



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:32 PM UTC

PDB ID : 6ZZ8 / pdb_00006zz8
Title : MB_CRS6-15 bound to CrSAS-6_6HR
Authors : Hatzopoulos, G.N.; Kukenshoner, T.; Banterle, N.; Favez, T.; Fluckiger, I.;
Hantschel, O.; Gonczy, P.
Deposited on : 2020-08-04
Resolution : 3.73 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

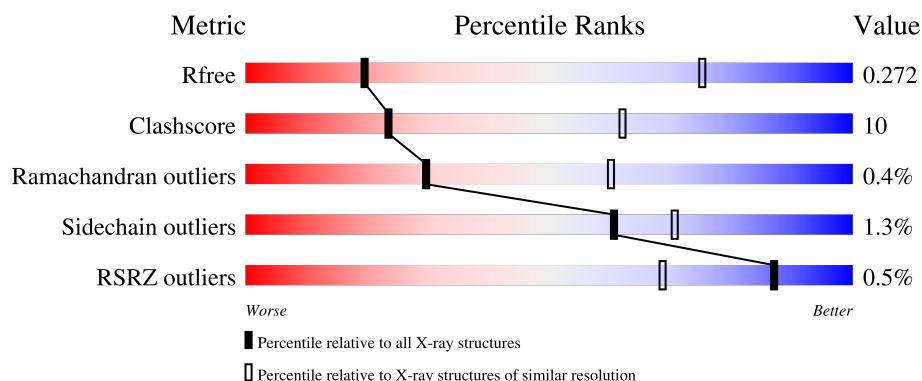
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

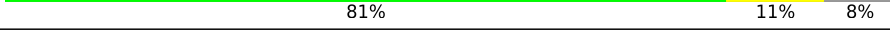
The reported resolution of this entry is 3.73 Å.

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	1234 (3.88-3.60)
Clashscore	190562	1274 (3.88-3.60)
Ramachandran outliers	187476	1226 (3.88-3.60)
Sidechain outliers	187428	1221 (3.88-3.60)
RSRZ outliers	180081	1233 (3.88-3.60)

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	227	
1	B	227	
1	C	227	
1	D	227	
1	E	227	

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Mol	Chain	Length	Quality of chain
1	F	227	69% 22% 8%
2	G	94	74% 26%
2	H	94	2% 64% 34% ..
2	I	94	2% 70% 29% .
2	J	94	% 83% 14% ..
2	K	94	67% 30% ..
2	L	94	2% 64% 32% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14335 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 Centriole protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	217	0	0
			1725	1088	305	328	4			
1	B	211	Total	C	N	O	S	163	0	0
			1692	1067	300	321	4			
1	C	211	Total	C	N	O	S	210	0	0
			1698	1073	301	320	4			
1	D	209	Total	C	N	O	S	196	0	0
			1684	1064	298	318	4			
1	E	207	Total	C	N	O	S	174	0	0
			1668	1055	295	314	4			
1	F	209	Total	C	N	O	S	168	0	0
			1684	1064	298	318	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A9CQL4
A	1	SER	-	expression tag	UNP A9CQL4
B	0	GLY	-	expression tag	UNP A9CQL4
B	1	SER	-	expression tag	UNP A9CQL4
C	0	GLY	-	expression tag	UNP A9CQL4
C	1	SER	-	expression tag	UNP A9CQL4
D	0	GLY	-	expression tag	UNP A9CQL4
D	1	SER	-	expression tag	UNP A9CQL4
E	0	GLY	-	expression tag	UNP A9CQL4
E	1	SER	-	expression tag	UNP A9CQL4
F	0	GLY	-	expression tag	UNP A9CQL4
F	1	SER	-	expression tag	UNP A9CQL4

