:HOH:O	2.19	0.42
1:H:159:ALA:HB3	1:H:160:PRO:CD	2.49	0.42
1:H:214:ASN:HD22	1:H:215:ASP:N	2.18	0.42
1:J:45:PHE:HD2	1:J:85:VAL:HA	1.82	0.42
1:A:214:ASN:HD22	1:A:215:ASP:N	2.17	0.42
1:B:76:MSE:HE3	1:B:277:LEU:HD21	2.00	0.42
1:B:281:ASP:OD2	1:B:281:ASP:C	2.62	0.42
1:D:159:ALA:HB3	1:D:160:PRO:CD	2.50	0.42
1:E:262:LEU:HD12	1:E:262:LEU:HA	1.93	0.42
1:F:125:MSE:CE	1:F:152:ASN:HB2	2.45	0.42
1:H:63:GLU:C	1:H:64:THR:O	2.62	0.42
1:J:28:ARG:HD3	1:J:100:ALA:HA	2.01	0.42
1:B:206:VAL:CG1	1:B:236:THR:HG23	2.50	0.42
1:C:33:ARG:HH11	1:C:33:ARG:CG	2.29	0.42
1:C:114:ASN:O	1:C:115:ARG:HD2	2.20	0.42
1:D:89:LEU:HD12	1:D:90:GLY:N	2.35	0.42
1:D:194:VAL:O	1:D:194:VAL:HG23	2.20	0.42
1:E:63:GLU:C	1:E:64:THR:O	2.62	0.42
1:E:206:VAL:CG1	1:E:236:THR:HG23	2.50	0.42
1:G:214:ASN:HD22	1:G:215:ASP:N	2.17	0.42
1:H:89:LEU:HD12	1:H:90:GLY:N	2.35	0.42
1:H:246:GLU:HG2	1:H:247:GLY:N	2.33	0.42
1:D:46:ILE:O	1:D:271:THR:HA	2.19	0.42
1:D:115:ARG:HB2	2:D:356:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:ILE:O	1:E:271:THR:HA	2.20	0.42
1:E:283:ASP:CG	1:E:286:ALA:HB2	2.45	0.42
1:I:184:PHE:O	1:I:185:MSE:HE2	2.20	0.42
1:J:45:PHE:CD2	1:J:85:VAL:HA	2.55	0.42
1:J:57:LEU:N	1:J:57:LEU:HD22	2.35	0.42
1:J:206:VAL:CG1	1:J:236:THR:HG23	2.50	0.42
1:A:32:ARG:HD2	1:A:104:LEU:HB3	2.01	0.42
1:A:92:PRO:HB2	2:H:468:HOH:O	2.19	0.42
1:A:112:SER:HA	1:A:146:LYS:HG3	2.01	0.42
1:C:194:VAL:O	1:C:194:VAL:HG23	2.20	0.42
1:D:246:GLU:HG2	1:D:247:GLY:N	2.33	0.42
1:F:44:LEU:O	1:F:269:GLY:HA3	2.19	0.42
1:B:65:ALA:O	1:B:66:MSE:HB2	2.19	0.42
1:C:10:SER:O	1:C:13:ALA:HB3	2.20	0.42
1:C:258:TRP:O	1:C:262:LEU:HB2	2.20	0.42
1:D:214:ASN:HD22	1:D:215:ASP:N	2.17	0.42
1:D:223:LEU:CD1	1:D:233:MSE:HE1	2.43	0.42
1:E:40:GLU:OE2	1:E:40:GLU:N	2.46	0.42
1:F:91:THR:HG23	1:F:94:ILE:HG12	2.01	0.42
1:J:47:VAL:HG11	1:J:76:MSE:HE1	2.02	0.42
1:J:194:VAL:O	1:J:194:VAL:HG23	2.20	0.42
1:A:68:ASN:C	1:A:68:ASN:ND2	2.67	0.42
1:A:223:LEU:CD1	1:A:233:MSE:HE1	2.43	0.42
1:G:184:PHE:O	1:G:185:MSE:HE2	2.20	0.42
1:I:206:VAL:CG1	1:I:236:THR:HG23	2.50	0.42
1:J:258:TRP:O	1:J:262:LEU:HB2	2.20	0.42
1:B:114:ASN:N	1:B:114:ASN:ND2	2.68	0.41
