



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:25 PM UTC

PDB ID : 8PKS / pdb_00008pks
Title : Low resolution crystal structure of Keap1-456, a repeat fragment from the human Keap1 beta-propeller
Authors : Wouters, S.M.L.
Deposited on : 2023-06-27
Resolution : 2.60 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

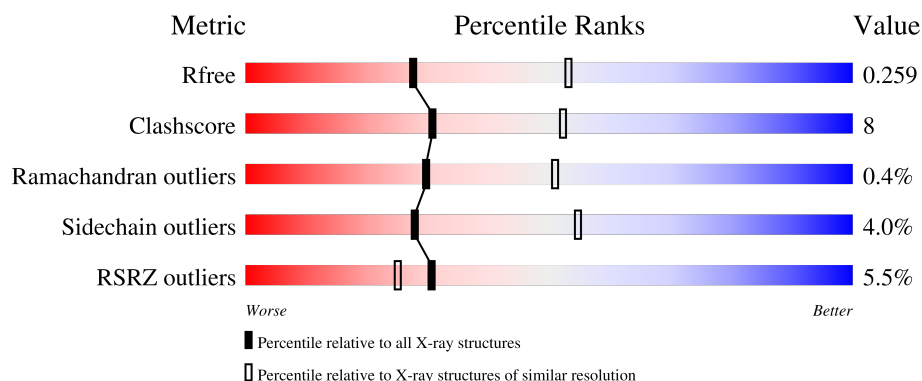
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	143	4% 81% 14% ..
1	B	143	3% 84% 13% .
1	C	143	78% 19% .
1	D	143	3% 81% 13% ..
1	E	143	3% 73% 22% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	143	4% 87% 11% .
1	G	143	6% 76% 18% ..
1	H	143	4% 78% 18% ...
1	I	143	3% 83% 13% ..
1	J	143	6% 79% 18% ..
1	K	143	8% 63% 34% ..
1	L	143	5% 78% 19% ..
1	M	143	13% 71% 23% 6%
1	N	143	13% 71% 24% ...

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15069 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1072	664	189	211	8			
1	B	138	Total	C	N	O	S	0	0	0
			1048	651	182	207	8			
1	C	139	Total	C	N	O	S	0	0	0
			1063	660	183	212	8			
1	D	138	Total	C	N	O	S	0	0	0
			1052	653	183	208	8			
1	E	139	Total	C	N	O	S	0	0	0
			1063	660	184	211	8			
1	F	140	Total	C	N	O	S	0	0	0
			1068	663	185	212	8			
1	G	139	Total	C	N	O	S	0	0	0
			1044	650	180	206	8			
1	H	140	Total	C	N	O	S	0	0	0
			1068	663	184	213	8			
1	I	140	Total	C	N	O	S	0	0	0
			1064	661	185	210	8			
1	J	140	Total	C	N	O	S	0	0	0
			1061	660	184	209	8			
1	K	140	Total	C	N	O	S	0	0	0
			1056	657	179	212	8			
1	L	141	Total	C	N	O	S	0	0	0
			1060	660	182	210	8			
1	M	134	Total	C	N	O	S	0	0	0
			998	623	171	197	7			
1	N	140	Total	C	N	O	S	0	0	0
			1047	652	177	210	8			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q14145

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	expression tag	UNP Q14145
A	3	HIS	-	expression tag	UNP Q14145
A	4	MET	-	expression tag	UNP Q14145
B	1	GLY	-	expression tag	UNP Q14145
B	2	SER	-	expression tag	UNP Q14145
B	3	HIS	-	expression tag	UNP Q14145
B	4	MET	-	expression tag	UNP Q14145
C	1	GLY	-	expression tag	UNP Q14145
C	2	SER	-	expression tag	UNP Q14145
C	3	HIS	-	expression tag	UNP Q14145
C	4	MET	-	expression tag	UNP Q14145
D	1	GLY	-	expression tag	UNP Q14145
D	2	SER	-	expression tag	UNP Q14145
D	3	HIS	-	expression tag	UNP Q14145
D	4	MET	-	expression tag	UNP Q14145
E	1	GLY	-	expression tag	UNP Q14145
E	2	SER	-	expression tag	UNP Q14145
E	3	HIS	-	expression tag	UNP Q14145
E	4	MET	-	expression tag	UNP Q14145
F	1	GLY	-	expression tag	UNP Q14145
F	2	SER	-	expression tag	UNP Q14145
F	3	HIS	-	expression tag	UNP Q14145
F	4	MET	-	expression tag	UNP Q14145
G	1	GLY	-	expression tag	UNP Q14145
G	2	SER	-	expression tag	UNP Q14145
G	3	HIS	-	expression tag	UNP Q14145
G	4	MET	-	expression tag	UNP Q14145
H	1	GLY	-	expression tag	UNP Q14145
H	2	SER	-	expression tag	UNP Q14145
H	3	HIS	-	expression tag	UNP Q14145
H	4	MET	-	expression tag	UNP Q14145
I	1	GLY	-	expression tag	UNP Q14145
I	2	SER	-	expression tag	UNP Q14145
I	3	HIS	-	expression tag	UNP Q14145
I	4	MET	-	expression tag	UNP Q14145
J	1	GLY	-	expression tag	UNP Q14145
J	2	SER	-	expression tag	UNP Q14145
J	3	HIS	-	expression tag	UNP Q14145
J	4	MET	-	expression tag	UNP Q14145
K	1	GLY	-	expression tag	UNP Q14145
K	2	SER	-	expression tag	UNP Q14145
K	3	HIS	-	expression tag	UNP Q14145

