



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:21 AM UTC

PDB ID : 7K7U / pdb_00007k7u
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

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

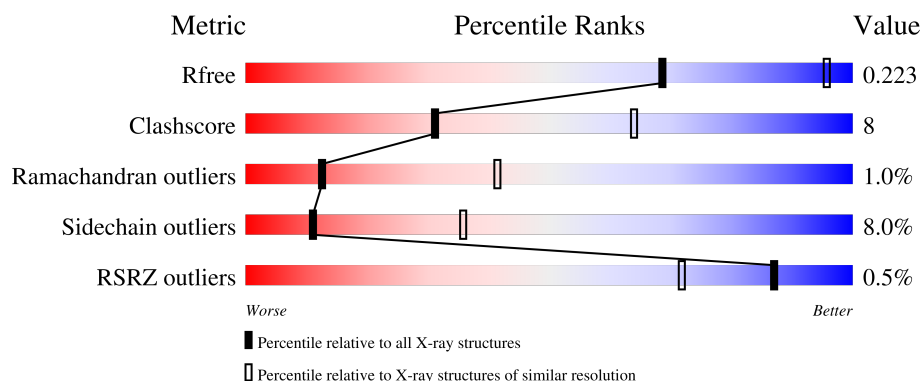
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (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 ≥ 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	
1	B	205	
1	C	205	
1	D	205	
1	E	205	

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Mol	Chain	Length	Quality of chain
1	F	205	67%21%10%
1	G	205	%71%14%10%
1	H	205	%76%12%11%
1	I	205	68%20%10%
1	J	205	70%19%9%
1	K	205	68%21%9%
1	L	205	63%23%10%

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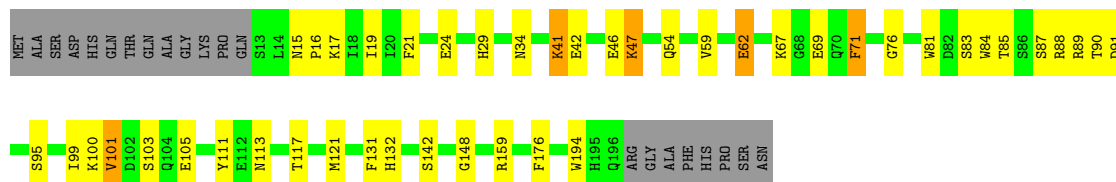
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	3	Total 3	O 3	0	0
2	L	4	Total 4	O 4	0	0
2	A	9	Total 9	O 9	0	0
2	C	9	Total 9	O 9	0	0
2	D	3	Total 3	O 3	0	0
2	E	5	Total 5	O 5	0	0
2	B	4	Total 4	O 4	0	0
2	F	5	Total 5	O 5	0	0
2	G	4	Total 4	O 4	0	0
2	H	9	Total 9	O 9	0	0

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.

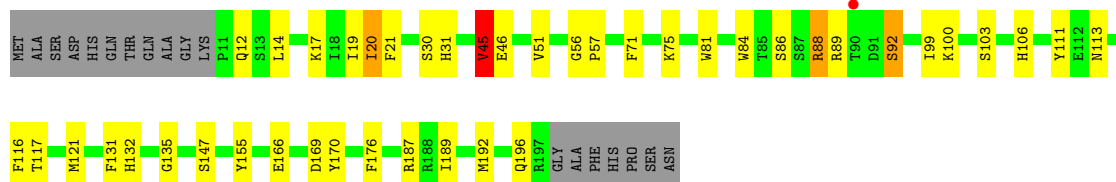
• Molecule 1: Beta-crystallin B2

Chain I: 



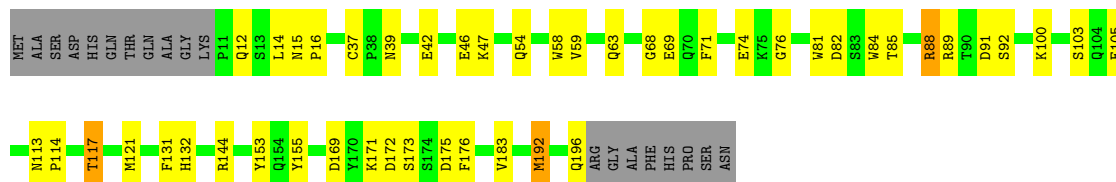
• Molecule 1: Beta-crystallin B2

Chain J: 



