



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:22 am BST

PDB ID : 5X47
Title : Crystal structure of dehydroquinase dehydratase from *Acinetobacter baumannii* at 2.5 Angstrom resolution
Authors : Iqbal, N.; Singh, P.K.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2017-02-10
Resolution : 2.54 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

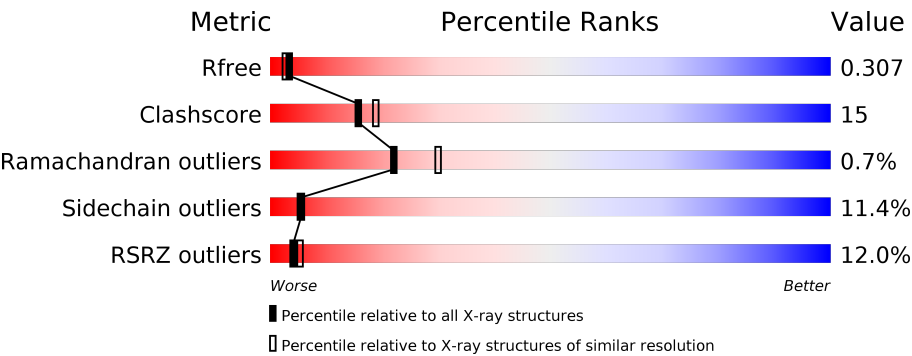
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 on 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	145	<div><div>7%</div><div>72%26%..</div></div>
1	B	145	<div><div>12%</div><div>72%24%. </div></div>
1	C	145	<div><div>8%</div><div>75%21%. </div></div>
1	D	145	<div><div>11%</div><div>68%25%6%. </div></div>
1	E	145	<div><div>8%</div><div>74%19%6%. </div></div>
1	F	145	<div><div>8%</div><div>72%25%. </div></div>

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Mol	Chain	Length	Quality of chain
1	G	145	<div> <div>10%</div> <div>73%</div> <div>24%</div> <div>•</div> </div>
1	H	145	<div> <div>10%</div> <div>66%</div> <div>28%</div> <div>6%</div> </div>
1	I	145	<div> <div>21%</div> <div>58%</div> <div>39%</div> <div>•</div> </div>
1	J	145	<div> <div>16%</div> <div>66%</div> <div>28%</div> <div>6%</div> </div>
1	K	145	<div> <div>14%</div> <div>72%</div> <div>24%</div> <div>• •</div> </div>
1	L	145	<div> <div>20%</div> <div>66%</div> <div>28%</div> <div>6%</div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13478 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 3-dehydroquinase dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	B	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	C	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	D	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	E	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	F	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	G	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	H	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	I	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	J	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	K	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			
1	L	145	Total	C	N	O	S	0	0	0
			1120	713	199	207	1			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	8	Total	O	0	0
			8	8		

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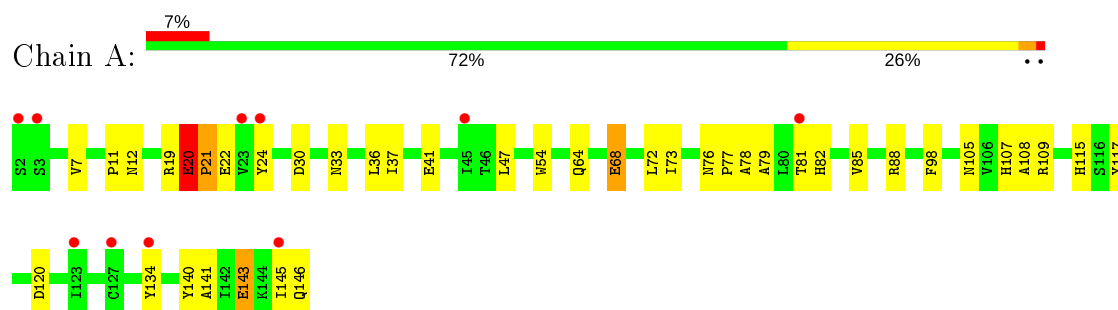
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	5	Total 5	O 5	0	0
2	D	2	Total 2	O 2	0	0
2	E	3	Total 3	O 3	0	0
2	F	2	Total 2	O 2	0	0
2	G	3	Total 3	O 3	0	0
2	H	4	Total 4	O 4	0	0
2	J	1	Total 1	O 1	0	0
2	L	2	Total 2	O 2	0	0

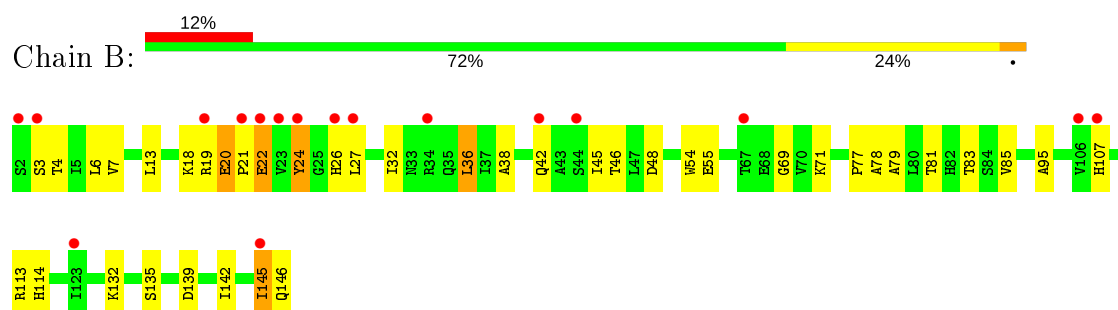
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

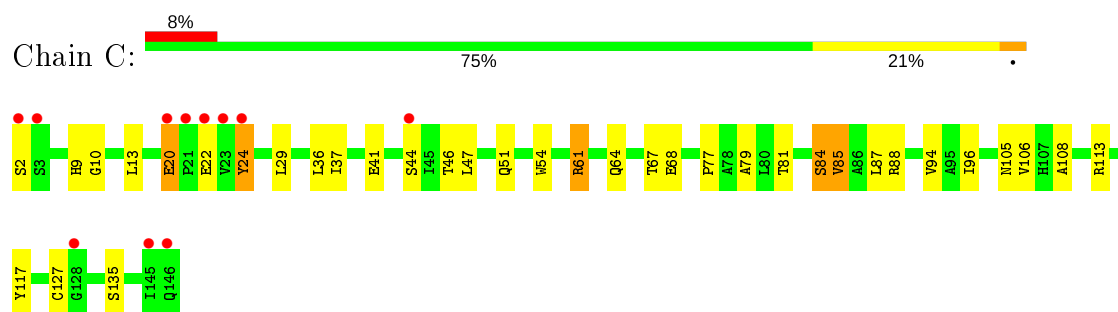
• Molecule 1: 3-dehydroquinase dehydratase



• Molecule 1: 3-dehydroquinase dehydratase

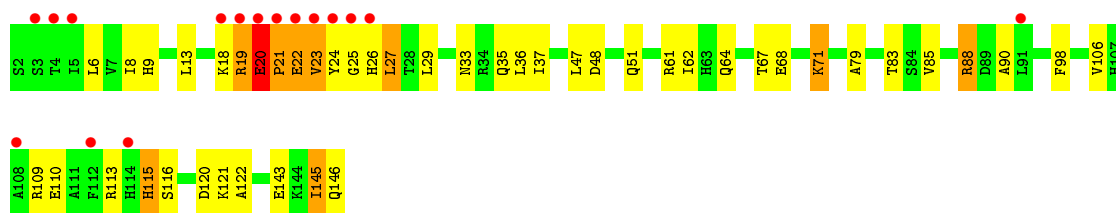


• Molecule 1: 3-dehydroquinase dehydratase

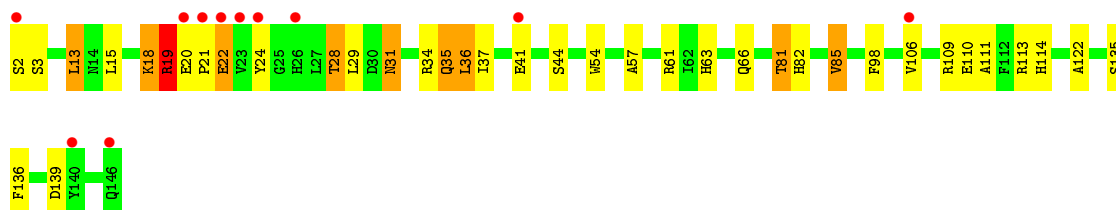
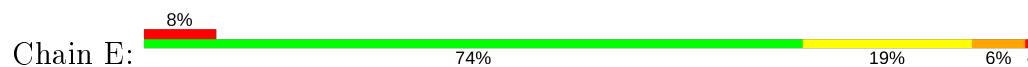


