



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:51 PM UTC

PDB ID : 4BWY / pdb_00004bwy
Title : P4 PROTEIN FROM BACTERIOPHAGE PHI8 (R32)
Authors : El Omari, K.; Meier, C.; Kainov, D.; Sutton, G.; Grimes, J.M.; Poranen, M.M.; Bamford, D.H.; Tuma, R.; Stuart, D.I.; Mancini, E.J.
Deposited on : 2013-07-05
Resolution : 3.10 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

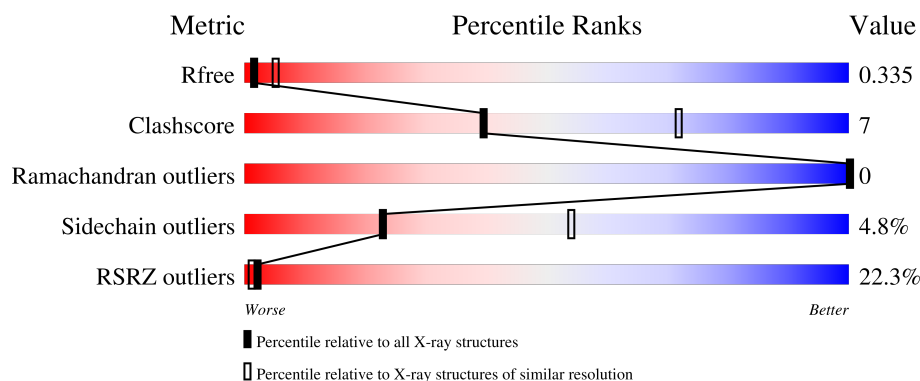
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	321	10% 76% 12% • 10%
1	B	321	17% 76% 13% • 10%
1	C	321	16% 75% 13% • 10%
1	D	321	31% 75% 13% • 10%
1	E	321	27% 69% 12% • 18%

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Mol	Chain	Length	Quality of chain
1	F	321	
1	G	321	
1	H	321	
1	I	321	
1	J	321	
1	K	321	
1	L	321	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25719 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.

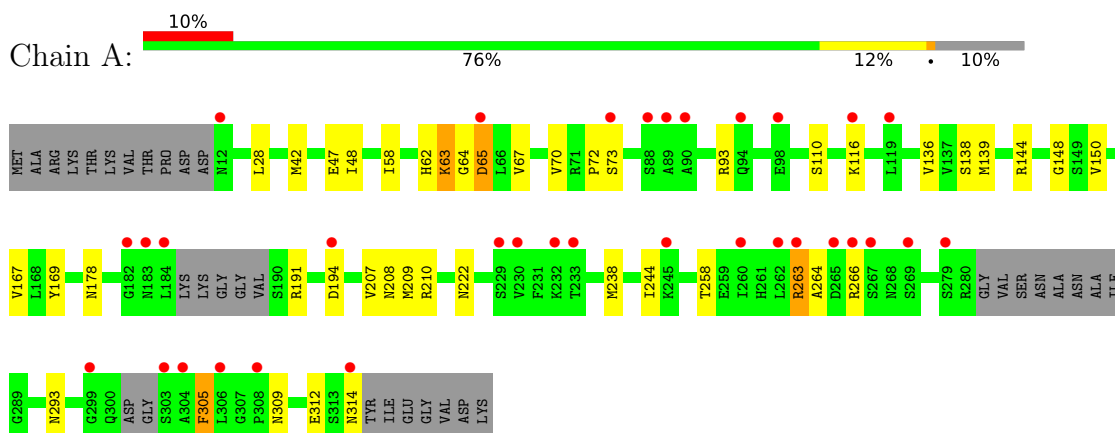
- Molecule 1 is a protein called P4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	B	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	C	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	D	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	E	264	Total	C	N	O	S	0	0	0
			1981	1233	357	381	10			
1	F	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	G	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	H	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	I	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	J	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	K	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			
1	L	288	Total	C	N	O	S	0	0	0
			2158	1347	386	415	10			

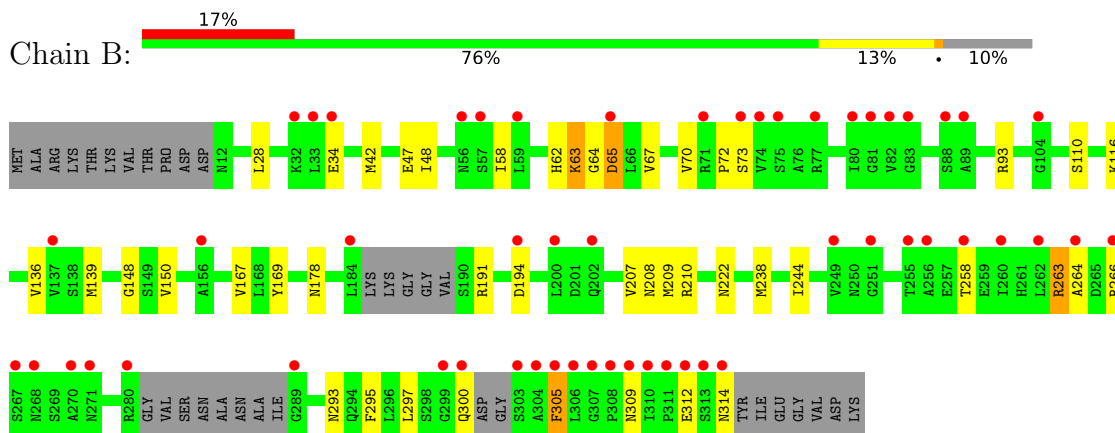
3 Residue-property plots [i](#)

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.

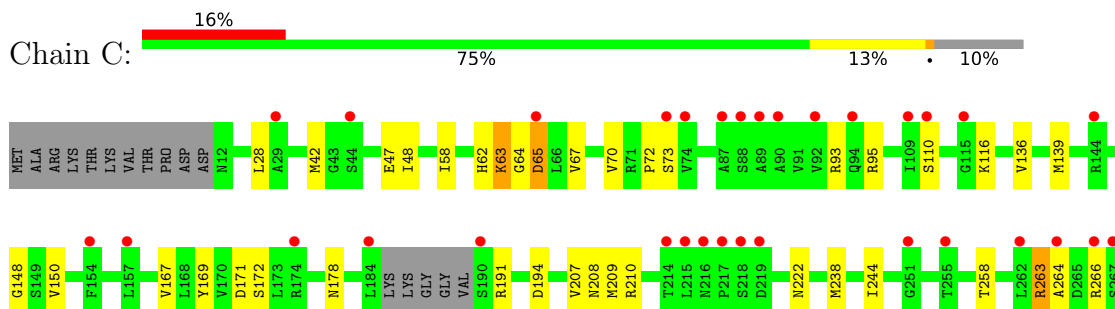
• Molecule 1: P4



• Molecule 1: P4

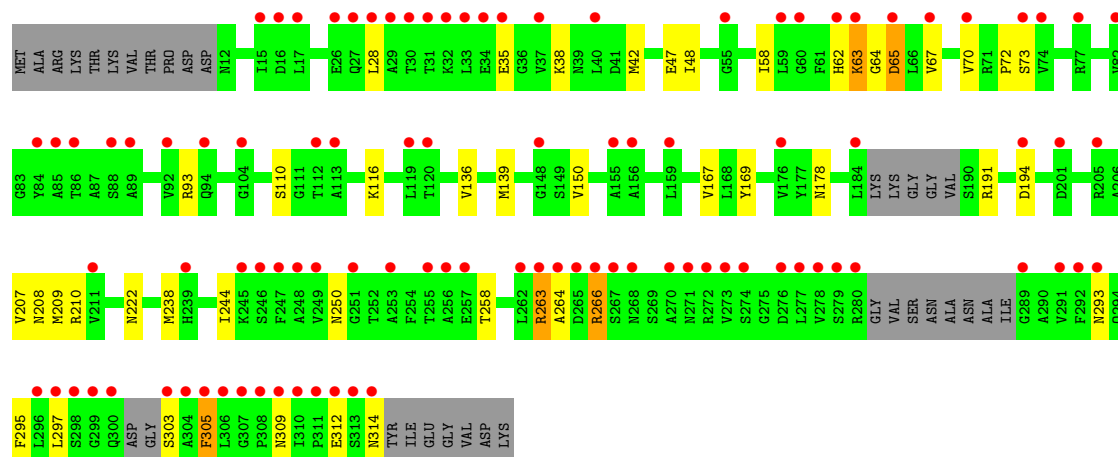
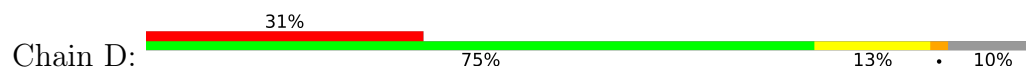


• Molecule 1: P4

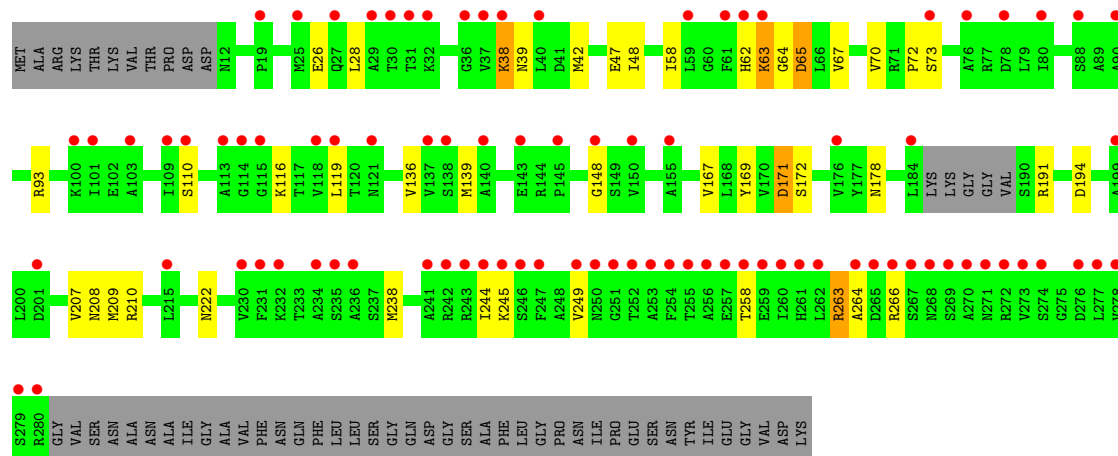




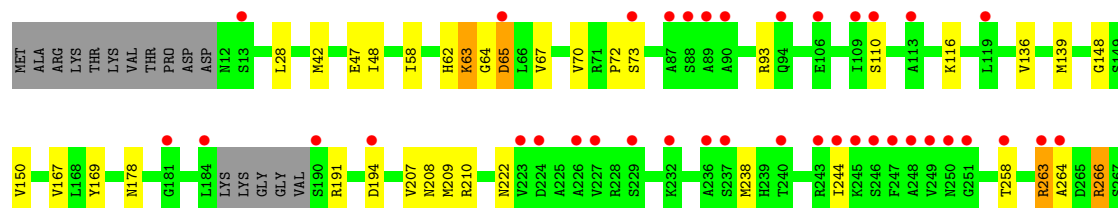
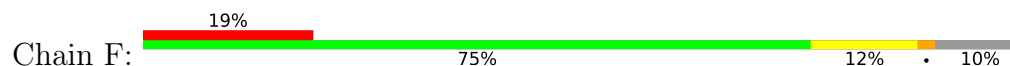
• Molecule 1: P4