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	4	MET	-	expression tag	UNP Q14145
L	1	GLY	-	expression tag	UNP Q14145
L	2	SER	-	expression tag	UNP Q14145
L	3	HIS	-	expression tag	UNP Q14145
L	4	MET	-	expression tag	UNP Q14145
M	1	GLY	-	expression tag	UNP Q14145
M	2	SER	-	expression tag	UNP Q14145
M	3	HIS	-	expression tag	UNP Q14145
M	4	MET	-	expression tag	UNP Q14145
N	1	GLY	-	expression tag	UNP Q14145
N	2	SER	-	expression tag	UNP Q14145
N	3	HIS	-	expression tag	UNP Q14145
N	4	MET	-	expression tag	UNP Q14145

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	37	Total O 37 37	0	0
2	C	27	Total O 27 27	0	0
2	D	29	Total O 29 29	0	0
2	E	17	Total O 17 17	0	0
2	F	29	Total O 29 29	0	0
2	G	26	Total O 26 26	0	0
2	H	20	Total O 20 20	0	0
2	I	18	Total O 18 18	0	0
2	J	7	Total O 7 7	0	0
2	K	12	Total O 12 12	0	0
2	L	21	Total O 21 21	0	0
2	M	14	Total O 14 14	0	0

Continued on next page...

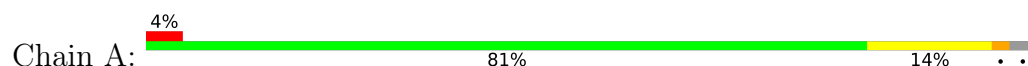
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	19	Total	O	0	0
			19	19		

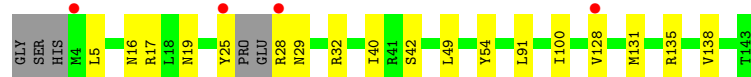
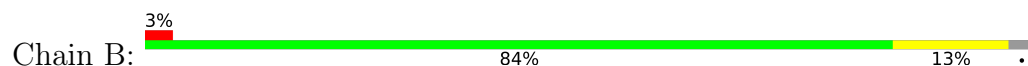
3 Residue-property plots [i](#)

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.

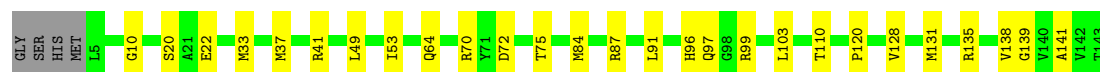
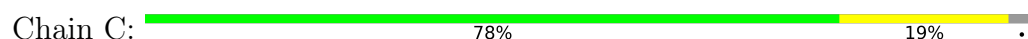
- Molecule 1: Kelch-like ECH-associated protein 1



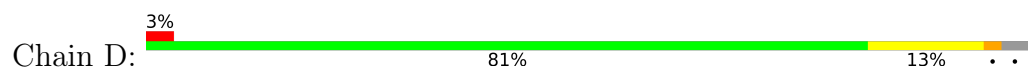
- Molecule 1: Kelch-like ECH-associated protein 1



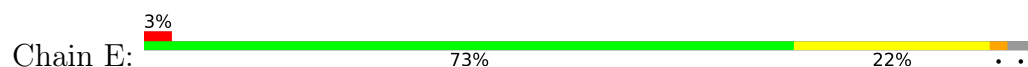
- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 1: Kelch-like ECH-associated protein 1

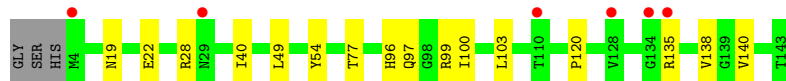
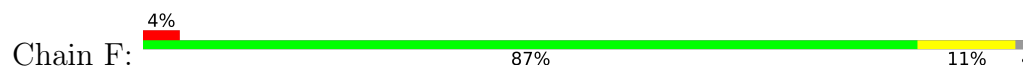


- Molecule 1: Kelch-like ECH-associated protein 1

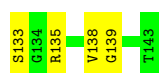
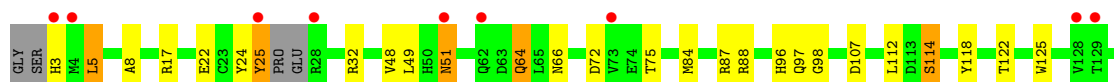
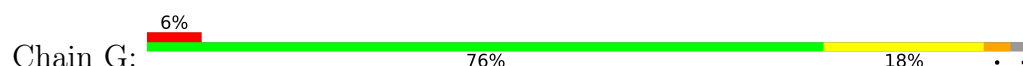




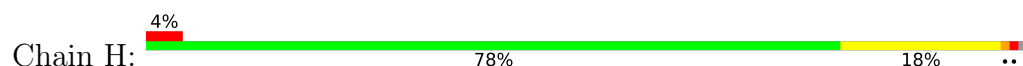
- Molecule 1: Kelch-like ECH-associated protein 1



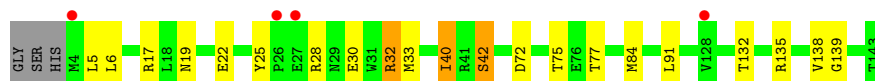
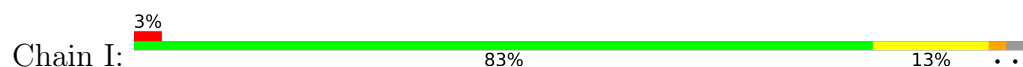
- Molecule 1: Kelch-like ECH-associated protein 1



