



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2022 – 12:46 PM EST

PDB ID : 7K7U  
Title : BetaB2-crystallin  
Authors : Tan, L.L.; Jackson, C.J.  
Deposited on : 2020-09-24  
Resolution : 3.03 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](mailto: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.

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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	:	2.26
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)	:	2.26

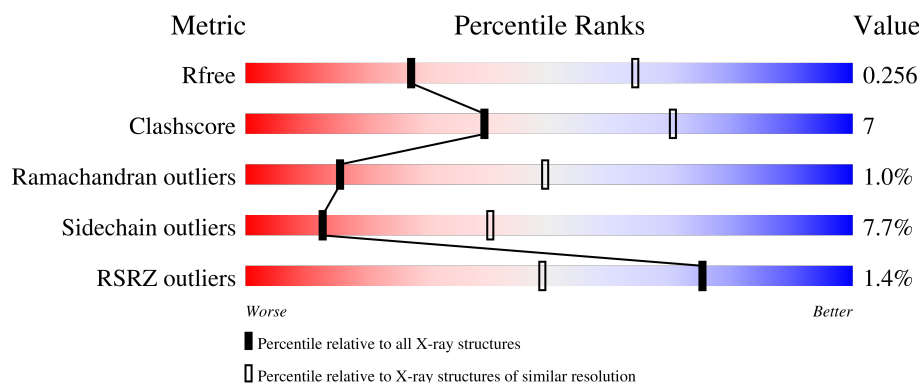
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.03 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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  $\geq 3$ , 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	205	<div> <div>72%</div> <div>18%</div> <div>9%</div> </div>
1	B	205	<div> <div>77%</div> <div>11%</div> <div>9%</div> </div>
1	C	205	<div> <div>69%</div> <div>19%</div> <div>9%</div> </div>
1	D	205	<div> <div>71%</div> <div>17%</div> <div>10%</div> </div>
1	E	205	<div> <div>69%</div> <div>20%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	205	<div><div><div>%</div><div><div></div><div>72%</div><div>17%</div><div>10%</div></div></div></div>
1	G	205	<div><div><div></div><div>73%</div><div>13%</div><div>•</div><div>10%</div></div></div>
1	H	205	<div><div><div>%</div><div><div></div><div>78%</div><div>11%</div><div>11%</div></div></div></div>
1	I	205	<div><div><div>4%</div><div><div></div><div>68%</div><div>20%</div><div>•</div><div>10%</div></div></div></div>
1	J	205	<div><div><div>2%</div><div><div></div><div>73%</div><div>17%</div><div>•</div><div>9%</div></div></div></div>
1	K	205	<div><div><div></div><div>69%</div><div>20%</div><div>•</div><div>9%</div></div></div>
1	L	205	<div><div><div>%</div><div><div></div><div>65%</div><div>22%</div><div>•</div><div>10%</div></div></div></div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18086 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 Beta-crystallin B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	184	Total	C	N	O	S	0	0	0
			1494	943	263	284	4			
1	J	187	Total	C	N	O	S	0	0	0
			1521	959	270	288	4			
1	K	186	Total	C	N	O	S	0	0	0
			1510	953	266	287	4			
1	L	184	Total	C	N	O	S	0	0	0
			1494	943	263	284	4			
1	A	186	Total	C	N	O	S	0	0	0
			1510	953	266	287	4			
1	C	186	Total	C	N	O	S	0	0	0
			1510	953	266	287	4			
1	D	185	Total	C	N	O	S	0	0	0
			1503	948	265	286	4			
1	E	185	Total	C	N	O	S	0	0	0
			1501	948	264	285	4			
1	B	187	Total	C	N	O	S	0	0	0
			1521	959	270	288	4			
1	F	184	Total	C	N	O	S	0	0	0
			1491	942	261	284	4			
1	G	184	Total	C	N	O	S	0	0	0
			1489	940	261	284	4			
1	H	183	Total	C	N	O	S	0	0	0
			1480	935	259	282	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	5	Total	O	0	0
			5	5		
2	J	2	Total	O	0	0
			2	2		

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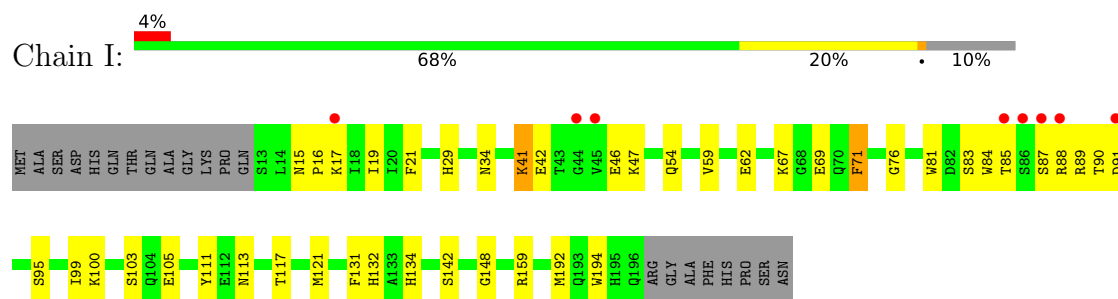
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	3	Total 3	O 3	0	0
2	L	4	Total 4	O 4	0	0
2	A	9	Total 9	O 9	0	0
2	C	9	Total 9	O 9	0	0
2	D	3	Total 3	O 3	0	0
2	E	5	Total 5	O 5	0	0
2	B	4	Total 4	O 4	0	0
2	F	5	Total 5	O 5	0	0
2	G	4	Total 4	O 4	0	0
2	H	9	Total 9	O 9	0	0

