



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:27 AM UTC

PDB ID : 3E2J / pdb_00003e2j
Title : Crystal structure of bovine coupling factor B
Authors : Stroud, R.M.; Lee, J.K.; Belogradov, G.I.
Deposited on : 2008-08-05
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

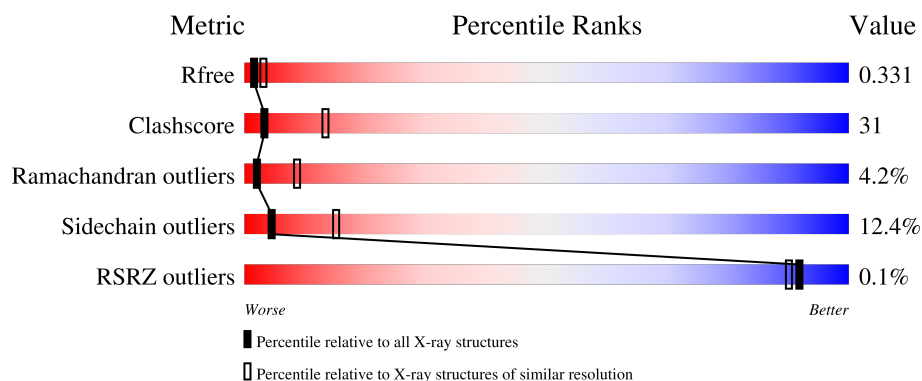
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	176	 48% 40% 11% ..
1	B	176	 57% 36% 5% ..
1	C	176	 36% 54% 9% ..
1	D	176	 38% 47% 13% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5623 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 ATP synthase subunit s, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	1	0
			1410	901	243	255	11			
1	B	175	Total	C	N	O	S	0	0	0
			1404	895	242	256	11			
1	C	175	Total	C	N	O	S	0	0	0
			1386	884	236	255	11			
1	D	175	Total	C	N	O	S	0	0	0
			1394	890	238	255	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P22027
B	0	SER	-	expression tag	UNP P22027
C	0	SER	-	expression tag	UNP P22027
D	0	SER	-	expression tag	UNP P22027

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

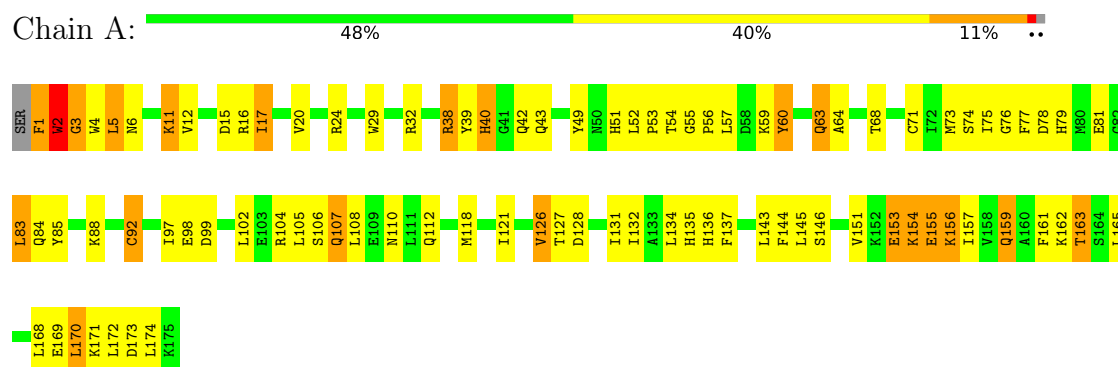
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total 10	O 10	0	0
3	B	10	Total 10	O 10	0	0
3	C	3	Total 3	O 3	0	0
3	D	2	Total 2	O 2	0	0