1:E:246:GLU:HG2	1:E:247:GLY:N	2.33	0.41
1:F:66:MSE:HG2	1:F:278:TYR:CE2	2.55	0.41
1:G:159:ALA:HB3	1:G:160:PRO:CD	2.50	0.41
1:D:63:GLU:C	1:D:64:THR:O	2.62	0.41
1:E:89:LEU:HD12	1:E:90:GLY:N	2.36	0.41
1:E:258:TRP:O	1:E:262:LEU:HB2	2.20	0.41
1:G:206:VAL:CG1	1:G:236:THR:HG23	2.50	0.41
1:H:194:VAL:O	1:H:194:VAL:HG23	2.19	0.41
1:I:12:GLU:HG3	1:I:16:ARG:NH1	2.21	0.41
1:I:63:GLU:C	1:I:64:THR:O	2.62	0.41
1:J:125:MSE:CE	1:J:152:ASN:HB2	2.44	0.41
1:C:206:VAL:CG1	1:C:236:THR:HG23	2.50	0.41
1:D:184:PHE:O	1:D:185:MSE:HE2	2.20	0.41
1:E:44:LEU:O	1:E:269:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:91:THR:HG23	1:H:94:ILE:HG12	2.03	0.41
1:H:125:MSE:CE	1:H:152:ASN:HB2	2.44	0.41
1:H:206:VAL:CG1	1:H:236:THR:HG23	2.50	0.41
1:I:3:PRO:HA	2:I:486:HOH:O	2.20	0.41
1:A:46:ILE:O	1:A:271:THR:HA	2.20	0.41
1:A:89:LEU:HD12	1:A:90:GLY:N	2.35	0.41
1:B:89:LEU:HD11	1:B:146:LYS:HG2	2.02	0.41
1:D:40:GLU:OE2	1:D:40:GLU:N	2.45	0.41
1:I:152:ASN:ND2	1:I:154:SER:H	2.18	0.41
1:A:98:LEU:HB3	1:A:104:LEU:CD1	2.51	0.41
1:B:214:ASN:HD22	1:B:215:ASP:N	2.18	0.41
1:E:125:MSE:CE	1:E:152:ASN:HB2	2.43	0.41
1:E:184:PHE:O	1:E:185:MSE:HE2	2.20	0.41
1:F:89:LEU:HD12	1:F:90:GLY:N	2.35	0.41
2:F:548:HOH:O	1:G:115:ARG:HB2	2.20	0.41
1:H:33:ARG:NH1	1:H:33:ARG:CG	2.83	0.41
1:I:85:VAL:HG23	1:I:107:LYS:HZ2	1.85	0.41
1:A:184:PHE:O	1:A:185:MSE:HE2	2.20	0.41
1:B:194:VAL:O	1:B:194:VAL:HG23	2.20	0.41
1:C:297:THR:OG1	1:C:299:ILE:HG13	2.20	0.41
1:F:65:ALA:O	1:F:66:MSE:HB2	2.19	0.41
1:G:223:LEU:CD1	1:G:233:MSE:HE1	2.43	0.41
1:H:66:MSE:HG2	1:H:278:TYR:CE2	2.56	0.41
1:J:37:LEU:HD13	1:J:38:LEU:HG	2.02	0.41
1:B:152:ASN:C	1:B:152:ASN:ND2	2.78	0.41
1:C:47:VAL:CB	1:C:76:MSE:HE1	2.50	0.41
1:C:89:LEU:HD12	1:C:90:GLY:N	2.35	0.41
1:I:258:TRP:O	1:I:262:LEU:HB2	2.20	0.41
1:B:125:MSE:CE	1:B:152:ASN:HB2	2.44	0.41
1:D:114:ASN:O	1:D:115:ARG:CD	2.69	0.41
1:G:152:ASN:ND2	1:G:154:SER:H	2.19	0.41
1:A:206:VAL:CG1	1:A:236:THR:HG23	2.50	0.41
1:B:54:ARG:NH2	1:B:150:ARG:HH12	2.18	0.41
1:B:220:TRP:CE3	1:B:239:PRO:HB2	2.56	0.41
1:B:258:TRP:O	1:B:262:LEU:HB2	2.20	0.41
1:C:63:GLU:C	1:C:64:THR:O	2.63	0.41