- Molecule 2 is a protein called Protein B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	94	Total	C	N	O	0	0	0
			699	446	110	143			
2	H	93	Total	C	N	O	0	0	0
			695	444	109	142			
2	I	93	Total	C	N	O	0	1	0
			704	452	109	143			
2	J	92	Total	C	N	O	0	0	0
			689	441	108	140			
2	K	92	Total	C	N	O	0	0	0
			689	441	108	140			
2	L	92	Total	C	N	O	0	0	0
			689	441	108	140			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	25	PRO	ARG	conflict	UNP M1E1G6
G	26	ALA	GLY	conflict	UNP M1E1G6
G	27	VAL	GLU	conflict	UNP M1E1G6
G	28	THR	TYR	conflict	UNP M1E1G6
G	30	TYR	VAL	conflict	UNP M1E1G6
G	31	LEU	TYR	conflict	UNP M1E1G6
G	33	VAL	ARG	conflict	UNP M1E1G6
G	49	GLU	THR	conflict	UNP M1E1G6
G	54	LYS	SER	conflict	UNP M1E1G6
G	63	LYS	SER	conflict	UNP M1E1G6
G	75	SER	ARG	conflict	UNP M1E1G6
G	77	LYS	TYR	conflict	UNP M1E1G6
G	78	HIS	TYR	conflict	UNP M1E1G6
G	79	SER	TRP	conflict	UNP M1E1G6
G	80	SER	GLY	conflict	UNP M1E1G6
G	81	ARG	TRP	conflict	UNP M1E1G6
G	83	ALA	-	insertion	UNP M1E1G6
H	25	PRO	ARG	conflict	UNP M1E1G6
H	26	ALA	GLY	conflict	UNP M1E1G6
H	27	VAL	GLU	conflict	UNP M1E1G6
H	28	THR	TYR	conflict	UNP M1E1G6
H	30	TYR	VAL	conflict	UNP M1E1G6
H	31	LEU	TYR	conflict	UNP M1E1G6
H	33	VAL	ARG	conflict	UNP M1E1G6
H	49	GLU	THR	conflict	UNP M1E1G6
H	54	LYS	SER	conflict	UNP M1E1G6
H	63	LYS	SER	conflict	UNP M1E1G6
H	75	SER	ARG	conflict	UNP M1E1G6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	77	LYS	TYR	conflict	UNP M1E1G6
H	78	HIS	TYR	conflict	UNP M1E1G6
H	79	SER	TRP	conflict	UNP M1E1G6
H	80	SER	GLY	conflict	UNP M1E1G6
H	81	ARG	TRP	conflict	UNP M1E1G6
H	83	ALA	-	insertion	UNP M1E1G6
I	25	PRO	ARG	conflict	UNP M1E1G6
I	26	ALA	GLY	conflict	UNP M1E1G6
I	27	VAL	GLU	conflict	UNP M1E1G6
I	28	THR	TYR	conflict	UNP M1E1G6
I	30	TYR	VAL	conflict	UNP M1E1G6
I	31	LEU	TYR	conflict	UNP M1E1G6
I	33	VAL	ARG	conflict	UNP M1E1G6
I	49	GLU	THR	conflict	UNP M1E1G6
I	54	LYS	SER	conflict	UNP M1E1G6
I	63	LYS	SER	conflict	UNP M1E1G6
I	75	SER	ARG	conflict	UNP M1E1G6
I	77	LYS	TYR	conflict	UNP M1E1G6
I	78	HIS	TYR	conflict	UNP M1E1G6
I	79	SER	TRP	conflict	UNP M1E1G6
I	80	SER	GLY	conflict	UNP M1E1G6
I	81	ARG	TRP	conflict	UNP M1E1G6
I	83	ALA	-	insertion	UNP M1E1G6
J	25	PRO	ARG	conflict	UNP M1E1G6
J	26	ALA	GLY	conflict	UNP M1E1G6
J	27	VAL	GLU	conflict	UNP M1E1G6
J	28	THR	TYR	conflict	UNP M1E1G6
J	30	TYR	VAL	conflict	UNP M1E1G6
J	31	LEU	TYR	conflict	UNP M1E1G6
J	33	VAL	ARG	conflict	UNP M1E1G6
J	49	GLU	THR	conflict	UNP M1E1G6
J	54	LYS	SER	conflict	UNP M1E1G6
J	63	LYS	SER	conflict	UNP M1E1G6
J	75	SER	ARG	conflict	UNP M1E1G6
J	77	LYS	TYR	conflict	UNP M1E1G6
J	78	HIS	TYR	conflict	UNP M1E1G6
J	79	SER	TRP	conflict	UNP M1E1G6
J	80	SER	GLY	conflict	UNP M1E1G6
J	81	ARG	TRP	conflict	UNP M1E1G6
J	83	ALA	-	insertion	UNP M1E1G6
K	25	PRO	ARG	conflict	UNP M1E1G6
K	26	ALA	GLY	conflict	UNP M1E1G6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	27	VAL	GLU	conflict	UNP M1E1G6
K	28	THR	TYR	conflict	UNP M1E1G6
K	30	TYR	VAL	conflict	UNP M1E1G6
K	31	LEU	TYR	conflict	UNP M1E1G6
K	33	VAL	ARG	conflict	UNP M1E1G6
K	49	GLU	THR	conflict	UNP M1E1G6
K	54	LYS	SER	conflict	UNP M1E1G6
K	63	LYS	SER	conflict	UNP M1E1G6
K	75	SER	ARG	conflict	UNP M1E1G6
K	77	LYS	TYR	conflict	UNP M1E1G6
K	78	HIS	TYR	conflict	UNP M1E1G6
K	79	SER	TRP	conflict	UNP M1E1G6
K	80	SER	GLY	conflict	UNP M1E1G6
K	81	ARG	TRP	conflict	UNP M1E1G6
K	83	ALA	-	insertion	UNP M1E1G6
L	25	PRO	ARG	conflict	UNP M1E1G6
L	26	ALA	GLY	conflict	UNP M1E1G6
L	27	VAL	GLU	conflict	UNP M1E1G6
L	28	THR	TYR	conflict	UNP M1E1G6
L	30	TYR	VAL	conflict	UNP M1E1G6
L	31	LEU	TYR	conflict	UNP M1E1G6
L	33	VAL	ARG	conflict	UNP M1E1G6
L	49	GLU	THR	conflict	UNP M1E1G6
L	54	LYS	SER	conflict	UNP M1E1G6
L	63	LYS	SER	conflict	UNP M1E1G6
L	75	SER	ARG	conflict	UNP M1E1G6
L	77	LYS	TYR	conflict	UNP M1E1G6
L	78	HIS	TYR	conflict	UNP M1E1G6
L	79	SER	TRP	conflict	UNP M1E1G6
L	80	SER	GLY	conflict	UNP M1E1G6
L	81	ARG	TRP	conflict	UNP M1E1G6
L	83	ALA	-	insertion	UNP M1E1G6

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0
3	B	4	Total O 4 4	0	0
3	C	2	Total O 2 2	0	0