• Molecule 1: P4

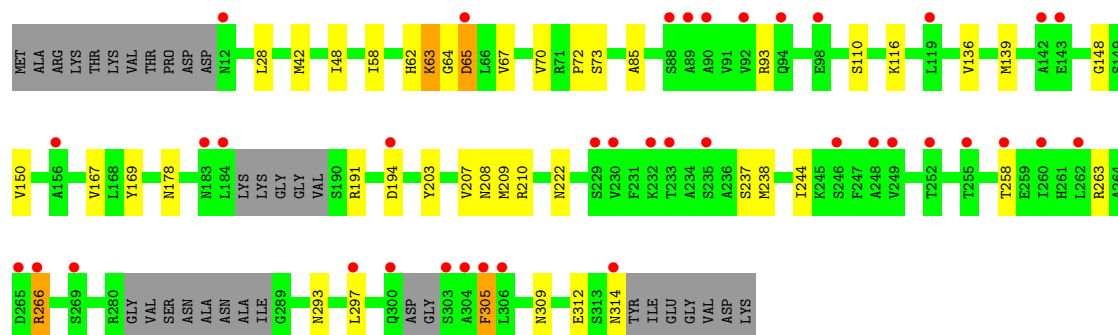
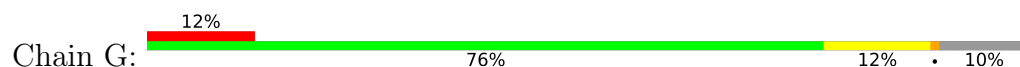


• Molecule 1: P4

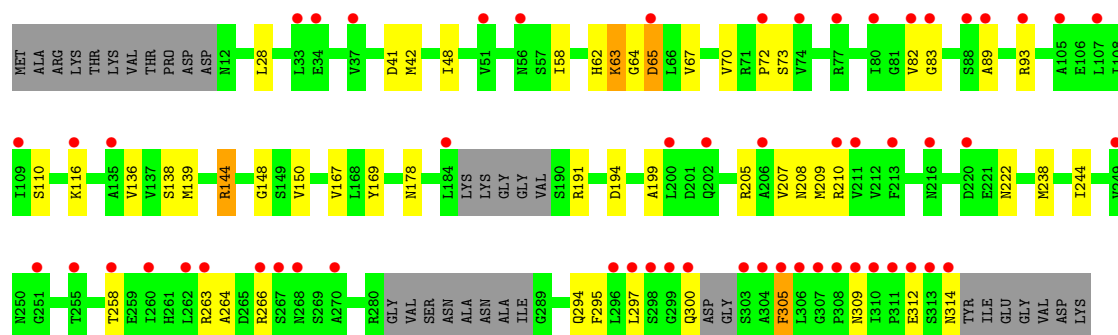
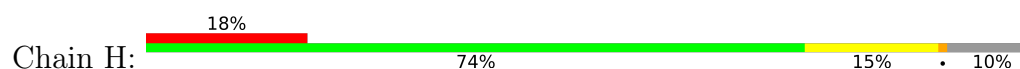




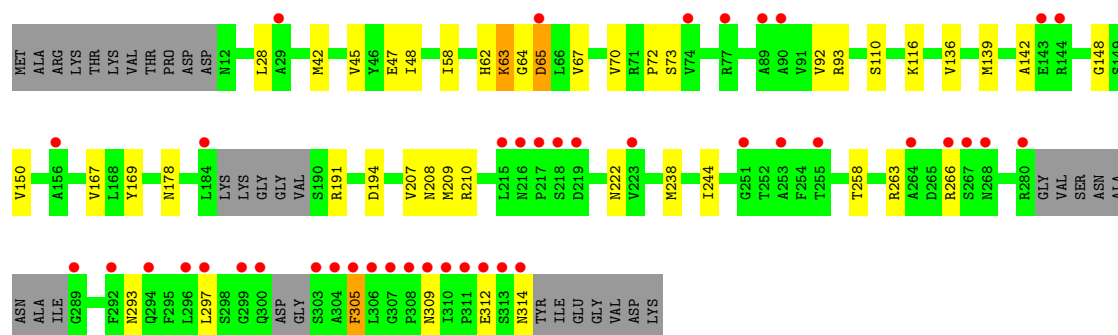
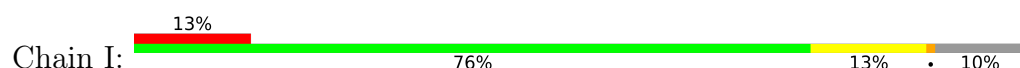
• Molecule 1: P4



• Molecule 1: P4

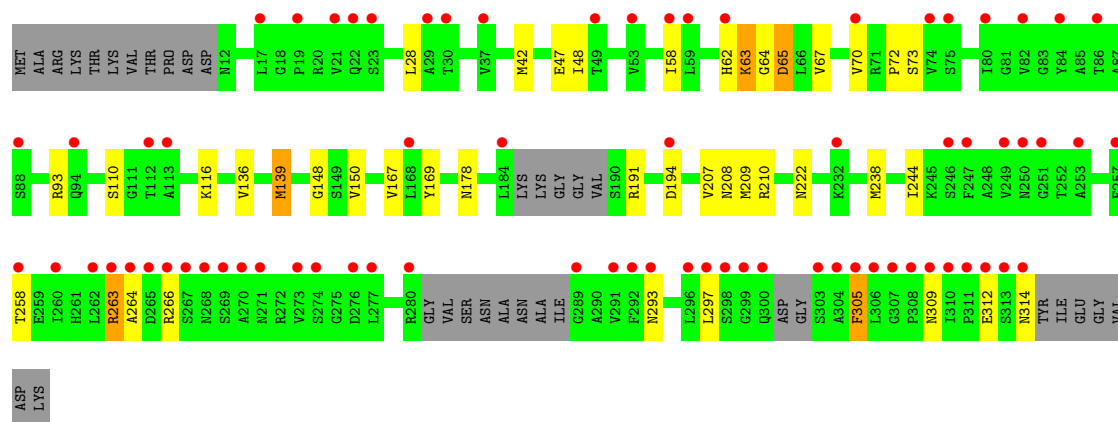


• Molecule 1: P4

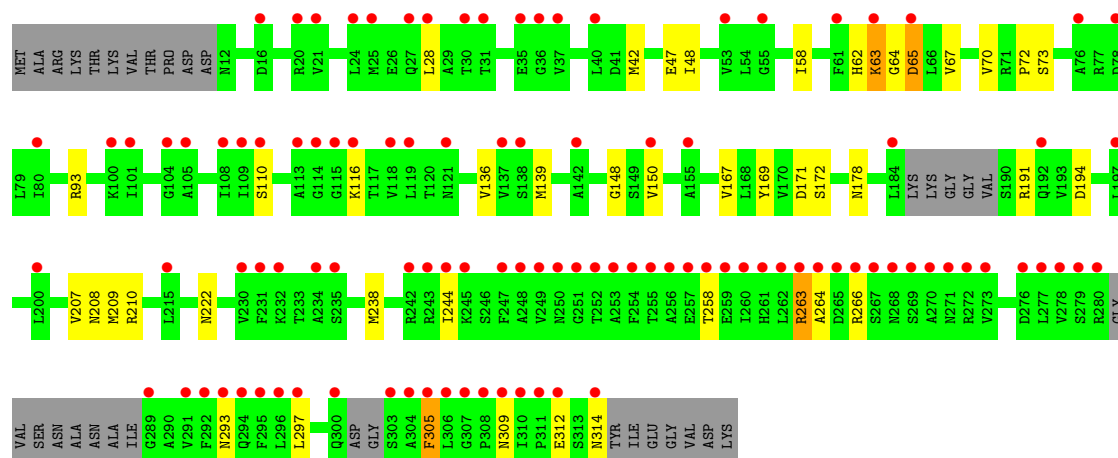
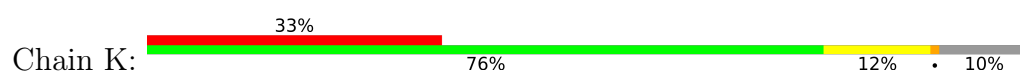


• Molecule 1: P4

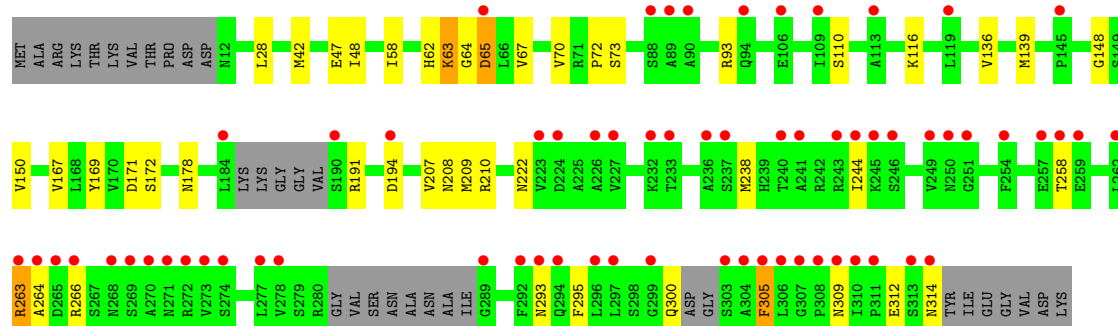
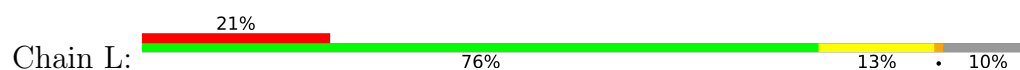




• Molecule 1: P4



• Molecule 1: P4



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	197.72Å 197.72Å 562.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.39 – 3.10 45.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.39-3.10) 99.8 (45.39-3.10)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.12Å)	Xtrriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.295 , 0.309 0.319 , 0.335	Depositor DCC
R_{free} test set	3870 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	25719	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3095e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.73	0/2183	1.32	9/2951 (0.3%)
1	B	0.74	0/2183	1.33	9/2951 (0.3%)
1	C	0.74	0/2183	1.32	9/2951 (0.3%)
1	D	0.75	0/2183	1.33	11/2951 (0.4%)
1	E	0.76	1/2003 (0.0%)	1.33	7/2709 (0.3%)
1	F	0.74	0/2183	1.32	9/2951 (0.3%)
1	G	0.73	0/2183	1.33	9/2951 (0.3%)
1	H	0.74	0/2183	1.33	7/2951 (0.2%)
1	I	0.74	0/2183	1.33	9/2951 (0.3%)
1	J	0.75	0/2183	1.32	11/2951 (0.4%)
1	K	0.75	0/2183	1.33	9/2951 (0.3%)
1	L	0.74	0/2183	1.32	9/2951 (0.3%)
All	All	0.74	1/26016 (0.0%)	1.33	108/35170 (0.3%)

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	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	249	VAL	C-N	5.54	1.44	1.34