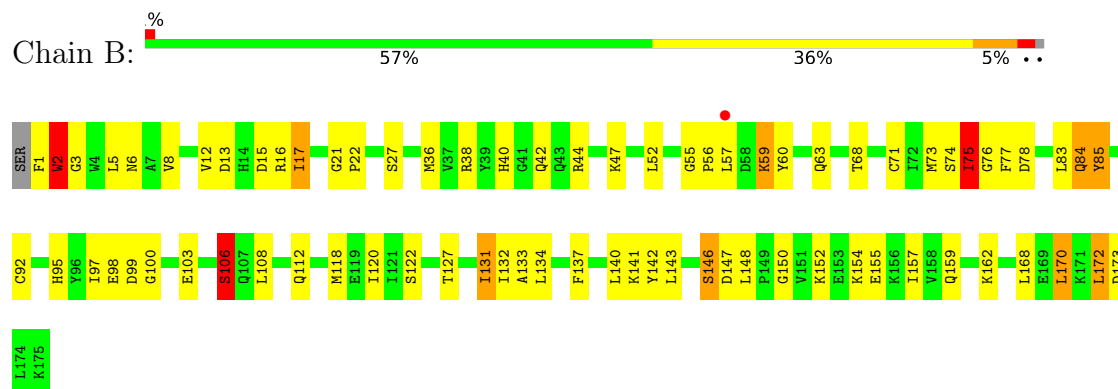
3 Residue-property plots

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.

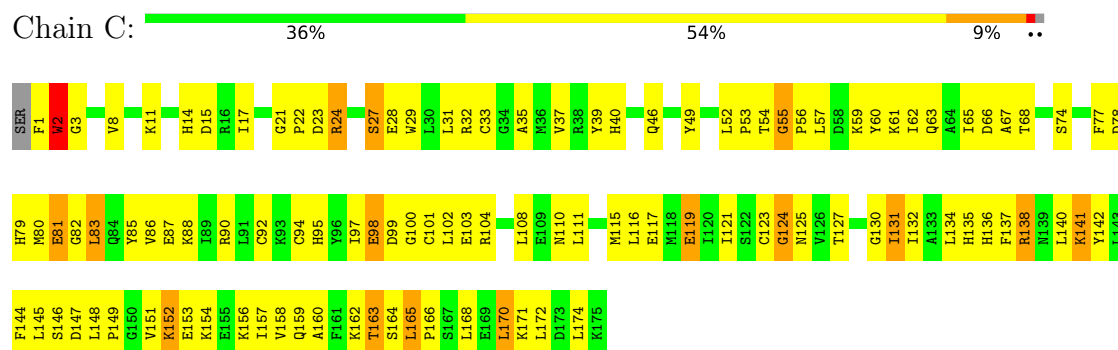
- Molecule 1: ATP synthase subunit s, mitochondrial



- Molecule 1: ATP synthase subunit s, mitochondrial



- Molecule 1: ATP synthase subunit s, mitochondrial



- Chain D:  38% 47% 13% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.56Å 133.94Å 115.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.9 (30.00-2.90) 95.8 (30.00-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.329 0.234 , 0.331	Depositor DCC
R_{free} test set	842 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5623	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.03	0/1444	1.16	7/1948 (0.4%)
1	B	1.01	0/1435	1.20	11/1938 (0.6%)
1	C	0.99	2/1417 (0.1%)	1.18	6/1918 (0.3%)
1	D	1.02	1/1425 (0.1%)	1.26	15/1926 (0.8%)
All	All	1.01	3/5721 (0.1%)	1.20	39/7730 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	35	ALA	CA-CB	-6.11	1.43	1.53
1	D	126	VAL	CA-CB	-6.10	1.48	1.54
1	C	8	VAL	CA-CB	-5.67	1.48	1.54