• Molecule 1: 3-dehydroquinase dehydratase

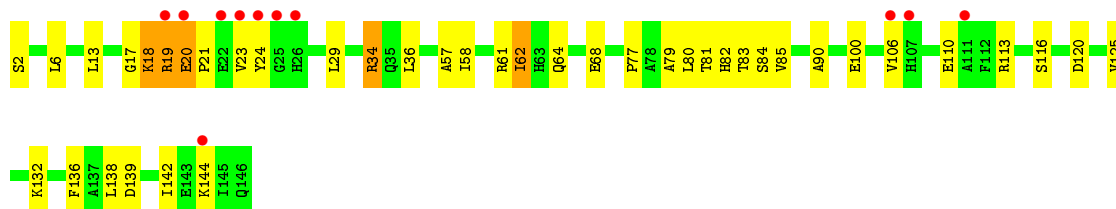




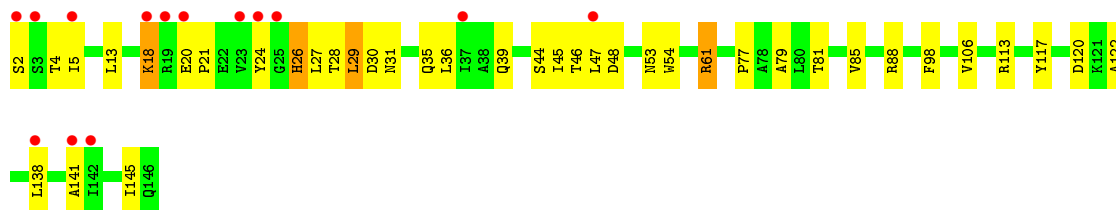
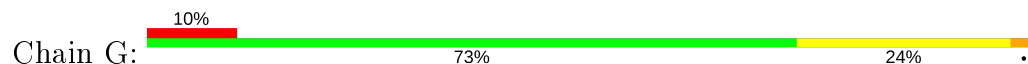
• Molecule 1: 3-dehydroquininate dehydratase



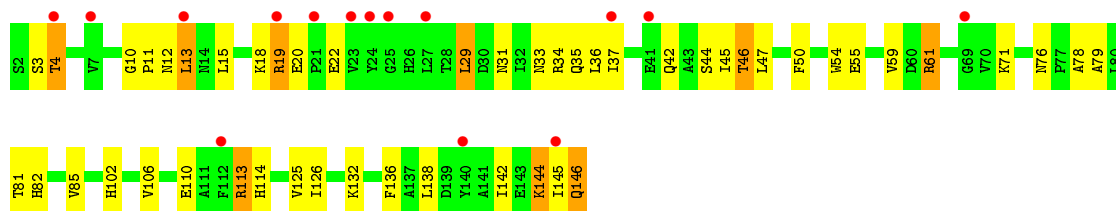
• Molecule 1: 3-dehydroquininate dehydratase



• Molecule 1: 3-dehydroquininate dehydratase

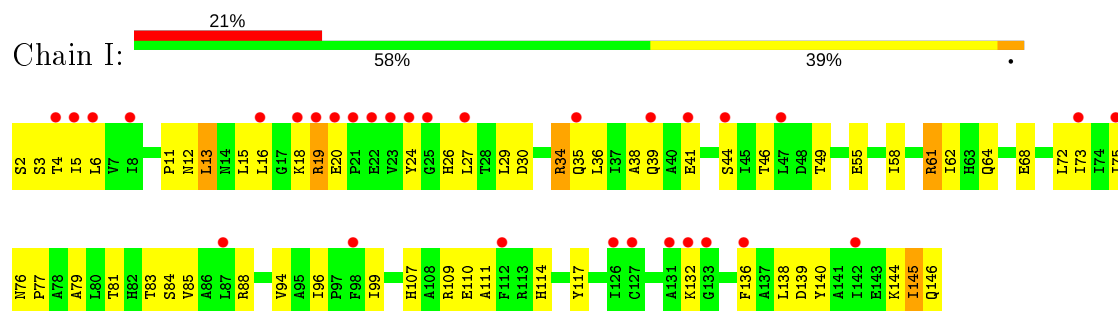


• Molecule 1: 3-dehydroquininate dehydratase



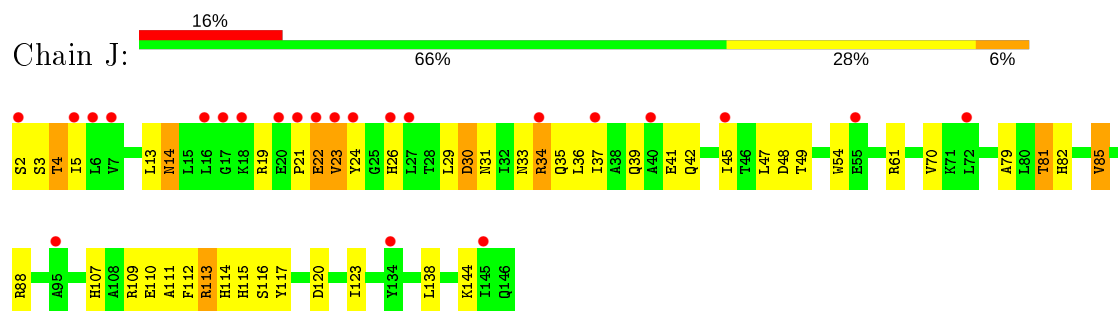
- Molecule 1: 3-dehydroquininate dehydratase

Chain I:



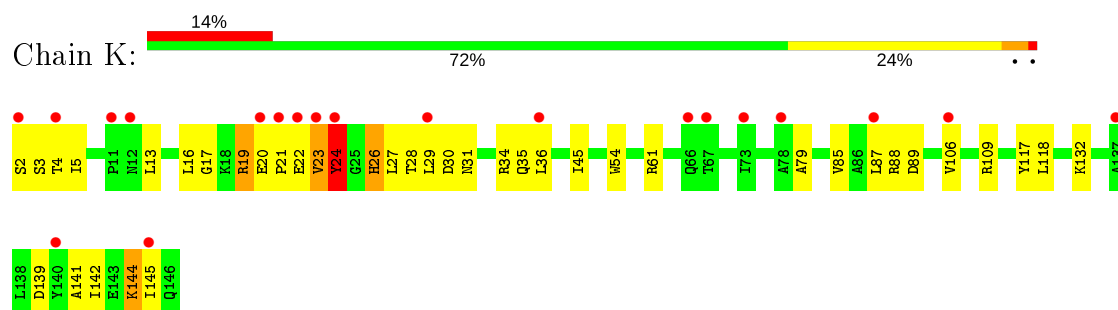
- Molecule 1: 3-dehydroquininate dehydratase

Chain J:



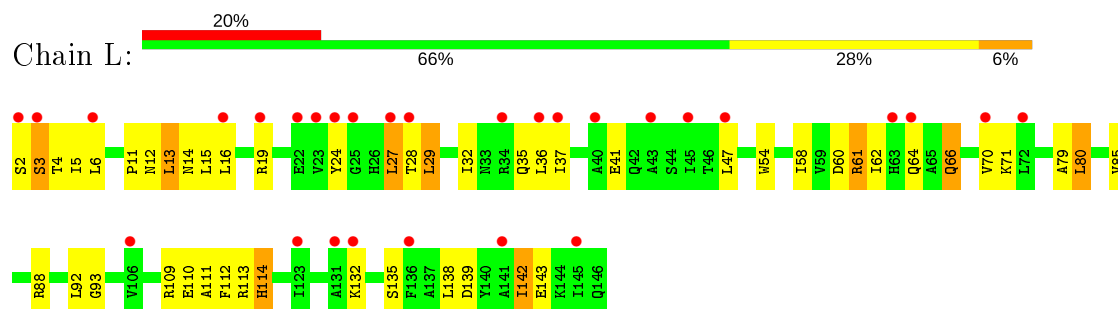
- Molecule 1: 3-dehydroquininate dehydratase

Chain K:



- Molecule 1: 3-dehydroquininate dehydratase

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.99Å 136.25Å 143.21Å 90.00° 97.59° 90.00°	Depositor
Resolution (Å)	47.93 – 2.54 49.15 – 2.54	Depositor EDS
% Data completeness (in resolution range)	70.3 (47.93-2.54) 70.3 (49.15-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.253 , 0.305 0.258 , 0.307	Depositor DCC
R_{free} test set	2142 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.784	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13478	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.21	0/1141	1.04	4/1551 (0.3%)
1	B	1.11	0/1141	0.99	3/1551 (0.2%)
1	C	1.17	0/1141	0.98	1/1551 (0.1%)
1	D	1.18	0/1141	1.01	1/1551 (0.1%)
1	E	1.16	0/1141	1.03	5/1551 (0.3%)
1	F	1.12	0/1141	1.02	3/1551 (0.2%)
1	G	1.11	0/1141	1.02	1/1551 (0.1%)
1	H	1.10	0/1141	1.09	5/1551 (0.3%)
1	I	1.18	0/1141	1.08	2/1551 (0.1%)
1	J	1.11	0/1141	1.04	1/1551 (0.1%)
1	K	1.17	0/1141	1.02	1/1551 (0.1%)
1	L	1.12	0/1141	1.08	2/1551 (0.1%)
All	All	1.14	0/13692	1.04	29/18612 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	19	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	H	19	ARG	N-CA-C	-7.07	91.91	111.00
1	A	20	GLU	C-N-CD	-6.62	106.04	120.60
1	A	109	ARG	NE-CZ-NH2	-6.51	117.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	19	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	J	22	GLU	C-N-CA	-6.36	105.79	121.70
1	E	20	GLU	N-CA-C	6.25	127.86	111.00
1	E	19	ARG	N-CA-C	-5.97	94.88	111.00
1	F	34	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	I	139	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	E	22	GLU	CA-CB-CG	5.70	125.94	113.40
1	B	139	ASP	CB-CG-OD2	5.67	123.40	118.30
1	G	61	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	I	19	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	K	139	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	E	139	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	113	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	H	144	LYS	CD-CE-NZ	5.31	123.91	111.70
1	B	55	GLU	OE1-CD-OE2	-5.28	116.96	123.30
1	E	61	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	68	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	F	139	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	L	139	ASP	CB-CG-OD1	5.21	122.98	118.30
1	H	145	ILE	C-N-CA	5.17	134.63	121.70
1	H	113	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	D	110	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	C	24	TYR	CB-CG-CD1	5.12	124.07	121.00
1	A	30	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	H	20	GLU	N-CA-C	5.11	124.80	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	22	GLU	Peptide
1	H	22	GLU	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	1120	0	1131	33	0
1	B	1120	0	1131	38	0
1	C	1120	0	1131	18	0
1	D	1120	0	1131	36	0
1	E	1120	0	1131	29	0
1	F	1120	0	1131	33	0
1	G	1120	0	1131	27	0
1	H	1120	0	1130	38	0
1	I	1120	0	1130	41	0
1	J	1120	0	1131	43	0
1	K	1120	0	1131	33	0
1	L	1120	0	1131	53	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
2	C	5	0	0	0	0
2	D	2	0	0	0	0
2	E	3	0	0	0	0
2	F	2	0	0	0	0
2	G	3	0	0	0	0
2	H	4	0	0	0	0
2	J	1	0	0	0	0
2	L	2	0	0	0	0
All	All	13478	0	13570	397	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 15.