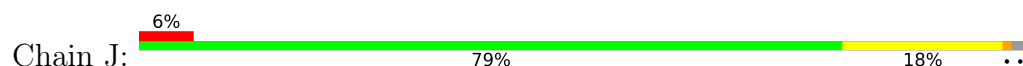
- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 1: Kelch-like ECH-associated protein 1

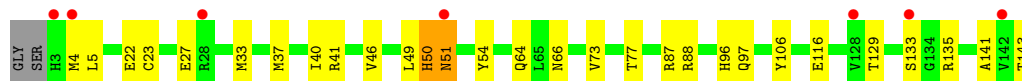
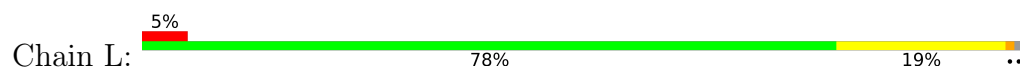


- Molecule 1: Kelch-like ECH-associated protein 1

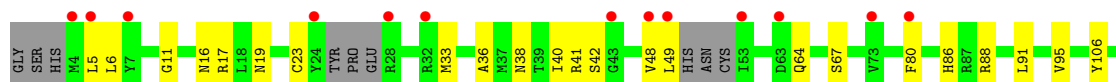




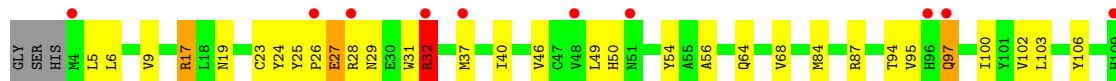
- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 1: Kelch-like ECH-associated protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.85Å 220.96Å 248.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 2.60 48.54 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.54-2.60) 95.5 (48.54-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.214 , 0.259 0.214 , 0.259	Depositor DCC
R_{free} test set	4032 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15069	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/1094	0.47	0/1485
1	B	0.31	0/1069	0.49	0/1453
1	C	0.22	0/1086	0.42	0/1478
1	D	0.29	0/1073	0.50	1/1458 (0.1%)
1	E	0.25	0/1086	0.44	0/1478
1	F	0.25	0/1091	0.43	0/1485
1	G	0.33	0/1065	0.54	1/1449 (0.1%)
1	H	0.28	0/1091	0.50	0/1485
1	I	0.35	0/1087	0.61	0/1480
1	J	0.37	0/1084	0.58	0/1476
1	K	0.43	0/1079	0.67	0/1471
1	L	0.28	0/1083	0.52	1/1476 (0.1%)
1	M	0.26	0/1017	0.44	0/1383
1	N	0.44	0/1069	0.67	0/1457
All	All	0.32	0/15074	0.53	3/20514 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	I	0	1
1	K	0	1
1	N	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	50	HIS	CA-C-O	-5.71	115.65	122.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	25	TYR	N-CA-CB	-5.59	101.00	110.50
1	G	25	TYR	CB-CA-C	5.04	119.68	110.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	ARG	Sidechain
1	I	32	ARG	Sidechain
1	K	99	ARG	Sidechain
1	N	32	ARG	Sidechain

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	1072	0	992	17	0
1	B	1048	0	964	16	0
1	C	1063	0	980	17	0
1	D	1052	0	970	15	0
1	E	1063	0	982	26	0
1	F	1068	0	984	11	0
1	G	1044	0	953	22	0
1	H	1068	0	982	20	0
1	I	1064	0	980	13	0
1	J	1061	0	976	18	0
1	K	1056	0	962	33	0
1	L	1060	0	967	17	0
1	M	998	0	913	18	0
1	N	1047	0	946	23	0
2	A	29	0	0	1	0
2	B	37	0	0	1	0
2	C	27	0	0	0	0
2	D	29	0	0	0	0
2	E	17	0	0	1	0
2	F	29	0	0	1	0
2	G	26	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	20	0	0	0	0
2	I	18	0	0	0	0
2	J	7	0	0	0	0
2	K	12	0	0	0	0
2	L	21	0	0	0	0
2	M	14	0	0	0	0
2	N	19	0	0	1	0
All	All	15069	0	13551	234	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 8.