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	305	PHE	CA-CB-CG	6.81	120.61	113.80
1	I	305	PHE	CA-CB-CG	6.77	120.57	113.80
1	A	305	PHE	CA-CB-CG	6.76	120.56	113.80
1	C	305	PHE	CA-CB-CG	6.75	120.55	113.80
1	K	305	PHE	CA-CB-CG	6.73	120.53	113.80
1	F	305	PHE	CA-CB-CG	6.72	120.52	113.80
1	G	305	PHE	CA-CB-CG	6.71	120.51	113.80
1	B	305	PHE	CA-CB-CG	6.70	120.50	113.80
1	D	305	PHE	CA-CB-CG	6.69	120.49	113.80
1	H	305	PHE	CA-CB-CG	6.68	120.48	113.80
1	L	305	PHE	CA-CB-CG	6.67	120.47	113.80
1	B	178	ASN	CA-C-N	5.59	127.78	120.28
1	B	178	ASN	C-N-CA	5.59	127.78	120.28
1	A	178	ASN	CA-C-N	5.54	127.71	120.28
1	A	178	ASN	C-N-CA	5.54	127.71	120.28
1	E	178	ASN	CA-C-N	5.53	127.69	120.28
1	E	178	ASN	C-N-CA	5.53	127.69	120.28
1	J	178	ASN	CA-C-N	5.53	127.69	120.28
1	J	178	ASN	C-N-CA	5.53	127.69	120.28
1	H	178	ASN	CA-C-N	5.53	127.69	120.28
1	H	178	ASN	C-N-CA	5.53	127.69	120.28
1	I	178	ASN	CA-C-N	5.52	127.67	120.28
1	I	178	ASN	C-N-CA	5.52	127.67	120.28
1	K	178	ASN	CA-C-N	5.52	127.67	120.28
1	K	178	ASN	C-N-CA	5.52	127.67	120.28
1	G	178	ASN	CA-C-N	5.51	127.66	120.28
1	G	178	ASN	C-N-CA	5.51	127.66	120.28
1	D	178	ASN	CA-C-N	5.48	127.62	120.28
1	D	178	ASN	C-N-CA	5.48	127.62	120.28
1	F	178	ASN	CA-C-N	5.47	127.61	120.28
1	F	178	ASN	C-N-CA	5.47	127.61	120.28
1	L	178	ASN	CA-C-N	5.45	127.59	120.28
1	L	178	ASN	C-N-CA	5.45	127.59	120.28
1	D	222	ASN	CA-C-N	5.41	127.38	120.56
1	D	222	ASN	C-N-CA	5.41	127.38	120.56
1	A	293	ASN	CA-C-N	5.40	127.51	120.28
1	A	293	ASN	C-N-CA	5.40	127.51	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	238	MET	CA-C-N	5.40	127.51	120.28
1	G	238	MET	C-N-CA	5.40	127.51	120.28
1	I	222	ASN	CA-C-N	5.39	127.35	120.56
1	I	222	ASN	C-N-CA	5.39	127.35	120.56
1	G	293	ASN	CA-C-N	5.37	127.47	120.28
1	G	293	ASN	C-N-CA	5.37	127.47	120.28
1	C	178	ASN	CA-C-N	5.37	127.47	120.28
1	C	178	ASN	C-N-CA	5.37	127.47	120.28
1	C	222	ASN	CA-C-N	5.37	127.32	120.56
1	C	222	ASN	C-N-CA	5.37	127.32	120.56
1	D	293	ASN	CA-C-N	5.36	127.46	120.28
1	D	293	ASN	C-N-CA	5.36	127.46	120.28
1	J	222	ASN	CA-C-N	5.36	127.31	120.56
1	J	222	ASN	C-N-CA	5.36	127.31	120.56
1	K	238	MET	CA-C-N	5.36	127.46	120.28
1	K	238	MET	C-N-CA	5.36	127.46	120.28
1	A	222	ASN	CA-C-N	5.36	127.31	120.56
1	A	222	ASN	C-N-CA	5.36	127.31	120.56
1	A	238	MET	CA-C-N	5.35	127.45	120.28
1	A	238	MET	C-N-CA	5.35	127.45	120.28
1	F	293	ASN	CA-C-N	5.35	127.45	120.28
1	F	293	ASN	C-N-CA	5.35	127.45	120.28
1	F	222	ASN	CA-C-N	5.34	127.29	120.56
1	F	222	ASN	C-N-CA	5.34	127.29	120.56
1	C	293	ASN	CA-C-N	5.34	127.43	120.28
1	C	293	ASN	C-N-CA	5.34	127.43	120.28
1	D	238	MET	CA-C-N	5.34	127.43	120.28
1	D	238	MET	C-N-CA	5.34	127.43	120.28
1	I	238	MET	CA-C-N	5.34	127.43	120.28
1	I	238	MET	C-N-CA	5.34	127.43	120.28
1	E	238	MET	CA-C-N	5.33	127.43	120.28
1	E	238	MET	C-N-CA	5.33	127.43	120.28
1	K	293	ASN	CA-C-N	5.33	127.42	120.28
1	K	293	ASN	C-N-CA	5.33	127.42	120.28
1	K	222	ASN	CA-C-N	5.32	127.26	120.56
1	K	222	ASN	C-N-CA	5.32	127.26	120.56
1	L	293	ASN	CA-C-N	5.31	127.40	120.28
1	L	293	ASN	C-N-CA	5.31	127.40	120.28
1	B	222	ASN	CA-C-N	5.31	127.34	120.70
1	B	222	ASN	C-N-CA	5.31	127.34	120.70
1	F	238	MET	CA-C-N	5.31	127.39	120.28
1	F	238	MET	C-N-CA	5.31	127.39	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	ASN	CA-C-N	5.31	127.39	120.28
1	B	293	ASN	C-N-CA	5.31	127.39	120.28
1	G	222	ASN	CA-C-N	5.30	127.24	120.56
1	G	222	ASN	C-N-CA	5.30	127.24	120.56
1	H	222	ASN	CA-C-N	5.29	127.23	120.56
1	H	222	ASN	C-N-CA	5.29	127.23	120.56
1	L	222	ASN	CA-C-N	5.29	127.22	120.56
1	L	222	ASN	C-N-CA	5.29	127.22	120.56
1	I	293	ASN	CA-C-N	5.29	127.36	120.28
1	I	293	ASN	C-N-CA	5.29	127.36	120.28
1	J	293	ASN	CA-C-N	5.28	127.36	120.28
1	J	293	ASN	C-N-CA	5.28	127.36	120.28
1	E	222	ASN	CA-C-N	5.27	127.20	120.56
1	E	222	ASN	C-N-CA	5.27	127.20	120.56
1	L	238	MET	CA-C-N	5.25	127.32	120.28
1	L	238	MET	C-N-CA	5.25	127.32	120.28
1	J	238	MET	CA-C-N	5.23	127.29	120.28
1	J	238	MET	C-N-CA	5.23	127.29	120.28
1	C	238	MET	CA-C-N	5.22	127.27	120.28
1	C	238	MET	C-N-CA	5.22	127.27	120.28
1	H	238	MET	CA-C-N	5.20	127.24	120.28
1	H	238	MET	C-N-CA	5.20	127.24	120.28
1	B	238	MET	CA-C-N	5.17	127.21	120.28
1	B	238	MET	C-N-CA	5.17	127.21	120.28
1	D	139	MET	CA-C-N	5.12	129.39	122.07
1	D	139	MET	C-N-CA	5.12	129.39	122.07
1	J	139	MET	CA-C-N	5.03	129.26	122.07
1	J	139	MET	C-N-CA	5.03	129.26	122.07
1	E	171	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	ASP	Peptide
1	B	65	ASP	Peptide
1	C	65	ASP	Peptide
1	D	65	ASP	Peptide
1	E	65	ASP	Peptide
1	F	65	ASP	Peptide
1	G	65	ASP	Peptide
1	H	65	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	I	65	ASP	Peptide
1	J	65	ASP	Peptide
1	K	65	ASP	Peptide
1	L	65	ASP	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	2158	0	2181	26	0
1	B	2158	0	2181	29	0
1	C	2158	0	2181	29	1
1	D	2158	0	2181	31	5
1	E	1981	0	2015	29	2
1	F	2158	0	2181	32	3
1	G	2158	0	2181	31	0
1	H	2158	0	2181	50	1
1	I	2158	0	2181	32	0
1	J	2158	0	2181	26	0
1	K	2158	0	2181	27	0
1	L	2158	0	2181	27	0
All	All	25719	0	26006	347	6

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 7.