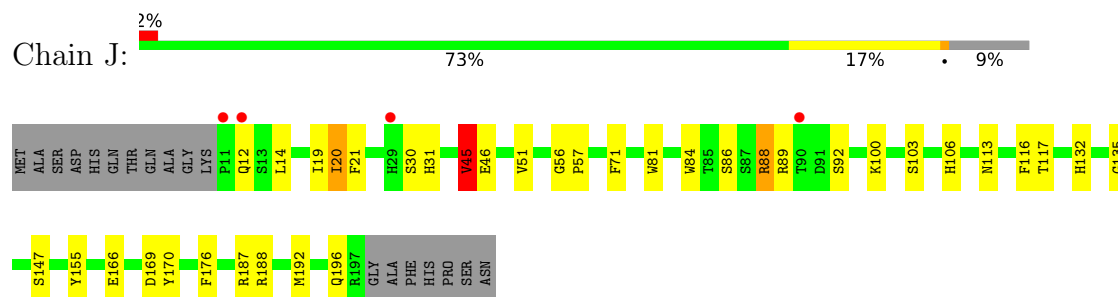
### 3 Residue-property plots [i](#)

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

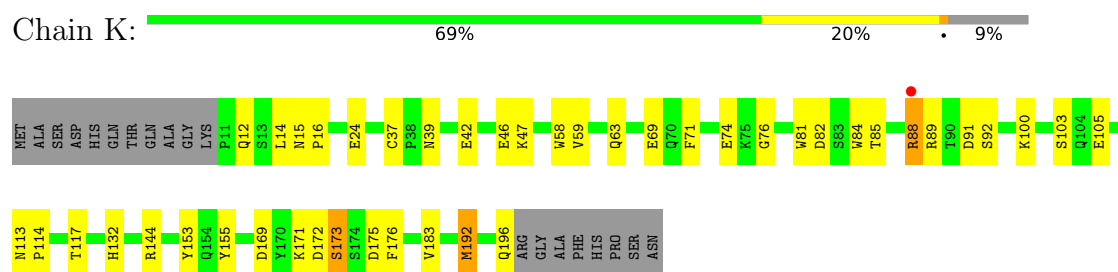
#### • Molecule 1: Beta-crystallin B2



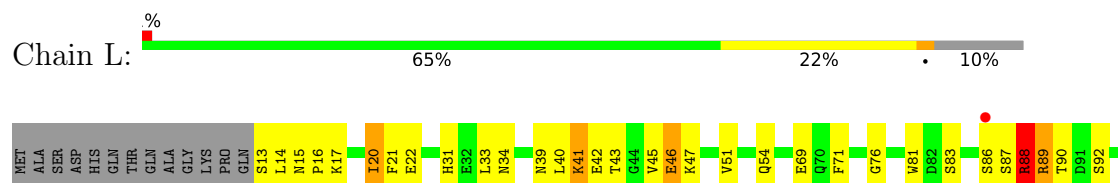
#### • Molecule 1: Beta-crystallin B2



#### • Molecule 1: Beta-crystallin B2

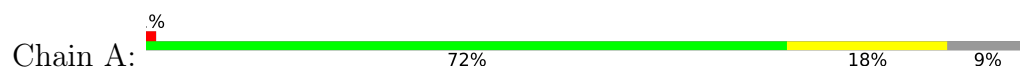


#### • Molecule 1: Beta-crystallin B2

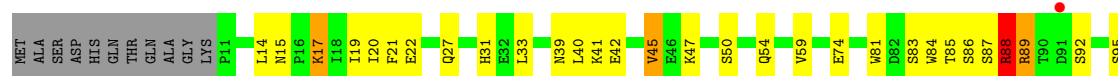




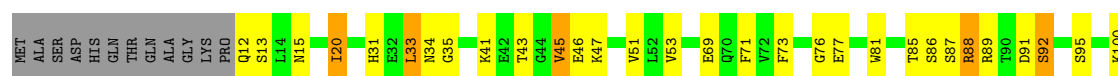
• Molecule 1: Beta-crystallin B2



• Molecule 1: Beta-crystallin B2



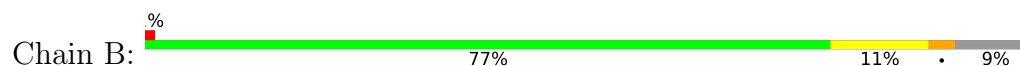
• Molecule 1: Beta-crystallin B2



• Molecule 1: Beta-crystallin B2

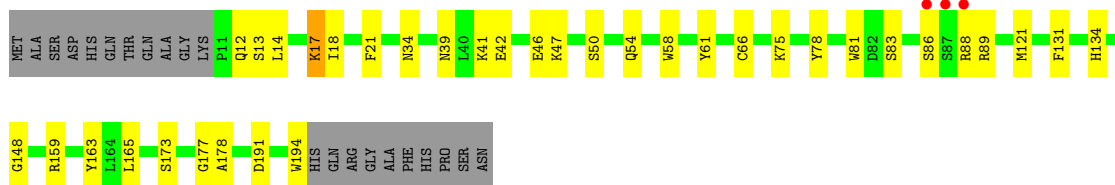


• Molecule 1: Beta-crystallin B2

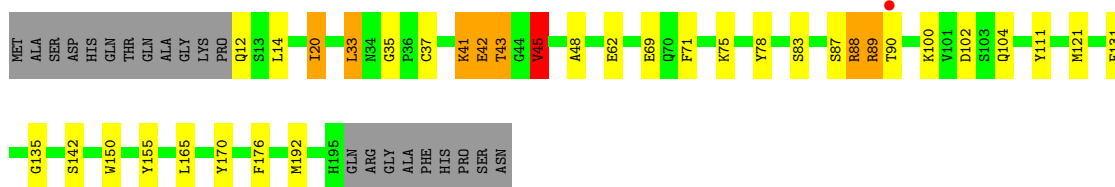




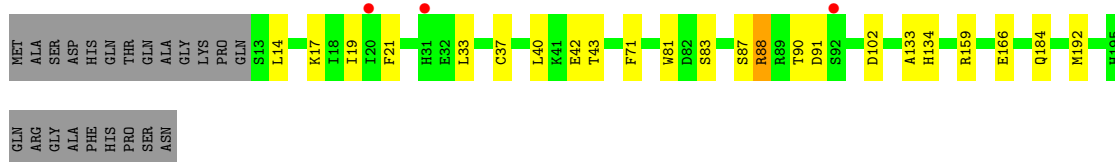
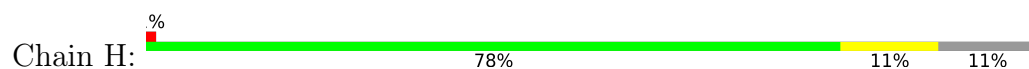
- Molecule 1: Beta-crystallin B2