All (397) 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:4:THR:HG23	1:H:46:THR:CG2	1.53	1.37
1:L:16:LEU:CD1	1:L:29:LEU:HB2	1.72	1.16
1:H:146:GLN:HA	1:H:146:GLN:HE21	1.14	1.13
1:L:16:LEU:HG	1:L:29:LEU:H	1.06	1.08
1:H:78:ALA:O	1:H:81:THR:HG22	1.54	1.06
1:L:16:LEU:HD23	1:L:28:THR:HB	1.34	1.04
1:L:16:LEU:HG	1:L:29:LEU:N	1.72	1.04
1:L:16:LEU:CD2	1:L:28:THR:HB	1.87	1.03
1:L:16:LEU:HD11	1:L:29:LEU:HB2	1.06	1.00
1:C:37:ILE:O	1:C:41:GLU:HG3	1.61	0.99
1:H:4:THR:HG23	1:H:46:THR:HG23	1.42	0.99
1:L:16:LEU:HD11	1:L:29:LEU:CB	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:16:LEU:CG	1:L:29:LEU:H	1.78	0.96
1:J:30:ASP:O	1:J:34:ARG:HG3	1.68	0.94
1:B:19:ARG:CZ	1:B:22:GLU:HG2	1.99	0.92
1:D:33:ASN:O	1:D:37:ILE:HG13	1.67	0.92
1:K:4:THR:HG21	1:K:45:ILE:HG23	1.51	0.92
1:I:64:GLN:O	1:I:68:GLU:HG3	1.70	0.92
1:H:4:THR:HG23	1:H:46:THR:HG22	1.49	0.92
1:H:10:GLY:N	1:H:13:LEU:HD23	1.84	0.91
1:K:19:ARG:HH21	1:K:19:ARG:HG2	1.34	0.90
1:L:60:ASP:O	1:L:64:GLN:HG3	1.71	0.90
1:B:20:GLU:HB3	1:B:21:PRO:CD	2.02	0.89
1:A:20:GLU:HB3	1:A:21:PRO:HD2	1.54	0.89
1:H:10:GLY:H	1:H:13:LEU:HD23	1.36	0.86
1:L:16:LEU:HD23	1:L:28:THR:CB	2.05	0.86
1:F:19:ARG:O	1:F:21:PRO:HD2	1.77	0.84
1:A:77:PRO:HG2	1:A:81:THR:HB	1.60	0.84
1:D:20:GLU:CB	1:D:21:PRO:CD	2.54	0.84
1:I:72:LEU:HD23	1:I:73:ILE:N	1.93	0.83
1:B:145:ILE:HD12	1:B:145:ILE:H	1.42	0.83
1:G:20:GLU:HG3	1:G:21:PRO:HD3	1.60	0.83
1:L:6:LEU:HD11	1:L:61:ARG:NH1	1.94	0.82
1:I:111:ALA:HA	1:I:114:HIS:HD2	1.43	0.82
1:H:146:GLN:HA	1:H:146:GLN:NE2	1.86	0.81
1:D:88:ARG:HG3	1:D:88:ARG:HH11	1.44	0.81
1:B:19:ARG:HG3	1:B:20:GLU:N	1.96	0.80
1:G:39:GLN:OE1	1:G:138:LEU:HD23	1.81	0.80
1:A:33:ASN:O	1:A:37:ILE:HG13	1.82	0.80
1:A:78:ALA:O	1:A:81:THR:HG22	1.81	0.80
1:B:20:GLU:HB3	1:B:21:PRO:HD3	1.63	0.80
1:I:39:GLN:HG2	1:I:138:LEU:HD23	1.61	0.79
1:D:145:ILE:HG22	1:D:146:GLN:OE1	1.81	0.79
1:K:19:ARG:HD2	1:K:23:VAL:HG23	1.65	0.78
1:D:20:GLU:CB	1:D:21:PRO:HD2	2.14	0.78
1:H:4:THR:CG2	1:H:46:THR:CG2	2.50	0.77
1:D:20:GLU:HB2	1:D:21:PRO:HD2	1.66	0.77
1:H:31:ASN:O	1:H:35:GLN:HG3	1.85	0.77
1:H:4:THR:HG23	1:H:46:THR:HG21	1.64	0.76
1:H:138:LEU:O	1:H:142:ILE:HG13	1.86	0.76
1:L:6:LEU:CD1	1:L:61:ARG:NH1	2.49	0.76
1:D:64:GLN:O	1:D:68:GLU:HG3	1.86	0.76
1:I:39:GLN:HG2	1:I:138:LEU:CD2	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:16:LEU:HD23	1:K:24:TYR:CE1	2.22	0.75
1:B:4:THR:HG21	1:B:45:ILE:HG23	1.67	0.75
1:D:20:GLU:HB2	1:D:21:PRO:CD	2.17	0.75
1:D:79:ALA:HB1	1:H:85:VAL:HG22	1.70	0.74
1:K:141:ALA:O	1:K:145:ILE:HD12	1.88	0.74
1:C:127:CYS:SG	1:F:125:VAL:HG13	2.28	0.73
1:L:6:LEU:HD11	1:L:61:ARG:HH11	1.54	0.73
1:J:19:ARG:CG	1:J:23:VAL:HG22	2.19	0.72
1:I:4:THR:HA	1:I:46:THR:HG23	1.72	0.72
1:F:6:LEU:HD13	1:F:61:ARG:HH21	1.53	0.72
1:J:33:ASN:O	1:J:37:ILE:HG13	1.89	0.72
1:K:144:LYS:N	1:K:144:LYS:HD2	2.02	0.72
1:C:77:PRO:HG2	1:C:81:THR:HB	1.72	0.72
1:B:19:ARG:HG2	1:B:22:GLU:HB2	1.72	0.71
1:A:20:GLU:HB3	1:A:21:PRO:CD	2.19	0.71
1:J:19:ARG:HB3	1:J:23:VAL:CG2	2.21	0.71
1:I:39:GLN:CG	1:I:138:LEU:HD23	2.20	0.71
1:B:20:GLU:CB	1:B:21:PRO:CD	2.66	0.70
1:B:145:ILE:HD12	1:B:145:ILE:N	2.06	0.70
1:I:85:VAL:HG22	1:K:79:ALA:HB1	1.74	0.70
1:J:31:ASN:HA	1:J:34:ARG:HD2	1.74	0.69
1:L:14:ASN:O	1:L:16:LEU:HD13	1.92	0.69
1:L:138:LEU:O	1:L:142:ILE:HG13	1.92	0.69
1:E:19:ARG:HG3	1:E:19:ARG:HH11	1.59	0.68
1:L:27:LEU:HD12	1:L:32:ILE:HG12	1.75	0.68
1:D:120:ASP:OD1	1:D:121:LYS:HG2	1.94	0.68
1:F:81:THR:HG22	1:F:116:SER:OG	1.93	0.68
1:K:19:ARG:HB3	1:K:24:TYR:HB2	1.75	0.67
1:F:81:THR:HG21	1:F:100:GLU:OE2	1.93	0.67
1:K:88:ARG:HB2	1:K:118:LEU:HD23	1.75	0.67
1:H:15:LEU:O	1:H:18:LYS:HG3	1.95	0.67
1:G:20:GLU:HG3	1:G:21:PRO:CD	2.24	0.67
1:L:16:LEU:HD23	1:L:28:THR:CG2	2.24	0.67
1:D:88:ARG:HG3	1:D:88:ARG:NH1	2.06	0.66
1:G:77:PRO:HG2	1:G:81:THR:HB	1.76	0.66
1:A:81:THR:HG23	1:A:82:HIS:CE1	2.30	0.66
1:I:4:THR:HA	1:I:46:THR:CG2	2.26	0.66
1:K:4:THR:CG2	1:K:45:ILE:HG23	2.25	0.66
1:B:20:GLU:HB3	1:B:21:PRO:HD2	1.78	0.65
1:H:132:LYS:HD2	1:H:136:PHE:CZ	2.32	0.65
1:F:64:GLN:O	1:F:68:GLU:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:ILE:HD12	1:G:45:ILE:HG21	1.77	0.64
1:J:19:ARG:HB3	1:J:23:VAL:HG22	1.80	0.64
1:L:16:LEU:CD1	1:L:29:LEU:H	2.11	0.64
1:I:58:ILE:O	1:I:62:ILE:HG13	1.97	0.63
1:L:16:LEU:HB3	1:L:28:THR:HG22	1.80	0.63
1:L:16:LEU:HD12	1:L:29:LEU:HB2	1.79	0.63
1:F:23:VAL:O	1:F:24:TYR:HB2	1.99	0.62
1:L:3:SER:HB3	1:L:71:LYS:HE2	1.81	0.62
1:K:20:GLU:N	1:K:21:PRO:CD	2.62	0.62
1:L:6:LEU:CD1	1:L:61:ARG:HH12	2.11	0.62
1:I:4:THR:OG1	1:I:46:THR:HG21	2.00	0.62
1:K:19:ARG:HH21	1:K:19:ARG:CG	2.09	0.62
1:J:39:GLN:CD	1:J:138:LEU:HD23	2.18	0.62
1:L:16:LEU:HG	1:L:28:THR:CA	2.31	0.61
1:H:4:THR:HA	1:H:46:THR:HG22	1.81	0.60
1:K:19:ARG:HD2	1:K:23:VAL:CG2	2.30	0.60
1:G:113:ARG:HG2	1:G:113:ARG:NH1	2.16	0.60
1:L:110:GLU:HG3	1:L:112:PHE:CE2	2.36	0.60
1:A:141:ALA:O	1:A:145:ILE:HG12	2.02	0.60
1:H:50:PHE:CE2	1:H:61:ARG:HG3	2.35	0.60
1:J:22:GLU:C	1:J:24:TYR:H	2.03	0.60
1:L:111:ALA:HA	1:L:114:HIS:CE1	2.36	0.60
1:J:107:HIS:HA	1:J:114:HIS:CD2	2.37	0.60
1:D:33:ASN:O	1:D:37:ILE:CG1	2.46	0.60
1:L:6:LEU:HD13	1:L:61:ARG:HH12	1.67	0.60
1:K:22:GLU:C	1:K:24:TYR:H	2.04	0.59
1:I:99:ILE:HD11	1:I:140:TYR:HD2	1.67	0.59
1:L:28:THR:O	1:L:29:LEU:C	2.39	0.59
1:F:18:LYS:N	1:F:18:LYS:HD2	2.18	0.59
1:G:48:ASP:OD2	1:G:61:ARG:NH2	2.35	0.59
1:H:18:LYS:HE3	1:L:93:GLY:O	2.03	0.59
1:A:7:VAL:HG23	1:A:47:LEU:HD11	1.84	0.59
1:D:143:GLU:HA	1:D:143:GLU:OE1	2.02	0.59
1:I:39:GLN:CD	1:I:138:LEU:HD23	2.24	0.59
1:E:15:LEU:O	1:E:18:LYS:HD2	2.03	0.59
1:G:141:ALA:O	1:G:145:ILE:HD12	2.03	0.58
1:A:37:ILE:O	1:A:41:GLU:HG3	2.03	0.58
1:A:76:ASN:CB	1:A:134:TYR:OH	2.51	0.58
1:D:115:HIS:ND1	1:D:116:SER:N	2.51	0.58
1:I:110:GLU:CD	1:I:110:GLU:H	2.06	0.58
1:F:23:VAL:HG12	1:F:24:TYR:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:VAL:HG13	1:E:113:ARG:HB3	1.85	0.58
1:F:19:ARG:C	1:F:21:PRO:HD2	2.23	0.58
1:F:79:ALA:HB1	1:G:85:VAL:HG22	1.85	0.58
1:E:81:THR:HG22	1:E:82:HIS:CE1	2.39	0.58
1:H:4:THR:CG2	1:H:46:THR:HG22	2.29	0.57
1:C:105:ASN:O	1:C:108:ALA:HB3	2.03	0.57
1:I:46:THR:O	1:I:46:THR:HG23	2.04	0.57
1:K:87:LEU:HD23	1:K:118:LEU:HD11	1.86	0.57
1:I:6:LEU:HD21	1:I:61:ARG:HE	1.69	0.57
1:L:58:ILE:O	1:L:62:ILE:HG13	2.05	0.57
1:A:105:ASN:O	1:A:108:ALA:HB3	2.05	0.57
1:H:76:ASN:HD21	1:H:102:HIS:HA	1.69	0.57
1:E:19:ARG:HH11	1:E:19:ARG:CG	2.18	0.57
1:B:145:ILE:CD1	1:B:145:ILE:H	2.17	0.56
1:B:78:ALA:O	1:B:81:THR:HG22	2.05	0.56
1:A:88:ARG:NH1	1:A:117:TYR:O	2.37	0.56
1:K:19:ARG:NE	1:K:21:PRO:HB2	2.19	0.56
1:H:54:TRP:N	1:H:54:TRP:CD1	2.73	0.56
1:F:58:ILE:O	1:F:62:ILE:HG22	2.04	0.56
1:G:39:GLN:CD	1:G:138:LEU:HD23	2.25	0.56
1:E:31:ASN:N	1:E:31:ASN:OD1	2.35	0.56
1:F:81:THR:CG2	1:F:100:GLU:OE2	2.54	0.56
1:F:77:PRO:HG2	1:F:81:THR:OG1	2.06	0.56
1:G:113:ARG:HH11	1:G:113:ARG:HG2	1.70	0.56
1:I:111:ALA:HA	1:I:114:HIS:CD2	2.31	0.56
1:J:19:ARG:CB	1:J:23:VAL:HG22	2.35	0.56
1:D:19:ARG:C	1:D:20:GLU:CG	2.74	0.55
1:A:76:ASN:HB2	1:A:134:TYR:OH	2.04	0.55
1:F:106:VAL:CG1	1:F:113:ARG:O	2.55	0.55
1:B:54:TRP:N	1:B:54:TRP:CD1	2.74	0.55
1:L:54:TRP:CD1	1:L:54:TRP:N	2.72	0.55
1:G:20:GLU:CG	1:G:21:PRO:HD3	2.34	0.55
1:A:54:TRP:CD1	1:A:54:TRP:N	2.75	0.55
1:K:20:GLU:N	1:K:21:PRO:HD2	2.22	0.55
1:A:19:ARG:HH12	1:B:95:ALA:HB3	1.71	0.55
1:E:81:THR:HG22	1:E:82:HIS:ND1	2.22	0.55
1:G:88:ARG:NH1	1:G:117:TYR:O	2.36	0.55
1:J:30:ASP:O	1:J:34:ARG:CG	2.51	0.55
1:F:17:GLY:C	1:F:18:LYS:HD2	2.27	0.55
1:E:66:GLN:NE2	1:G:18:LYS:HE2	2.22	0.55
1:L:4:THR:HG23	1:L:70:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:54:TRP:N	1:J:54:TRP:CD1	2.75	0.54
1:D:20:GLU:HB3	1:D:21:PRO:CD	2.38	0.54
1:F:19:ARG:O	1:F:21:PRO:CD	2.50	0.54
1:I:99:ILE:HD11	1:I:140:TYR:CD2	2.43	0.53
1:J:112:PHE:CE1	1:J:113:ARG:HG2	2.43	0.53
1:J:4:THR:HG22	1:J:5:ILE:N	2.23	0.53
1:B:20:GLU:CB	1:B:21:PRO:HD2	2.37	0.53
1:F:19:ARG:C	1:F:21:PRO:CD	2.77	0.53
1:G:27:LEU:O	1:G:27:LEU:HD12	2.09	0.53
1:D:20:GLU:HB3	1:D:21:PRO:HD2	1.90	0.53
1:A:85:VAL:HG22	1:C:79:ALA:HB1	1.91	0.53
1:J:19:ARG:HG2	1:J:23:VAL:HG22	1.90	0.53
1:I:38:ALA:HA	1:I:41:GLU:CD	2.30	0.52
1:F:138:LEU:O	1:F:142:ILE:HG12	2.09	0.52
1:I:38:ALA:O	1:I:41:GLU:HG2	2.10	0.52
1:C:88:ARG:NH1	1:C:117:TYR:O	2.42	0.52
1:C:20:GLU:O	1:C:22:GLU:N	2.42	0.52
1:H:79:ALA:HB1	1:L:85:VAL:HG22	1.91	0.52
1:B:79:ALA:HB1	1:C:85:VAL:HG22	1.91	0.52
1:G:28:THR:O	1:G:31:ASN:HB2	2.09	0.52
1:E:106:VAL:CG1	1:E:113:ARG:O	2.58	0.52
1:L:110:GLU:HG2	1:L:113:ARG:HG3	1.92	0.52
1:J:107:HIS:HA	1:J:114:HIS:HD2	1.74	0.51
1:J:22:GLU:C	1:J:24:TYR:N	2.62	0.51
1:B:19:ARG:CG	1:B:22:GLU:HB2	2.40	0.51
1:B:3:SER:HB2	1:B:48:ASP:HB2	1.91	0.51
1:C:94:VAL:HG23	1:C:96:ILE:HG13	1.93	0.51
1:H:50:PHE:CD2	1:H:61:ARG:HG3	2.45	0.51
1:J:3:SER:OG	1:J:4:THR:N	2.42	0.51
1:L:27:LEU:CD1	1:L:32:ILE:HG12	2.41	0.51
1:A:20:GLU:CB	1:A:21:PRO:HD2	2.25	0.51
1:B:6:LEU:HD12	1:B:7:VAL:N	2.26	0.51