1:D:206:VAL:CG1	1:D:236:THR:HG23	2.50	0.41
1:E:119:ARG:HD3	2:E:324:HOH:O	2.21	0.41
1:E:223:LEU:CD1	1:E:233:MSE:HE1	2.43	0.41
1:F:46:ILE:O	1:F:271:THR:HA	2.20	0.41
1:F:158:THR:HB	1:G:123:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:LEU:HD12	1:G:90:GLY:N	2.36	0.41
1:G:110:VAL:HG13	1:G:144:PHE:HB3	2.03	0.41
1:J:229:MSE:O	1:J:233:MSE:HG2	2.21	0.41
1:A:258:TRP:O	1:A:262:LEU:HB2	2.21	0.41
1:D:125:MSE:CE	1:D:152:ASN:HB2	2.44	0.41
1:H:47:VAL:CB	1:H:76:MSE:HE1	2.51	0.41
1:I:232:VAL:O	1:I:235:SER:HB2	2.21	0.41
1:A:47:VAL:CB	1:A:76:MSE:HE1	2.51	0.40
1:B:63:GLU:C	1:B:64:THR:O	2.62	0.40
1:B:184:PHE:O	1:B:185:MSE:HE2	2.20	0.40
1:D:47:VAL:CB	1:D:76:MSE:HE1	2.51	0.40
1:F:152:ASN:ND2	1:F:154:SER:H	2.19	0.40
1:G:258:TRP:O	1:G:262:LEU:HB2	2.20	0.40
1:I:33:ARG:NH1	1:I:33:ARG:CG	2.84	0.40
1:I:89:LEU:HD11	1:I:146:LYS:HG2	2.03	0.40
1:A:220:TRP:CE3	1:A:239:PRO:HB2	2.56	0.40
1:B:47:VAL:CB	1:B:76:MSE:HE1	2.51	0.40
1:C:220:TRP:CE3	1:C:239:PRO:HB2	2.56	0.40
1:D:297:THR:C	1:D:299:ILE:N	2.78	0.40
1:G:101:LEU:HD12	1:G:101:LEU:HA	1.91	0.40
1:H:114:ASN:ND2	1:H:147:THR:HG23	2.37	0.40
1:H:220:TRP:CE3	1:H:239:PRO:HB2	2.57	0.40
1:I:12:GLU:OE1	1:I:16:ARG:NH2	2.55	0.40
1:J:105:ASP:O	1:J:107:LYS:HG2	2.20	0.40
1:A:83:PRO:HG2	2:A:319:HOH:O	2.22	0.40
1:B:115:ARG:HD2	1:B:115:ARG:HA	1.57	0.40
1:C:110:VAL:HG13	1:C:144:PHE:HB3	2.02	0.40
1:E:194:VAL:O	1:E:194:VAL:HG23	2.20	0.40
1:G:33:ARG:HH11	1:G:33:ARG:CG	2.29	0.40
1:G:98:LEU:HB3	1:G:104:LEU:HD11	2.03	0.40
1:A:75:ARG:NH2	1:A:278:TYR:HA	2.37	0.40
1:A:296:HIS:C	1:A:298:ASP:N	2.79	0.40
1:I:281:ASP:O	1:I:283:ASP:N	2.54	0.40
1:J:129:TYR:OH	1:J:147:THR:CG2	2.70	0.40
1:B:47:VAL:HB	1:B:76:MSE:HE1	2.03	0.40
1:B:89:LEU:HD12	1:B:90:GLY:N	2.36	0.40
1:C:229:MSE:O	1:C:233:MSE:HG2	2.22	0.40
1:D:258:TRP:O	1:D:262:LEU:HB2	2.21	0.40
1:E:95:ILE:HD12	1:E:109:VAL:HG13	2.03	0.40
1:E:220:TRP:CE3	1:E:239:PRO:HB2	2.57	0.40
1:F:194:VAL:O	1:F:194:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:258:TRP:O	1:H:262:LEU:HB2	2.21	0.40
1:J:94:ILE:HD13	1:J:94:ILE:HA	1.98	0.40
1:J:115:ARG:HA	1:J:115:ARG:HD2	1.56	0.40
1:J:246:GLU:HG2	1:J:247:GLY:N	2.33	0.40