- Molecule 1: Beta-crystallin B2



- Molecule 1: Beta-crystallin B2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.66Å 113.19Å 340.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 3.03 47.12 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.00-3.03) 99.4 (47.12-3.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.189 , 0.250 0.194 , 0.256	Depositor DCC
$R_{free}$ test set	2973 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 32.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.71	0/1554	0.95	0/2103
1	B	0.71	0/1565	0.94	0/2117
1	C	0.72	0/1554	0.95	0/2103
1	D	0.72	0/1546	0.97	0/2092
1	E	0.71	0/1545	0.96	0/2091
1	F	0.71	0/1534	0.92	0/2076
1	G	0.73	0/1531	0.94	0/2072
1	H	0.72	0/1522	0.95	0/2060
1	I	0.69	0/1537	0.96	0/2080
1	J	0.71	0/1565	0.95	0/2117
1	K	0.71	0/1554	0.94	0/2103
1	L	0.68	0/1537	0.97	0/2080
All	All	0.71	0/18544	0.95	0/25094

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	2
1	D	0	2
1	G	0	2
1	J	0	1
1	L	0	1
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ASN	Peptide
1	A	135	GLY	Peptide
1	D	46	GLU	Peptide
1	D	86	SER	Peptide
1	G	135	GLY	Peptide
1	G	88	ARG	Peptide
1	J	135	GLY	Peptide
1	L	88	ARG	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	1510	0	1433	21	0
1	B	1521	0	1446	20	0
1	C	1510	0	1433	28	0
1	D	1503	0	1425	22	0
1	E	1501	0	1425	27	0
1	F	1491	0	1418	17	0
1	G	1489	0	1412	30	0
1	H	1480	0	1404	13	0
1	I	1494	0	1417	28	0
1	J	1521	0	1446	21	0
1	K	1510	0	1433	25	0
1	L	1494	0	1417	38	0
2	A	9	0	0	1	0
2	B	4	0	0	1	0
2	C	9	0	0	1	0
2	D	3	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	1	0
2	G	4	0	0	0	0
2	H	9	0	0	1	0
2	I	5	0	0	0	0
2	J	2	0	0	0	0
2	K	3	0	0	0	0
2	L	4	0	0	2	0
All	All	18086	0	17109	260	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 7.