1:K:17:GLY:HA3	1:K:28:THR:HG22	1.93	0.51
1:I:15:LEU:O	1:I:16:LEU:C	2.47	0.51
1:E:54:TRP:CD1	1:E:54:TRP:N	2.79	0.50
1:K:26:HIS:CG	1:K:27:LEU:N	2.79	0.50
1:K:5:ILE:HD12	1:K:45:ILE:HG21	1.92	0.50
1:E:57:ALA:HB2	1:G:54:TRP:CH2	2.47	0.50
1:B:6:LEU:HD12	1:B:7:VAL:H	1.76	0.50
1:J:88:ARG:NH1	1:J:120:ASP:OD2	2.44	0.50
1:I:72:LEU:C	1:I:72:LEU:HD23	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:GLN:O	1:C:68:GLU:HG3	2.12	0.49
1:A:81:THR:HG23	1:A:82:HIS:ND1	2.25	0.49
1:J:110:GLU:O	1:J:113:ARG:N	2.42	0.49
1:D:8:ILE:HD11	1:D:62:ILE:HG22	1.93	0.49
1:D:88:ARG:CG	1:D:88:ARG:HH11	2.14	0.49
1:G:120:ASP:OD1	1:G:120:ASP:N	2.37	0.49
1:J:110:GLU:HB2	1:J:113:ARG:HG3	1.93	0.49
1:D:6:LEU:HD12	1:D:48:ASP:O	2.12	0.49
1:I:132:LYS:O	1:I:136:PHE:CD2	2.66	0.49
1:B:4:THR:HG21	1:B:45:ILE:CG2	2.41	0.49
1:J:115:HIS:CD2	1:J:116:SER:N	2.81	0.49
1:L:4:THR:HG23	1:L:70:VAL:HA	1.94	0.49
1:F:110:GLU:HB2	1:F:113:ARG:HG3	1.95	0.49
1:D:62:ILE:HD11	1:D:90:ALA:HB3	1.95	0.48
1:G:106:VAL:HG12	1:G:113:ARG:HB3	1.94	0.48
1:D:85:VAL:HG22	1:L:79:ALA:HB1	1.94	0.48
1:K:54:TRP:N	1:K:54:TRP:CD1	2.81	0.48
1:A:19:ARG:HG3	1:A:20:GLU:N	2.29	0.48
1:B:27:LEU:HD21	1:B:32:ILE:CG1	2.43	0.48
1:J:4:THR:HG22	1:J:5:ILE:H	1.78	0.48
1:J:5:ILE:HD12	1:J:45:ILE:HG21	1.96	0.48
1:B:19:ARG:NH2	1:B:22:GLU:HG2	2.26	0.48
1:F:62:ILE:HD11	1:F:90:ALA:O	2.13	0.48
1:K:2:SER:O	1:K:2:SER:OG	2.30	0.48
1:H:55:GLU:O	1:H:59:VAL:HG23	2.14	0.48
1:L:11:PRO:O	1:L:12:ASN:HB2	2.14	0.48
1:A:140:TYR:C	1:A:140:TYR:CD1	2.86	0.48
1:G:26:HIS:N	1:G:26:HIS:ND1	2.60	0.48
1:A:72:LEU:HD22	1:A:141:ALA:HB2	1.95	0.47
1:I:94:VAL:HG21	1:I:96:ILE:HD12	1.96	0.47
1:E:37:ILE:O	1:E:41:GLU:HG3	2.14	0.47
1:L:47:LEU:HD23	1:L:47:LEU:O	2.14	0.47
1:B:69:GLY:O	1:B:71:LYS:HE2	2.14	0.47
1:A:72:LEU:HD22	1:A:141:ALA:CB	2.45	0.47
1:C:9:HIS:HB2	1:C:51:GLN:CG	2.44	0.47
1:D:22:GLU:HB3	1:D:23:VAL:HA	1.96	0.47
1:B:142:ILE:HA	1:B:145:ILE:HD13	1.97	0.47
1:E:98:PHE:CE1	1:E:122:ALA:HB2	2.50	0.47
1:H:33:ASN:O	1:H:37:ILE:CG1	2.62	0.47
1:J:113:ARG:NH1	1:K:89:ASP:OD1	2.38	0.47
1:I:77:PRO:HG2	1:I:81:THR:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33:ASN:O	1:H:37:ILE:HG13	2.14	0.47
1:L:16:LEU:HG	1:L:28:THR:HA	1.97	0.47
1:E:35:GLN:NE2	1:E:135:SER:OG	2.43	0.46
1:E:111:ALA:HA	1:E:114:HIS:CE1	2.50	0.46
1:J:41:GLU:O	1:J:42:GLN:C	2.52	0.46
1:K:31:ASN:O	1:K:35:GLN:HG3	2.16	0.46
1:L:37:ILE:O	1:L:41:GLU:HB2	2.15	0.46
1:A:143:GLU:OE1	1:A:143:GLU:HA	2.16	0.46
1:G:18:LYS:O	1:G:24:TYR:HB2	2.16	0.46
1:L:16:LEU:HG	1:L:28:THR:C	2.31	0.46
1:A:81:THR:CG2	1:A:82:HIS:CE1	2.99	0.46
1:G:53:ASN:HD22	1:G:53:ASN:N	2.14	0.46
1:H:29:LEU:HA	1:H:29:LEU:HD23	1.77	0.46
1:A:79:ALA:HB1	1:B:85:VAL:HG22	1.97	0.46
1:D:19:ARG:C	1:D:20:GLU:HG2	2.35	0.46
1:L:138:LEU:O	1:L:142:ILE:CG1	2.63	0.46
1:L:47:LEU:HD23	1:L:47:LEU:C	2.37	0.46
1:E:35:GLN:HG3	1:E:36:LEU:N	2.31	0.45
1:L:66:GLN:HB3	1:L:66:GLN:HE21	1.69	0.45
1:D:62:ILE:HD11	1:D:90:ALA:CB	2.46	0.45
1:I:55:GLU:OE2	1:I:84:SER:HB2	2.16	0.45
1:C:106:VAL:HG13	1:C:113:ARG:HB3	1.97	0.45
1:D:19:ARG:O	1:D:20:GLU:CG	2.65	0.45
1:F:120:ASP:N	1:F:120:ASP:OD1	2.49	0.45
1:H:11:PRO:O	1:H:12:ASN:HB2	2.16	0.45
1:D:27:LEU:HA	1:D:27:LEU:HD22	1.64	0.45
1:H:110:GLU:OE1	1:H:113:ARG:NE	2.47	0.45
1:I:30:ASP:OD1	1:I:34:ARG:HD2	2.17	0.45
1:L:60:ASP:O	1:L:64:GLN:CG	2.55	0.45
1:G:98:PHE:CE2	1:G:122:ALA:HB2	2.51	0.45
1:I:107:HIS:ND1	1:I:114:HIS:ND1	2.62	0.45
1:J:14:ASN:N	1:J:14:ASN:OD1	2.47	0.45
1:L:114:HIS:ND1	1:L:114:HIS:N	2.64	0.45
1:E:81:THR:CG2	1:E:82:HIS:CE1	3.00	0.45
1:F:23:VAL:O	1:F:24:TYR:CB	2.60	0.45
1:H:106:VAL:HG13	1:H:113:ARG:HB3	1.99	0.45
1:J:19:ARG:CB	1:J:23:VAL:CG2	2.92	0.45
1:J:110:GLU:O	1:J:113:ARG:HB2	2.17	0.45
1:D:64:GLN:O	1:D:67:THR:OG1	2.32	0.45
1:I:20:GLU:HG2	1:I:26:HIS:HA	1.98	0.45
1:I:72:LEU:HD23	1:I:73:ILE:CA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:ILE:HG12	1:I:76:ASN:N	2.32	0.45
1:I:79:ALA:HB1	1:J:85:VAL:HG22	1.99	0.45
1:J:88:ARG:HG3	1:J:117:TYR:O	2.16	0.45
1:I:4:THR:CG2	1:I:5:ILE:N	2.80	0.45
1:A:64:GLN:O	1:A:68:GLU:HG3	2.17	0.44
1:J:48:ASP:OD1	1:J:49:THR:N	2.50	0.44
1:B:21:PRO:HA	1:B:24:TYR:O	2.17	0.44
1:D:98:PHE:CE2	1:D:122:ALA:HB2	2.52	0.44
1:H:125:VAL:HG12	1:H:126:ILE:N	2.32	0.44
1:H:15:LEU:HD23	1:H:15:LEU:HA	1.64	0.44
1:J:22:GLU:O	1:J:24:TYR:N	2.49	0.44
1:E:13:LEU:HA	1:E:13:LEU:HD12	1.75	0.44
1:H:10:GLY:H	1:H:13:LEU:CD2	2.16	0.44
1:J:109:ARG:HB3	1:J:113:ARG:HD2	1.99	0.44
1:A:7:VAL:CG2	1:A:47:LEU:HD11	2.47	0.44
1:L:15:LEU:O	1:L:16:LEU:C	2.53	0.44
1:E:110:GLU:OE1	1:E:113:ARG:NE	2.25	0.43
1:I:27:LEU:O	1:I:27:LEU:HD12	2.18	0.43
1:D:19:ARG:O	1:D:20:GLU:HG3	2.18	0.43
1:K:88:ARG:NH1	1:K:117:TYR:O	2.44	0.43
1:A:36:LEU:HD21	1:A:134:TYR:HB3	1.99	0.43
1:F:81:THR:CG2	1:F:116:SER:OG	2.62	0.43
1:E:28:THR:HG23	1:E:31:ASN:HD21	1.82	0.43
1:B:19:ARG:CG	1:B:20:GLU:N	2.77	0.43
1:F:80:LEU:O	1:F:82:HIS:N	2.51	0.43
1:E:85:VAL:HG22	1:G:79:ALA:HB1	2.01	0.43
1:L:143:GLU:OE1	1:L:143:GLU:HA	2.19	0.43
1:J:26:HIS:O	1:J:26:HIS:ND1	2.52	0.43
1:L:3:SER:CB	1:L:71:LYS:HE2	2.47	0.43
1:C:106:VAL:CG1	1:C:113:ARG:O	2.67	0.43
1:F:20:GLU:N	1:F:21:PRO:CD	2.82	0.43
1:I:88:ARG:NH1	1:I:117:TYR:O	2.45	0.43
1:I:13:LEU:HD12	1:I:13:LEU:HA	1.86	0.43
1:K:142:ILE:HA	1:K:145:ILE:HD12	1.99	0.43
1:A:115:HIS:ND1	1:A:115:HIS:C	2.71	0.43
1:E:136:PHE:HB3	1:H:136:PHE:CD2	2.53	0.43
1:F:61:ARG:HD2	1:F:61:ARG:O	2.18	0.43
1:I:132:LYS:HB3	1:I:136:PHE:CE2	2.53	0.43
1:L:16:LEU:CG	1:L:28:THR:HB	2.43	0.43
1:B:13:LEU:HA	1:B:13:LEU:HD23	1.80	0.42
1:E:81:THR:CG2	1:E:82:HIS:ND1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:LEU:HD13	1:F:61:ARG:NH2	2.29	0.42
1:J:111:ALA:O	1:J:112:PHE:C	2.56	0.42
1:D:25:GLY:O	1:D:27:LEU:N	2.51	0.42
1:E:111:ALA:HA	1:E:114:HIS:ND1	2.34	0.42
1:J:79:ALA:HB1	1:K:85:VAL:HG22	2.01	0.42
1:B:83:THR:CG2	1:C:85:VAL:HG13	2.48	0.42
1:J:19:ARG:HG2	1:J:23:VAL:CG2	2.49	0.42
1:K:20:GLU:CB	1:K:21:PRO:HD3	2.48	0.42
1:I:109:ARG:HB3	1:I:110:GLU:OE2	2.19	0.42
1:J:109:ARG:HD3	1:J:113:ARG:HD3	2.01	0.42
1:G:29:LEU:HA	1:G:29:LEU:HD23	1.85	0.42
1:F:83:THR:CG2	1:G:85:VAL:HG13	2.50	0.42
1:D:71:LYS:HD2	1:D:71:LYS:HA	1.72	0.42
1:I:145:ILE:HG12	1:I:145:ILE:H	1.66	0.42
1:L:13:LEU:HA	1:L:13:LEU:HD12	1.78	0.42
1:D:106:VAL:CG1	1:D:113:ARG:O	2.67	0.42
1:F:80:LEU:O	1:F:81:THR:C	2.58	0.42
1:K:19:ARG:NH2	1:K:19:ARG:HG2	2.13	0.42
1:A:11:PRO:O	1:A:12:ASN:HB2	2.20	0.42
1:B:107:HIS:HA	1:B:114:HIS:NE2	2.35	0.42
1:C:10:GLY:O	1:C:51:GLN:NE2	2.37	0.42
1:C:54:TRP:CD1	1:C:54:TRP:N	2.88	0.42
1:C:84:SER:OG	1:C:87:LEU:HB2	2.19	0.42
1:D:145:ILE:HD13	1:D:145:ILE:HA	1.63	0.42
1:E:109:ARG:HB3	1:E:113:ARG:HD2	2.02	0.41
1:J:81:THR:HG22	1:J:82:HIS:CE1	2.55	0.41
1:E:54:TRP:CH2	1:F:57:ALA:HB2	2.55	0.41
1:I:11:PRO:O	1:I:12:ASN:HB2	2.19	0.41
1:J:85:VAL:O	1:J:88:ARG:HB3	2.21	0.41
1:A:19:ARG:NH1	1:B:95:ALA:HB3	2.34	0.41
1:E:63:HIS:CE1	1:G:53:ASN:OD1	2.74	0.41
1:A:73:ILE:O	1:A:98:PHE:HA	2.21	0.41
1:D:9:HIS:HB2	1:D:51:GLN:HG2	2.02	0.41
1:H:4:THR:CG2	1:H:46:THR:HG23	2.29	0.41
1:K:20:GLU:HB2	1:K:21:PRO:HD3	2.03	0.41
1:K:19:ARG:CG	1:K:19:ARG:NH2	2.74	0.41
1:L:88:ARG:O	1:L:92:LEU:HG	2.20	0.41
1:B:19:ARG:O	1:B:20:GLU:O	2.38	0.41
1:F:132:LYS:HD2	1:F:136:PHE:CZ	2.55	0.41
1:F:18:LYS:CD	1:F:18:LYS:N	2.83	0.41
1:H:146:GLN:CA	1:H:146:GLN:NE2	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:11:PRO:CD	1:L:80:LEU:HD22	2.51	0.41
1:H:45:ILE:HA	1:H:45:ILE:HD13	1.80	0.41
1:K:19:ARG:CD	1:K:23:VAL:HG23	2.44	0.41
1:A:120:ASP:N	1:A:120:ASP:OD1	2.53	0.41
1:J:113:ARG:NH1	1:K:89:ASP:OD2	2.54	0.41
1:B:132:LYS:O	1:B:135:SER:HB2	2.21	0.40
1:I:83:THR:CG2	1:J:85:VAL:HG12	2.51	0.40
1:E:19:ARG:NH1	1:E:19:ARG:CG	2.79	0.40
1:B:38:ALA:O	1:B:42:GLN:HG3	2.21	0.40
1:H:82:HIS:CE1	1:H:113:ARG:HA	2.55	0.40
1:B:19:ARG:HG2	1:B:22:GLU:CB	2.47	0.40
1:B:36:LEU:HA	1:B:36:LEU:HD12	1.95	0.40
1:B:77:PRO:HG2	1:B:81:THR:HB	2.04	0.40
1:C:61:ARG:HH11	1:C:61:ARG:HD3	1.77	0.40
1:D:106:VAL:HG13	1:D:113:ARG:HB3	2.03	0.40
1:E:28:THR:H	1:E:31:ASN:ND2	2.20	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	143/145 (99%)	135 (94%)	6 (4%)	2 (1%)	11	15
1	B	143/145 (99%)	137 (96%)	5 (4%)	1 (1%)	22	30
1	C	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
1	D	143/145 (99%)	136 (95%)	5 (4%)	2 (1%)	11	15
1	E	143/145 (99%)	136 (95%)	5 (4%)	2 (1%)	11	15
1	F	143/145 (99%)	137 (96%)	6 (4%)	0	100	100
1	G	143/145 (99%)	139 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
1	I	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
1	J	143/145 (99%)	135 (94%)	6 (4%)	2 (1%)	11	15
1	K	143/145 (99%)	137 (96%)	3 (2%)	3 (2%)	7	7
1	L	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
All	All	1716/1740 (99%)	1633 (95%)	71 (4%)	12 (1%)	22	30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	GLU
1	D	20	GLU
1	D	26	HIS
1	K	24	TYR
1	A	21	PRO
1	E	21	PRO
1	K	23	VAL
1	A	20	GLU
1	E	22	GLU
1	J	23	VAL
1	K	3	SER
1	J	21	PRO