There are no symmetry-related clashes.

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	291/307 (95%)	266 (91%)	19 (6%)	6 (2%)	5	9
1	B	291/307 (95%)	269 (92%)	17 (6%)	5 (2%)	7	13
1	C	291/307 (95%)	269 (92%)	17 (6%)	5 (2%)	7	13
1	D	291/307 (95%)	266 (91%)	18 (6%)	7 (2%)	4	8
1	E	291/307 (95%)	267 (92%)	19 (6%)	5 (2%)	7	13
1	F	291/307 (95%)	266 (91%)	19 (6%)	6 (2%)	5	9
1	G	291/307 (95%)	268 (92%)	18 (6%)	5 (2%)	7	13
1	H	291/307 (95%)	266 (91%)	19 (6%)	6 (2%)	5	9
1	I	291/307 (95%)	268 (92%)	16 (6%)	7 (2%)	4	8
1	J	291/307 (95%)	265 (91%)	19 (6%)	7 (2%)	4	8
All	All	2910/3070 (95%)	2670 (92%)	181 (6%)	59 (2%)	6	10

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	B	64	THR
1	C	64	THR

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Mol	Chain	Res	Type
1	D	64	THR
1	D	298	ASP
1	E	64	THR
1	F	64	THR
1	G	64	THR
1	H	64	THR
1	I	64	THR
1	J	62	ASN
1	A	62	ASN
1	A	63	GLU
1	A	245	GLY
1	B	62	ASN
1	B	63	GLU
1	B	245	GLY
1	C	62	ASN
1	C	63	GLU
1	C	245	GLY
1	D	62	ASN
1	D	63	GLU
1	D	245	GLY
1	E	62	ASN
1	E	63	GLU
1	E	245	GLY
1	F	62	ASN
1	F	63	GLU
1	F	245	GLY
1	G	62	ASN
1	G	63	GLU
1	G	245	GLY
1	H	62	ASN
1	H	63	GLU
1	H	245	GLY
1	I	62	ASN
1	I	63	GLU
1	I	245	GLY
1	I	282	GLY
1	I	297	THR
1	J	245	GLY
1	A	297	THR
1	D	297	THR
1	F	297	THR
1	J	59	VAL

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Mol	Chain	Res	Type
1	J	297	THR
1	A	60	GLY
1	B	60	GLY
1	C	60	GLY
1	D	60	GLY
1	E	60	GLY
1	F	60	GLY
1	G	60	GLY
1	H	60	GLY
1	H	297	THR
1	I	60	GLY
1	J	63	GLU
1	J	65	ALA
1	J	60	GLY

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	230/229 (100%)	208 (90%)	22 (10%)	8	17
1	B	230/229 (100%)	206 (90%)	24 (10%)	7	14
1	C	230/229 (100%)	206 (90%)	24 (10%)	7	14
1	D	230/229 (100%)	206 (90%)	24 (10%)	7	14
1	E	230/229 (100%)	207 (90%)	23 (10%)	7	15
1	F	230/229 (100%)	207 (90%)	23 (10%)	7	15
1	G	230/229 (100%)	207 (90%)	23 (10%)	7	15
1	H	230/229 (100%)	206 (90%)	24 (10%)	7	14
1	I	230/229 (100%)	209 (91%)	21 (9%)	9	19
1	J	230/229 (100%)	206 (90%)	24 (10%)	7	14
All	All	2300/2290 (100%)	2068 (90%)	232 (10%)	7	15

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	61	ASP
1	A	68	ASN
1	A	72	LEU
1	A	74	GLU
1	A	76	MSE
1	A	91	THR
1	A	101	LEU
1	A	114	ASN
1	A	115	ARG
1	A	144	PHE
1	A	146	LYS
1	A	148	LEU
1	A	152	ASN
1	A	214	ASN
1	A	216	SER
1	A	219	THR
1	A	262	LEU
1	A	264	LEU
1	A	270	LEU
1	A	274	ARG
1	A	299	ILE
1	B	37	LEU
1	B	61	ASP
1	B	68	ASN
1	B	72	LEU
1	B	74	GLU
1	B	76	MSE
1	B	91	THR
1	B	101	LEU
1	B	104	LEU
1	B	114	ASN
1	B	115	ARG
1	B	144	PHE
1	B	146	LYS
1	B	148	LEU
1	B	152	ASN
1	B	214	ASN
1	B	216	SER
1	B	219	THR
1	B	262	LEU
1	B	264	LEU
1	B	270	LEU