All (234) 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:N:9:VAL:HG13	1:N:37:MET:HE1	1.48	0.96
1:N:100:ILE:HB	1:N:118:TYR:HB3	1.62	0.80
1:D:17:ARG:HG2	1:D:42:SER:HB2	1.65	0.79
1:B:16:ASN:HD21	1:G:17:ARG:HG3	1.50	0.77
1:D:25:TYR:HE2	1:D:32:ARG:HB2	1.47	0.76
1:N:84:MET:HE2	1:N:102:VAL:HG21	1.68	0.75
1:C:72:ASP:HB3	1:C:75:THR:HG22	1.67	0.75
1:G:88:ARG:HH22	1:G:114:SER:HB2	1.52	0.73
1:I:72:ASP:HB3	1:I:75:THR:HG22	1.70	0.72
1:N:17:ARG:NH1	2:N:201:HOH:O	2.22	0.72
1:E:19:ASN:HB3	1:E:40:ILE:HD13	1.72	0.72
1:J:128:VAL:HG13	1:J:129:THR:HG22	1.71	0.71
1:K:49:LEU:HD22	1:K:100:ILE:HG13	1.71	0.71
1:K:20:SER:HB2	1:K:33:MET:HE1	1.73	0.69
1:H:72:ASP:HB3	1:H:75:THR:HG22	1.73	0.69
1:J:28:ARG:HB2	1:J:30:GLU:HG2	1.76	0.67
1:G:25:TYR:HE2	1:G:32:ARG:HB2	1.60	0.66
1:E:17:ARG:NH1	2:E:201:HOH:O	2.29	0.64
1:C:64:GLN:O	1:C:87:ARG:NH1	2.29	0.63
1:F:99:ARG:NH1	2:F:202:HOH:O	2.33	0.62
1:J:19:ASN:HB3	1:J:40:ILE:HG12	1.82	0.61
1:E:17:ARG:HG2	1:E:42:SER:HB3	1.83	0.60
1:K:88:ARG:HG3	1:K:91:LEU:HD22	1.86	0.58
1:H:28:ARG:HG3	1:H:30:GLU:HG2	1.85	0.58
1:I:91:LEU:H	1:I:91:LEU:HD23	1.68	0.58
1:L:66:ASN:HB3	1:L:87:ARG:HG2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:ASN:HB3	1:G:87:ARG:HG2	1.87	0.57
1:K:64:GLN:HG3	1:K:107:ASP:C	2.30	0.56
1:M:19:ASN:HB3	1:M:40:ILE:HA	1.88	0.56
1:C:49:LEU:HD21	1:C:120:PRO:HG3	1.88	0.56
1:B:17:ARG:NH2	2:B:201:HOH:O	2.30	0.55
1:K:33:MET:HE2	1:M:36:ALA:HB3	1.87	0.55
1:L:5:LEU:HB3	1:L:23:CYS:SG	2.47	0.55
1:N:28:ARG:O	1:N:29:ASN:C	2.50	0.55
1:M:6:LEU:HD21	1:N:103:LEU:HD11	1.90	0.54
1:B:49:LEU:HD22	1:B:100:ILE:HG13	1.90	0.54
1:E:64:GLN:HG3	1:E:107:ASP:C	2.33	0.54
1:J:49:LEU:HD11	1:J:98:GLY:HA2	1.90	0.53
1:A:113:ASP:HB3	1:A:134:GLY:HA2	1.90	0.53
1:D:25:TYR:O	1:D:28:ARG:N	2.41	0.53
1:K:31:TRP:HE1	1:L:129:THR:CG2	2.22	0.53
1:A:113:ASP:CG	1:A:130:ARG:HG2	2.34	0.53
1:G:64:GLN:HG3	1:G:107:ASP:C	2.34	0.53
1:B:16:ASN:ND2	1:G:17:ARG:H	2.05	0.52
1:B:16:ASN:HD22	1:G:17:ARG:H	1.56	0.52
1:F:135:ARG:HG3	1:F:138:VAL:HG22	1.91	0.52
1:E:135:ARG:NH2	1:F:22:GLU:OE2	2.42	0.52
1:M:129:THR:OG1	1:M:130:ARG:N	2.41	0.52
1:B:91:LEU:HD23	1:B:91:LEU:H	1.75	0.52
1:H:135:ARG:HG3	1:H:138:VAL:HG11	1.91	0.52
1:B:25:TYR:HE1	1:B:32:ARG:HB3	1.75	0.52
1:C:141:ALA:HB1	1:D:48:VAL:HG23	1.92	0.52
1:E:5:LEU:HD13	1:E:23:CYS:SG	2.50	0.52
1:M:91:LEU:HD23	1:M:91:LEU:H	1.74	0.51
1:E:28:ARG:HB2	1:E:30:GLU:OE1	2.10	0.51
1:J:54:TYR:OH	1:J:70:ARG:NH1	2.42	0.51
1:G:3:HIS:CB	1:H:143:THR:HA	2.40	0.51
1:K:17:ARG:H	1:M:16:ASN:HD22	1.59	0.51
1:B:17:ARG:HG3	1:B:42:SER:HB2	1.92	0.51
1:E:91:LEU:HD23	1:E:91:LEU:H	1.75	0.51
1:I:28:ARG:HB3	1:I:30:GLU:HG3	1.93	0.51
1:M:49:LEU:HD21	1:M:120:PRO:HG3	1.93	0.51
1:G:5:LEU:HD12	1:G:24:TYR:O	2.11	0.50
1:D:91:LEU:H	1:D:91:LEU:HD23	1.77	0.50
1:B:135:ARG:HG3	1:B:138:VAL:CG1	2.42	0.50
1:I:22:GLU:OE1	1:J:132:THR:OG1	2.26	0.50
1:N:5:LEU:HB3	1:N:23:CYS:SG	2.51	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ILE:HB	1:D:118:TYR:HB3	1.93	0.50
1:K:70:ARG:HD3	1:K:81:VAL:HG21	1.94	0.50
1:E:117:CYS:HB2	1:E:128:VAL:HG22	1.93	0.50
1:K:23:CYS:SG	1:K:34:ILE:HG21	2.52	0.50
1:K:37:MET:HE1	1:K:41:ARG:HD2	1.94	0.50
1:B:16:ASN:ND2	1:G:17:ARG:HG3	2.22	0.50
1:C:135:ARG:HG3	1:C:138:VAL:CG1	2.42	0.49
1:N:26:PRO:O	1:N:27:GLU:C	2.56	0.49
1:M:17:ARG:HB3	1:M:40:ILE:CG2	2.43	0.49
1:G:22:GLU:OE2	1:H:135:ARG:NH2	2.46	0.48
1:K:19:ASN:HB3	1:K:40:ILE:HD13	1.94	0.48
1:L:51:ASN:HD22	1:L:73:VAL:HG12	1.79	0.48
1:L:49:LEU:O	1:L:50:HIS:C	2.57	0.48
1:I:135:ARG:HG3	1:I:138:VAL:HB	1.94	0.48
1:C:96:HIS:CD2	1:C:97:GLN:HG3	2.49	0.48
1:H:88:ARG:NH2	1:H:114:SER:OG	2.47	0.48
1:J:88:ARG:NH2	1:J:116:GLU:OE2	2.47	0.48
1:E:100:ILE:HB	1:E:118:TYR:HB3	1.95	0.48
1:L:33:MET:HE2	1:L:33:MET:HB2	1.78	0.47
1:K:31:TRP:HE1	1:L:129:THR:HG21	1.79	0.47
1:B:135:ARG:HG3	1:B:138:VAL:HG11	1.96	0.47
1:J:19:ASN:HB3	1:J:40:ILE:HA	1.95	0.47
1:A:113:ASP:CG	1:A:130:ARG:HE	2.22	0.47
1:B:28:ARG:O	1:B:29:ASN:C	2.57	0.47
1:C:37:MET:HE1	1:C:41:ARG:HB2	1.96	0.47
1:J:129:THR:OG1	1:J:130:ARG:N	2.47	0.47
1:J:71:TYR:HB2	1:J:78:TRP:CD2	2.50	0.47
1:L:27:GLU:H	1:L:27:GLU:CD	2.22	0.47
1:G:72:ASP:OD1	1:G:75:THR:HG22	2.15	0.47
1:H:116:GLU:HG2	1:H:127:GLU:HG3	1.97	0.47
1:H:49:LEU:HD22	1:H:100:ILE:HG13	1.96	0.47
1:M:64:GLN:HG2	1:M:106:TYR:O	2.14	0.47
1:A:29:ASN:HA	2:A:208:HOH:O	2.15	0.47
1:K:37:MET:HG2	1:K:78:TRP:CD2	2.50	0.47
1:D:25:TYR:CE2	1:D:32:ARG:HB2	2.37	0.46
1:E:19:ASN:CB	1:E:40:ILE:HD13	2.43	0.46
1:E:113:ASP:O	1:E:131:MET:HG2	2.16	0.46
1:K:135:ARG:HG3	1:K:138:VAL:HG11	1.96	0.46
1:E:103:LEU:HD23	1:E:131:MET:HE1	1.97	0.46
1:B:49:LEU:HB3	1:B:54:TYR:CE1	2.51	0.46
1:N:64:GLN:O	1:N:87:ARG:NH1	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:56:ALA:HA	1:N:68:VAL:HG22	1.98	0.46
1:M:86:HIS:HB2	1:M:88:ARG:HH21	1.80	0.46
1:B:25:TYR:CE1	1:B:32:ARG:HB3	2.51	0.46
1:L:96:HIS:CE1	1:L:97:GLN:HG3	2.51	0.45
1:N:97:GLN:HE21	1:N:97:GLN:HB2	1.39	0.45
1:C:22:GLU:OE1	1:D:132:THR:OG1	2.29	0.45
1:K:41:ARG:HH21	1:K:69:GLU:HG2	1.81	0.45
1:F:49:LEU:HD21	1:F:120:PRO:HG3	1.98	0.45