All (347) 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:H:205:ARG:NH1	1:H:263:ARG:NH2	1.80	1.27
1:H:82:VAL:HG21	1:H:199:ALA:HB2	1.36	1.04
1:H:205:ARG:HH12	1:H:263:ARG:HH22	1.00	0.99
1:H:82:VAL:HG21	1:H:199:ALA:CB	1.94	0.97
1:A:138:SER:HB3	1:A:144:ARG:HG2	1.48	0.96
1:D:62:HIS:HB3	1:D:65:ASP:OD1	1.67	0.95
1:H:205:ARG:HH12	1:H:263:ARG:NH2	1.44	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:HIS:HB3	1:H:65:ASP:OD1	1.67	0.95
1:G:62:HIS:HB3	1:G:65:ASP:OD1	1.67	0.94
1:I:62:HIS:HB3	1:I:65:ASP:OD1	1.67	0.94
1:B:62:HIS:HB3	1:B:65:ASP:OD1	1.67	0.94
1:A:62:HIS:HB3	1:A:65:ASP:OD1	1.67	0.94
1:F:62:HIS:HB3	1:F:65:ASP:OD1	1.67	0.94
1:E:62:HIS:HB3	1:E:65:ASP:OD1	1.67	0.93
1:K:62:HIS:HB3	1:K:65:ASP:OD1	1.67	0.93
1:L:62:HIS:HB3	1:L:65:ASP:OD1	1.67	0.93
1:J:62:HIS:HB3	1:J:65:ASP:OD1	1.67	0.93
1:H:205:ARG:NH1	1:H:263:ARG:HH21	1.58	0.92
1:C:62:HIS:HB3	1:C:65:ASP:OD1	1.67	0.92
1:F:298:SER:HB2	1:H:41:ASP:HB2	1.50	0.92
1:A:63:LYS:H	1:A:63:LYS:HD2	1.35	0.92
1:G:63:LYS:H	1:G:63:LYS:HD2	1.35	0.92
1:H:205:ARG:NH1	1:H:263:ARG:HH22	1.55	0.92
1:B:63:LYS:H	1:B:63:LYS:HD2	1.35	0.91
1:H:138:SER:HB3	1:H:144:ARG:HG2	1.50	0.91
1:I:63:LYS:H	1:I:63:LYS:HD2	1.35	0.91
1:H:144:ARG:HG3	1:H:144:ARG:HH11	1.35	0.91
1:C:63:LYS:HD2	1:C:63:LYS:H	1.35	0.91
1:J:63:LYS:H	1:J:63:LYS:HD2	1.35	0.90
1:H:63:LYS:H	1:H:63:LYS:HD2	1.35	0.90
1:F:63:LYS:H	1:F:63:LYS:HD2	1.35	0.90
1:D:63:LYS:H	1:D:63:LYS:HD2	1.35	0.89
1:E:63:LYS:H	1:E:63:LYS:HD2	1.35	0.89
1:L:63:LYS:H	1:L:63:LYS:HD2	1.35	0.89
1:K:63:LYS:H	1:K:63:LYS:HD2	1.35	0.87
1:H:205:ARG:CZ	1:H:263:ARG:NH2	2.41	0.83
1:H:82:VAL:CG2	1:H:199:ALA:HB2	2.11	0.80
1:G:266:ARG:HA	1:G:266:ARG:NE	1.97	0.79
1:H:82:VAL:HG23	1:H:83:GLY:H	1.48	0.78
1:F:298:SER:HB2	1:H:41:ASP:CB	2.15	0.75
1:D:48:ILE:O	1:D:63:LYS:HB3	1.86	0.75
1:G:48:ILE:O	1:G:63:LYS:HB3	1.87	0.75
1:J:48:ILE:O	1:J:63:LYS:HB3	1.86	0.74
1:B:48:ILE:O	1:B:63:LYS:HB3	1.88	0.74
1:E:48:ILE:O	1:E:63:LYS:HB3	1.88	0.74
1:L:48:ILE:O	1:L:63:LYS:HB3	1.88	0.74
1:A:48:ILE:O	1:A:63:LYS:HB3	1.87	0.73
1:I:48:ILE:O	1:I:63:LYS:HB3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:VAL:CG2	1:H:199:ALA:CB	2.67	0.73
1:K:48:ILE:O	1:K:63:LYS:HB3	1.88	0.73
1:F:48:ILE:O	1:F:63:LYS:HB3	1.88	0.73
1:C:48:ILE:O	1:C:63:LYS:HB3	1.89	0.72
1:H:48:ILE:O	1:H:63:LYS:HB3	1.89	0.72
1:H:144:ARG:HG3	1:H:144:ARG:NH1	2.07	0.70
1:H:82:VAL:HG23	1:H:83:GLY:N	2.07	0.70
1:E:62:HIS:CB	1:E:65:ASP:OD1	2.40	0.70
1:J:62:HIS:CB	1:J:65:ASP:OD1	2.40	0.70
1:K:62:HIS:CB	1:K:65:ASP:OD1	2.40	0.69
1:I:62:HIS:CB	1:I:65:ASP:OD1	2.40	0.69
1:F:62:HIS:CB	1:F:65:ASP:OD1	2.40	0.69
1:G:62:HIS:CB	1:G:65:ASP:OD1	2.40	0.69
1:H:62:HIS:CB	1:H:65:ASP:OD1	2.40	0.69
1:D:62:HIS:CB	1:D:65:ASP:OD1	2.40	0.69
1:A:62:HIS:CB	1:A:65:ASP:OD1	2.40	0.68
1:L:62:HIS:CB	1:L:65:ASP:OD1	2.40	0.68
1:C:62:HIS:CB	1:C:65:ASP:OD1	2.40	0.67
1:B:62:HIS:CB	1:B:65:ASP:OD1	2.40	0.66
1:E:136:VAL:HG22	1:E:169:TYR:HB2	1.78	0.65
1:K:136:VAL:HG22	1:K:169:TYR:HB2	1.79	0.65
1:A:136:VAL:HG22	1:A:169:TYR:HB2	1.79	0.65
1:B:136:VAL:HG22	1:B:169:TYR:HB2	1.79	0.65
1:E:38:LYS:HD2	1:H:294:GLN:HE22	1.61	0.65
1:H:136:VAL:HG22	1:H:169:TYR:HB2	1.79	0.64
1:D:38:LYS:HG2	1:I:45:VAL:HG13	1.79	0.64
1:L:136:VAL:HG22	1:L:169:TYR:HB2	1.79	0.64
1:F:136:VAL:HG22	1:F:169:TYR:HB2	1.79	0.64
1:G:136:VAL:HG22	1:G:169:TYR:HB2	1.79	0.64
1:J:136:VAL:HG22	1:J:169:TYR:HB2	1.79	0.64
1:H:205:ARG:CZ	1:H:263:ARG:HH22	2.06	0.64
1:C:136:VAL:HG22	1:C:169:TYR:HB2	1.79	0.64
1:D:63:LYS:O	1:D:63:LYS:HG2	1.99	0.63
1:K:63:LYS:O	1:K:63:LYS:HG2	1.99	0.63
1:C:63:LYS:HG2	1:C:63:LYS:O	1.99	0.62
1:E:63:LYS:O	1:E:63:LYS:HG2	1.99	0.62
1:H:63:LYS:HG2	1:H:63:LYS:O	1.99	0.62
1:D:136:VAL:HG22	1:D:169:TYR:HB2	1.79	0.62
1:A:63:LYS:O	1:A:63:LYS:HG2	1.99	0.62
1:L:63:LYS:O	1:L:63:LYS:HG2	1.99	0.62
1:I:63:LYS:O	1:I:63:LYS:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LYS:O	1:B:63:LYS:HG2	1.99	0.62
1:G:63:LYS:O	1:G:63:LYS:HG2	1.99	0.62
1:F:63:LYS:O	1:F:63:LYS:HG2	1.99	0.61
1:J:63:LYS:O	1:J:63:LYS:HG2	1.99	0.61
1:G:266:ARG:O	1:G:266:ARG:NH1	2.34	0.60
1:I:136:VAL:HG22	1:I:169:TYR:HB2	1.84	0.59
1:F:266:ARG:H	1:F:266:ARG:CD	2.16	0.58
1:K:63:LYS:H	1:K:63:LYS:CD	2.15	0.57
1:I:63:LYS:H	1:I:63:LYS:CD	2.15	0.57
1:A:63:LYS:H	1:A:63:LYS:CD	2.15	0.57
1:D:38:LYS:HD3	1:I:45:VAL:CG1	2.34	0.57
1:G:63:LYS:H	1:G:63:LYS:CD	2.15	0.56
1:F:272:ARG:NH1	1:F:274:SER:OG	2.38	0.56
1:B:63:LYS:H	1:B:63:LYS:CD	2.15	0.56
1:C:63:LYS:H	1:C:63:LYS:CD	2.15	0.55
1:G:63:LYS:HD2	1:G:63:LYS:N	2.15	0.55
1:D:38:LYS:CG	1:I:45:VAL:HG13	2.37	0.55
1:D:63:LYS:H	1:D:63:LYS:CD	2.15	0.55
1:J:63:LYS:HD2	1:J:63:LYS:N	2.15	0.54
1:C:63:LYS:HD2	1:C:63:LYS:N	2.15	0.54
1:A:63:LYS:HD2	1:A:63:LYS:N	2.15	0.53
1:F:63:LYS:H	1:F:63:LYS:CD	2.15	0.53
1:H:82:VAL:CG2	1:H:83:GLY:H	2.18	0.53
1:E:62:HIS:CE1	1:F:297:LEU:HD21	2.44	0.53
1:J:63:LYS:H	1:J:63:LYS:CD	2.15	0.52
1:C:62:HIS:HB3	1:C:65:ASP:CG	2.35	0.52
1:I:62:HIS:HB3	1:I:65:ASP:CG	2.35	0.52
1:K:62:HIS:HB3	1:K:65:ASP:CG	2.35	0.51
1:L:63:LYS:H	1:L:63:LYS:CD	2.15	0.51
1:A:62:HIS:HB3	1:A:65:ASP:CG	2.35	0.51
1:D:38:LYS:HD3	1:I:45:VAL:HG13	1.93	0.51
1:E:28:LEU:HD11	1:E:67:VAL:HG11	1.93	0.51
1:G:62:HIS:HB3	1:G:65:ASP:CG	2.35	0.51
1:K:63:LYS:HD2	1:K:63:LYS:N	2.15	0.51
1:C:28:LEU:HD11	1:C:67:VAL:HG11	1.93	0.51
1:E:63:LYS:H	1:E:63:LYS:CD	2.15	0.51
1:E:63:LYS:HD2	1:E:63:LYS:N	2.15	0.51
1:E:62:HIS:HB3	1:E:65:ASP:CG	2.35	0.50
1:I:28:LEU:HD11	1:I:67:VAL:HG11	1.93	0.50
1:J:62:HIS:HB3	1:J:65:ASP:CG	2.35	0.50
1:L:62:HIS:HB3	1:L:65:ASP:CG	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:62:HIS:O	1:J:64:GLY:N	2.45	0.50
1:L:42:MET:HB2	1:L:64:GLY:HA2	1.94	0.50
1:I:62:HIS:O	1:I:64:GLY:N	2.45	0.50
1:I:63:LYS:HD2	1:I:63:LYS:N	2.15	0.50
1:B:62:HIS:HB3	1:B:65:ASP:CG	2.35	0.49
1:F:42:MET:HB2	1:F:64:GLY:HA2	1.93	0.49
1:K:28:LEU:HD11	1:K:67:VAL:HG11	1.94	0.49
1:B:62:HIS:O	1:B:64:GLY:N	2.45	0.49
1:F:62:HIS:O	1:F:64:GLY:N	2.45	0.49
1:B:63:LYS:HD2	1:B:63:LYS:N	2.15	0.49
1:H:28:LEU:HD11	1:H:67:VAL:HG11	1.93	0.49
1:J:28:LEU:HD11	1:J:67:VAL:HG11	1.94	0.49
1:K:42:MET:HB2	1:K:64:GLY:HA2	1.95	0.49
1:L:28:LEU:HD11	1:L:67:VAL:HG11	1.94	0.49
1:D:28:LEU:HD11	1:D:67:VAL:HG11	1.94	0.49
1:F:62:HIS:HB3	1:F:65:ASP:CG	2.35	0.49
1:B:28:LEU:HD11	1:B:67:VAL:HG11	1.94	0.49
1:F:28:LEU:HD11	1:F:67:VAL:HG11	1.94	0.49
1:B:42:MET:HB2	1:B:64:GLY:HA2	1.94	0.49
1:D:62:HIS:O	1:D:64:GLY:N	2.45	0.49
1:G:62:HIS:O	1:G:64:GLY:N	2.45	0.49
1:C:167:VAL:HG13	1:C:210:ARG:HG3	1.95	0.48
1:E:42:MET:HB2	1:E:64:GLY:HA2	1.95	0.48
1:A:62:HIS:O	1:A:64:GLY:N	2.45	0.48
1:B:58:ILE:HB	1:B:70:VAL:HG22	1.95	0.48
1:J:65:ASP:OD1	1:J:65:ASP:N	2.47	0.48
1:G:28:LEU:HD11	1:G:67:VAL:HG11	1.94	0.48
1:K:62:HIS:O	1:K:64:GLY:N	2.45	0.48
1:A:28:LEU:HD11	1:A:67:VAL:HG11	1.94	0.48
1:D:42:MET:HB2	1:D:64:GLY:HA2	1.96	0.48
1:E:167:VAL:HG13	1:E:210:ARG:HG3	1.95	0.48
1:H:63:LYS:H	1:H:63:LYS:CD	2.15	0.48
1:L:65:ASP:OD1	1:L:65:ASP:N	2.47	0.48
1:H:42:MET:HB2	1:H:64:GLY:HA2	1.96	0.48
1:I:207:VAL:HG12	1:I:209:MET:HB2	1.96	0.48
1:K:167:VAL:HG13	1:K:210:ARG:HG3	1.96	0.48
1:L:167:VAL:HG13	1:L:210:ARG:HG3	1.95	0.48
1:A:167:VAL:HG13	1:A:210:ARG:HG3	1.95	0.48
1:D:62:HIS:HB3	1:D:65:ASP:CG	2.35	0.48
1:A:62:HIS:CE1	1:C:297:LEU:HD21	2.49	0.48
1:B:65:ASP:OD1	1:B:65:ASP:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ASP:OD1	1:D:65:ASP:N	2.47	0.48
1:F:110:SER:HB2	1:F:244:ILE:HD12	1.96	0.48
1:B:167:VAL:HG13	1:B:210:ARG:HG3	1.96	0.48