• Molecule 1: Beta-crystallin B2

Chain K: 

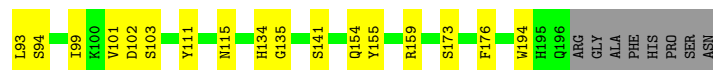
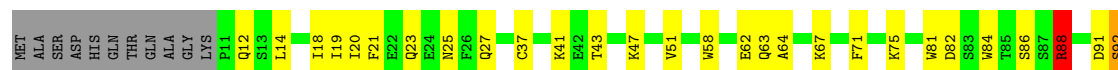


• Molecule 1: Beta-crystallin B2

Chain L: 



- Molecule 1: Beta-crystallin B2



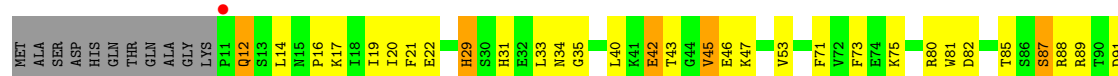
- Molecule 1: Beta-crystallin B2



- Molecule 1: Beta-crystallin B2



- Molecule 1: Beta-crystallin B2

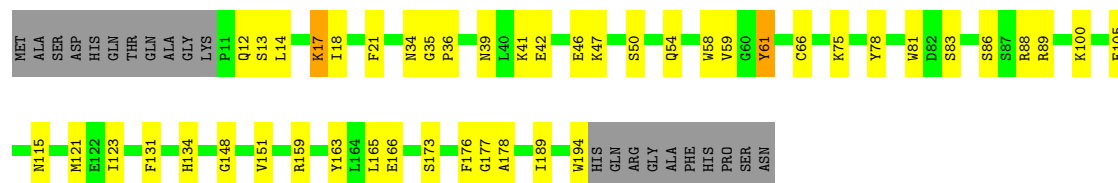


- Molecule 1: Beta-crystallin B2

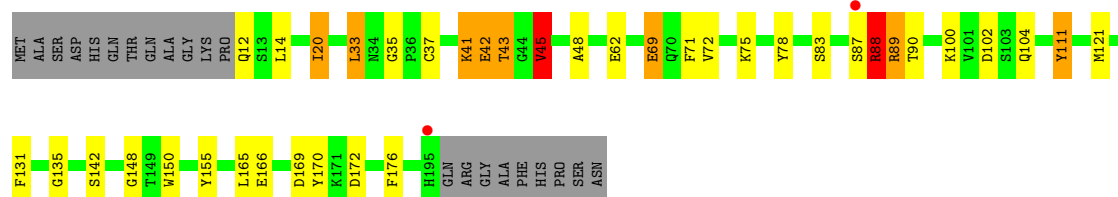




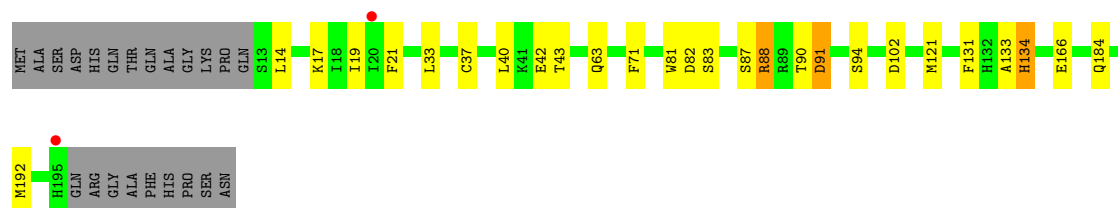
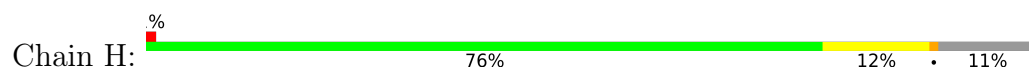
• Molecule 1: Beta-crystallin B2



• Molecule 1: Beta-crystallin B2



• Molecule 1: Beta-crystallin B2



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	78.66Å 113.19Å 340.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 3.03 45.00 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.00-3.03) 99.3 (45.00-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.189 , 0.250 (Not available) , 0.223	Depositor DCC
R_{free} test set	2973 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	66.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