All (260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:113:ASN:HB2	1:J:117:THR:HG23	1.47	0.95
1:G:42:GLU:O	1:G:43:THR:OG1	1.84	0.94
1:G:20:ILE:HD13	1:G:48:ALA:HB2	1.51	0.93
1:K:88:ARG:O	1:K:88:ARG:HG2	1.69	0.92
1:J:113:ASN:HB2	1:J:117:THR:CG2	2.07	0.84
1:B:86:SER:O	1:B:88:ARG:N	2.13	0.81
1:L:69:GLU:HB2	1:L:89:ARG:HH12	1.47	0.79
1:G:69:GLU:HG2	1:G:89:ARG:CZ	2.14	0.78
1:L:43:THR:HG22	1:L:45:VAL:O	1.82	0.77
1:D:81:TRP:CZ3	1:D:88:ARG:HB3	2.21	0.75
1:H:40:LEU:O	1:H:43:THR:OG1	2.05	0.75
1:A:63:GLN:C	1:A:94:SER:OG	2.25	0.73
1:L:20:ILE:HG22	1:L:51:VAL:HG22	1.73	0.71
1:E:80:ARG:NH1	1:E:82:ASP:OD1	2.24	0.71
1:J:113:ASN:CB	1:J:117:THR:HG23	2.20	0.71
1:L:43:THR:CG2	1:L:45:VAL:HB	2.20	0.70
1:L:22:GLU:HG3	1:L:45:VAL:CG2	2.22	0.70
1:E:89:ARG:HD2	1:E:89:ARG:O	1.91	0.70
1:G:102:ASP:OD1	1:G:104:GLN:NE2	2.24	0.70
1:C:22:GLU:HG2	1:C:45:VAL:HG12	1.74	0.70
1:F:148:GLY:N	1:H:102:ASP:OD2	2.26	0.69
1:L:113:ASN:HB2	1:L:117:THR:HG23	1.73	0.68
1:I:83:SER:HB2	1:K:155:TYR:CD2	2.29	0.68
1:D:20:ILE:HG22	1:D:51:VAL:HG22	1.76	0.68
1:E:31:HIS:CG	1:E:45:VAL:HG22	2.29	0.67
1:J:31:HIS:ND1	1:J:45:VAL:HG23	2.10	0.67
1:G:69:GLU:HG2	1:G:89:ARG:NH1	2.10	0.67
1:E:31:HIS:CD2	1:E:45:VAL:HG22	2.30	0.67
1:I:83:SER:HB2	1:K:155:TYR:CE2	2.30	0.66
1:K:113:ASN:HB2	1:K:117:THR:HG23	1.77	0.66
1:C:88:ARG:H	1:C:88:ARG:HD3	1.59	0.66
1:L:88:ARG:HB2	2:L:301:HOH:O	1.95	0.66
1:L:22:GLU:CG	1:L:45:VAL:HG22	2.26	0.65
1:A:23:GLN:HB2	1:A:27:GLN:HB2	1.77	0.65
1:K:144:ARG:HG3	1:K:169:ASP:OD1	1.97	0.64
1:I:113:ASN:HB2	1:I:117:THR:OG1	1.98	0.64
1:J:31:HIS:CE1	1:J:45:VAL:HG23	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:TRP:CD1	1:H:88:ARG:HD3	2.32	0.64
1:B:88:ARG:O	1:B:88:ARG:HG2	1.98	0.64
1:J:113:ASN:CB	1:J:117:THR:CG2	2.76	0.64
1:K:69:GLU:OE2	1:K:89:ARG:NH1	2.29	0.64
1:C:88:ARG:HD3	1:C:88:ARG:N	2.13	0.63
1:B:69:GLU:OE1	1:B:89:ARG:HB2	1.97	0.63
2:C:309:HOH:O	1:E:104:GLN:HG2	1.97	0.63
1:L:22:GLU:HG3	1:L:45:VAL:HG22	1.80	0.62
1:E:33:LEU:HD22	1:E:35:GLY:O	1.99	0.62
1:G:33:LEU:HD22	1:G:35:GLY:O	1.99	0.62
1:C:27:GLN:OE1	1:C:27:GLN:HA	1.99	0.62
1:G:20:ILE:CD1	1:G:48:ALA:HB2	2.28	0.61
1:B:43:THR:O	1:B:45:VAL:N	2.34	0.61
1:L:88:ARG:N	2:L:301:HOH:O	2.33	0.60
1:J:20:ILE:HG22	1:J:51:VAL:HG22	1.83	0.60
1:E:40:LEU:O	1:E:45:VAL:O	2.20	0.60
1:D:69:GLU:OE2	1:D:89:ARG:CB	2.49	0.60
1:E:16:PRO:HG2	1:E:34:ASN:O	2.02	0.60
1:D:69:GLU:OE2	1:D:89:ARG:HB2	2.01	0.60
1:L:113:ASN:HB2	1:L:117:THR:CG2	2.31	0.60
1:C:81:TRP:HA	1:C:84:TRP:CH2	2.37	0.59
1:E:89:ARG:O	1:E:89:ARG:CD	2.50	0.59
1:L:31:HIS:CE1	1:L:45:VAL:HG23	2.37	0.59
1:G:69:GLU:HB3	1:G:89:ARG:NH2	2.19	0.58
1:F:18:ILE:HG22	1:F:58:TRP:CZ2	2.40	0.57
1:G:42:GLU:O	1:G:43:THR:CB	2.52	0.57
1:A:86:SER:OG	1:C:159:ARG:CZ	2.53	0.57
1:K:172:ASP:O	1:K:175:ASP:HB2	2.04	0.56
1:D:43:THR:OG1	1:D:45:VAL:HG23	2.04	0.56
1:A:47:LYS:NZ	1:A:91:ASP:OD1	2.37	0.56
1:C:17:LYS:HG2	1:C:54:GLN:HB2	1.87	0.56
1:D:88:ARG:O	1:D:88:ARG:HG2	2.06	0.56
1:E:22:GLU:HG3	1:E:29:HIS:O	2.04	0.56
1:E:46:GLU:OE1	1:E:46:GLU:N	2.37	0.56
1:A:19:ILE:HG22	1:A:21:PHE:CE1	2.40	0.56
1:H:81:TRP:NE1	1:H:88:ARG:HD3	2.20	0.56
1:A:88:ARG:O	1:A:88:ARG:HD3	2.06	0.55
1:C:39:ASN:OD1	1:C:41:LYS:HB2	2.06	0.55
1:D:81:TRP:CH2	1:D:88:ARG:HB3	2.42	0.55
1:G:33:LEU:CD2	1:G:35:GLY:O	2.55	0.55
1:E:12:GLN:N	1:E:12:GLN:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:LYS:HD3	1:G:42:GLU:H	1.72	0.55
1:I:41:LYS:HD2	1:I:41:LYS:N	2.22	0.54
1:B:59:VAL:HG13	1:B:59:VAL:O	2.07	0.54
1:L:43:THR:HG22	1:L:45:VAL:HB	1.89	0.54
1:E:16:PRO:O	1:E:34:ASN:HA	2.07	0.54
1:G:155:TYR:CE2	1:H:83:SER:HB2	2.43	0.54
1:G:155:TYR:CD2	1:H:83:SER:HB2	2.43	0.54
1:I:16:PRO:O	1:I:34:ASN:HA	2.08	0.54
1:I:148:GLY:HA2	1:L:102:ASP:O	2.08	0.54
1:E:81:TRP:CH2	1:E:88:ARG:HB2	2.41	0.54
1:E:106:HIS:HA	1:E:147:SER:OG	2.07	0.54
1:H:88:ARG:CZ	1:H:91:ASP:HB3	2.37	0.53
1:K:37:CYS:SG	1:K:39:ASN:O	2.66	0.53
1:L:41:LYS:HA	1:L:46:GLU:OE2	2.08	0.53