1:B:207:VAL:HG12	1:B:209:MET:HB2	1.96	0.48
1:H:62:HIS:HB3	1:H:65:ASP:CG	2.35	0.48
1:J:42:MET:HB2	1:J:64:GLY:HA2	1.95	0.48
1:C:62:HIS:O	1:C:64:GLY:N	2.45	0.48
1:E:58:ILE:HB	1:E:70:VAL:HG22	1.96	0.48
1:F:207:VAL:HG12	1:F:209:MET:HB2	1.96	0.48
1:H:62:HIS:O	1:H:64:GLY:N	2.45	0.47
1:L:62:HIS:O	1:L:64:GLY:N	2.45	0.47
1:G:65:ASP:OD1	1:G:65:ASP:N	2.46	0.47
1:C:58:ILE:HB	1:C:70:VAL:HG22	1.96	0.47
1:I:42:MET:HB2	1:I:64:GLY:HA2	1.96	0.47
1:I:58:ILE:HB	1:I:70:VAL:HG22	1.97	0.47
1:I:65:ASP:OD1	1:I:65:ASP:N	2.47	0.47
1:A:65:ASP:OD1	1:A:65:ASP:N	2.47	0.47
1:E:65:ASP:OD1	1:E:65:ASP:N	2.47	0.47
1:G:62:HIS:CE1	1:I:297:LEU:HD21	2.49	0.47
1:I:167:VAL:HG13	1:I:210:ARG:HG3	1.96	0.47
1:C:65:ASP:OD1	1:C:65:ASP:N	2.47	0.47
1:H:65:ASP:OD1	1:H:65:ASP:N	2.46	0.47
1:A:58:ILE:HB	1:A:70:VAL:HG22	1.97	0.47
1:E:62:HIS:O	1:E:64:GLY:N	2.45	0.47
1:G:58:ILE:HB	1:G:70:VAL:HG22	1.97	0.47
1:G:110:SER:HB2	1:G:244:ILE:HD12	1.97	0.47
1:J:110:SER:HB2	1:J:244:ILE:HD12	1.97	0.47
1:L:207:VAL:HG12	1:L:209:MET:HB2	1.96	0.47
1:C:110:SER:HB2	1:C:244:ILE:HD12	1.97	0.47
1:C:207:VAL:HG12	1:C:209:MET:HB2	1.96	0.47
1:D:110:SER:HB2	1:D:244:ILE:HD12	1.97	0.47
1:D:207:VAL:HG12	1:D:209:MET:HB2	1.96	0.47
1:H:167:VAL:HG13	1:H:210:ARG:HG3	1.96	0.47
1:J:167:VAL:HG13	1:J:210:ARG:HG3	1.97	0.47
1:J:207:VAL:HG12	1:J:209:MET:HB2	1.96	0.47
1:A:207:VAL:HG12	1:A:209:MET:HB2	1.96	0.47
1:G:42:MET:HB2	1:G:64:GLY:HA2	1.97	0.47
1:G:167:VAL:HG13	1:G:210:ARG:HG3	1.96	0.47
1:H:207:VAL:HG12	1:H:209:MET:HB2	1.95	0.47
1:J:150:VAL:HG11	1:J:314:ASN:HD22	1.80	0.47
1:K:110:SER:HB2	1:K:244:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:150:VAL:HG11	1:K:314:ASN:HD22	1.80	0.47
1:A:42:MET:HB2	1:A:64:GLY:HA2	1.96	0.46
1:G:150:VAL:HG11	1:G:314:ASN:HD22	1.80	0.46
1:H:58:ILE:HB	1:H:70:VAL:HG22	1.97	0.46
1:K:58:ILE:HB	1:K:70:VAL:HG22	1.97	0.46
1:A:150:VAL:HG11	1:A:314:ASN:HD22	1.80	0.46
1:C:150:VAL:HG11	1:C:314:ASN:HD22	1.80	0.46
1:E:207:VAL:HG12	1:E:209:MET:HB2	1.96	0.46
1:F:58:ILE:HB	1:F:70:VAL:HG22	1.97	0.46
1:G:207:VAL:HG12	1:G:209:MET:HB2	1.95	0.46
1:K:207:VAL:HG12	1:K:209:MET:HB2	1.96	0.46
1:C:42:MET:HB2	1:C:64:GLY:HA2	1.97	0.46
1:E:110:SER:HB2	1:E:244:ILE:HD12	1.96	0.46
1:F:167:VAL:HG13	1:F:210:ARG:HG3	1.96	0.46
1:H:110:SER:HB2	1:H:244:ILE:HD12	1.97	0.46
1:L:63:LYS:HD2	1:L:63:LYS:N	2.15	0.46
1:A:110:SER:HB2	1:A:244:ILE:HD12	1.97	0.46
1:L:58:ILE:HB	1:L:70:VAL:HG22	1.96	0.46
1:L:110:SER:HB2	1:L:244:ILE:HD12	1.97	0.46
1:E:39:ASN:HB2	1:H:294:GLN:HG2	1.97	0.46
1:B:150:VAL:HG11	1:B:314:ASN:HD22	1.80	0.46
1:F:150:VAL:HG11	1:F:314:ASN:HD22	1.81	0.46
1:G:266:ARG:HA	1:G:266:ARG:CZ	2.46	0.46
1:H:139:MET:HB2	1:H:148:GLY:HA2	1.97	0.46
1:H:205:ARG:NH2	1:H:263:ARG:HH22	2.13	0.46
1:D:150:VAL:HG11	1:D:314:ASN:HD22	1.80	0.46
1:J:58:ILE:HB	1:J:70:VAL:HG22	1.97	0.46
1:D:167:VAL:HG13	1:D:210:ARG:HG3	1.96	0.46
1:I:150:VAL:HG11	1:I:314:ASN:HD22	1.81	0.46
1:L:150:VAL:HG11	1:L:314:ASN:HD22	1.80	0.46
1:D:38:LYS:CD	1:I:45:VAL:HG13	2.46	0.45
1:H:150:VAL:HG11	1:H:314:ASN:HD22	1.80	0.45
1:I:93:ARG:HG3	1:I:208:ASN:O	2.16	0.45
1:D:47:GLU:HA	1:D:63:LYS:HG3	1.99	0.45
1:F:65:ASP:OD1	1:F:65:ASP:N	2.47	0.45
1:F:272:ARG:C	1:F:272:ARG:HD3	2.41	0.45
1:J:93:ARG:HG3	1:J:208:ASN:O	2.17	0.45
1:H:297:LEU:HD21	1:I:62:HIS:CE1	2.51	0.45
1:K:93:ARG:HG3	1:K:208:ASN:O	2.17	0.45
1:K:139:MET:HB2	1:K:148:GLY:HA2	1.99	0.45
1:I:139:MET:HB2	1:I:148:GLY:HA2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ARG:HG3	1:A:208:ASN:O	2.17	0.45
1:E:139:MET:HB2	1:E:148:GLY:HA2	1.99	0.45
1:C:93:ARG:HG3	1:C:208:ASN:O	2.17	0.45
1:A:263:ARG:HA	1:A:264:ALA:HA	1.75	0.45
1:B:110:SER:HB2	1:B:244:ILE:HD12	1.97	0.45
1:B:139:MET:HB2	1:B:148:GLY:HA2	1.99	0.45
1:E:93:ARG:HG3	1:E:208:ASN:O	2.17	0.45
1:C:139:MET:HB2	1:C:148:GLY:HA2	1.99	0.44
1:H:63:LYS:HD2	1:H:63:LYS:N	2.15	0.44
1:L:93:ARG:HG3	1:L:208:ASN:O	2.17	0.44
1:G:93:ARG:HG3	1:G:208:ASN:O	2.17	0.44
1:H:62:HIS:CE1	1:J:297:LEU:HD21	2.52	0.44
1:K:65:ASP:OD1	1:K:65:ASP:N	2.47	0.44
1:A:70:VAL:HG23	1:A:72:PRO:HD3	2.00	0.44
1:D:93:ARG:HG3	1:D:208:ASN:O	2.17	0.44
1:E:171:ASP:HA	1:E:172:SER:HA	1.83	0.44
1:B:70:VAL:HG23	1:B:72:PRO:HD3	1.98	0.44
1:F:93:ARG:HG3	1:F:208:ASN:O	2.17	0.44
1:G:70:VAL:HG23	1:G:72:PRO:HD3	2.00	0.44
1:A:139:MET:HB2	1:A:148:GLY:HA2	2.00	0.44
1:L:70:VAL:HG23	1:L:72:PRO:HD3	2.00	0.44
1:G:297:LEU:HD21	1:L:62:HIS:CE1	2.53	0.44
1:H:70:VAL:HG23	1:H:72:PRO:HD3	1.99	0.44
1:L:263:ARG:HA	1:L:264:ALA:HA	1.74	0.44
1:G:139:MET:HB2	1:G:148:GLY:HA2	2.00	0.44
1:I:110:SER:HB2	1:I:244:ILE:HD12	1.99	0.44
1:H:144:ARG:NH1	1:H:144:ARG:CG	2.73	0.43
1:I:70:VAL:HG23	1:I:72:PRO:HD3	2.00	0.43
1:L:139:MET:HB2	1:L:148:GLY:HA2	1.99	0.43
1:F:70:VAL:HG23	1:F:72:PRO:HD3	2.00	0.43
1:F:139:MET:HB2	1:F:148:GLY:HA2	1.99	0.43
1:H:93:ARG:HG3	1:H:208:ASN:O	2.17	0.43
1:D:35:GLU:CD	1:I:92:VAL:CG1	2.91	0.43
1:F:266:ARG:H	1:F:266:ARG:NE	2.16	0.43
1:E:70:VAL:HG23	1:E:72:PRO:HD3	1.99	0.43
1:F:263:ARG:HA	1:F:264:ALA:HA	1.74	0.43
1:D:58:ILE:HB	1:D:70:VAL:HG22	2.01	0.43
1:J:47:GLU:HA	1:J:63:LYS:HG3	2.01	0.43
1:J:70:VAL:HG23	1:J:72:PRO:HD3	2.00	0.43
1:K:70:VAL:HG23	1:K:72:PRO:HD3	2.01	0.43
1:F:63:LYS:HD2	1:F:63:LYS:N	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:VAL:HG23	1:C:72:PRO:HD3	2.00	0.43
1:K:171:ASP:HA	1:K:172:SER:HA	1.85	0.43
1:B:93:ARG:HG3	1:B:208:ASN:O	2.19	0.42
1:B:297:LEU:HD21	1:C:62:HIS:CE1	2.54	0.42
1:J:139:MET:HB2	1:J:148:GLY:HA2	2.00	0.42
1:B:34:GLU:HB3	1:D:303:SER:N	2.35	0.42
1:B:62:HIS:CE1	1:D:297:LEU:HD21	2.55	0.42
1:D:263:ARG:HA	1:D:264:ALA:HA	1.74	0.42
1:H:263:ARG:HA	1:H:264:ALA:HA	1.72	0.42
1:K:47:GLU:HA	1:K:63:LYS:HG3	2.02	0.42
1:K:62:HIS:CG	1:K:65:ASP:OD1	2.73	0.42
1:J:263:ARG:HA	1:J:264:ALA:HA	1.74	0.42
1:D:70:VAL:HG23	1:D:72:PRO:HD3	2.02	0.42
1:E:47:GLU:HA	1:E:63:LYS:HG3	2.01	0.42
1:L:47:GLU:HA	1:L:63:LYS:HG3	2.02	0.42
1:E:62:HIS:CG	1:E:65:ASP:OD1	2.73	0.42
1:C:171:ASP:HA	1:C:172:SER:HA	1.85	0.42
1:G:62:HIS:CG	1:G:65:ASP:OD1	2.73	0.41
1:I:47:GLU:HA	1:I:63:LYS:HG3	2.02	0.41
1:G:266:ARG:NE	1:G:266:ARG:CA	2.78	0.41
1:A:62:HIS:CG	1:A:65:ASP:OD1	2.73	0.41
1:E:263:ARG:HA	1:E:264:ALA:HA	1.74	0.41
1:J:62:HIS:CE1	1:K:297:LEU:HD21	2.56	0.41
1:C:263:ARG:HA	1:C:264:ALA:HA	1.74	0.41
1:F:47:GLU:HA	1:F:63:LYS:HG3	2.02	0.41
1:G:85:ALA:HB2	1:G:203:TYR:CE2	2.55	0.41
1:H:205:ARG:NH2	1:H:263:ARG:NH2	2.68	0.41
1:B:70:VAL:HG12	1:D:295:PHE:CE1	2.56	0.41
1:B:263:ARG:HA	1:B:264:ALA:HA	1.74	0.41
1:B:295:PHE:CE2	1:B:300:GLN:HG2	2.56	0.41
1:C:62:HIS:C	1:C:65:ASP:OD1	2.64	0.41
1:D:62:HIS:CG	1:D:65:ASP:OD1	2.73	0.41
1:E:62:HIS:C	1:E:65:ASP:OD1	2.64	0.41
1:H:295:PHE:CE2	1:H:300:GLN:HG2	2.56	0.41
1:I:62:HIS:C	1:I:65:ASP:OD1	2.64	0.41
1:K:263:ARG:HA	1:K:264:ALA:HA	1.74	0.41
1:L:171:ASP:HA	1:L:172:SER:HA	1.84	0.41
1:A:47:GLU:HA	1:A:63:LYS:HG3	2.03	0.41
1:C:47:GLU:HA	1:C:63:LYS:HG3	2.02	0.40
1:F:62:HIS:C	1:F:65:ASP:OD1	2.64	0.40
1:K:62:HIS:C	1:K:65:ASP:OD1	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:HIS:CG	1:C:65:ASP:OD1	2.73	0.40
1:F:295:PHE:CE2	1:F:300:GLN:HG2	2.56	0.40
1:G:237:SER:HA	1:I:142:ALA:HB1	2.04	0.40
1:H:62:HIS:C	1:H:65:ASP:OD1	2.64	0.40
1:L:295:PHE:CE2	1:L:300:GLN:HG2	2.56	0.40
1:C:295:PHE:CE2	1:C:300:GLN:HG2	2.56	0.40
1:G:62:HIS:C	1:G:65:ASP:OD1	2.64	0.40
1:J:62:HIS:C	1:J:65:ASP:OD1	2.64	0.40
1:L:62:HIS:C	1:L:65:ASP:OD1	2.64	0.40
1:B:47:GLU:HA	1:B:63:LYS:HG3	2.03	0.40
1:B:62:HIS:C	1:B:65:ASP:OD1	2.64	0.40
1:E:119:LEU:HD23	1:E:119:LEU:HA	1.96	0.40