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	TYR	N-CA-C	7.25	120.23	108.63
1	A	43	GLN	N-CA-C	-6.67	105.15	113.55
1	A	165	LEU	CA-C-N	6.57	126.01	118.85
1	A	165	LEU	C-N-CA	6.57	126.01	118.85
1	D	165	LEU	CA-C-N	6.53	126.30	119.05
1	D	165	LEU	C-N-CA	6.53	126.30	119.05
1	D	98	GLU	N-CA-C	6.46	116.38	107.73
1	D	132	ILE	CB-CA-C	-6.21	103.65	112.22
1	C	95	HIS	N-CA-C	6.19	118.03	111.28
1	C	115	MET	N-CA-C	6.09	118.58	109.25
1	B	8	VAL	CB-CA-C	-6.03	104.16	111.88
1	D	25	ALA	N-CA-C	-5.91	104.53	110.97
1	C	165	LEU	CA-C-N	5.88	125.35	119.24
1	C	165	LEU	C-N-CA	5.88	125.35	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	151	VAL	CB-CA-C	-5.83	104.94	111.23
1	D	115	MET	N-CA-C	5.79	118.72	110.10
1	B	100	GLY	N-CA-C	-5.78	105.50	112.49
1	D	97	ILE	CB-CA-C	-5.74	102.78	111.33
1	B	21	GLY	CA-C-N	5.74	125.21	119.24
1	B	21	GLY	C-N-CA	5.74	125.21	119.24
1	D	64	ALA	N-CA-C	5.69	118.73	109.06
1	B	27	SER	N-CA-C	-5.67	105.24	111.82
1	B	85	TYR	N-CA-C	5.65	119.49	112.59
1	B	52	LEU	CA-C-N	5.58	125.59	119.90
1	B	52	LEU	C-N-CA	5.58	125.59	119.90
1	B	95	HIS	N-CA-C	5.37	117.82	111.33
1	C	65	ILE	CB-CA-C	-5.30	103.24	110.77
1	A	107	GLN	N-CA-C	-5.26	104.87	113.19
1	D	170	LEU	N-CA-C	5.24	116.55	109.11
1	D	55	GLY	CA-C-N	5.22	126.36	119.84
1	D	55	GLY	C-N-CA	5.22	126.36	119.84
1	A	40	HIS	N-CA-C	-5.20	102.60	110.24
1	C	60	TYR	N-CA-C	5.19	117.75	109.96
1	B	142	TYR	N-CA-C	5.19	116.83	108.32
1	D	60	TYR	N-CA-C	5.15	117.69	109.96
1	A	169	GLU	N-CA-C	-5.11	102.30	109.96
1	D	39	TYR	N-CA-C	5.11	117.06	109.25
1	D	114	SER	N-CA-C	5.10	117.58	111.71
1	B	84	GLN	N-CA-C	5.03	116.57	111.14

There are no chirality outliers.

There are no planarity outliers.

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	1410	0	1394	84	0
1	B	1404	0	1375	68	0
1	C	1386	0	1337	102	0
1	D	1394	0	1359	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
All	All	5623	0	5465	338	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 31.