1:B:132:HIS:HB3	1:F:75:LYS:HG2	1.90	0.53
1:L:39:ASN:CG	1:L:41:LYS:HD2	2.29	0.52
1:A:64:ALA:N	1:A:94:SER:OG	2.42	0.52
1:D:77:GLU:H	1:E:184:GLN:HE22	1.56	0.52
1:G:20:ILE:HD11	1:G:45:VAL:HG22	1.91	0.52
1:L:40:LEU:O	1:L:43:THR:HB	2.10	0.52
1:I:121:MET:HE1	1:I:131:PHE:CG	2.45	0.52
1:I:47:LYS:HE3	1:I:91:ASP:CG	2.30	0.52
1:I:76:GLY:HA2	1:K:132:HIS:ND1	2.25	0.52
1:K:14:LEU:HD12	1:D:33:LEU:HD22	1.92	0.52
1:A:37:CYS:SG	1:A:43:THR:HG21	2.49	0.52
1:D:138:GLU:N	1:D:138:GLU:OE2	2.43	0.51
1:L:41:LYS:HG2	1:L:42:GLU:N	2.26	0.51
1:C:74:GLU:OE2	1:E:187:ARG:NH2	2.41	0.51
1:E:19:ILE:HG22	1:E:21:PHE:CE1	2.46	0.51
1:L:22:GLU:HG3	1:L:45:VAL:HG23	1.93	0.51
1:J:155:TYR:CD2	1:L:83:SER:HB2	2.45	0.51
1:E:20:ILE:HG13	1:E:45:VAL:HG11	1.92	0.51
1:E:81:TRP:HH2	1:E:88:ARG:HB2	1.76	0.50
1:I:85:THR:HB	1:I:87:SER:O	2.12	0.50
1:I:15:ASN:HD21	1:I:34:ASN:HB3	1.75	0.50
1:H:81:TRP:HE1	1:H:88:ARG:HD3	1.77	0.50
1:I:47:LYS:CE	1:I:91:ASP:CG	2.80	0.50
1:D:47:LYS:HD2	1:D:92:SER:HA	1.94	0.50
1:I:69:GLU:OE2	1:I:89:ARG:HB2	2.11	0.50
1:K:114:PRO:O	1:K:117:THR:HG22	2.12	0.49
1:K:46:GLU:HG3	1:K:47:LYS:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:PHE:HB2	1:F:50:SER:OG	2.13	0.49
1:J:46:GLU:O	1:J:46:GLU:HG3	2.11	0.49
1:L:108:ILE:HD12	1:L:145:VAL:HG22	1.94	0.49
1:H:19:ILE:HG22	1:H:21:PHE:CE1	2.47	0.49
1:H:37:CYS:SG	1:H:40:LEU:HD12	2.53	0.49
1:D:133:ALA:HA	1:E:75:LYS:HD3	1.95	0.49
1:G:42:GLU:C	1:G:43:THR:OG1	2.51	0.48
1:G:45:VAL:O	1:G:45:VAL:CG1	2.61	0.48
1:I:194:TRP:CZ2	1:L:98:PRO:HB2	2.49	0.48
1:B:159:ARG:NH2	1:F:86:SER:OG	2.46	0.48
1:I:81:TRP:HA	1:I:84:TRP:CH2	2.48	0.48
1:K:15:ASN:HD21	1:D:34:ASN:H	1.62	0.48
1:E:81:TRP:O	1:E:85:THR:HG22	2.14	0.48
1:K:16:PRO:HB2	1:K:58:TRP:CZ2	2.49	0.48
1:G:20:ILE:HD11	1:G:45:VAL:CG2	2.43	0.48
1:B:89:ARG:CZ	1:B:89:ARG:HB3	2.43	0.48
1:I:88:ARG:CZ	1:I:91:ASP:HB3	2.43	0.48
1:L:41:LYS:HE2	1:L:42:GLU:OE1	2.13	0.48
1:A:81:TRP:CH2	1:A:88:ARG:HG3	2.49	0.48
1:B:14:LEU:C	2:B:302:HOH:O	2.51	0.48
1:B:20:ILE:HG22	1:B:51:VAL:HG22	1.96	0.47
1:H:184:GLN:NE2	2:H:303:HOH:O	2.46	0.47
1:K:46:GLU:CG	1:K:47:LYS:N	2.77	0.47
1:F:46:GLU:HG3	1:F:47:LYS:N	2.29	0.47
1:A:102:ASP:O	1:D:148:GLY:HA2	2.15	0.47
1:L:43:THR:HG22	1:L:45:VAL:CB	2.44	0.47
1:G:78:TYR:HB3	1:G:83:SER:OG	2.15	0.47
1:D:53:VAL:HG21	1:D:73:PHE:HB3	1.97	0.47
1:E:116:PHE:CD2	1:E:144:ARG:NH2	2.83	0.47
1:C:85:THR:OG1	1:C:87:SER:O	2.33	0.47
1:J:100:LYS:HA	1:K:192:MET:SD	2.55	0.46
1:J:170:TYR:CD2	1:J:176:PHE:HB3	2.51	0.46
1:J:45:VAL:HG12	1:J:45:VAL:O	2.16	0.46
1:A:62:GLU:HA	1:A:92:SER:O	2.16	0.46
1:K:14:LEU:HD12	1:D:33:LEU:CD2	2.46	0.45
1:A:37:CYS:SG	1:A:43:THR:CG2	3.04	0.45
1:A:194:TRP:CG	1:A:194:TRP:O	2.69	0.45
1:G:45:VAL:O	1:G:45:VAL:HG13	2.17	0.45
1:G:111:TYR:HB2	1:G:142:SER:OG	2.16	0.45
1:I:62:GLU:HG3	1:I:90:THR:HG21	1.98	0.45
1:A:155:TYR:CD2	1:C:83:SER:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:HIS:HB3	1:C:45:VAL:HG21	1.98	0.45
1:C:59:VAL:HG13	1:C:59:VAL:O	2.16	0.45
1:D:154:GLN:HG3	1:D:161:LEU:HB2	1.98	0.45
1:G:89:ARG:CD	1:G:89:ARG:H	2.30	0.45
1:D:33:LEU:HD12	1:D:35:GLY:O	2.17	0.45
1:I:71:PHE:CE1	1:I:85:THR:HG22	2.52	0.45
1:C:113:ASN:HB2	1:C:117:THR:HG23	1.98	0.45
1:C:19:ILE:HG22	1:C:21:PHE:CE1	2.52	0.45
1:C:27:GLN:OE1	1:C:27:GLN:CA	2.65	0.45
1:C:173:SER:HA	1:C:176:PHE:CE2	2.52	0.45
1:K:59:VAL:HG13	1:K:59:VAL:O	2.17	0.45
1:A:75:LYS:O	1:C:130:SER:OG	2.30	0.45
1:C:153:TYR:CG	1:C:158:TYR:HA	2.51	0.45
1:D:173:SER:HA	1:D:176:PHE:CE2	2.52	0.45
1:I:71:PHE:HA	1:L:162:GLN:OE1	2.17	0.44
1:F:17:LYS:HB3	1:F:34:ASN:OD1	2.18	0.44
1:A:18:ILE:HG22	1:A:58:TRP:CZ2	2.52	0.44
1:L:45:VAL:O	1:L:45:VAL:HG12	2.18	0.44
1:C:81:TRP:HA	1:C:84:TRP:CZ2	2.53	0.44
1:G:41:LYS:HD3	1:G:42:GLU:N	2.32	0.44
1:L:39:ASN:OD1	1:L:41:LYS:HB3	2.17	0.44
1:F:177:GLY:HA3	2:F:302:HOH:O	2.18	0.44
1:G:33:LEU:HD21	1:G:37:CYS:HB2	2.00	0.44
1:L:47:LYS:HD2	1:L:92:SER:HA	1.99	0.44
1:I:19:ILE:HG22	1:I:21:PHE:CE1	2.53	0.43