All (6) 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:D:250:ASN:ND2	1:F:272:ARG:NH2[4_555]	0.76	1.44
1:D:266:ARG:NH1	1:E:245:LYS:NZ[4_555]	1.49	0.71
1:D:250:ASN:CG	1:F:272:ARG:NH2[4_555]	1.65	0.55
1:D:250:ASN:ND2	1:F:272:ARG:CZ[4_555]	1.89	0.31
1:D:266:ARG:CZ	1:E:245:LYS:NZ[4_555]	1.99	0.21
1:C:95:ARG:NH2	1:H:89:ALA:CB[2_665]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	B	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	C	280/321 (87%)	269 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	E	260/321 (81%)	250 (96%)	10 (4%)	0	100	100
1	F	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	G	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	H	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	I	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	J	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	K	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	L	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
All	All	3340/3852 (87%)	3209 (96%)	131 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	B	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	C	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	D	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	E	213/257 (83%)	203 (95%)	10 (5%)	23	55
1	F	232/257 (90%)	219 (94%)	13 (6%)	19	49
1	G	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	H	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	I	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	J	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	K	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	L	232/257 (90%)	221 (95%)	11 (5%)	23	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2765/3084 (90%)	2632 (95%)	133 (5%)	23 54

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	73	SER
1	A	116	LYS
1	A	191	ARG
1	A	194	ASP
1	A	258	THR
1	A	263	ARG
1	A	266	ARG
1	A	305	PHE
1	A	309	ASN
1	A	312	GLU
1	B	63	LYS
1	B	73	SER
1	B	116	LYS
1	B	191	ARG
1	B	194	ASP
1	B	258	THR
1	B	263	ARG
1	B	266	ARG
1	B	305	PHE
1	B	309	ASN
1	B	312	GLU
1	C	63	LYS
1	C	73	SER
1	C	116	LYS
1	C	191	ARG
1	C	194	ASP
1	C	258	THR
1	C	263	ARG
1	C	266	ARG
1	C	305	PHE
1	C	309	ASN
1	C	312	GLU
1	D	63	LYS
1	D	73	SER
1	D	116	LYS
1	D	191	ARG

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Mol	Chain	Res	Type
1	D	194	ASP
1	D	258	THR
1	D	263	ARG
1	D	266	ARG
1	D	305	PHE
1	D	309	ASN
1	D	312	GLU
1	E	26	GLU
1	E	38	LYS
1	E	63	LYS
1	E	73	SER
1	E	116	LYS
1	E	191	ARG
1	E	194	ASP
1	E	258	THR
1	E	263	ARG
1	E	266	ARG
1	F	63	LYS
1	F	73	SER
1	F	116	LYS
1	F	191	ARG
1	F	194	ASP
1	F	258	THR
1	F	263	ARG
1	F	266	ARG
1	F	272	ARG
1	F	298	SER
1	F	305	PHE
1	F	309	ASN
1	F	312	GLU
1	G	63	LYS
1	G	73	SER
1	G	116	LYS
1	G	191	ARG
1	G	194	ASP
1	G	258	THR
1	G	263	ARG
1	G	266	ARG
1	G	305	PHE
1	G	309	ASN
1	G	312	GLU
1	H	63	LYS

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Mol	Chain	Res	Type
1	H	73	SER
1	H	116	LYS
1	H	144	ARG
1	H	191	ARG
1	H	194	ASP
1	H	258	THR
1	H	266	ARG
1	H	305	PHE
1	H	309	ASN
1	H	312	GLU
1	I	63	LYS
1	I	73	SER
1	I	116	LYS
1	I	191	ARG
1	I	194	ASP
1	I	258	THR
1	I	263	ARG
1	I	266	ARG
1	I	305	PHE
1	I	309	ASN
1	I	312	GLU
1	J	63	LYS
1	J	73	SER
1	J	116	LYS
1	J	191	ARG
1	J	194	ASP
1	J	258	THR
1	J	263	ARG
1	J	266	ARG
1	J	305	PHE
1	J	309	ASN
1	J	312	GLU
1	K	63	LYS
1	K	73	SER
1	K	116	LYS
1	K	191	ARG
1	K	194	ASP
1	K	258	THR
1	K	263	ARG
1	K	266	ARG
1	K	305	PHE
1	K	309	ASN

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Mol	Chain	Res	Type
1	K	312	GLU
1	L	63	LYS
1	L	73	SER
1	L	116	LYS
1	L	191	ARG
1	L	194	ASP
1	L	258	THR
1	L	263	ARG
1	L	266	ARG
1	L	305	PHE
1	L	309	ASN
1	L	312	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	309	ASN
1	A	314	ASN
1	B	122	HIS
1	B	202	GLN
1	B	309	ASN
1	B	314	ASN
1	C	122	HIS
1	C	202	GLN
1	C	271	ASN
1	C	309	ASN
1	C	314	ASN
1	D	122	HIS
1	D	178	ASN
1	D	202	GLN
1	D	271	ASN
1	D	309	ASN
1	D	314	ASN
1	E	39	ASN
1	E	122	HIS
1	E	271	ASN
1	F	122	HIS
1	F	309	ASN
1	F	314	ASN
1	G	122	HIS
1	G	271	ASN

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Mol	Chain	Res	Type
1	G	309	ASN
1	G	314	ASN
1	H	39	ASN
1	H	122	HIS
1	H	202	GLN
1	H	294	GLN
1	H	309	ASN
1	H	314	ASN
1	I	122	HIS
1	I	271	ASN
1	I	309	ASN
1	I	314	ASN
1	J	122	HIS
1	J	178	ASN
1	J	309	ASN
1	J	314	ASN
1	K	122	HIS
1	K	309	ASN
1	K	314	ASN
1	L	309	ASN
1	L	314	ASN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	288/321 (89%)	0.93	33 (11%) 9 5	34, 53, 78, 109	0
1	B	288/321 (89%)	1.33	54 (18%) 3 1	39, 61, 99, 124	0
1	C	288/321 (89%)	1.19	50 (17%) 4 2	29, 54, 102, 137	0
1	D	288/321 (89%)	1.72	98 (34%) 1 0	40, 69, 120, 155	0
1	E	264/321 (82%)	1.69	88 (33%) 1 0	44, 70, 109, 135	0
1	F	288/321 (89%)	1.26	61 (21%) 2 1	41, 59, 100, 137	0
1	G	288/321 (89%)	0.97	38 (13%) 7 4	32, 53, 85, 127	0
1	H	288/321 (89%)	1.32	57 (19%) 3 1	36, 58, 102, 149	0
1	I	288/321 (89%)	1.20	43 (14%) 5 3	35, 55, 112, 156	0
1	J	288/321 (89%)	1.56	73 (25%) 1 1	36, 68, 119, 152	0
1	K	288/321 (89%)	1.85	106 (36%) 1 0	44, 75, 123, 162	0
1	L	288/321 (89%)	1.26	66 (22%) 2 1	40, 61, 119, 147	0
All	All	3432/3852 (89%)	1.35	767 (22%) 2 1	29, 61, 110, 162	0