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Mol	Chain	Res	Type
1	B	274	ARG
1	B	294	LEU
1	B	299	ILE
1	C	37	LEU
1	C	61	ASP
1	C	68	ASN
1	C	72	LEU
1	C	74	GLU
1	C	76	MSE
1	C	91	THR
1	C	101	LEU
1	C	104	LEU
1	C	114	ASN
1	C	115	ARG
1	C	144	PHE
1	C	146	LYS
1	C	148	LEU
1	C	152	ASN
1	C	214	ASN
1	C	216	SER
1	C	219	THR
1	C	262	LEU
1	C	264	LEU
1	C	270	LEU
1	C	274	ARG
1	C	280	GLN
1	C	294	LEU
1	D	37	LEU
1	D	61	ASP
1	D	68	ASN
1	D	72	LEU
1	D	74	GLU
1	D	76	MSE
1	D	91	THR
1	D	101	LEU
1	D	104	LEU
1	D	114	ASN
1	D	115	ARG
1	D	144	PHE
1	D	146	LYS
1	D	148	LEU
1	D	152	ASN

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Mol	Chain	Res	Type
1	D	214	ASN
1	D	216	SER
1	D	219	THR
1	D	262	LEU
1	D	264	LEU
1	D	270	LEU
1	D	274	ARG
1	D	280	GLN
1	D	294	LEU
1	E	37	LEU
1	E	61	ASP
1	E	68	ASN
1	E	72	LEU
1	E	74	GLU
1	E	76	MSE
1	E	91	THR
1	E	101	LEU
1	E	104	LEU
1	E	114	ASN
1	E	115	ARG
1	E	144	PHE
1	E	146	LYS
1	E	148	LEU
1	E	152	ASN
1	E	214	ASN
1	E	216	SER
1	E	219	THR
1	E	262	LEU
1	E	264	LEU
1	E	270	LEU
1	E	274	ARG
1	E	299	ILE
1	F	37	LEU
1	F	61	ASP
1	F	68	ASN
1	F	72	LEU
1	F	74	GLU
1	F	76	MSE
1	F	91	THR
1	F	101	LEU
1	F	104	LEU
1	F	114	ASN

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Mol	Chain	Res	Type
1	F	115	ARG
1	F	144	PHE
1	F	146	LYS
1	F	148	LEU
1	F	152	ASN
1	F	214	ASN
1	F	216	SER
1	F	219	THR
1	F	262	LEU
1	F	264	LEU
1	F	270	LEU
1	F	274	ARG
1	F	283	ASP
1	G	37	LEU
1	G	61	ASP
1	G	68	ASN
1	G	72	LEU
1	G	74	GLU
1	G	76	MSE
1	G	91	THR
1	G	101	LEU
1	G	114	ASN
1	G	115	ARG
1	G	144	PHE
1	G	146	LYS
1	G	148	LEU
1	G	152	ASN
1	G	214	ASN
1	G	216	SER
1	G	219	THR
1	G	262	LEU
1	G	264	LEU
1	G	270	LEU
1	G	274	ARG
1	G	276	LEU
1	G	294	LEU
1	H	9	GLU
1	H	37	LEU
1	H	61	ASP
1	H	68	ASN
1	H	72	LEU
1	H	74	GLU

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Mol	Chain	Res	Type
1	H	76	MSE
1	H	91	THR
1	H	101	LEU
1	H	104	LEU
1	H	114	ASN
1	H	115	ARG
1	H	144	PHE
1	H	146	LYS
1	H	148	LEU
1	H	152	ASN
1	H	214	ASN
1	H	216	SER
1	H	219	THR
1	H	262	LEU
1	H	264	LEU
1	H	270	LEU
1	H	274	ARG
1	H	294	LEU
1	I	37	LEU
1	I	61	ASP
1	I	68	ASN
1	I	72	LEU
1	I	74	GLU
1	I	76	MSE
1	I	91	THR
1	I	114	ASN
1	I	115	ARG
1	I	144	PHE
1	I	146	LYS
1	I	148	LEU
1	I	152	ASN
1	I	214	ASN
1	I	216	SER
1	I	219	THR
1	I	262	LEU
1	I	264	LEU
1	I	270	LEU
1	I	274	ARG
1	I	281	ASP
1	J	33	ARG
1	J	37	LEU
1	J	47	VAL