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	1.05	1/1554 (0.1%)	1.40	5/2103 (0.2%)
1	B	1.05	0/1565	1.38	3/2117 (0.1%)
1	C	1.06	0/1554	1.44	4/2103 (0.2%)
1	D	1.06	1/1546 (0.1%)	1.44	3/2092 (0.1%)
1	E	1.05	0/1545	1.47	4/2091 (0.2%)
1	F	1.06	1/1534 (0.1%)	1.42	7/2076 (0.3%)
1	G	1.10	1/1531 (0.1%)	1.41	6/2072 (0.3%)
1	H	1.09	1/1522 (0.1%)	1.43	2/2060 (0.1%)
1	I	1.04	0/1537	1.43	3/2080 (0.1%)
1	J	1.06	1/1565 (0.1%)	1.45	4/2117 (0.2%)
1	K	1.04	0/1554	1.43	4/2103 (0.2%)
1	L	1.03	0/1537	1.45	4/2080 (0.2%)
All	All	1.06	6/18544 (0.0%)	1.43	49/25094 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	2
1	G	0	2
1	J	0	1
1	L	0	1
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189	ILE	C-O	6.93	1.30	1.24
1	G	72	VAL	C-O	5.46	1.30	1.24
1	H	134	HIS	CE1-NE2	5.43	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	HIS	CE1-NE2	5.35	1.38	1.32
1	J	189	ILE	C-O	5.20	1.29	1.24
1	F	189	ILE	C-O	5.17	1.30	1.24

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ASP	CA-CB-CG	7.81	120.41	112.60
1	L	148	GLY	CA-C-O	-7.41	116.67	122.52
1	E	125	ASP	CA-CB-CG	6.78	119.38	112.60
1	F	176	PHE	CA-CB-CG	6.66	120.45	113.80
1	E	29	HIS	CB-CA-C	6.32	120.14	109.84
1	D	176	PHE	CA-CB-CG	6.23	120.03	113.80
1	K	117	THR	CA-CB-OG1	-6.05	100.52	109.60
1	H	82	ASP	CA-CB-CG	5.95	118.55	112.60
1	F	59	VAL	CA-C-N	5.88	126.62	122.33
1	F	59	VAL	C-N-CA	5.88	126.62	122.33
1	A	111	TYR	CA-C-N	5.83	128.01	120.44
1	A	111	TYR	C-N-CA	5.83	128.01	120.44
1	B	176	PHE	CA-CB-CG	5.66	119.46	113.80
1	F	61	TYR	CA-C-N	5.46	127.92	120.54
1	F	61	TYR	C-N-CA	5.46	127.92	120.54
1	B	131	PHE	N-CA-C	-5.43	105.26	111.07
1	E	176	PHE	CA-CB-CG	5.38	119.19	113.80
1	I	101	VAL	N-CA-CB	5.36	116.38	110.53
1	B	122	GLU	CB-CA-C	-5.35	101.53	110.19
1	A	176	PHE	CA-CB-CG	5.32	119.12	113.80
1	C	131	PHE	N-CA-C	-5.32	105.49	111.28
1	L	195	HIS	CA-CB-CG	5.31	119.11	113.80
1	D	36	PRO	CA-C-O	-5.30	115.30	121.34
1	H	91	ASP	CA-CB-CG	5.27	117.87	112.60
1	F	151	VAL	CA-C-N	5.27	125.35	120.34
1	F	151	VAL	C-N-CA	5.27	125.35	120.34
1	C	54	GLN	N-CA-C	-5.27	106.98	113.41
1	K	54	GLN	N-CA-C	-5.25	107.42	113.88
1	C	127	ASP	CA-CB-CG	5.23	117.83	112.60
1	K	68	GLY	CA-C-N	5.21	128.25	120.90
1	K	68	GLY	C-N-CA	5.21	128.25	120.90
1	C	25	ASN	CA-CB-CG	-5.18	107.42	112.60
1	I	24	GLU	CB-CG-CD	5.18	121.40	112.60
1	G	172	ASP	CA-C-N	5.17	127.92	120.38
1	G	172	ASP	C-N-CA	5.17	127.92	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	154	GLN	CB-CG-CD	-5.15	103.84	112.60
1	L	85	THR	CA-C-N	5.15	127.63	120.63
1	L	85	THR	C-N-CA	5.15	127.63	120.63
1	J	92	SER	CA-C-N	5.14	128.53	121.33
1	J	92	SER	C-N-CA	5.14	128.53	121.33
1	I	176	PHE	CA-CB-CG	5.12	118.92	113.80
1	D	87	SER	CA-C-O	-5.11	115.43	120.80
1	G	148	GLY	CA-C-O	-5.07	118.19	122.29
1	G	111	TYR	CA-C-N	5.03	126.98	120.44
1	G	111	TYR	C-N-CA	5.03	126.98	120.44
1	G	169	ASP	CB-CA-C	5.03	118.04	109.75
1	J	111	TYR	CA-C-N	5.01	126.96	120.44
1	J	111	TYR	C-N-CA	5.01	126.96	120.44
1	A	99	ILE	O-C-N	5.01	128.59	123.03