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	119/119 (100%)	114 (96%)	5 (4%)	30	40
1	B	119/119 (100%)	111 (93%)	8 (7%)	16	21
1	C	119/119 (100%)	105 (88%)	14 (12%)	5	5
1	D	119/119 (100%)	100 (84%)	19 (16%)	2	2
1	E	119/119 (100%)	104 (87%)	15 (13%)	4	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	119/119 (100%)	108 (91%)	11 (9%)	9	11
1	G	119/119 (100%)	107 (90%)	12 (10%)	7	8
1	H	119/119 (100%)	103 (87%)	16 (13%)	4	3
1	I	119/119 (100%)	103 (87%)	16 (13%)	4	3
1	J	119/119 (100%)	102 (86%)	17 (14%)	3	3
1	K	119/119 (100%)	106 (89%)	13 (11%)	6	6
1	L	119/119 (100%)	102 (86%)	17 (14%)	3	3
All	All	1428/1428 (100%)	1265 (89%)	163 (11%)	5	5

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	24	TYR
1	A	107	HIS
1	A	143	GLU
1	A	146	GLN
1	B	18	LYS
1	B	22	GLU
1	B	24	TYR
1	B	26	HIS
1	B	36	LEU
1	B	46	THR
1	B	145	ILE
1	B	146	GLN
1	C	2	SER
1	C	13	LEU
1	C	20	GLU
1	C	24	TYR
1	C	29	LEU
1	C	36	LEU
1	C	44	SER
1	C	46	THR
1	C	47	LEU
1	C	61	ARG
1	C	67	THR
1	C	84	SER
1	C	85	VAL
1	C	135	SER
1	D	13	LEU