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Mol	Chain	Res	Type
1	J	57	LEU
1	J	68	ASN
1	J	74	GLU
1	J	76	MSE
1	J	88	VAL
1	J	89	LEU
1	J	91	THR
1	J	104	LEU
1	J	114	ASN
1	J	115	ARG
1	J	144	PHE
1	J	146	LYS
1	J	148	LEU
1	J	152	ASN
1	J	214	ASN
1	J	216	SER
1	J	219	THR
1	J	262	LEU
1	J	264	LEU
1	J	270	LEU
1	J	274	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	68	ASN
1	A	114	ASN
1	A	152	ASN
1	A	170	ASN
1	A	187	ASN
1	A	190	ASN
1	A	204	GLN
1	A	214	ASN
1	A	280	GLN
1	A	296	HIS
1	B	68	ASN
1	B	114	ASN
1	B	152	ASN
1	B	167	HIS
1	B	170	ASN
1	B	176	GLN

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Mol	Chain	Res	Type
1	B	187	ASN
1	B	190	ASN
1	B	204	GLN
1	B	214	ASN
1	B	280	GLN
1	B	296	HIS
1	C	31	GLN
1	C	68	ASN
1	C	114	ASN
1	C	152	ASN
1	C	170	ASN
1	C	176	GLN
1	C	187	ASN
1	C	204	GLN
1	C	214	ASN
1	C	280	GLN
1	C	296	HIS
1	D	31	GLN
1	D	68	ASN
1	D	114	ASN
1	D	152	ASN
1	D	170	ASN
1	D	176	GLN
1	D	190	ASN
1	D	204	GLN
1	D	214	ASN
1	D	296	HIS
1	E	31	GLN
1	E	68	ASN
1	E	114	ASN
1	E	152	ASN
1	E	170	ASN
1	E	176	GLN
1	E	187	ASN
1	E	190	ASN
1	E	204	GLN
1	E	214	ASN
1	E	260	HIS
1	E	280	GLN
1	E	296	HIS
1	F	31	GLN
1	F	68	ASN

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Mol	Chain	Res	Type
1	F	114	ASN
1	F	152	ASN
1	F	170	ASN
1	F	176	GLN
1	F	187	ASN
1	F	190	ASN
1	F	204	GLN
1	F	214	ASN
1	F	260	HIS
1	F	280	GLN
1	F	296	HIS
1	G	31	GLN
1	G	68	ASN
1	G	114	ASN
1	G	152	ASN
1	G	170	ASN
1	G	176	GLN
1	G	204	GLN
1	G	214	ASN
1	G	280	GLN
1	G	296	HIS
1	H	31	GLN
1	H	68	ASN
1	H	114	ASN
1	H	152	ASN
1	H	167	HIS
1	H	170	ASN
1	H	176	GLN
1	H	190	ASN
1	H	204	GLN
1	H	214	ASN
1	H	280	GLN
1	H	296	HIS
1	I	31	GLN
1	I	68	ASN
1	I	114	ASN
1	I	152	ASN
1	I	170	ASN
1	I	176	GLN
1	I	204	GLN
1	I	214	ASN
1	I	280	GLN