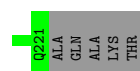
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total 2	O 2	0	0
3	E	1	Total 1	O 1	0	0
3	F	2	Total 2	O 2	0	0
3	G	2	Total 2	O 2	0	0
3	H	1	Total 1	O 1	0	0
3	I	1	Total 1	O 1	0	0
3	L	1	Total 1	O 1	0	0

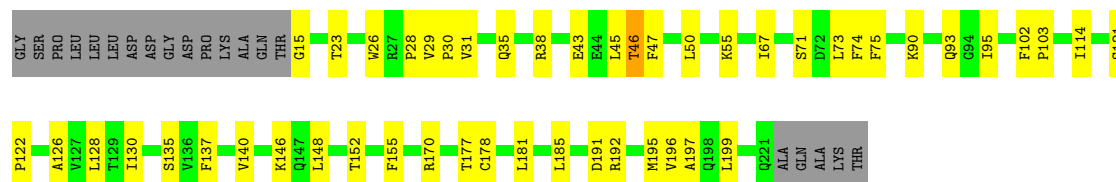
- Molecule 1: Centriole protein





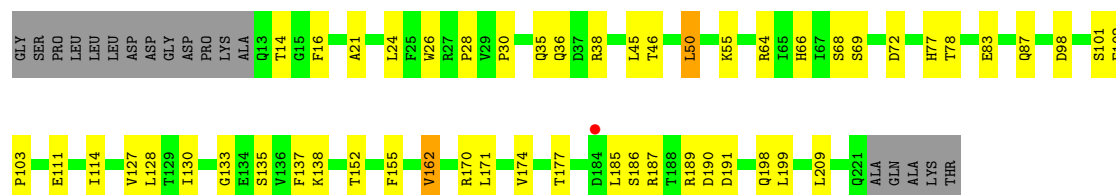
• Molecule 1: Centriole protein

Chain E:  70% 21% 9%



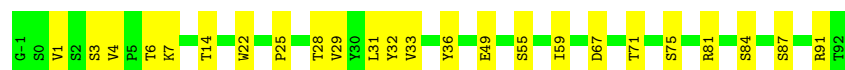
• Molecule 1: Centriole protein

Chain F:  69% 22% 8%



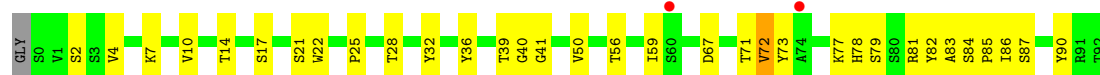
• Molecule 2: Protein B

Chain G:  74% 26%



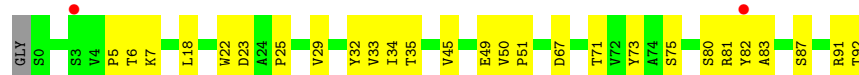
• Molecule 2: Protein B

Chain H:  2% 64% 34% 2%



• Molecule 2: Protein B

Chain I:  2% 70% 29% 1%

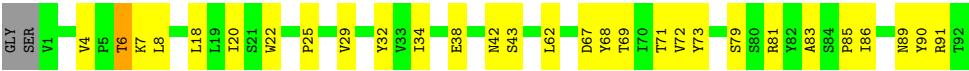


• Molecule 2: Protein B

Chain J:  1% 83% 14% 2%



● Molecule 2: Protein B



● Molecule 2: Protein B



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	257.16Å 257.16Å 125.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.73 49.63 – 3.73	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.63-3.73) 99.0 (49.63-3.73)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.225 , 0.267 0.229 , 0.272	Depositor DCC
R_{free} test set	2184 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	140.1	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 144.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14335	wwPDB-VP
Average B, all atoms (Å ²)	227.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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	0.17	0/1756	0.41	0/2373
1	B	0.14	0/1723	0.37	0/2328
1	C	0.16	0/1728	0.38	0/2334
1	D	0.14	0/1714	0.39	0/2316
1	E	0.14	0/1698	0.39	0/2294
1	F	0.15	0/1714	0.40	0/2316
2	G	0.15	0/716	0.41	0/982
2	H	0.19	0/712	0.49	0/977
2	I	0.15	0/725	0.36	0/995
2	J	0.14	0/706	0.45	0/969
2	K	0.16	0/706	0.45	0/969
2	L	0.14	0/706	0.46	0/969
All	All	0.15	0/14604	0.40	0/19822

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1725	0	1717	40	0
1	B	1692	0	1683	32	0
1	C	1698	0	1699	27	0
1	D	1684	0	1681	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1668	0	1665	29	0
1	F	1684	0	1680	35	0
2	G	699	0	698	17	0
2	H	695	0	695	24	0
2	I	704	0	704	18	0
2	J	689	0	690	9	0
2	K	689	0	690	19	0
2	L	689	0	690	31	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	1	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
All	All	14335	0	14292	269	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 10.