1:B:62:GLU:O	1:B:94:SER:OG	2.26	0.43
1:G:75:LYS:HD3	1:H:133:ALA:HA	1.99	0.43
1:K:14:LEU:HD21	1:D:31:HIS:HB3	2.01	0.43
1:C:119:LYS:NZ	1:C:135:GLY:O	2.49	0.43
1:L:31:HIS:HE1	1:L:45:VAL:HG23	1.84	0.43
1:D:76:GLY:HA2	1:E:132:HIS:ND1	2.33	0.43
1:B:14:LEU:O	1:B:14:LEU:HD22	2.18	0.43
1:L:22:GLU:HG2	1:L:45:VAL:HG22	1.99	0.43
1:K:81:TRP:CE3	1:K:91:ASP:HB3	2.54	0.43
1:I:84:TRP:CD1	1:I:85:THR:HG23	2.53	0.43
1:B:14:LEU:N	1:B:14:LEU:HD13	2.34	0.43
1:F:163:TYR:O	1:F:165:LEU:HG	2.18	0.43
1:A:141:SER:O	1:A:173:SER:N	2.51	0.43
1:B:41:LYS:O	1:B:43:THR:N	2.52	0.43
1:F:61:TYR:CG	1:F:66:CYS:HA	2.54	0.43
1:I:111:TYR:HB2	1:I:142:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASN:OD1	1:B:41:LYS:HB2	2.19	0.43
1:F:46:GLU:HG3	1:F:47:LYS:H	1.82	0.43
1:I:62:GLU:OE2	1:I:90:THR:HG21	2.18	0.42
1:J:88:ARG:H	1:J:88:ARG:HD3	1.83	0.42
1:C:88:ARG:O	1:C:89:ARG:C	2.56	0.42
1:I:17:LYS:HG2	1:I:54:GLN:HB2	2.01	0.42
1:A:81:TRP:HA	1:A:84:TRP:CH2	2.53	0.42
1:B:53:VAL:HG21	1:B:73:PHE:HB3	2.01	0.42
1:G:89:ARG:H	1:G:89:ARG:HD3	1.84	0.42
1:C:121:MET:HE1	1:C:131:PHE:CD2	2.54	0.42
1:G:62:GLU:HG3	1:G:90:THR:HG21	2.02	0.42
1:G:150:TRP:HB2	1:G:165:LEU:HB2	2.01	0.42
1:L:41:LYS:HG2	1:L:42:GLU:HG3	2.01	0.42
1:F:173:SER:O	1:F:178:ALA:HB3	2.19	0.42
1:I:121:MET:HE1	1:I:131:PHE:CD2	2.55	0.42
1:B:141:SER:O	1:B:173:SER:N	2.53	0.42
1:F:81:TRP:HH2	1:F:88:ARG:HG2	1.85	0.42
1:C:121:MET:CE	1:C:131:PHE:CE2	3.03	0.42
1:E:81:TRP:HZ3	1:E:88:ARG:HA	1.85	0.42
1:C:121:MET:CE	1:C:131:PHE:CD2	3.02	0.42
1:F:78:TYR:HB3	1:F:83:SER:OG	2.19	0.41
1:L:17:LYS:HE2	1:L:54:GLN:OE1	2.21	0.41
1:B:12:GLN:O	1:B:12:GLN:HG3	2.20	0.41
1:F:121:MET:HE1	1:F:131:PHE:CE1	2.54	0.41
1:J:132:HIS:ND1	1:L:76:GLY:HA2	2.34	0.41
1:L:43:THR:HG22	1:L:45:VAL:CA	2.51	0.41
1:J:19:ILE:HG22	1:J:21:PHE:CE1	2.56	0.41
1:J:106:HIS:HA	1:J:147:SER:OG	2.20	0.41
1:C:121:MET:HE3	1:C:131:PHE:CZ	2.55	0.41
1:D:85:THR:O	1:E:159:ARG:NH2	2.53	0.41
1:J:116:PHE:HZ	1:J:169:ASP:HB3	1.84	0.41
1:C:20:ILE:CD1	1:C:40:LEU:HD22	2.50	0.41
1:J:81:TRP:HA	1:J:84:TRP:CH2	2.56	0.41
1:L:16:PRO:O	1:L:34:ASN:HA	2.20	0.41
1:L:81:TRP:CZ3	1:L:88:ARG:HG3	2.55	0.41
1:L:153:TYR:CG	1:L:158:TYR:HA	2.55	0.41
1:B:62:GLU:OE2	1:B:90:THR:HG21	2.20	0.41
1:I:42:GLU:N	1:I:42:GLU:OE1	2.54	0.41
1:I:132:HIS:ND1	1:K:76:GLY:HA2	2.36	0.41
1:G:89:ARG:HD3	1:G:89:ARG:N	2.36	0.41
1:H:90:THR:O	1:H:91:ASP:OD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:56:GLY:HA3	1:J:57:PRO:HA	1.85	0.41
1:K:81:TRP:HA	1:K:84:TRP:CH2	2.56	0.41
1:K:153:TYR:O	1:K:183:VAL:HA	2.21	0.41
1:A:154:GLN:HG2	2:A:302:HOH:O	2.20	0.41
1:F:39:ASN:OD1	1:F:41:LYS:HB2	2.21	0.41
1:I:59:VAL:HB	1:I:99:ILE:HD11	2.03	0.41
1:K:173:SER:HA	1:K:176:PHE:CE2	2.56	0.40
1:E:53:VAL:HG21	1:E:73:PHE:HB3	2.03	0.40
1:B:43:THR:C	1:B:45:VAL:H	2.24	0.40
1:A:20:ILE:HG22	1:A:51:VAL:HG22	2.02	0.40
1:G:170:TYR:CD2	1:G:176:PHE:HB3	2.56	0.40
1:L:170:TYR:CD2	1:L:176:PHE:HB3	2.57	0.40
1:F:17:LYS:CE	1:F:54:GLN:OE1	2.69	0.40
1:J:20:ILE:HG13	1:J:45:VAL:HG11	2.02	0.40
1:J:187:ARG:NH2	1:K:74:GLU:OE2	2.43	0.40
1:A:81:TRP:CH2	1:A:88:ARG:CG	3.05	0.40
1:C:121:MET:HE3	1:C:131:PHE:CE1	2.56	0.40
1:G:121:MET:HE1	1:G:131:PHE:CE2	2.56	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	184/205 (90%)	173 (94%)	9 (5%)	2 (1%)	14	47
1	B	185/205 (90%)	169 (91%)	10 (5%)	6 (3%)	4	20
1	C	184/205 (90%)	170 (92%)	11 (6%)	3 (2%)	9	37
1	D	183/205 (89%)	171 (93%)	12 (7%)	0	100	100
1	E	183/205 (89%)	171 (93%)	10 (6%)	2 (1%)	14	47
1	F	182/205 (89%)	167 (92%)	14 (8%)	1 (0%)	29	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	182/205 (89%)	169 (93%)	10 (6%)	3 (2%)	9	37
1	H	181/205 (88%)	170 (94%)	10 (6%)	1 (1%)	25	60
1	I	182/205 (89%)	174 (96%)	8 (4%)	0	100	100
1	J	185/205 (90%)	171 (92%)	12 (6%)	2 (1%)	14	47
1	K	184/205 (90%)	172 (94%)	11 (6%)	1 (0%)	29	65
1	L	182/205 (89%)	170 (93%)	10 (6%)	2 (1%)	14	47
All	All	2197/2460 (89%)	2047 (93%)	127 (6%)	23 (1%)	15	49