1:H:29:ASN:O	1:H:29:ASN:ND2	2.49	0.45
1:L:46:VAL:HA	1:L:54:TYR:O	2.17	0.45
1:H:135:ARG:HG3	1:H:138:VAL:CG1	2.46	0.45
1:I:17:ARG:HG2	1:I:42:SER:HB3	1.97	0.45
1:N:25:TYR:CE2	1:N:32:ARG:HB2	2.52	0.45
1:A:135:ARG:HG3	1:A:138:VAL:CG1	2.46	0.45
1:K:84:MET:HE2	1:K:102:VAL:HG11	1.98	0.45
1:N:37:MET:HE2	1:N:37:MET:HB3	1.80	0.45
1:N:100:ILE:O	1:N:117:CYS:HA	2.16	0.45
1:C:131:MET:HE1	1:C:138:VAL:HG21	1.99	0.45
1:F:49:LEU:HD22	1:F:100:ILE:HG13	1.99	0.45
1:K:56:ALA:HB1	1:K:84:MET:CE	2.46	0.45
1:A:114:SER:HA	1:A:130:ARG:HG3	1.99	0.44
1:H:26:PRO:C	1:H:28:ARG:H	2.25	0.44
1:K:72:ASP:HB3	1:K:75:THR:OG1	2.16	0.44
1:K:135:ARG:HG3	1:K:138:VAL:CG1	2.47	0.44
1:L:64:GLN:HG2	1:L:106:TYR:O	2.17	0.44
1:K:25:TYR:O	1:K:29:ASN:N	2.50	0.44
1:C:135:ARG:HG3	1:C:138:VAL:HG11	1.99	0.44
1:D:49:LEU:HD22	1:D:100:ILE:HG13	1.99	0.44
1:H:75:THR:O	1:H:77:THR:HG23	2.18	0.44
1:A:113:ASP:OD1	1:A:130:ARG:NE	2.51	0.44
1:B:131:MET:HE2	1:B:135:ARG:HD2	1.99	0.44
1:C:103:LEU:HD23	1:C:131:MET:HE3	1.99	0.44
1:E:129:THR:OG1	1:E:130:ARG:N	2.40	0.44
1:C:10:GLY:O	1:D:135:ARG:NH1	2.48	0.44
1:G:49:LEU:HD11	1:G:98:GLY:HA2	1.99	0.44
1:H:5:LEU:HB3	1:H:23:CYS:SG	2.57	0.44
1:M:11:GLY:HA3	1:N:135:ARG:HG3	1.99	0.44
1:F:19:ASN:HB3	1:F:40:ILE:HG13	1.98	0.44
1:F:103:LEU:HD13	1:F:140:VAL:HG21	1.98	0.44
1:M:88:ARG:NH2	1:M:116:GLU:OE2	2.50	0.44
1:M:48:VAL:HG21	1:N:143:THR:HB	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:LEU:O	1:G:51:ASN:N	2.50	0.43
1:J:91:LEU:HD23	1:J:91:LEU:H	1.83	0.43
1:E:49:LEU:HD22	1:E:100:ILE:HG13	2.00	0.43
1:K:48:VAL:CG2	1:L:141:ALA:HB1	2.48	0.43
1:E:48:VAL:O	1:E:95:VAL:HG11	2.19	0.43
1:F:96:HIS:CD2	1:F:97:GLN:HG3	2.54	0.43
1:K:7:TYR:CE1	1:K:23:CYS:SG	3.08	0.43
1:K:49:LEU:HD11	1:K:98:GLY:HA2	1.98	0.43
1:G:96:HIS:CE1	1:G:97:GLN:HG3	2.53	0.43
1:K:96:HIS:HB3	1:K:101:TYR:CE1	2.54	0.43
1:L:37:MET:HE1	1:L:41:ARG:HB2	1.99	0.43
1:E:88:ARG:HG3	1:E:91:LEU:HD13	2.00	0.43
1:G:84:MET:HE3	1:G:84:MET:HB2	1.88	0.43
1:K:48:VAL:HG11	1:L:143:THR:HB	1.99	0.43
1:J:71:TYR:HB2	1:J:78:TRP:CE2	2.54	0.43
1:G:107:ASP:HB3	1:G:112:LEU:HD21	2.00	0.43
1:B:19:ASN:HB3	1:B:40:ILE:HD13	2.00	0.43
1:K:71:TYR:HB2	1:K:78:TRP:CD2	2.53	0.43
1:M:139:GLY:HA3	1:N:46:VAL:HG21	2.01	0.43
1:N:49:LEU:HB3	1:N:54:TYR:CE2	2.53	0.43
1:K:12:PHE:CD1	1:K:17:ARG:HG3	2.54	0.42
1:A:5:LEU:HB3	1:A:23:CYS:SG	2.60	0.42
1:F:49:LEU:HB3	1:F:54:TYR:CE1	2.54	0.42
1:I:6:LEU:HD21	1:J:103:LEU:HD11	2.01	0.42
1:N:132:THR:OG1	1:N:133:SER:N	2.53	0.42
1:D:107:ASP:HB3	1:D:112:LEU:HD21	2.00	0.42
1:A:64:GLN:HG2	1:A:106:TYR:O	2.20	0.42
1:E:135:ARG:HH21	1:F:22:GLU:CD	2.26	0.42
1:G:8:ALA:HB1	1:H:131:MET:HE3	2.01	0.42
1:G:139:GLY:HA3	1:H:46:VAL:HG21	2.00	0.42
1:I:84:MET:HE3	1:I:84:MET:HB2	1.86	0.42
1:L:133:SER:H	1:L:135:ARG:HH21	1.66	0.42
1:H:64:GLN:HG3	1:H:89:SER:HB3	2.02	0.42
1:M:38:ASN:HB2	1:M:80:PHE:HE1	1.84	0.42
1:E:131:MET:HE2	1:E:131:MET:HB3	1.73	0.42
1:A:118:TYR:HB2	1:A:125:TRP:CH2	2.55	0.42
1:A:25:TYR:CE2	1:A:32:ARG:HB2	2.54	0.42
1:C:139:GLY:HA3	1:D:46:VAL:HG21	2.02	0.42
1:D:82:ALA:HA	1:D:83:PRO:HD3	1.95	0.42
1:I:25:TYR:CD2	1:I:32:ARG:HB2	2.55	0.42
1:L:88:ARG:NH1	1:L:116:GLU:OE2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:24:TYR:HB2	1:N:31:TRP:CE2	2.55	0.42
1:A:113:ASP:HB3	1:A:134:GLY:CA	2.50	0.41
1:D:71:TYR:CZ	1:D:76:GLU:HA	2.55	0.41
1:I:139:GLY:HA3	1:J:46:VAL:HG21	2.02	0.41
1:C:84:MET:HE3	1:C:84:MET:HB2	1.89	0.41
1:E:24:TYR:OH	1:E:29:ASN:OD1	2.37	0.41
1:J:66:ASN:HB3	1:J:87:ARG:HG2	2.02	0.41
1:K:49:LEU:HD21	1:K:120:PRO:HG3	2.03	0.41
1:N:64:GLN:HG2	1:N:106:TYR:O	2.21	0.41
1:A:25:TYR:HE2	1:A:32:ARG:HB2	1.85	0.41
1:M:135:ARG:HG3	1:M:138:VAL:HG11	2.01	0.41
1:A:107:ASP:HB3	1:A:112:LEU:HD11	2.00	0.41
1:E:25:TYR:O	1:E:30:GLU:HG2	2.20	0.41
1:E:122:THR:O	1:E:123:ASP:C	2.64	0.41
1:G:88:ARG:NH2	1:G:114:SER:HB2	2.26	0.41
1:I:19:ASN:HB3	1:I:40:ILE:HA	2.01	0.41
1:I:75:THR:HG23	1:I:77:THR:H	1.86	0.41
1:K:132:THR:OG1	1:L:22:GLU:OE1	2.37	0.41
1:G:48:VAL:HG23	1:H:141:ALA:HB1	2.03	0.41
1:H:46:VAL:HA	1:H:54:TYR:O	2.19	0.41
1:K:46:VAL:HA	1:K:54:TYR:O	2.20	0.41
1:E:25:TYR:HB2	1:E:30:GLU:HG2	2.03	0.41
1:H:19:ASN:HB3	1:H:40:ILE:HG12	2.02	0.41
1:I:132:THR:OG1	1:J:22:GLU:OE1	2.22	0.41
1:A:49:LEU:HD21	1:A:120:PRO:HG3	2.03	0.41
1:A:64:GLN:O	1:A:87:ARG:HD3	2.21	0.41
1:E:30:GLU:HB2	1:E:32:ARG:CZ	2.51	0.41
1:H:19:ASN:HB3	1:H:40:ILE:HA	2.03	0.41
1:K:6:LEU:C	1:K:7:TYR:HD1	2.29	0.41
1:N:19:ASN:HB3	1:N:40:ILE:HA	2.02	0.41
1:A:29:ASN:HB3	1:A:30:GLU:H	1.76	0.41
1:C:20:SER:HB2	1:C:33:MET:HE2	2.03	0.41
1:K:103:LEU:HD22	1:K:131:MET:SD	2.61	0.41
1:C:53:ILE:O	1:C:70:ARG:HA	2.21	0.40
1:D:99:ARG:NH2	1:D:119:ASP:OD2	2.54	0.40
1:E:103:LEU:HD13	1:E:140:VAL:HG21	2.01	0.40
1:C:91:LEU:H	1:C:91:LEU:HD23	1.86	0.40
1:N:25:TYR:HE2	1:N:32:ARG:HB2	1.85	0.40
1:E:6:LEU:HD21	1:F:103:LEU:HD21	2.03	0.40
1:M:41:ARG:NH2	1:M:67:SER:OG	2.52	0.40
1:G:118:TYR:HB2	1:G:125:TRP:CD2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:28:ARG:O	1:J:29:ASN:C	2.63	0.40
1:J:96:HIS:HB3	1:J:101:TYR:HE2	1.87	0.40
1:K:17:ARG:H	1:M:16:ASN:ND2	2.19	0.40