All (269) 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:A:141:GLU:HB2	1:A:150:HIS:HE1	1.30	0.96
2:I:5:PRO:HB3	2:I:25:PRO:HD3	1.52	0.91
1:E:199:LEU:HD21	1:F:199:LEU:HA	1.60	0.84
2:G:3:SER:HB3	2:G:25:PRO:HB2	1.61	0.83
1:F:68:SER:HB2	1:F:170:ARG:HH21	1.48	0.78
1:A:141:GLU:HB2	1:A:150:HIS:CE1	2.17	0.77
1:B:30:PRO:HD2	1:B:114:ILE:HG22	1.69	0.74
1:A:93:GLN:O	1:C:146:LYS:NZ	2.21	0.72
1:A:128:LEU:HD11	1:A:135:SER:HB3	1.72	0.71
1:F:138:LYS:HB3	1:F:152:THR:HG22	1.71	0.70
1:F:128:LEU:HD11	1:F:135:SER:HB3	1.74	0.69
2:K:34:ILE:HG13	2:K:72:VAL:HG12	1.74	0.69
2:L:35:THR:HB	2:L:47:GLU:HG2	1.74	0.68
1:C:93:GLN:NE2	1:C:152:THR:O	2.26	0.67
1:E:29:VAL:HG22	1:E:114:ILE:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:PRO:HD2	1:C:114:ILE:HG22	1.80	0.64
2:J:67:ASP:HA	2:J:91:ARG:HG2	1.80	0.64
1:E:67:ILE:HG22	1:E:75:PHE:HE1	1.63	0.63
2:G:31:LEU:H	2:G:75:SER:HG	1.47	0.63
2:K:8:LEU:HD21	2:K:86:ILE:HB	1.79	0.63
2:G:1:VAL:HG12	2:G:3:SER:H	1.64	0.63
2:L:18:LEU:HD13	2:L:62:LEU:HD12	1.80	0.62
1:C:162:VAL:HA	1:C:165:GLN:NE2	2.14	0.62
2:G:4:VAL:HG12	2:G:84:SER:HB2	1.81	0.62
1:D:35:GLN:HB2	1:D:38:ARG:HB2	1.82	0.62
2:G:71:THR:HG22	2:G:87:SER:HB3	1.80	0.62
1:C:34:LYS:HB2	1:C:129:THR:HG22	1.83	0.61
2:H:84:SER:H	2:L:89:ASN:HD21	1.49	0.61
1:E:45:LEU:HD12	1:E:128:LEU:HD21	1.82	0.61
1:B:23:THR:O	2:H:81:ARG:NH1	2.34	0.60
1:C:159:ASN:OD1	1:C:160:ASP:N	2.34	0.60
1:A:32:HIS:HB2	1:A:127:VAL:HG12	1.83	0.60
1:E:90:LYS:HB2	1:E:95:ILE:HB	1.84	0.60
1:B:14:THR:HA	1:B:55:LYS:HD3	1.84	0.59
1:C:43:GLU:OE1	1:C:71:SER:OG	2.17	0.59
2:G:31:LEU:N	2:G:75:SER:OG	2.33	0.59
1:B:128:LEU:HD11	1:B:135:SER:HB3	1.85	0.58
2:K:73:TYR:HB3	2:K:81:ARG:O	2.03	0.58
1:A:28:PRO:HG3	1:A:46:THR:HG22	1.85	0.58
2:J:73:TYR:CE2	2:J:85:PRO:HB3	2.38	0.58
2:K:6:THR:OG1	2:K:7:LYS:HD2	2.03	0.58
1:A:64:ARG:HD3	1:A:66:HIS:NE2	2.19	0.57
1:E:15:GLY:O	1:E:55:LYS:N	2.37	0.57
1:E:185:LEU:HD13	1:F:185:LEU:HA	1.87	0.56
2:L:10:VAL:HG21	2:L:90:TYR:HD2	1.70	0.56
2:G:91:ARG:NH1	3:G:101:HOH:O	2.37	0.56
2:I:75:SER:HB3	2:I:81:ARG:HA	1.86	0.56
1:D:185:LEU:HD12	1:D:188:THR:HB	1.86	0.56
1:C:128:LEU:HD11	1:C:135:SER:HB3	1.86	0.56
1:F:128:LEU:HD13	1:F:137:PHE:HB2	1.89	0.55
2:H:7:LYS:O	2:H:22:TRP:HA	2.06	0.55
1:A:73:LEU:HG	1:A:73:LEU:O	2.05	0.55
2:L:29:VAL:HG11	2:L:32:TYR:CZ	2.41	0.55
2:H:71:THR:HG22	2:H:87:SER:HB3	1.87	0.55
1:B:192:ARG:NH2	1:B:193:ASP:OD1	2.40	0.55
1:A:48:ARG:HG2	1:A:50:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:VAL:HG13	2:H:86:ILE:HG22	1.90	0.54
1:D:194:SER:O	1:D:198:GLN:HG2	2.07	0.54
2:H:83:ALA:HB1	2:L:89:ASN:ND2	2.22	0.54
1:D:26:TRP:HB3	2:J:31:LEU:HD12	1.90	0.54
1:A:46:THR:HG1	1:A:68:SER:HG	1.49	0.54
1:A:185:LEU:HD11	1:B:185:LEU:HB3	1.90	0.54
1:B:67:ILE:HG22	1:B:75:PHE:HE1	1.73	0.54
2:G:67:ASP:HA	2:G:91:ARG:HA	1.89	0.54
1:A:73:LEU:HD22	1:A:170:ARG:HG2	1.90	0.54
1:F:64:ARG:HE	1:F:66:HIS:CE1	2.26	0.54
1:E:23:THR:HA	1:E:50:LEU:HD23	1.89	0.53
2:K:62:LEU:HB2	2:K:68:TYR:HE2	1.72	0.53
1:F:30:PRO:HD2	1:F:114:ILE:HG12	1.88	0.53
1:C:28:PRO:HA	1:C:46:THR:HA	1.91	0.53
2:L:15:PRO:HB3	2:L:64:PRO:HB3	1.89	0.53