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Mol	Chain	Res	Type
1	D	18	LYS
1	D	19	ARG
1	D	20	GLU
1	D	21	PRO
1	D	23	VAL
1	D	24	TYR
1	D	27	LEU
1	D	29	LEU
1	D	35	GLN
1	D	36	LEU
1	D	47	LEU
1	D	61	ARG
1	D	71	LYS
1	D	83	THR
1	D	88	ARG
1	D	109	ARG
1	D	115	HIS
1	D	145	ILE
1	E	2	SER
1	E	3	SER
1	E	13	LEU
1	E	18	LYS
1	E	19	ARG
1	E	24	TYR
1	E	28	THR
1	E	29	LEU
1	E	31	ASN
1	E	34	ARG
1	E	35	GLN
1	E	36	LEU
1	E	44	SER
1	E	81	THR
1	E	85	VAL
1	F	2	SER
1	F	13	LEU
1	F	18	LYS
1	F	20	GLU
1	F	29	LEU
1	F	34	ARG
1	F	36	LEU
1	F	62	ILE
1	F	84	SER

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Mol	Chain	Res	Type
1	F	85	VAL
1	F	144	LYS
1	G	2	SER
1	G	4	THR
1	G	13	LEU
1	G	18	LYS
1	G	26	HIS
1	G	29	LEU
1	G	30	ASP
1	G	35	GLN
1	G	36	LEU
1	G	44	SER
1	G	46	THR
1	G	47	LEU
1	H	3	SER
1	H	4	THR
1	H	13	LEU
1	H	19	ARG
1	H	29	LEU
1	H	34	ARG
1	H	36	LEU
1	H	42	GLN
1	H	44	SER
1	H	46	THR
1	H	47	LEU
1	H	61	ARG
1	H	71	LYS
1	H	114	HIS
1	H	144	LYS
1	H	146	GLN
1	I	2	SER
1	I	3	SER
1	I	13	LEU
1	I	18	LYS
1	I	19	ARG
1	I	24	TYR
1	I	29	LEU
1	I	34	ARG
1	I	35	GLN
1	I	36	LEU
1	I	44	SER
1	I	49	THR

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Mol	Chain	Res	Type
1	I	61	ARG
1	I	144	LYS
1	I	145	ILE
1	I	146	GLN
1	J	2	SER
1	J	4	THR
1	J	13	LEU
1	J	14	ASN
1	J	29	LEU
1	J	30	ASP
1	J	34	ARG
1	J	35	GLN
1	J	36	LEU
1	J	47	LEU
1	J	61	ARG
1	J	70	VAL
1	J	81	THR
1	J	85	VAL
1	J	113	ARG
1	J	123	ILE
1	J	144	LYS
1	K	13	LEU
1	K	19	ARG
1	K	24	TYR
1	K	26	HIS
1	K	29	LEU
1	K	30	ASP
1	K	34	ARG
1	K	36	LEU
1	K	61	ARG
1	K	106	VAL
1	K	109	ARG
1	K	132	LYS
1	K	144	LYS
1	L	2	SER
1	L	3	SER
1	L	5	ILE
1	L	13	LEU
1	L	24	TYR
1	L	27	LEU
1	L	29	LEU
1	L	35	GLN