There are no symmetry-related clashes.

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	135/143 (94%)	127 (94%)	7 (5%)	1 (1%)	18	38
1	B	134/143 (94%)	128 (96%)	6 (4%)	0	100	100
1	C	137/143 (96%)	130 (95%)	7 (5%)	0	100	100
1	D	134/143 (94%)	129 (96%)	5 (4%)	0	100	100
1	E	137/143 (96%)	130 (95%)	6 (4%)	1 (1%)	18	38
1	F	138/143 (96%)	129 (94%)	8 (6%)	1 (1%)	18	38
1	G	135/143 (94%)	127 (94%)	7 (5%)	1 (1%)	18	38
1	H	138/143 (96%)	129 (94%)	8 (6%)	1 (1%)	18	38
1	I	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
1	J	138/143 (96%)	133 (96%)	5 (4%)	0	100	100
1	K	138/143 (96%)	129 (94%)	9 (6%)	0	100	100
1	L	139/143 (97%)	132 (95%)	6 (4%)	1 (1%)	18	38
1	M	128/143 (90%)	124 (97%)	4 (3%)	0	100	100
1	N	138/143 (96%)	128 (93%)	9 (6%)	1 (1%)	18	38
All	All	1907/2002 (95%)	1810 (95%)	90 (5%)	7 (0%)	30	51