2:L:6:THR:HB	2:L:23:ASP:HB2	1.91	0.52
2:L:39:THR:OG1	2:L:67:ASP:O	2.23	0.52
1:C:102:PHE:HB3	1:C:103:PRO:HD3	1.92	0.51
1:E:146:LYS:HE3	1:E:148:LEU:HD11	1.91	0.51
1:C:111:GLU:HA	1:C:114:ILE:HG12	1.91	0.51
2:L:1:VAL:HG23	2:L:2:SER:H	1.75	0.51
1:A:30:PRO:HA	1:A:44:GLU:HA	1.93	0.51
2:H:2:SER:HB2	2:H:4:VAL:HG12	1.91	0.51
1:F:187:ARG:NH1	1:F:190:ASP:OD2	2.36	0.51
2:J:14:THR:O	2:J:92:THR:OG1	2.28	0.51
1:B:185:LEU:HA	1:B:188:THR:HG22	1.92	0.51
1:F:16:PHE:HE2	1:F:21:ALA:HB2	1.75	0.51
2:H:78:HIS:CG	2:L:90:TYR:HE1	2.28	0.51
2:I:7:LYS:O	2:I:22:TRP:HA	2.11	0.50
1:A:183:ASP:O	1:A:186:SER:OG	2.27	0.50
1:E:35:GLN:HB3	1:E:38:ARG:HG2	1.93	0.50
2:L:91:ARG:O	2:L:92:THR:OG1	2.28	0.50
1:F:127:VAL:HG13	1:F:138:LYS:HG3	1.92	0.50
2:I:6:THR:OG1	2:I:7:LYS:N	2.40	0.50
1:F:26:TRP:CE2	2:L:51:PRO:HG3	2.45	0.50
1:F:72:ASP:OD2	1:F:72:ASP:N	2.44	0.50
1:A:187:ARG:HH22	2:G:14:THR:HG21	1.76	0.49
2:K:7:LYS:O	2:K:22:TRP:HA	2.12	0.49
1:C:66:HIS:CD2	1:C:78:THR:HG23	2.48	0.49
1:B:23:THR:HA	1:B:50:LEU:HD23	1.95	0.49
1:D:128:LEU:HD11	1:D:135:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:67:ASP:HA	2:K:91:ARG:HA	1.95	0.49
2:K:4:VAL:O	2:K:25:PRO:HB3	2.13	0.48
1:C:21:ALA:HB1	1:C:50:LEU:HD23	1.95	0.48
2:L:69:THR:HG22	2:L:89:ASN:HB3	1.95	0.48
1:D:79:LEU:HB2	1:D:155:PHE:CD1	2.48	0.48
1:E:35:GLN:CD	1:E:130:ILE:HD11	2.39	0.48
1:A:14:THR:HA	1:A:55:LYS:HD3	1.95	0.48
1:C:135:SER:HB2	1:C:155:PHE:HB2	1.94	0.48
1:E:67:ILE:HG22	1:E:75:PHE:CE1	2.45	0.48
1:F:45:LEU:HD22	1:F:69:SER:HB2	1.96	0.48
2:K:67:ASP:HA	2:K:90:TYR:O	2.13	0.48
1:A:122:PRO:HB2	1:A:141:GLU:HG3	1.94	0.48
1:A:73:LEU:CD2	1:A:170:ARG:HG2	2.44	0.48
1:C:48:ARG:HG2	1:C:50:LEU:CD1	2.45	0.47
2:J:67:ASP:HB2	2:J:91:ARG:HE	1.79	0.47
1:C:48:ARG:HB3	1:C:66:HIS:HB2	1.97	0.47
1:D:79:LEU:HD22	1:D:155:PHE:HE1	1.79	0.47
1:F:111:GLU:OE1	2:L:77:LYS:HD3	2.15	0.47
2:G:75:SER:HB3	2:G:81:ARG:HG2	1.96	0.47
1:A:181:LEU:HB2	1:B:181:LEU:HD21	1.96	0.47
1:D:122:PRO:HB2	1:D:141:GLU:HG3	1.97	0.47
1:E:28:PRO:HA	1:E:46:THR:HA	1.95	0.47
1:E:31:VAL:HG11	1:E:128:LEU:HD23	1.96	0.47
2:G:75:SER:CB	2:G:81:ARG:HG2	2.45	0.47
2:H:32:TYR:HB2	2:H:50:VAL:CG1	2.44	0.47
2:I:71:THR:HG22	2:I:87:SER:HB3	1.96	0.47
2:J:6:THR:OG1	2:J:7:LYS:N	2.48	0.47
2:K:18:LEU:HD13	2:K:20:ILE:HG23	1.95	0.47
1:B:64:ARG:HD3	1:B:80:GLU:HG2	1.95	0.47
2:H:67:ASP:OD1	2:H:67:ASP:N	2.47	0.47
2:I:73:TYR:HD2	2:I:82[B]:TYR:HD1	1.63	0.47
2:K:6:THR:OG1	2:K:7:LYS:N	2.48	0.47
1:B:102:PHE:HB3	1:B:103:PRO:HD3	1.97	0.46
2:H:81:ARG:HG3	2:H:82:TYR:CD2	2.50	0.46
1:A:138:LYS:HB3	1:A:152:THR:HG22	1.96	0.46
1:C:26:TRP:HE1	2:I:51:PRO:HD3	1.80	0.46
2:G:36:TYR:HB3	2:G:59:ILE:HD13	1.98	0.46
2:H:73:TYR:CD1	2:H:85:PRO:HB3	2.49	0.46
2:G:67:ASP:OD1	2:G:67:ASP:N	2.49	0.46
1:A:124:PHE:HE1	1:A:150:HIS:CE1	2.34	0.46
1:E:192:ARG:HD2	1:F:191:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:77:LYS:HD2	2:L:78:HIS:H	1.80	0.46
1:B:28:PRO:HA	1:B:46:THR:HA	1.96	0.46
1:B:90:LYS:HG3	1:B:95:ILE:HB	1.97	0.46
1:C:35:GLN:OE1	1:C:38:ARG:HD2	2.15	0.46
1:E:30:PRO:HD2	1:E:114:ILE:HG12	1.97	0.46
1:B:110:LEU:O	1:B:114:ILE:HG23	2.15	0.46