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Mol	Chain	Res	Type
1	I	296	HIS
1	J	31	GLN
1	J	62	ASN
1	J	68	ASN
1	J	114	ASN
1	J	152	ASN
1	J	170	ASN
1	J	176	GLN
1	J	190	ASN
1	J	204	GLN
1	J	214	ASN
1	J	260	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 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	282/307 (91%)	0.45	19 (6%)	24	21	10, 23, 47, 62	0
1	B	282/307 (91%)	0.40	20 (7%)	22	19	12, 22, 43, 65	0
1	C	282/307 (91%)	0.42	22 (7%)	19	17	10, 23, 43, 61	0
1	D	282/307 (91%)	0.54	27 (9%)	13	11	12, 23, 45, 67	0
1	E	282/307 (91%)	0.51	22 (7%)	19	17	11, 24, 48, 65	0
1	F	282/307 (91%)	0.47	18 (6%)	25	22	12, 25, 48, 66	0
1	G	282/307 (91%)	0.44	21 (7%)	20	18	13, 26, 45, 67	0
1	H	282/307 (91%)	0.56	29 (10%)	12	10	11, 24, 45, 70	0
1	I	282/307 (91%)	0.65	18 (6%)	25	22	13, 27, 51, 73	0
1	J	282/307 (91%)	0.54	21 (7%)	20	18	12, 29, 51, 68	0
All	All	2820/3070 (91%)	0.50	217 (7%)	19	17	10, 24, 49, 73	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	ILE	10.3
1	H	282	GLY	7.5
1	A	282	GLY	6.9
1	D	282	GLY	6.9
1	H	299	ILE	6.8
1	E	299	ILE	6.8
1	D	64	THR	6.7
1	A	64	THR	6.5
1	A	60	GLY	6.5
1	B	248	GLY	6.5
1	A	299	ILE	6.4
1	J	248	GLY	6.2
1	C	64	THR	6.1