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	4	MET
1	A	30	GLU
1	H	28	ARG
1	G	51	ASN
1	N	50	HIS
1	E	129	THR
1	F	28	ARG

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	111/117 (95%)	108 (97%)	3 (3%)	39	67
1	B	107/117 (92%)	105 (98%)	2 (2%)	50	75
1	C	110/117 (94%)	107 (97%)	3 (3%)	39	67
1	D	108/117 (92%)	105 (97%)	3 (3%)	38	66
1	E	110/117 (94%)	106 (96%)	4 (4%)	31	58
1	F	110/117 (94%)	109 (99%)	1 (1%)	70	87
1	G	105/117 (90%)	98 (93%)	7 (7%)	15	33
1	H	110/117 (94%)	106 (96%)	4 (4%)	31	58
1	I	109/117 (93%)	105 (96%)	4 (4%)	30	57
1	J	108/117 (92%)	105 (97%)	3 (3%)	38	66
1	K	108/117 (92%)	101 (94%)	7 (6%)	15	35
1	L	107/117 (92%)	104 (97%)	3 (3%)	38	66
1	M	100/117 (86%)	92 (92%)	8 (8%)	11	25
1	N	105/117 (90%)	97 (92%)	8 (8%)	12	27
All	All	1508/1638 (92%)	1448 (96%)	60 (4%)	28	55