2:I:22:TRP:CH2	2:I:34:ILE:HD11	2.51	0.46
2:I:32:TYR:HB2	2:I:50:VAL:HG23	1.98	0.46
2:I:67:ASP:N	2:I:67:ASP:OD1	2.47	0.45
2:K:79:SER:CB	2:K:83:ALA:HB2	2.46	0.45
1:A:117:GLN:HG2	1:A:118:PRO:HD2	1.98	0.45
1:A:146:LYS:HE3	1:C:93:GLN:O	2.16	0.45
2:L:17:SER:C	2:L:18:LEU:HD12	2.40	0.45
2:H:10:VAL:HG21	2:H:90:TYR:CE1	2.51	0.45
2:L:66:VAL:C	2:L:91:ARG:HG3	2.41	0.45
1:F:83:GLU:O	1:F:87:GLN:HG2	2.16	0.45
1:B:148:LEU:HD13	1:D:148:LEU:HD13	1.99	0.45
1:B:114:ILE:HD11	2:H:28:THR:HG21	1.99	0.45
1:B:133:GLY:O	1:B:157:PRO:HD3	2.16	0.45
1:A:28:PRO:HA	1:A:46:THR:HA	1.98	0.45
1:D:28:PRO:HG3	1:D:46:THR:HG22	1.99	0.45
1:C:48:ARG:HE	1:C:50:LEU:HD11	1.81	0.45
1:E:74:PHE:CE1	1:F:171:LEU:HD22	2.51	0.45
1:F:36:GLN:C	1:F:38:ARG:H	2.24	0.45
1:A:126:ALA:HB1	1:A:137:PHE:CE1	2.52	0.44
1:B:111:GLU:HA	1:B:114:ILE:HG12	1.98	0.44
2:H:21:SER:HB2	2:H:56:THR:HG22	1.98	0.44
1:C:35:GLN:HG2	1:C:130:ILE:HG13	1.99	0.44
1:E:43:GLU:OE1	1:E:71:SER:OG	2.26	0.44
1:B:48:ARG:HB2	1:B:66:HIS:HB2	1.98	0.44
1:D:28:PRO:HA	1:D:46:THR:HA	2.00	0.44
1:D:126:ALA:HB1	1:D:137:PHE:HE1	1.82	0.44
1:F:28:PRO:HA	1:F:46:THR:HA	1.98	0.44
2:L:34:ILE:HG13	2:L:72:VAL:HG13	1.99	0.44
1:A:146:LYS:NZ	1:C:93:GLN:OE1	2.48	0.44
1:A:184:ASP:OD2	1:B:189:ARG:NH2	2.51	0.44
2:H:71:THR:HG22	2:H:87:SER:CB	2.47	0.44
1:E:26:TRP:HA	1:E:47:PHE:O	2.18	0.44
1:E:102:PHE:HB3	1:E:103:PRO:HD3	1.99	0.44
1:E:199:LEU:HD13	1:F:198:GLN:HB3	1.99	0.44
2:I:33:VAL:HG21	2:I:81:ARG:HH21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ASP:OD1	1:D:93:GLN:N	2.51	0.43
2:J:69:THR:OG1	2:J:89:ASN:OD1	2.26	0.43
2:I:35:THR:CG2	2:I:45:VAL:HB	2.48	0.43
1:D:66:HIS:ND1	1:D:78:THR:HG22	2.33	0.43
2:L:67:ASP:OD1	2:L:67:ASP:N	2.52	0.43
1:B:69:SER:O	1:B:69:SER:OG	2.36	0.43
1:B:128:LEU:HD13	1:B:137:PHE:HB2	2.00	0.43
1:C:128:LEU:HD13	1:C:137:PHE:HB2	2.00	0.43
1:C:102:PHE:O	1:C:106:ILE:HG12	2.18	0.43
2:H:79:SER:O	2:L:91:ARG:HD3	2.17	0.43
2:I:29:VAL:HG21	2:I:32:TYR:CZ	2.52	0.43
2:I:33:VAL:HG22	2:I:49:GLU:HG2	2.00	0.43
1:A:78:THR:HG21	1:A:158:GLY:HA2	2.01	0.43
2:K:68:TYR:O	2:K:89:ASN:HA	2.18	0.43
1:F:66:HIS:CE1	1:F:78:THR:HG23	2.54	0.43
1:A:175:LYS:HD2	1:B:73:LEU:HD12	2.00	0.43
1:B:122:PRO:HB2	1:B:141:GLU:HG3	1.99	0.43
1:C:175:LYS:HE2	1:C:175:LYS:HB3	1.90	0.43
1:E:135:SER:HB2	1:E:155:PHE:HB2	2.01	0.42
1:F:138:LYS:CB	1:F:152:THR:HG22	2.45	0.42
2:H:4:VAL:O	2:H:25:PRO:HB3	2.19	0.42
1:A:48:ARG:HG2	1:A:50:LEU:CD1	2.48	0.42
1:A:159:ASN:HB3	1:A:162:VAL:HG22	2.01	0.42
2:K:79:SER:HB3	2:K:83:ALA:HB2	2.01	0.42
1:B:76:LEU:HD23	1:B:163:VAL:HG22	2.00	0.42
2:H:77:LYS:HD3	2:H:78:HIS:CG	2.54	0.42
1:A:25:PHE:O	1:A:48:ARG:HA	2.19	0.42
2:G:22:TRP:O	2:G:55:SER:HB2	2.19	0.42
2:K:71:THR:HG22	2:K:85:PRO:HB2	2.01	0.42
2:L:38:GLU:HB2	2:L:43:SER:HB2	2.02	0.42
1:E:199:LEU:HA	1:E:199:LEU:HD23	1.63	0.42
1:C:140:VAL:HG11	1:C:147:GLN:HG2	2.01	0.42
1:D:185:LEU:O	1:D:185:LEU:HG	2.19	0.42
1:D:26:TRP:HA	1:D:47:PHE:O	2.20	0.42
1:F:135:SER:HB2	1:F:155:PHE:HB2	2.01	0.42
1:A:21:ALA:HB1	1:A:50:LEU:HD23	2.01	0.42
1:F:98:ASP:OD1	1:F:101:SER:OG	2.34	0.42
2:K:62:LEU:HB2	2:K:68:TYR:CE2	2.53	0.42