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	86	SER
1	L	195	HIS
1	C	47	LYS
1	B	42	GLU
1	B	43	THR
1	B	87	SER
1	B	88	ARG
1	G	43	THR
1	H	87	SER
1	C	88	ARG
1	C	89	ARG
1	E	87	SER
1	B	44	GLY
1	G	87	SER
1	A	88	ARG
1	E	42	GLU
1	J	45	VAL
1	L	116	PHE
1	B	86	SER
1	K	12	GLN
1	A	25	ASN
1	F	13	SER
1	G	45	VAL

### 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	165/179 (92%)	156 (94%)	9 (6%)	21	54
1	B	166/179 (93%)	159 (96%)	7 (4%)	30	64
1	C	165/179 (92%)	150 (91%)	15 (9%)	9	32
1	D	164/179 (92%)	147 (90%)	17 (10%)	7	25
1	E	164/179 (92%)	152 (93%)	12 (7%)	14	42
1	F	163/179 (91%)	154 (94%)	9 (6%)	21	54
1	G	162/179 (90%)	150 (93%)	12 (7%)	13	42
1	H	161/179 (90%)	151 (94%)	10 (6%)	18	49
1	I	163/179 (91%)	151 (93%)	12 (7%)	13	42
1	J	166/179 (93%)	152 (92%)	14 (8%)	11	36
1	K	165/179 (92%)	150 (91%)	15 (9%)	9	32
1	L	163/179 (91%)	143 (88%)	20 (12%)	4	19
All	All	1967/2148 (92%)	1815 (92%)	152 (8%)	13	40