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 [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	1510	0	1433	22	0
1	B	1521	0	1446	23	0
1	C	1510	0	1433	30	0
1	D	1503	0	1425	26	0
1	E	1501	0	1425	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1491	0	1418	22	0
1	G	1489	0	1412	32	0
1	H	1480	0	1404	16	0
1	I	1494	0	1417	30	0
1	J	1521	0	1446	24	0
1	K	1510	0	1433	28	0
1	L	1494	0	1417	39	0
2	A	9	0	0	1	0
2	B	4	0	0	1	0
2	C	9	0	0	2	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	287	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 (287) 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:A:63:GLN:C	1:A:94:SER:OG	2.25	0.78
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:121:MET:HE1	1:C:131:PHE:CD2	2.29	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:C:121:MET:HE1	1:C:131:PHE:CG	2.33	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
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:F:121:MET:HE3	1:F:123:ILE:HD11	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:39:ASN:CG	1:L:41:LYS:HD2	2.29	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:I:47:LYS:HE3	1:I:91:ASP:CG	2.30	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:J:121:MET:HE1	1:J:131:PHE:CD2	2.40	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
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:I:47:LYS:CE	1:I:91:ASP:CG	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:ARG:CZ	1:H:91:ASP:HB3	2.37	0.53
1:I:121:MET:HE1	1:I:131:PHE:CG	2.44	0.53
1:K:37:CYS:SG	1:K:39:ASN:O	2.66	0.53
1:G:42:GLU:C	1:G:43:THR:OG1	2.51	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: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:B:14:LEU:C	2:B:302:HOH:O	2.51	0.52
1:B:62:GLU:O	1:B:94:SER:OG	2.26	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: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:G:121:MET:HE1	1:G:131:PHE:CD2	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:F:121:MET:HE1	1:F:131:PHE:CE2	2.47	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:F:121:MET:HE1	1:F:131:PHE:CD2	2.46	0.50
1:H:81:TRP:HE1	1:H:88:ARG:HD3	1.77	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:45:VAL:O	1:G:45:VAL:CG1	2.61	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:K:121:MET:HE1	1:K:131:PHE:CD2	2.49	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: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:J:121:MET:HE1	1:J:131:PHE:CG	2.50	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:C:88:ARG:O	1:C:89:ARG:C	2.56	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:H:121:MET:HE1	1:H:131:PHE:CG	2.50	0.46
1:A:62:GLU:HA	1:A:92:SER:O	2.16	0.46
1:J:75:LYS:O	1:L:130:SER:OG	2.31	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:O	1:A:194:TRP:CG	2.69	0.45
1:K:121:MET:HE1	1:K:131:PHE:CE2	2.52	0.45
1:G:45:VAL:O	1:G:45:VAL:HG13	2.17	0.45
1:F:121:MET:HE1	1:F:131:PHE:CG	2.52	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
1:B:43:THR:C	1:B:45:VAL:H	2.24	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:45:VAL:C	2:C:302:HOH:O	2.60	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:B:131:PHE:O	1:B:132:HIS:C	2.59	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:45:VAL:O	1:L:45:VAL:HG12	2.18	0.44
1:L:39:ASN:OD1	1:L:41:LYS:HB3	2.17	0.44
1:F:121:MET:HE1	1:F:131:PHE:CZ	2.53	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:H:63:GLN:C	1:H:94:SER:HB2	2.43	0.44
1:I:19:ILE:HG22	1:I:21:PHE:CE1	2.53	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:D:74:GLU:O	1:D:75:LYS:C	2.60	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:I:121:MET:HE1	1:I:131:PHE:CD1	2.54	0.43
1:G:88:ARG:HD2	1:G:90:THR:C	2.44	0.43
1:K:81:TRP:CE3	1:K:91:ASP:HB3	2.54	0.43
1:H:81:TRP:NE1	1:H:88:ARG:HH21	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:17:LYS:HG2	1:I:54:GLN:HB2	2.01	0.42
1:K:121:MET:HE1	1:K:131:PHE:CG	2.54	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: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:D:63:GLN:C	1:D:94:SER:HB2	2.45	0.42
1:L:41:LYS:HG2	1:L:42:GLU:HG3	2.01	0.42
1:D:69:GLU:CD	1:D:89:ARG:HB2	2.44	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:87:SER:C	1:C:89:ARG:H	2.28	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:A:101:VAL:HB	1:D:192:MET:HE2	2.01	0.41
1:C:121:MET:HE1	1:C:131:PHE:CE2	2.54	0.41
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: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: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:I:47:LYS:HE2	1:I:91:ASP:CG	2.45	0.41
1:J:81:TRP:HA	1:J:84:TRP:CH2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:121:MET:HE1	1:G:131:PHE:CG	2.56	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
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:86:SER:C	1:B:88:ARG:N	2.79	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:B:74:GLU:O	1:B:75:LYS:C	2.64	0.40
1:F:35:GLY:O	1:F:36:PRO:C	2.65	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%)	11	39
1	B	185/205 (90%)	169 (91%)	10 (5%)	6 (3%)	3	16
1	C	184/205 (90%)	170 (92%)	11 (6%)	3 (2%)	7	30
1	D	183/205 (89%)	171 (93%)	12 (7%)	0	100	100
1	E	183/205 (89%)	171 (93%)	10 (6%)	2 (1%)	11	39
1	F	182/205 (89%)	167 (92%)	14 (8%)	1 (0%)	24	57
1	G	182/205 (89%)	169 (93%)	10 (6%)	3 (2%)	7	30
1	H	181/205 (88%)	170 (94%)	10 (6%)	1 (1%)	21	53
1	I	182/205 (89%)	174 (96%)	8 (4%)	0	100	100
1	J	185/205 (90%)	171 (92%)	12 (6%)	2 (1%)	11	39
1	K	184/205 (90%)	172 (94%)	11 (6%)	1 (0%)	24	57
1	L	182/205 (89%)	170 (93%)	10 (6%)	2 (1%)	11	39
All	All	2197/2460 (89%)	2047 (93%)	127 (6%)	23 (1%)	12	41