All (767) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	310	ILE	7.5
1	C	310	ILE	7.0
1	K	314	ASN	6.8
1	I	306	LEU	6.6
1	J	303	SER	6.5
1	K	303	SER	6.4
1	B	309	ASN	6.4
1	J	304	ALA	6.2
1	B	303	SER	6.2
1	D	303	SER	6.1
1	J	314	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
1	K	110	SER	6.0
1	D	304	ALA	6.0
1	I	314	ASN	6.0
1	E	115	GLY	5.9
1	F	303	SER	5.9
1	L	310	ILE	5.8
1	H	309	ASN	5.7
1	C	314	ASN	5.7
1	K	264	ALA	5.7
1	D	307	GLY	5.6
1	C	306	LEU	5.6
1	J	307	GLY	5.5
1	E	30	THR	5.5
1	B	306	LEU	5.5
1	J	308	PRO	5.4
1	J	251	GLY	5.4
1	E	110	SER	5.4
1	B	255	THR	5.4
1	J	296	LEU	5.4
1	B	308	PRO	5.4
1	H	308	PRO	5.3
1	D	251	GLY	5.2
1	E	268	ASN	5.2
1	H	303	SER	5.2
1	K	310	ILE	5.1
1	E	264	ALA	5.1
1	K	244	ILE	5.0
1	D	306	LEU	5.0
1	K	115	GLY	5.0
1	C	308	PRO	4.9
1	J	306	LEU	4.8
1	D	249	VAL	4.8
1	E	31	THR	4.8
1	K	304	ALA	4.8
1	I	309	ASN	4.7
1	E	255	THR	4.7
1	H	255	THR	4.7
1	C	218	SER	4.7
1	L	194	ASP	4.7
1	K	311	PRO	4.7
1	F	314	ASN	4.7
1	G	232	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	H	310	ILE	4.6
1	D	62	HIS	4.6
1	I	308	PRO	4.6
1	E	252	THR	4.6
1	J	249	VAL	4.5
1	F	113	ALA	4.5
1	F	311	PRO	4.5
1	E	280	ARG	4.5
1	F	310	ILE	4.5
1	H	306	LEU	4.5
1	G	229	SER	4.5
1	J	309	ASN	4.5
1	L	308	PRO	4.5
1	B	77	ARG	4.5
1	D	268	ASN	4.4
1	H	300	GLN	4.4
1	D	296	LEU	4.4
1	E	279	SER	4.4
1	L	293	ASN	4.4
1	E	277	LEU	4.3
1	E	150	VAL	4.3
1	I	311	PRO	4.2
1	L	303	SER	4.2
1	E	244	ILE	4.2
1	H	307	GLY	4.2
1	D	305	PHE	4.2
1	D	308	PRO	4.2
1	L	113	ALA	4.2
1	E	119	LEU	4.2
1	F	306	LEU	4.2
1	J	305	PHE	4.2
1	J	310	ILE	4.2
1	K	278	VAL	4.2
1	L	314	ASN	4.2
1	B	304	ALA	4.2
1	C	312	GLU	4.1
1	B	65	ASP	4.1
1	H	314	ASN	4.1
1	K	276	ASP	4.1
1	K	309	ASN	4.1
1	L	292	PHE	4.1
1	D	267	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	K	291	VAL	4.1
1	C	311	PRO	4.1
1	I	313	SER	4.1
1	D	277	LEU	4.1
1	F	109	ILE	4.1
1	F	236	ALA	4.1
1	L	306	LEU	4.0
1	F	194	ASP	4.0
1	K	292	PHE	4.0
1	L	311	PRO	4.0
1	D	313	SER	4.0
1	B	256	ALA	4.0
1	H	312	GLU	4.0
1	D	311	PRO	4.0
1	I	218	SER	4.0
1	J	266	ARG	3.9
1	E	140	ALA	3.9
1	H	184	LEU	3.9
1	K	296	LEU	3.9
1	L	246	SER	3.9
1	D	314	ASN	3.9
1	E	278	VAL	3.9
1	K	255	THR	3.9
1	D	293	ASN	3.9
1	J	313	SER	3.9
1	B	34	GLU	3.8
1	B	310	ILE	3.8
1	F	88	SER	3.8
1	H	65	ASP	3.8
1	B	184	LEU	3.8
1	E	273	VAL	3.8
1	B	314	ASN	3.8
1	K	253	ALA	3.8
1	D	292	PHE	3.8
1	J	59	LEU	3.8
1	C	313	SER	3.8
1	E	231	PHE	3.8
1	K	306	LEU	3.8
1	F	304	ALA	3.8
1	K	268	ASN	3.8
1	D	265	ASP	3.8
1	I	219	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	305	PHE	3.8
1	E	270	ALA	3.7
1	F	245	LYS	3.7
1	F	237	SER	3.7
1	J	292	PHE	3.7
1	J	250	ASN	3.7
1	B	305	PHE	3.7
1	D	65	ASP	3.6
1	D	300	GLN	3.6
1	K	308	PRO	3.6
1	D	273	VAL	3.6
1	I	255	THR	3.6
1	I	305	PHE	3.6
1	E	114	GLY	3.6
1	C	309	ASN	3.6
1	J	267	SER	3.6
1	A	232	LYS	3.6
1	C	219	ASP	3.6
1	G	265	ASP	3.6
1	K	261	HIS	3.5
1	B	307	GLY	3.5
1	I	90	ALA	3.5
1	E	109	ILE	3.5
1	J	62	HIS	3.5
1	K	273	VAL	3.5
1	E	262	LEU	3.5
1	K	230	VAL	3.5
1	E	256	ALA	3.5
1	D	55	GLY	3.5
1	J	298	SER	3.5
1	B	89	ALA	3.5
1	J	311	PRO	3.5
1	D	310	ILE	3.5
1	E	101	ILE	3.5
1	K	280	ARG	3.5
1	F	250	ASN	3.5
1	I	184	LEU	3.5
1	J	113	ALA	3.5
1	L	226	ALA	3.5
1	C	280	ARG	3.5
1	J	84	TYR	3.4
1	F	227	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	255	THR	3.4
1	L	88	SER	3.4
1	A	98	GLU	3.4
1	G	184	LEU	3.4
1	L	251	GLY	3.4
1	G	98	GLU	3.4
1	I	143	GLU	3.4
1	I	264	ALA	3.4
1	D	271	ASN	3.4
1	D	88	SER	3.4
1	F	264	ALA	3.4
1	K	256	ALA	3.4
1	G	65	ASP	3.4
1	H	251	GLY	3.4
1	L	245	LYS	3.4
1	J	184	LEU	3.3
1	K	312	GLU	3.3
1	H	202	GLN	3.3
1	J	293	ASN	3.3
1	G	92	VAL	3.3
1	F	246	SER	3.3
1	B	311	PRO	3.3
1	J	22	GLN	3.3
1	K	300	GLN	3.3
1	E	36	GLY	3.3
1	K	101	ILE	3.3
1	K	270	ALA	3.3
1	L	313	SER	3.3
1	I	280	ARG	3.3
1	B	262	LEU	3.3
1	E	234	ALA	3.3
1	E	253	ALA	3.3
1	E	242	ARG	3.3
1	C	215	LEU	3.3
1	E	37	VAL	3.3
1	K	249	VAL	3.3
1	E	271	ASN	3.3
1	F	226	ALA	3.3
1	I	312	GLU	3.3
1	K	252	THR	3.2
1	K	277	LEU	3.2
1	G	194	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	289	GLY	3.2
1	F	296	LEU	3.2
1	E	276	ASP	3.2
1	I	65	ASP	3.2
1	L	264	ALA	3.2
1	J	268	ASN	3.2
1	K	293	ASN	3.2
1	L	309	ASN	3.2
1	J	300	GLN	3.2
1	B	266	ARG	3.2
1	F	258	THR	3.2
1	G	266	ARG	3.2
1	B	83	GLY	3.2
1	K	114	GLY	3.2
1	D	184	LEU	3.2
1	H	51	VAL	3.2
1	J	273	VAL	3.2
1	G	235	SER	3.2
1	G	90	ALA	3.2
1	F	65	ASP	3.1
1	C	305	PHE	3.1
1	E	261	HIS	3.1
1	B	270	ALA	3.1
1	C	303	SER	3.1
1	H	105	ALA	3.1
1	D	276	ASP	3.1
1	K	28	LEU	3.1
1	G	305	PHE	3.1
1	L	227	VAL	3.1
1	G	314	ASN	3.1
1	C	264	ALA	3.1
1	G	262	LEU	3.1
1	K	272	ARG	3.1
1	B	300	GLN	3.1
1	F	240	THR	3.1
1	G	255	THR	3.1
1	I	303	SER	3.1
1	D	247	PHE	3.1
1	E	249	VAL	3.1
1	J	276	ASP	3.1
1	K	109	ILE	3.1
1	A	314	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	297	LEU	3.1
1	D	148	GLY	3.1
1	K	36	GLY	3.1
1	D	291	VAL	3.1
1	K	305	PHE	3.1
1	K	265	ASP	3.1
1	C	268	ASN	3.0
1	E	113	ALA	3.0
1	E	272	ARG	3.0
1	L	265	ASP	3.0
1	A	184	LEU	3.0
1	B	56	ASN	3.0
1	C	92	VAL	3.0
1	L	258	THR	3.0
1	H	34	GLU	3.0
1	H	88	SER	3.0
1	L	237	SER	3.0
1	K	119	LEU	3.0
1	K	184	LEU	3.0
1	L	296	LEU	3.0
1	D	256	ALA	3.0
1	E	63	LYS	3.0
1	L	305	PHE	3.0
1	J	277	LEU	3.0
1	D	155	ALA	3.0
1	H	266	ARG	3.0
1	D	74	VAL	3.0
1	H	268	ASN	3.0
1	K	231	PHE	3.0
1	D	298	SER	3.0
1	A	65	ASP	3.0
1	H	83	GLY	3.0
1	G	12	ASN	3.0
1	L	250	ASN	2.9
1	K	30	THR	2.9
1	D	264	ALA	2.9
1	L	304	ALA	2.9
1	D	84	TYR	2.9
1	G	88	SER	2.9
1	L	274	SER	2.9
1	K	242	ARG	2.9
1	K	262	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	56	ASN	2.9
1	J	30	THR	2.9
1	J	253	ALA	2.9
1	B	251	GLY	2.9
1	F	305	PHE	2.9
1	A	262	LEU	2.9
1	L	266	ARG	2.9
1	D	248	ALA	2.9
1	J	271	ASN	2.9
1	L	89	ALA	2.9
1	D	70	VAL	2.9
1	A	266	ARG	2.9
1	C	184	LEU	2.9
1	J	58	ILE	2.9
1	J	274	SER	2.9
1	K	235	SER	2.9
1	A	304	ALA	2.9
1	D	30	THR	2.9
1	H	311	PRO	2.9
1	L	257	GLU	2.9
1	F	249	VAL	2.9
1	D	299	GLY	2.9
1	I	77	ARG	2.9
1	E	184	LEU	2.9
1	E	246	SER	2.8
1	D	194	ASP	2.8
1	E	250	ASN	2.8
1	K	271	ASN	2.8
1	L	272	ARG	2.8
1	A	229	SER	2.8
1	H	267	SER	2.8
1	D	270	ALA	2.8
1	K	142	ALA	2.8
1	L	236	ALA	2.8
1	I	217	PRO	2.8
1	E	265	ASP	2.8
1	L	224	ASP	2.8
1	B	249	VAL	2.8
1	D	37	VAL	2.8
1	L	232	LYS	2.8
1	G	306	LEU	2.8
1	K	260	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	274	SER	2.8
1	J	264	ALA	2.8
1	K	279	SER	2.8
1	F	243	ARG	2.8
1	B	312	GLU	2.8
1	J	258	THR	2.8
1	J	247	PHE	2.8
1	K	61	PHE	2.8
1	K	250	ASN	2.8
1	K	251	GLY	2.8
1	K	307	GLY	2.8
1	B	202	GLN	2.8
1	D	89	ALA	2.8
1	D	274	SER	2.8
1	F	73	SER	2.8
1	D	312	GLU	2.8
1	L	65	ASP	2.8
1	I	307	GLY	2.8
1	A	90	ALA	2.8
1	C	89	ALA	2.8
1	C	144	ARG	2.8
1	L	90	ALA	2.8
1	A	303	SER	2.8
1	D	59	LEU	2.8
1	F	313	SER	2.8
1	C	65	ASP	2.7
1	C	307	GLY	2.7
1	B	71	ARG	2.7
1	H	77	ARG	2.7
1	K	100	LYS	2.7
1	K	105	ALA	2.7
1	C	94	GLN	2.7
1	B	267	SER	2.7
1	K	78	ASP	2.7