1:B:191:ASP:O	1:B:195:MET:HG2	2.20	0.42
1:E:73:LEU:HG	1:E:170:ARG:HH21	1.84	0.42
1:F:24:LEU:HD11	2:L:81:ARG:NE	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:LEU:HD12	1:F:64:ARG:HB3	2.02	0.42
2:K:38:GLU:HG2	2:K:68:TYR:CE1	2.55	0.42
1:A:18:LEU:HD12	1:A:18:LEU:H	1.85	0.41
1:F:174:VAL:HA	1:F:177:THR:OG1	2.20	0.41
2:L:80:SER:C	2:L:81:ARG:HG3	2.45	0.41
1:B:43:GLU:OE2	1:B:71:SER:OG	2.21	0.41
2:G:29:VAL:HG21	2:G:32:TYR:CZ	2.54	0.41
2:H:39:THR:O	2:H:41:GLY:N	2.53	0.41
1:A:127:VAL:HG23	1:A:138:LYS:HG3	2.01	0.41
1:E:93:GLN:NE2	1:E:152:THR:O	2.40	0.41
1:F:186:SER:O	1:F:189:ARG:HG2	2.20	0.41
1:B:29:VAL:HG12	1:B:31:VAL:HG23	2.03	0.41
2:K:29:VAL:HG11	2:K:32:TYR:OH	2.20	0.41
2:L:18:LEU:HD11	2:L:92:THR:CG2	2.51	0.41
1:A:73:LEU:CD2	1:B:171:LEU:HD21	2.51	0.41
1:F:14:THR:H	1:F:55:LYS:HD2	1.84	0.41
2:J:38:GLU:HA	2:J:68:TYR:HD1	1.86	0.41
2:J:73:TYR:HE2	2:J:85:PRO:HB3	1.86	0.41
1:C:130:ILE:HG22	1:C:135:SER:OG	2.20	0.41
2:G:33:VAL:HG22	2:G:49:GLU:HG2	2.01	0.41
2:I:80:SER:H	2:I:83:ALA:HB3	1.84	0.41
1:F:102:PHE:HB3	1:F:103:PRO:HD3	2.03	0.41
2:H:78:HIS:O	2:L:91:ARG:HB3	2.21	0.41
1:E:121:SER:HA	1:E:122:PRO:HA	1.91	0.41
2:H:36:TYR:HB3	2:H:59:ILE:HD13	2.03	0.41
2:I:18:LEU:HD23	2:I:92:THR:HG22	2.03	0.41
1:A:30:PRO:HD2	1:A:114:ILE:HG13	2.03	0.41
2:G:7:LYS:HA	2:G:7:LYS:HD2	1.88	0.41
1:A:84:GLU:H	1:A:84:GLU:CD	2.28	0.40
1:F:77:HIS:HB3	1:F:155:PHE:HB3	2.02	0.40
2:H:83:ALA:HB1	2:L:89:ASN:HD21	1.85	0.40
2:L:66:VAL:HB	2:L:68:TYR:HE1	1.85	0.40
1:A:124:PHE:CE1	1:A:150:HIS:CE1	3.10	0.40
1:B:33:VAL:HG12	1:B:41:VAL:O	2.21	0.40
1:E:191:ASP:O	1:E:195:MET:HG2	2.21	0.40
1:F:26:TRP:CZ2	2:L:51:PRO:HG3	2.56	0.40
2:I:67:ASP:HB3	2:I:91:ARG:NE	2.37	0.40
2:L:38:GLU:OE1	2:L:43:SER:HB2	2.21	0.40
2:L:67:ASP:HB3	2:L:91:ARG:HD2	2.03	0.40
1:E:126:ALA:HB1	1:E:137:PHE:CE1	2.56	0.40
2:H:14:THR:HG22	2:H:17:SER:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:7:LYS:HD3	2:I:23:ASP:OD2	2.21	0.40
1:A:93:GLN:NE2	1:A:152:THR:O	2.52	0.40
1:E:178:CYS:HA	1:E:181:LEU:HG	2.04	0.40
2:K:42:ASN:OD1	2:K:43:SER:N	2.54	0.40
1:B:164:LYS:HB3	1:B:164:LYS:HE2	1.87	0.40
1:D:65:ILE:HD12	1:D:79:LEU:HD23	2.03	0.40
1:F:35:GLN:HG2	1:F:130:ILE:HD11	2.02	0.40
1:F:64:ARG:NH2	1:F:162:VAL:HG12	2.36	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	213/227 (94%)	202 (95%)	9 (4%)	2 (1%)	14	45
1	B	209/227 (92%)	202 (97%)	7 (3%)	0	100	100
1	C	209/227 (92%)	200 (96%)	9 (4%)	0	100	100
1	D	207/227 (91%)	199 (96%)	8 (4%)	0	100	100
1	E	205/227 (90%)	196 (96%)	7 (3%)	2 (1%)	12	43
1	F	207/227 (91%)	198 (96%)	8 (4%)	1 (0%)	24	56
2	G	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
2	H	91/94 (97%)	88 (97%)	2 (2%)	1 (1%)	11	41
2	I	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
2	J	90/94 (96%)	85 (94%)	4 (4%)	1 (1%)	11	41
2	K	90/94 (96%)	80 (89%)	10 (11%)	0	100	100
2	L	90/94 (96%)	88 (98%)	2 (2%)	0	100	100
All	All	1795/1926 (93%)	1715 (96%)	73 (4%)	7 (0%)	30	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	40	GLY
1	E	197	ALA
1	E	196	VAL
2	J	41	GLY
1	A	133	GLY
1	F	133	GLY
1	A	196	VAL