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

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Mol	Chain	Res	Type
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%)	155 (94%)	10 (6%)	17	46
1	B	166/179 (93%)	158 (95%)	8 (5%)	23	54
1	C	165/179 (92%)	150 (91%)	15 (9%)	9	31
1	D	164/179 (92%)	149 (91%)	15 (9%)	9	31
1	E	164/179 (92%)	151 (92%)	13 (8%)	11	36
1	F	163/179 (91%)	151 (93%)	12 (7%)	13	39
1	G	162/179 (90%)	149 (92%)	13 (8%)	11	36
1	H	161/179 (90%)	152 (94%)	9 (6%)	19	49
1	I	163/179 (91%)	150 (92%)	13 (8%)	11	36
1	J	166/179 (93%)	151 (91%)	15 (9%)	9	31
1	K	165/179 (92%)	152 (92%)	13 (8%)	11	36
1	L	163/179 (91%)	142 (87%)	21 (13%)	4	17
All	All	1967/2148 (92%)	1810 (92%)	157 (8%)	11	36

All (157) 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	47	LYS
1	I	62	GLU
1	I	67	LYS
1	I	71	PHE
1	I	95	SER
1	I	100	LYS

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Mol	Chain	Res	Type
1	I	101	VAL
1	I	103	SER
1	I	105	GLU
1	I	159	ARG
1	J	12	GLN
1	J	14	LEU
1	J	17	LYS
1	J	20	ILE
1	J	30	SER
1	J	45	VAL
1	J	71	PHE
1	J	88	ARG
1	J	89	ARG
1	J	92	SER
1	J	99	ILE
1	J	103	SER
1	J	166	GLU
1	J	192	MET
1	J	196	GLN
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	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	43	THR
1	L	45	VAL
1	L	46	GLU