1	F	270	ALA	2.7
1	H	304	ALA	2.7
1	D	176	VAL	2.7
1	J	70	VAL	2.7
1	J	94	GLN	2.7
1	K	294	GLN	2.7
1	B	33	LEU	2.7
1	E	40	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	260	ILE	2.7
1	B	313	SER	2.7
1	I	251	GLY	2.7
1	J	269	SER	2.7
1	K	267	SER	2.7
1	H	135	ALA	2.7
1	J	270	ALA	2.7
1	B	82	VAL	2.7
1	F	94	GLN	2.7
1	E	80	ILE	2.7
1	B	32	LYS	2.7
1	K	269	SER	2.7
1	B	264	ALA	2.7
1	I	304	ALA	2.7
1	G	230	VAL	2.7
1	K	40	LEU	2.7
1	H	80	ILE	2.7
1	F	247	PHE	2.7
1	J	289	GLY	2.7
1	D	120	THR	2.7
1	I	267	SER	2.7
1	D	309	ASN	2.7
1	K	80	ILE	2.6
1	K	63	LYS	2.6
1	F	299	GLY	2.6
1	H	89	ALA	2.6
1	H	206	ALA	2.6
1	J	74	VAL	2.6
1	K	76	ALA	2.6
1	L	249	VAL	2.6
1	C	216	ASN	2.6
1	E	266	ARG	2.6
1	D	94	GLN	2.6
1	K	247	PHE	2.6
1	I	299	GLY	2.6
1	D	33	LEU	2.6
1	E	176	VAL	2.6
1	E	235	SER	2.6
1	H	313	SER	2.6
1	C	266	ARG	2.6
1	H	260	ILE	2.6
1	C	217	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	268	ASN	2.6
1	H	299	GLY	2.6
1	C	90	ALA	2.6
1	E	76	ALA	2.6
1	I	156	ALA	2.6
1	A	279	SER	2.6
1	D	73	SER	2.6
1	K	27	GLN	2.6
1	F	293	ASN	2.6
1	D	159	LEU	2.6
1	D	262	LEU	2.6
1	F	106	GLU	2.6
1	F	87	ALA	2.6
1	I	29	ALA	2.6
1	K	155	ALA	2.6
1	K	234	ALA	2.6
1	C	174	ARG	2.6
1	D	32	LYS	2.6
1	E	247	PHE	2.6
1	F	269	SER	2.6
1	G	269	SER	2.6
1	G	303	SER	2.6
1	J	88	SER	2.6
1	A	194	ASP	2.6
1	I	216	ASN	2.6
1	J	265	ASP	2.6
1	L	271	ASN	2.6
1	L	119	LEU	2.6
1	D	85	ALA	2.6
1	D	278	VAL	2.6
1	E	230	VAL	2.6
1	J	37	VAL	2.6
1	L	240	THR	2.6
1	E	62	HIS	2.5
1	J	19	PRO	2.5
1	A	88	SER	2.5
1	D	104	GLY	2.5
1	F	251	GLY	2.5
1	F	300	GLN	2.5
1	F	184	LEU	2.5
1	A	265	ASP	2.5
1	F	224	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	121	ASN	2.5
1	K	248	ALA	2.5
1	F	308	PRO	2.5
1	B	75	SER	2.5
1	F	119	LEU	2.5
1	J	297	LEU	2.5
1	D	63	LYS	2.5
1	F	223	VAL	2.5
1	K	37	VAL	2.5
1	K	254	PHE	2.5
1	C	267	SER	2.5
1	F	190	SER	2.5
1	K	138	SER	2.5
1	J	291	VAL	2.5
1	E	155	ALA	2.5
1	B	268	ASN	2.5
1	I	215	LEU	2.5
1	J	17	LEU	2.5
1	K	24	LEU	2.5
1	E	251	GLY	2.5
1	I	289	GLY	2.5
1	D	29	ALA	2.5
1	D	279	SER	2.5
1	E	29	ALA	2.5
1	C	109	ILE	2.5
1	D	34	GLU	2.5
1	J	257	GLU	2.5
1	K	257	GLU	2.5
1	D	280	ARG	2.5
1	B	260	ILE	2.4
1	D	35	GLU	2.4
1	E	121	ASN	2.4
1	K	232	LYS	2.4
1	J	168	LEU	2.4
1	D	92	VAL	2.4
1	F	90	ALA	2.4
1	J	29	ALA	2.4
1	L	294	GLN	2.4
1	L	109	ILE	2.4
1	B	88	SER	2.4
1	D	266	ARG	2.4
1	G	233	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	258	THR	2.4
1	D	211	VAL	2.4
1	F	273	VAL	2.4
1	K	137	VAL	2.4
1	L	307	GLY	2.4
1	L	94	GLN	2.4
1	D	263	ARG	2.4
1	F	312	GLU	2.4
1	I	266	ARG	2.4
1	J	263	ARG	2.4
1	L	106	GLU	2.4
1	L	269	SER	2.4
1	K	215	LEU	2.4
1	H	72	PRO	2.4
1	H	74	VAL	2.4
1	E	236	ALA	2.4
1	G	142	ALA	2.4
1	G	156	ALA	2.4
1	G	248	ALA	2.4
1	L	263	ARG	2.4
1	K	295	PHE	2.4
1	H	211	VAL	2.4
1	A	299	GLY	2.4
1	E	148	GLY	2.4
1	B	80	ILE	2.4
1	H	270	ALA	2.4
1	E	32	LYS	2.4
1	K	25	MET	2.4
1	D	17	LEU	2.4
1	D	119	LEU	2.4
1	H	200	LEU	2.4
1	L	184	LEU	2.4
1	A	269	SER	2.4
1	B	73	SER	2.4
1	F	110	SER	2.4
1	F	248	ALA	2.3
1	F	268	ASN	2.3
1	L	268	ASN	2.3
1	E	243	ARG	2.3
1	D	297	LEU	2.3
1	E	61	PHE	2.3
1	I	292	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	74	VAL	2.3
1	E	138	SER	2.3
1	L	145	PRO	2.3
1	A	182	GLY	2.3
1	D	86	THR	2.3
1	F	181	GLY	2.3
1	H	263	ARG	2.3
1	L	299	GLY	2.3
1	A	89	ALA	2.3
1	G	304	ALA	2.3
1	H	107	LEU	2.3
1	L	262	LEU	2.3
1	K	35	GLU	2.3
1	A	116	LYS	2.3
1	H	116	LYS	2.3
1	K	20	ARG	2.3
1	B	81	GLY	2.3
1	C	299	GLY	2.3
1	B	258	THR	2.3
1	C	304	ALA	2.3
1	L	190	SER	2.3
1	I	300	GLN	2.3
1	D	60	GLY	2.3
1	J	260	ILE	2.3
1	E	199	ALA	2.3
1	A	233	THR	2.3
1	E	73	SER	2.3
1	G	252	THR	2.3
1	J	86	THR	2.3
1	L	277	LEU	2.3
1	F	271	ASN	2.3
1	H	220	ASP	2.3
1	K	65	ASP	2.3
1	K	192	GLN	2.3
1	K	116	LYS	2.3
1	J	280	ARG	2.3
1	K	243	ARG	2.3
1	C	251	GLY	2.3
1	E	103	ALA	2.3
1	C	262	LEU	2.3
1	E	59	LEU	2.3
1	K	200	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	88	SER	2.3
1	F	13	SER	2.3
1	G	300	GLN	2.3
1	J	194	ASP	2.3
1	L	278	VAL	2.3
1	J	312	GLU	2.2
1	D	15	ILE	2.2
1	I	253	ALA	2.2
1	D	40	LEU	2.2
1	I	297	LEU	2.2
1	D	31	THR	2.2
1	E	258	THR	2.2
1	C	44	SER	2.2
1	C	88	SER	2.2
1	B	74	VAL	2.2
1	G	94	GLN	2.2
1	K	53	VAL	2.2
1	L	223	VAL	2.2
1	E	260	ILE	2.2
1	L	244	ILE	2.2
1	E	145	PRO	2.2
1	C	157	LEU	2.2
1	L	289	GLY	2.2
1	F	232	LYS	2.2
1	L	254	PHE	2.2
1	J	246	SER	2.2
1	D	67	VAL	2.2
1	A	308	PRO	2.2
1	B	59	LEU	2.2
1	E	25	MET	2.2
1	E	215	LEU	2.2
1	E	38	LYS	2.2
1	E	232	LYS	2.2
1	J	112	THR	2.2
1	E	118	VAL	2.2
1	F	278	VAL	2.2
1	A	267	SER	2.2
1	H	298	SER	2.2
1	K	108	ILE	2.2
1	B	271	ASN	2.2
1	B	200	LEU	2.2
1	G	119	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	296	LEU	2.2
1	C	87	ALA	2.2
1	C	115	GLY	2.2
1	K	55	GLY	2.2
1	L	270	ALA	2.2
1	B	194	ASP	2.2
1	J	232	LYS	2.2
1	D	77	ARG	2.2
1	H	210	ARG	2.2
1	K	258	THR	2.2
1	E	137	VAL	2.2
1	A	94	GLN	2.2
1	B	57	SER	2.2
1	G	260	ILE	2.2
1	J	75	SER	2.2
1	A	119	LEU	2.2
1	C	296	LEU	2.2
1	I	296	LEU	2.2
1	K	297	LEU	2.2
1	D	26	GLU	2.2
1	D	257	GLU	2.2
1	K	104	GLY	2.2
1	A	263	ARG	2.2
1	K	31	THR	2.1
1	H	33	LEU	2.1
1	J	262	LEU	2.1
1	K	197	LEU	2.1
1	C	29	ALA	2.1
1	C	73	SER	2.1
1	E	90	ALA	2.1
1	E	267	SER	2.1
1	F	229	SER	2.1
1	B	289	GLY	2.1
1	D	272	ARG	2.1
1	I	144	ARG	2.1
1	L	259	GLU	2.1
1	F	276	ASP	2.1
1	C	74	VAL	2.1
1	H	82	VAL	2.1
1	K	21	VAL	2.1
1	L	273	VAL	2.1
1	A	306	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	297	LEU	2.1
1	B	280	ARG	2.1
1	C	300	GLN	2.1
1	D	27	GLN	2.1
1	I	294	GLN	2.1
1	F	89	ALA	2.1
1	K	113	ALA	2.1
1	B	299	GLY	2.1
1	E	19	PRO	2.1
1	J	23	SER	2.1
1	C	154	PHE	2.1
1	G	183	ASN	2.1
1	H	213	PHE	2.1
1	J	21	VAL	2.1
1	J	82	VAL	2.1
1	K	16	ASP	2.1
1	K	118	VAL	2.1
1	C	214	THR	2.1
1	E	245	LYS	2.1
1	J	49	THR	2.1
1	B	156	ALA	2.1
1	D	253	ALA	2.1
1	E	257	GLU	2.1
1	C	110	SER	2.1
1	D	246	SER	2.1
1	E	254	PHE	2.1
1	E	269	SER	2.1
1	D	16	ASP	2.1
1	E	100	LYS	2.1
1	F	244	ILE	2.1
1	D	205	ARG	2.1
1	F	263	ARG	2.1
1	D	156	ALA	2.1
1	E	241	ALA	2.1
1	G	89	ALA	2.1
1	B	104	GLY	2.1
1	G	246	SER	2.1
1	A	230	VAL	2.1
1	D	82	VAL	2.1
1	G	249	VAL	2.1
1	K	150	VAL	2.1
1	H	216	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	263	ARG	2.1
1	E	78	ASP	2.1
1	C	255	THR	2.1
1	I	89	ALA	2.1
1	L	241	ALA	2.1
1	E	143	GLU	2.1
1	G	143	GLU	2.1
1	K	245	LYS	2.0
1	A	73	SER	2.0
1	C	190	SER	2.0
1	C	277	LEU	2.0
1	G	297	LEU	2.0
1	J	80	ILE	2.0
1	L	243	ARG	2.0
1	D	239	HIS	2.0
1	D	112	THR	2.0
1	D	113	ALA	2.0
1	E	201	ASP	2.0
1	G	258	THR	2.0
1	L	233	THR	2.0
1	E	27	GLN	2.0
1	D	245	LYS	2.0
1	E	259	GLU	2.0
1	K	259	GLU	2.0
1	H	37	VAL	2.0
1	I	223	VAL	2.0
1	J	53	VAL	2.0
1	D	28	LEU	2.0
1	H	262	LEU	2.0
1	H	297	LEU	2.0
1	A	12	ASN	2.0
1	A	183	ASN	2.0
1	D	201	ASP	2.0
1	F	292	PHE	2.0
1	J	299	GLY	2.0
1	K	289	GLY	2.0
1	A	245	LYS	2.0
1	B	137	VAL	2.0
1	H	93	ARG	2.0
1	H	249	VAL	2.0
1	K	266	ARG	2.0
1	H	109	ILE	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.