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	29	HIS
1	I	41	LYS
1	I	46	GLU
1	I	67	LYS
1	I	71	PHE
1	I	95	SER
1	I	100	LYS
1	I	103	SER
1	I	105	GLU
1	I	134	HIS
1	I	159	ARG
1	I	192	MET
1	J	12	GLN
1	J	14	LEU
1	J	20	ILE
1	J	30	SER
1	J	45	VAL
1	J	71	PHE
1	J	88	ARG

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Mol	Chain	Res	Type
1	J	89	ARG
1	J	92	SER
1	J	103	SER
1	J	166	GLU
1	J	188	ARG
1	J	192	MET
1	J	196	GLN
1	K	24	GLU
1	K	42	GLU
1	K	63	GLN
1	K	71	PHE
1	K	82	ASP
1	K	85	THR
1	K	88	ARG
1	K	92	SER
1	K	100	LYS
1	K	103	SER
1	K	105	GLU
1	K	171	LYS
1	K	173	SER
1	K	192	MET
1	K	196	GLN
1	L	13	SER
1	L	14	LEU
1	L	15	ASN
1	L	20	ILE
1	L	21	PHE
1	L	33	LEU
1	L	41	LYS
1	L	46	GLU
1	L	71	PHE
1	L	86	SER
1	L	87	SER
1	L	88	ARG
1	L	89	ARG
1	L	90	THR
1	L	95	SER
1	L	96	LEU
1	L	101	VAL
1	L	121	MET
1	L	134	HIS
1	L	192	MET

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Mol	Chain	Res	Type
1	A	12	GLN
1	A	41	LYS
1	A	67	LYS
1	A	71	PHE
1	A	88	ARG
1	A	92	SER
1	A	93	LEU
1	A	103	SER
1	A	159	ARG
1	C	14	LEU
1	C	15	ASN
1	C	17	LYS
1	C	33	LEU
1	C	42	GLU
1	C	45	VAL
1	C	50	SER
1	C	86	SER
1	C	88	ARG
1	C	92	SER
1	C	95	SER
1	C	100	LYS
1	C	117	THR
1	C	159	ARG
1	C	192	MET
1	D	12	GLN
1	D	13	SER
1	D	15	ASN
1	D	20	ILE
1	D	33	LEU
1	D	41	LYS
1	D	45	VAL
1	D	71	PHE
1	D	87	SER
1	D	88	ARG
1	D	91	ASP
1	D	92	SER
1	D	95	SER
1	D	100	LYS
1	D	119	LYS
1	D	134	HIS
1	D	196	GLN
1	E	14	LEU

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Mol	Chain	Res	Type
1	E	17	LYS
1	E	42	GLU
1	E	43	THR
1	E	45	VAL
1	E	47	LYS
1	E	71	PHE
1	E	87	SER
1	E	95	SER
1	E	120	LYS
1	E	180	HIS
1	E	194	TRP
1	B	12	GLN
1	B	14	LEU
1	B	41	LYS
1	B	95	SER
1	B	100	LYS
1	B	134	HIS
1	B	180	HIS
1	F	12	GLN
1	F	14	LEU
1	F	17	LYS
1	F	42	GLU
1	F	89	ARG
1	F	134	HIS
1	F	159	ARG
1	F	191	ASP
1	F	194	TRP
1	G	12	GLN
1	G	14	LEU
1	G	20	ILE
1	G	33	LEU
1	G	41	LYS
1	G	42	GLU
1	G	45	VAL
1	G	71	PHE
1	G	88	ARG
1	G	89	ARG
1	G	100	LYS
1	G	192	MET
1	H	14	LEU
1	H	17	LYS
1	H	33	LEU

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Mol	Chain	Res	Type
1	H	42	GLU
1	H	71	PHE
1	H	88	ARG
1	H	134	HIS
1	H	159	ARG
1	H	166	GLU
1	H	192	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	15	ASN
1	J	12	GLN
1	J	15	ASN
1	K	15	ASN
1	K	162	GLN
1	K	195	HIS
1	L	134	HIS
1	L	184	GLN
1	A	23	GLN
1	E	184	GLN
1	B	31	HIS
1	B	104	GLN
1	F	12	GLN
1	F	15	ASN
1	G	31	HIS
1	G	104	GLN
1	H	70	GLN
1	H	184	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 [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	186/205 (90%)	-0.26	3 (1%) 72 44	33, 61, 127, 146	0
1	B	187/205 (91%)	-0.22	3 (1%) 72 44	44, 73, 125, 161	0
1	C	186/205 (90%)	-0.39	2 (1%) 80 56	39, 61, 111, 154	0
1	D	185/205 (90%)	-0.26	0 100 100	42, 62, 114, 189	0
1	E	185/205 (90%)	-0.25	2 (1%) 80 56	38, 65, 120, 172	0
1	F	184/205 (89%)	-0.28	3 (1%) 72 44	50, 74, 116, 182	0
1	G	184/205 (89%)	-0.28	1 (0%) 91 75	41, 72, 119, 192	0
1	H	183/205 (89%)	-0.12	3 (1%) 72 44	39, 69, 127, 180	0
1	I	184/205 (89%)	-0.14	8 (4%) 35 14	36, 67, 124, 163	0
1	J	187/205 (91%)	-0.26	4 (2%) 63 34	42, 67, 128, 231	0
1	K	186/205 (90%)	-0.33	1 (0%) 91 75	43, 67, 119, 166	0
1	L	184/205 (89%)	-0.28	2 (1%) 80 56	42, 63, 122, 182	0
All	All	2221/2460 (90%)	-0.26	32 (1%) 75 49	33, 67, 124, 231	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	88	ARG	3.4
1	H	31	HIS	3.3
1	I	44	GLY	3.2
1	E	89	ARG	3.2
1	F	87	SER	3.1
1	H	20	ILE	3.0
1	B	46	GLU	2.9
1	F	86	SER	2.8
1	J	12	GLN	2.8
1	K	88	ARG	2.6
1	I	86	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	86	SER	2.6
1	B	88	ARG	2.6
1	I	91	ASP	2.5
1	I	17	LYS	2.4
1	H	92	SER	2.4
1	J	90	THR	2.4
1	G	90	THR	2.3
1	J	11	PRO	2.2
1	I	45	VAL	2.2
1	A	46	GLU	2.2
1	A	11	PRO	2.2
1	I	85	THR	2.2
1	B	89	ARG	2.2
1	I	87	SER	2.1
1	J	29	HIS	2.1
1	A	12	GLN	2.1
1	C	194	TRP	2.1
1	E	90	THR	2.1
1	F	88	ARG	2.0
1	C	91	ASP	2.0
1	L	194	TRP	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 monosaccharides 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.