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Mol	Chain	Res	Type
1	L	86	SER
1	L	87	SER
1	L	88	ARG
1	L	90	THR
1	L	95	SER
1	L	96	LEU
1	L	101	VAL
1	L	109	ILE
1	L	121	MET
1	L	124	ILE
1	L	192	MET
1	A	12	GLN
1	A	14	LEU
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	22	GLU
1	C	33	LEU
1	C	42	GLU
1	C	45	VAL
1	C	50	SER
1	C	86	SER
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	42	GLU

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Mol	Chain	Res	Type
1	D	45	VAL
1	D	87	SER
1	D	88	ARG
1	D	91	ASP
1	D	92	SER
1	D	95	SER
1	D	119	LYS
1	D	134	HIS
1	D	196	GLN
1	E	12	GLN
1	E	14	LEU
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	91	ASP
1	E	95	SER
1	E	120	LYS
1	E	180	HIS
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	171	LYS
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	100	LYS
1	F	105	GLU
1	F	115	ASN
1	F	134	HIS
1	F	159	ARG
1	F	166	GLU
1	F	194	TRP

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Mol	Chain	Res	Type
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	69	GLU
1	G	71	PHE
1	G	88	ARG
1	G	89	ARG
1	G	100	LYS
1	G	166	GLU
1	H	14	LEU
1	H	17	LYS
1	H	33	LEU
1	H	42	GLU
1	H	71	PHE
1	H	88	ARG
1	H	134	HIS
1	H	166	GLU
1	H	192	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	15	ASN
1	I	34	ASN
1	I	113	ASN
1	I	195	HIS
1	J	12	GLN
1	J	15	ASN
1	J	154	GLN
1	J	195	HIS
1	K	15	ASN
1	K	23	GLN
1	K	195	HIS
1	L	29	HIS
1	L	34	ASN
1	L	134	HIS
1	L	180	HIS
1	L	184	GLN

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Mol	Chain	Res	Type
1	L	195	HIS
1	A	23	GLN
1	C	34	ASN
1	C	65	ASN
1	C	154	GLN
1	C	162	GLN
1	D	25	ASN
1	E	25	ASN
1	E	184	GLN
1	B	31	HIS
1	B	34	ASN
1	B	65	ASN
1	B	104	GLN
1	B	115	ASN
1	B	162	GLN
1	F	15	ASN
1	F	25	ASN
1	F	31	HIS
1	G	34	ASN
1	G	65	ASN
1	G	104	GLN
1	H	34	ASN
1	H	70	GLN
1	H	113	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	186/205 (90%)	-0.60	0 100 100	33, 61, 127, 146	0
1	B	187/205 (91%)	-0.57	1 (0%) 87 72	44, 73, 125, 161	0
1	C	186/205 (90%)	-0.53	1 (0%) 87 72	39, 61, 111, 154	0
1	D	185/205 (90%)	-0.54	2 (1%) 78 56	42, 62, 114, 189	0
1	E	185/205 (90%)	-0.50	1 (0%) 87 72	38, 65, 120, 172	0
1	F	184/205 (89%)	-0.50	0 100 100	50, 74, 116, 182	0
1	G	184/205 (89%)	-0.46	2 (1%) 78 56	41, 72, 119, 192	0
1	H	183/205 (89%)	-0.49	2 (1%) 78 56	39, 69, 127, 180	0
1	I	184/205 (89%)	-0.52	0 100 100	36, 67, 124, 163	0
1	J	187/205 (91%)	-0.42	1 (0%) 87 72	42, 67, 128, 231	0
1	K	186/205 (90%)	-0.58	0 100 100	43, 67, 119, 166	0
1	L	184/205 (89%)	-0.61	0 100 100	42, 63, 122, 182	0
All	All	2221/2460 (90%)	-0.53	10 (0%) 87 72	33, 67, 124, 231	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	195	HIS	4.9
1	J	90	THR	3.0
1	E	11	PRO	3.0
1	B	46	GLU	2.6
1	H	195	HIS	2.5
1	D	196	GLN	2.5
1	H	20	ILE	2.4
1	G	87	SER	2.1
1	C	91	ASP	2.1
1	D	90	THR	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.