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Mol	Chain	Res	Type	RSRZ
1	H	64	THR	6.1
1	C	248	GLY	6.0
1	B	64	THR	6.0
1	B	63	GLU	6.0
1	H	63	GLU	5.9
1	C	299	ILE	5.7
1	I	299	ILE	5.7
1	F	63	GLU	5.7
1	B	60	GLY	5.6
1	D	60	GLY	5.5
1	D	248	GLY	5.5
1	B	282	GLY	5.4
1	H	60	GLY	5.4
1	H	248	GLY	5.3
1	I	64	THR	5.3
1	F	299	ILE	5.2
1	G	64	THR	5.2
1	C	63	GLU	5.2
1	D	299	ILE	5.1
1	D	28	ARG	5.1
1	H	216	SER	5.0
1	D	63	GLU	5.0
1	G	299	ILE	5.0
1	J	64	THR	4.9
1	C	246	GLU	4.9
1	B	247	GLY	4.9
1	E	60	GLY	4.9
1	F	64	THR	4.8
1	E	282	GLY	4.8
1	D	65	ALA	4.8
1	G	248	GLY	4.8
1	D	246	GLU	4.7
1	H	29	PHE	4.7
1	F	282	GLY	4.6
1	C	247	GLY	4.6
1	A	248	GLY	4.6
1	B	216	SER	4.6
1	C	216	SER	4.5
1	B	244	GLY	4.5
1	F	248	GLY	4.5
1	J	282	GLY	4.5
1	I	216	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	H	33	ARG	4.5
1	E	216	SER	4.4
1	C	60	GLY	4.4
1	J	60	GLY	4.3
1	F	230	GLU	4.3
1	J	65	ALA	4.3
1	D	216	SER	4.3
1	F	216	SER	4.3
1	D	247	GLY	4.2
1	C	65	ALA	4.2
1	J	216	SER	4.2
1	I	230	GLU	4.2
1	A	247	GLY	4.2
1	J	299	ILE	4.1
1	G	247	GLY	4.0
1	H	251	PRO	4.0
1	B	251	PRO	4.0
1	I	251	PRO	4.0
1	F	60	GLY	4.0
1	C	244	GLY	3.9
1	E	64	THR	3.9
1	G	246	GLU	3.8
1	D	29	PHE	3.8
1	J	247	GLY	3.8
1	A	65	ALA	3.8
1	E	244	GLY	3.8
1	A	216	SER	3.7
1	C	251	PRO	3.7
1	G	60	GLY	3.7
1	E	280	GLN	3.7
1	A	63	GLU	3.6
1	I	248	GLY	3.6
1	E	248	GLY	3.6
1	I	60	GLY	3.6
1	A	244	GLY	3.6
1	J	251	PRO	3.6
1	E	61	ASP	3.6
1	D	30	LYS	3.5
1	B	65	ALA	3.5
1	A	246	GLU	3.5
1	H	246	GLU	3.5
1	G	251	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	246	GLU	3.4
1	D	61	ASP	3.4
1	F	251	PRO	3.4
1	J	246	GLU	3.4
1	G	63	GLU	3.4
1	E	63	GLU	3.3
1	I	63	GLU	3.3
1	H	65	ALA	3.3
1	G	65	ALA	3.3
1	E	251	PRO	3.2
1	I	3	PRO	3.2
1	B	62	ASN	3.2
1	J	63	GLU	3.2
1	I	244	GLY	3.2
1	C	62	ASN	3.2
1	H	244	GLY	3.2
1	B	230	GLU	3.1
1	C	3	PRO	3.1
1	D	251	PRO	3.1
1	C	298	ASP	3.1
1	G	190	ASN	3.1
1	C	245	GLY	3.1
1	F	247	GLY	3.1
1	F	65	ALA	3.0
1	A	251	PRO	3.0
1	C	230	GLU	3.0
1	D	62	ASN	3.0
1	H	62	ASN	3.0
1	E	246	GLU	3.0
1	H	230	GLU	3.0
1	C	190	ASN	3.0
1	E	65	ALA	2.9
1	A	230	GLU	2.9
1	F	40	GLU	2.9
1	F	246	GLU	2.9
1	D	230	GLU	2.9
1	B	190	ASN	2.9
1	I	247	GLY	2.9
1	H	26	ALA	2.9
1	E	40	GLU	2.9
1	D	140	ARG	2.8
1	A	61	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	62	ASN	2.8
1	G	216	SER	2.7
1	B	59	VAL	2.7
1	C	61	ASP	2.7
1	H	61	ASP	2.7
1	B	61	ASP	2.7
1	D	244	GLY	2.7
1	E	62	ASN	2.7
1	H	247	GLY	2.6
1	G	226	VAL	2.6
1	I	297	THR	2.6
1	A	298	ASP	2.6
1	J	190	ASN	2.6
1	D	3	PRO	2.6
1	J	294	LEU	2.6
1	A	59	VAL	2.6
1	J	62	ASN	2.6
1	H	34	LYS	2.5
1	G	36	GLU	2.5
1	I	298	ASP	2.5
1	D	26	ALA	2.5
1	H	27	GLU	2.5
1	J	244	GLY	2.5
1	C	59	VAL	2.5
1	G	245	GLY	2.4
1	E	298	ASP	2.4
1	A	280	GLN	2.4
1	I	65	ALA	2.4
1	C	21	GLU	2.4
1	H	40	GLU	2.4
1	D	31	GLN	2.4
1	E	230	GLU	2.4
1	B	245	GLY	2.4
1	F	253	ALA	2.4
1	G	230	GLU	2.4
1	G	61	ASP	2.3
1	I	61	ASP	2.3
1	I	246	GLU	2.3
1	J	230	GLU	2.3
1	A	40	GLU	2.3
1	A	62	ASN	2.3
1	G	244	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	139	ASP	2.3
1	D	190	ASN	2.3
1	J	3	PRO	2.3
1	H	275	THR	2.3
1	C	277	LEU	2.3
1	F	61	ASP	2.3
1	J	298	ASP	2.3
1	D	59	VAL	2.3
1	F	280	GLN	2.2
1	E	235	SER	2.2
1	B	298	ASP	2.2
1	G	298	ASP	2.2
1	G	40	GLU	2.2
1	C	226	VAL	2.2
1	E	36	GLU	2.1
1	E	3	PRO	2.1
1	G	62	ASN	2.1
1	F	244	GLY	2.1
1	B	40	GLU	2.1
1	J	274	ARG	2.1
1	G	3	PRO	2.1
1	I	253	ALA	2.1
1	H	298	ASP	2.1
1	H	59	VAL	2.1
1	I	59	VAL	2.1
1	J	276	LEU	2.1
1	D	36	GLU	2.1
1	H	252	ASP	2.1
1	E	59	VAL	2.0
1	D	27	GLU	2.0
1	H	297	THR	2.0
1	D	252	ASP	2.0
1	H	280	GLN	2.0
1	J	226	VAL	2.0
1	H	277	LEU	2.0
1	E	252	ASP	2.0

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

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.