5.3.2 Protein sidechains [i](#)

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	194/203 (96%)	191 (98%)	3 (2%)	57	68
1	B	190/203 (94%)	187 (98%)	3 (2%)	55	68
1	C	191/203 (94%)	191 (100%)	0	100	100
1	D	190/203 (94%)	189 (100%)	1 (0%)	81	80
1	E	188/203 (93%)	185 (98%)	3 (2%)	55	68
1	F	190/203 (94%)	187 (98%)	3 (2%)	55	68
2	G	80/80 (100%)	78 (98%)	2 (2%)	42	61
2	H	80/80 (100%)	79 (99%)	1 (1%)	61	71
2	I	81/80 (101%)	81 (100%)	0	100	100
2	J	79/80 (99%)	78 (99%)	1 (1%)	61	71
2	K	79/80 (99%)	77 (98%)	2 (2%)	42	61
2	L	79/80 (99%)	77 (98%)	2 (2%)	42	61
All	All	1621/1698 (96%)	1600 (99%)	21 (1%)	61	71

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	140	VAL

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Mol	Chain	Res	Type
1	A	152	THR
1	B	46	THR
1	B	140	VAL
1	B	162	VAL
1	D	177	THR
1	E	46	THR
1	E	140	VAL
1	E	177	THR
1	F	50	LEU
1	F	162	VAL
1	F	209	LEU
2	G	6	THR
2	G	28	THR
2	H	72	VAL
2	J	14	THR
2	K	6	THR
2	K	69	THR
2	L	1	VAL
2	L	39	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	HIS
1	B	147	GLN
1	B	165	GLN
1	E	77	HIS
1	F	147	GLN
1	F	179	HIS
2	L	89	ASN

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 [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	189/227 (83%)	-0.38	0  	91, 168, 352, 507	0
1	B	192/227 (84%)	-0.31	0  	79, 169, 393, 451	0
1	C	186/227 (81%)	-0.35	0  	106, 173, 408, 621	0
1	D	186/227 (81%)	-0.35	0  	96, 161, 397, 572	0
1	E	187/227 (82%)	-0.46	0  	147, 210, 373, 628	0
1	F	190/227 (83%)	-0.30	1 (0%)  	125, 205, 401, 461	0
2	G	94/94 (100%)	-0.44	0  	115, 174, 231, 290	0
2	H	93/94 (98%)	0.00	2 (2%)  	114, 161, 208, 276	0
2	I	93/94 (98%)	-0.19	2 (2%)  	82, 165, 215, 243	1 (1%)
2	J	92/94 (97%)	-0.30	1 (1%)  	142, 195, 257, 303	0
2	K	92/94 (97%)	-0.39	0  	189, 279, 340, 372	0
2	L	92/94 (97%)	0.02	2 (2%)  	105, 164, 230, 310	0
All	All	1686/1926 (87%)	-0.31	8 (0%)  	79, 181, 363, 628	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	82[A]	TYR	6.1
2	H	60	SER	2.3
2	J	73	TYR	2.3
2	I	3	SER	2.3
1	F	184	ASP	2.3
2	H	74	ALA	2.2
2	L	4	VAL	2.2
2	L	56	THR	2.1

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.