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Mol	Chain	Res	Type
1	L	36	LEU
1	L	61	ARG
1	L	66	GLN
1	L	80	LEU
1	L	109	ARG
1	L	114	HIS
1	L	132	LYS
1	L	135	SER
1	L	142	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	51	GLN
1	H	146	GLN
1	J	115	HIS
1	L	66	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	145/145 (100%)	0.55	10 (6%) 16 20	25, 35, 76, 110	0
1	B	145/145 (100%)	0.63	17 (11%) 4 6	25, 35, 72, 115	0
1	C	145/145 (100%)	0.73	11 (7%) 13 17	25, 34, 72, 145	0
1	D	145/145 (100%)	0.78	16 (11%) 5 7	28, 46, 90, 124	0
1	E	145/145 (100%)	0.66	11 (7%) 13 17	27, 40, 82, 118	0
1	F	145/145 (100%)	0.50	11 (7%) 13 17	25, 34, 75, 122	0
1	G	145/145 (100%)	0.71	14 (9%) 7 9	29, 50, 91, 144	0
1	H	145/145 (100%)	0.74	15 (10%) 6 8	31, 51, 93, 144	0
1	I	145/145 (100%)	1.07	31 (21%) 0 0	34, 64, 104, 148	0
1	J	145/145 (100%)	0.93	23 (15%) 1 2	36, 53, 100, 144	0
1	K	145/145 (100%)	0.93	20 (13%) 2 3	30, 44, 85, 156	0
1	L	145/145 (100%)	1.11	29 (20%) 1 1	32, 57, 100, 127	0
All	All	1740/1740 (100%)	0.78	208 (11%) 4 5	25, 45, 95, 156	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	24	TYR	15.5
1	K	23	VAL	15.1
1	A	2	SER	13.2
1	C	24	TYR	13.1
1	L	23	VAL	10.6
1	F	24	TYR	9.0
1	K	106	VAL	8.9
1	G	3	SER	8.2
1	C	22	GLU	7.9
1	J	24	TYR	7.9
1	H	21	PRO	7.7

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Mol	Chain	Res	Type	RSRZ
1	C	21	PRO	7.4
1	J	21	PRO	7.1
1	K	24	TYR	7.0
1	K	21	PRO	7.0
1	C	2	SER	6.8
1	I	22	GLU	6.6
1	J	2	SER	6.4
1	L	24	TYR	6.2
1	K	87	LEU	6.1
1	C	23	VAL	5.9
1	H	23	VAL	5.6
1	L	145	ILE	5.3
1	L	27	LEU	5.3
1	B	24	TYR	5.2
1	L	37	ILE	5.1
1	G	18	LYS	5.1
1	I	23	VAL	5.1
1	I	47	LEU	5.1
1	C	146	GLN	5.0
1	J	23	VAL	5.0
1	F	26	HIS	4.9
1	I	24	TYR	4.9
1	G	25	GLY	4.8
1	L	34	ARG	4.8
1	I	73	ILE	4.8
1	C	3	SER	4.7
1	E	23	VAL	4.7
1	I	75	ILE	4.7
1	K	22	GLU	4.7
1	I	27	LEU	4.7
1	D	23	VAL	4.6
1	I	5	ILE	4.6
1	B	22	GLU	4.6
1	E	24	TYR	4.5
1	A	123	ILE	4.4
1	J	145	ILE	4.3
1	L	36	LEU	4.3
1	L	25	GLY	4.2
1	K	36	LEU	4.2
1	I	39	GLN	4.1
1	E	22	GLU	4.1
1	K	20	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	I	126	ILE	4.1
1	D	22	GLU	4.1
1	D	4	THR	4.1
1	G	2	SER	4.0
1	L	40	ALA	4.0
1	F	20	GLU	4.0
1	F	23	VAL	4.0
1	J	7	VAL	3.9
1	B	2	SER	3.8
1	A	23	VAL	3.8
1	J	22	GLU	3.7
1	J	18	LYS	3.6
1	J	6	LEU	3.6
1	L	72	LEU	3.5
1	I	4	THR	3.5
1	K	4	THR	3.5
1	L	22	GLU	3.4
1	I	35	GLN	3.4
1	D	18	LYS	3.4
1	F	107	HIS	3.4
1	H	19	ARG	3.4
1	D	19	ARG	3.4
1	G	24	TYR	3.4
1	I	127	CYS	3.4
1	B	19	ARG	3.4
1	I	133	GLY	3.3
1	A	3	SER	3.3
1	I	136	PHE	3.3
1	F	25	GLY	3.3
1	D	3	SER	3.3
1	J	45	ILE	3.2
1	H	25	GLY	3.2
1	F	106	VAL	3.2
1	I	16	LEU	3.2
1	L	2	SER	3.2
1	B	107	HIS	3.1
1	E	106	VAL	3.1
1	K	73	ILE	3.1
1	H	112	PHE	3.1
1	H	145	ILE	3.0
1	E	26	HIS	3.0
1	B	34	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	70	VAL	3.0
1	E	140	TYR	3.0
1	D	26	HIS	2.9
1	L	136	PHE	2.9
1	H	24	TYR	2.9
1	J	95	ALA	2.9
1	E	2	SER	2.9
1	G	5	ILE	2.9
1	J	20	GLU	2.9
1	J	27	LEU	2.9
1	B	23	VAL	2.9
1	E	21	PRO	2.9
1	L	63	HIS	2.9
1	B	145	ILE	2.8
1	I	21	PRO	2.8
1	L	132	LYS	2.8
1	G	142	ILE	2.8
1	L	45	ILE	2.8
1	L	131	ALA	2.8
1	L	141	ALA	2.8
1	H	140	TYR	2.8
1	I	18	LYS	2.7
1	B	44	SER	2.7
1	F	22	GLU	2.7
1	L	19	ARG	2.7
1	B	67	THR	2.7
1	D	21	PRO	2.7
1	I	132	LYS	2.7
1	H	41	GLU	2.6
1	J	34	ARG	2.6
1	D	5	ILE	2.6
1	I	112	PHE	2.6
1	A	134	TYR	2.6
1	K	11	PRO	2.6
1	L	3	SER	2.6
1	L	6	LEU	2.6
1	G	23	VAL	2.6
1	J	40	ALA	2.6
1	A	145	ILE	2.6
1	I	41	GLU	2.6
1	L	43	ALA	2.6
1	I	19	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	37	ILE	2.5
1	G	47	LEU	2.5
1	I	131	ALA	2.5
1	B	21	PRO	2.5
1	E	146	GLN	2.5
1	E	20	GLU	2.5
1	D	114	HIS	2.5
1	I	44	SER	2.5
1	J	72	LEU	2.5
1	L	47	LEU	2.5
1	B	26	HIS	2.4
1	F	19	ARG	2.4
1	F	144	LYS	2.4
1	G	20	GLU	2.4
1	L	28	THR	2.4
1	K	2	SER	2.4
1	J	134	TYR	2.4
1	F	111	ALA	2.4
1	H	7	VAL	2.4
1	L	106	VAL	2.4
1	D	112	PHE	2.4
1	H	27	LEU	2.4
1	G	138	LEU	2.4
1	J	16	LEU	2.3
1	D	25	GLY	2.3
1	K	140	TYR	2.3
1	I	87	LEU	2.3
1	C	145	ILE	2.3
1	D	91	LEU	2.3
1	D	108	ALA	2.2
1	J	5	ILE	2.2
1	L	123	ILE	2.2
1	D	20	GLU	2.2
1	H	13	LEU	2.2
1	B	3	SER	2.2
1	B	123	ILE	2.2
1	H	37	ILE	2.2
1	I	142	ILE	2.2
1	K	78	ALA	2.2
1	G	141	ALA	2.2
1	J	37	ILE	2.2
1	K	12	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	8	ILE	2.2
1	A	127	CYS	2.2
1	C	128	GLY	2.2
1	I	6	LEU	2.2
1	C	20	GLU	2.2
1	J	26	HIS	2.1
1	K	67	THR	2.1
1	H	4	THR	2.1
1	K	66	GLN	2.1
1	L	16	LEU	2.1
1	A	81	THR	2.1
1	B	106	VAL	2.1
1	I	98	PHE	2.1
1	B	42	GLN	2.1
1	G	19	ARG	2.1
1	K	145	ILE	2.1
1	A	24	TYR	2.0
1	A	45	ILE	2.0
1	B	27	LEU	2.0
1	E	41	GLU	2.0
1	I	20	GLU	2.0
1	I	25	GLY	2.0
1	J	55	GLU	2.0
1	C	44	SER	2.0
1	H	69	GLY	2.0
1	K	29	LEU	2.0
1	K	137	ALA	2.0
1	L	64	GLN	2.0
1	J	17	GLY	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.