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	109	HIS
1	A	130	ARG
1	B	5	LEU
1	B	128	VAL
1	C	99	ARG
1	C	110	THR
1	C	128	VAL
1	D	28	ARG
1	D	32	ARG
1	D	138	VAL
1	E	23	CYS
1	E	110	THR
1	E	126	SER
1	E	131	MET
1	F	77	THR
1	G	5	LEU
1	G	64	GLN
1	G	114	SER
1	G	122	THR
1	G	133	SER
1	G	135	ARG
1	G	138	VAL
1	H	28	ARG
1	H	75	THR
1	H	110	THR
1	H	128	VAL
1	I	5	LEU
1	I	33	MET
1	I	40	ILE
1	I	42	SER
1	J	5	LEU
1	J	28	ARG
1	J	121	ASP
1	K	5	LEU
1	K	33	MET
1	K	39	THR
1	K	51	ASN
1	K	95	VAL
1	K	126	SER
1	K	133	SER
1	L	40	ILE
1	L	51	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	77	THR
1	M	5	LEU
1	M	23	CYS
1	M	33	MET
1	M	42	SER
1	M	95	VAL
1	M	110	THR
1	M	124	THR
1	M	126	SER
1	N	6	LEU
1	N	17	ARG
1	N	27	GLU
1	N	32	ARG
1	N	94	THR
1	N	95	VAL
1	N	97	GLN
1	N	131	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	B	16	ASN
1	B	19	ASN
1	C	16	ASN
1	C	38	ASN
1	D	97	GLN
1	E	96	HIS
1	F	29	ASN
1	H	29	ASN
1	K	51	ASN
1	K	62	GLN
1	K	97	GLN
1	L	51	ASN
1	L	97	GLN
1	M	16	ASN
1	N	38	ASN
1	N	97	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	139/143 (97%)	-0.03	6 (4%) 40 34	39, 56, 83, 107	0
1	B	138/143 (96%)	-0.04	4 (2%) 53 48	39, 54, 77, 116	0
1	C	139/143 (97%)	-0.22	0 100 100	33, 48, 74, 116	0
1	D	138/143 (96%)	0.04	4 (2%) 53 48	40, 59, 91, 136	0
1	E	139/143 (97%)	0.23	5 (3%) 46 40	48, 66, 106, 132	0
1	F	140/143 (97%)	0.04	6 (4%) 40 34	44, 56, 82, 97	0
1	G	139/143 (97%)	0.44	9 (6%) 25 19	47, 71, 107, 125	0
1	H	140/143 (97%)	0.20	6 (4%) 40 34	45, 63, 106, 137	0
1	I	140/143 (97%)	0.15	4 (2%) 53 48	40, 59, 104, 153	0
1	J	140/143 (97%)	0.41	8 (5%) 29 24	47, 68, 115, 125	0
1	K	140/143 (97%)	0.72	12 (8%) 16 12	50, 84, 112, 144	0
1	L	141/143 (98%)	0.16	7 (4%) 34 28	41, 62, 92, 127	0
1	M	134/143 (93%)	0.80	18 (13%) 7 5	59, 84, 125, 151	0
1	N	140/143 (97%)	0.70	18 (12%) 7 6	50, 85, 119, 152	0
All	All	1947/2002 (97%)	0.26	107 (5%) 30 25	33, 65, 110, 153	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	4	MET	4.9
1	M	141	ALA	4.3
1	M	4	MET	4.3
1	M	28	ARG	4.2
1	J	128	VAL	4.0
1	E	128	VAL	3.9
1	E	30	GLU	3.7
1	G	51	ASN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	128	VAL	3.6
1	N	51	ASN	3.6
1	K	122	THR	3.6
1	I	4	MET	3.5
1	B	4	MET	3.4
1	J	4	MET	3.4
1	M	128	VAL	3.4
1	M	49	LEU	3.3
1	J	51	ASN	3.3
1	M	53	ILE	3.2
1	H	4	MET	3.1
1	H	142	VAL	3.1
1	N	129	THR	3.0
1	J	124	THR	3.0
1	G	3	HIS	2.9
1	L	4	MET	2.9
1	M	115	VAL	2.9
1	K	4	MET	2.8
1	G	25	TYR	2.8
1	M	63	ASP	2.8
1	G	128	VAL	2.8
1	K	128	VAL	2.8
1	D	28	ARG	2.8
1	N	141	ALA	2.7
1	A	128	VAL	2.7
1	M	32	ARG	2.7
1	N	133	SER	2.6
1	J	96	HIS	2.6
1	L	128	VAL	2.6
1	H	129	THR	2.6
1	L	3	HIS	2.6
1	L	133	SER	2.6
1	G	129	THR	2.5
1	N	138	VAL	2.5
1	M	5	LEU	2.5
1	J	26	PRO	2.5
1	G	4	MET	2.5
1	L	28	ARG	2.5
1	N	97	GLN	2.5
1	F	134	GLY	2.4
1	M	80	PHE	2.4
1	L	51	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	24	TYR	2.4
1	N	128	VAL	2.4
1	F	4	MET	2.4
1	N	109	HIS	2.4
1	N	127	GLU	2.3
1	N	130	ARG	2.3
1	B	128	VAL	2.3
1	E	26	PRO	2.3
1	F	29	ASN	2.3
1	A	130	ARG	2.3
1	D	25	TYR	2.3
1	I	27	GLU	2.3
1	J	127	GLU	2.3
1	N	48	VAL	2.3
1	K	85	LYS	2.2
1	E	29	ASN	2.2
1	B	28	ARG	2.2
1	K	28	ARG	2.2
1	G	62	GLN	2.2
1	J	98	GLY	2.2
1	F	128	VAL	2.2
1	K	23	CYS	2.2
1	M	127	GLU	2.2
1	H	26	PRO	2.2
1	G	73	VAL	2.2
1	I	128	VAL	2.2
1	M	73	VAL	2.2
1	E	129	THR	2.2
1	G	28	ARG	2.2
1	N	32	ARG	2.2
1	M	7	TYR	2.2
1	F	135	ARG	2.2
1	B	25	TYR	2.2
1	M	24	TYR	2.2
1	N	26	PRO	2.2
1	M	43	GLY	2.2
1	A	29	ASN	2.1
1	H	51	ASN	2.1
1	N	37	MET	2.1
1	A	25	TYR	2.1
1	K	54	TYR	2.1
1	K	130	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	75	THR	2.1
1	H	128	VAL	2.1
1	F	110	THR	2.1
1	M	129	THR	2.1
1	N	96	HIS	2.1
1	M	48	VAL	2.1
1	A	28	ARG	2.0
1	N	28	ARG	2.0
1	K	124	THR	2.0
1	I	26	PRO	2.0
1	K	5	LEU	2.0
1	L	142	VAL	2.0
1	D	4	MET	2.0
1	A	134	GLY	2.0
1	N	139	GLY	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.