All (338) 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:B:55:GLY:O	1:B:57:LEU:HD12	1.42	1.19
1:A:2:TRP:N	1:A:2:TRP:HE3	1.51	1.07
1:D:170:LEU:HG	1:D:170:LEU:O	1.59	1.02
1:C:146:SER:O	1:C:148:LEU:HG	1.61	0.99
1:D:1:PHE:O	1:D:3:GLY:N	1.95	0.98
1:A:170:LEU:O	1:A:170:LEU:HG	1.64	0.95
1:C:2:TRP:HE3	1:C:2:TRP:N	1.67	0.93
1:A:38:ARG:HG2	1:A:38:ARG:HH11	1.33	0.92
1:B:132:ILE:HD11	1:B:157:ILE:HG12	1.52	0.91
1:B:2:TRP:HE3	1:B:2:TRP:N	1.68	0.91
1:C:2:TRP:HE3	1:C:2:TRP:H	1.18	0.91
1:B:2:TRP:N	1:B:2:TRP:CE3	2.38	0.89
1:A:73:MET:HE1	1:B:73:MET:HE1	1.56	0.88
1:B:1:PHE:O	1:B:3:GLY:N	2.07	0.86
1:A:55:GLY:O	1:A:57:LEU:HD12	1.73	0.86
1:A:2:TRP:N	1:A:2:TRP:CE3	2.31	0.85
1:C:1:PHE:CG	1:C:1:PHE:O	2.30	0.85
1:D:5:LEU:H	1:D:5:LEU:HD22	1.42	0.84
1:B:2:TRP:HE3	1:B:2:TRP:H	0.85	0.83
1:C:2:TRP:N	1:C:2:TRP:CE3	2.47	0.82
1:B:1:PHE:O	1:B:1:PHE:CG	2.32	0.82
1:C:28:GLU:O	1:C:32:ARG:HG2	1.80	0.81
1:D:40:HIS:HE1	1:D:87:GLU:OE2	1.65	0.80
1:A:132:ILE:HD11	1:A:157:ILE:HG12	1.64	0.80
1:D:55:GLY:O	1:D:57:LEU:HD12	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:HIS:HE1	1:C:87:GLU:OE2	1.65	0.79
1:C:55:GLY:O	1:C:57:LEU:HD12	1.82	0.78
1:A:1:PHE:CG	1:A:1:PHE:O	2.37	0.77
1:C:170:LEU:O	1:C:170:LEU:HG	1.84	0.76
1:C:77:PHE:CB	1:C:104:ARG:HD2	2.16	0.75
1:A:159:GLN:HE22	1:A:162:LYS:HE3	1.50	0.75
1:A:73:MET:CE	1:B:73:MET:HE1	2.18	0.74
1:B:59:LYS:HD3	1:B:60:TYR:CE1	2.23	0.74
1:A:2:TRP:HE3	1:A:2:TRP:H	0.79	0.73
1:A:154:LYS:HG2	1:A:155:GLU:H	1.51	0.73
1:D:40:HIS:CE1	1:D:87:GLU:OE2	2.40	0.73
1:D:141:LYS:O	1:D:168:LEU:HD12	1.88	0.73
1:A:170:LEU:O	1:A:170:LEU:CG	2.37	0.73
1:A:99:ASP:OD2	1:A:127:THR:OG1	2.06	0.72
1:A:146:SER:HB2	1:A:173:ASP:HB3	1.72	0.72
1:A:73:MET:HE1	1:B:73:MET:CE	2.18	0.72
1:A:154:LYS:HG2	1:A:155:GLU:N	2.06	0.71
1:A:40:HIS:CE1	1:A:63:GLN:HB2	2.26	0.70
1:D:68:THR:O	1:D:69:ASP:HB2	1.92	0.70
1:B:36:MET:HG2	1:B:47:LYS:HA	1.74	0.70
1:D:5:LEU:H	1:D:5:LEU:CD2	2.04	0.69
1:D:77:PHE:CE1	1:D:101:CYS:HB3	2.28	0.69
1:A:1:PHE:CE1	1:B:71:CYS:SG	2.84	0.69
1:B:146:SER:HB2	1:B:173:ASP:HB3	1.75	0.69
1:D:143:LEU:HD11	1:D:145:LEU:HD21	1.76	0.68
1:C:77:PHE:HB2	1:C:104:ARG:HD2	1.75	0.68
1:D:61:LYS:HG3	1:D:85:TYR:CE2	2.29	0.68
1:C:1:PHE:O	1:C:3:GLY:N	2.25	0.68
1:B:108:LEU:O	1:B:112:GLN:HG3	1.95	0.67
1:B:132:ILE:CD1	1:B:157:ILE:HG12	2.24	0.67
1:D:31:LEU:O	1:D:34:GLY:N	2.25	0.67
1:D:99:ASP:O	1:D:103:GLU:HG2	1.95	0.67
1:B:74:SER:C	1:B:76:GLY:H	2.02	0.67
1:A:24:ARG:HH12	1:A:52:LEU:HB3	1.60	0.66
1:A:71:CYS:SG	1:B:1:PHE:CE1	2.84	0.66
1:D:77:PHE:HE1	1:D:101:CYS:HB3	1.58	0.66
1:A:154:LYS:CG	1:A:155:GLU:N	2.59	0.66
1:B:154:LYS:O	1:B:157:ILE:N	2.30	0.65
1:D:83:LEU:O	1:D:110:ASN:ND2	2.23	0.65
1:A:71:CYS:SG	1:B:1:PHE:CD1	2.89	0.65
1:D:67:ALA:O	1:D:94:CYS:SG	2.55	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HG2	1:A:38:ARG:NH1	2.08	0.64
1:A:63:GLN:HG3	1:A:64:ALA:N	2.11	0.64
1:D:38:ARG:HD2	1:D:42:GLN:O	1.97	0.63
1:D:5:LEU:HD22	1:D:5:LEU:N	2.14	0.63
1:A:52:LEU:O	1:A:54:THR:HG23	2.00	0.62
1:D:39:TYR:HD1	1:D:61:LYS:O	1.82	0.62
1:D:59:LYS:HD2	1:D:60:TYR:CE2	2.34	0.62
1:B:74:SER:C	1:B:76:GLY:N	2.56	0.62
1:C:87:GLU:HG2	1:C:116:LEU:HD12	1.82	0.62
1:D:158:VAL:O	1:D:162:LYS:HB2	2.00	0.62
1:D:31:LEU:N	1:D:31:LEU:HD12	2.15	0.61
1:C:108:LEU:HD12	1:C:111:LEU:HD12	1.83	0.61
1:D:146:SER:HB2	1:D:173:ASP:HB3	1.82	0.61
1:C:22:PRO:HB2	1:C:83:LEU:HD23	1.83	0.61
1:D:141:LYS:C	1:D:168:LEU:HD12	2.26	0.61
1:C:135:HIS:O	1:C:137:PHE:N	2.35	0.60
1:B:74:SER:O	1:B:76:GLY:N	2.34	0.60
1:D:63:GLN:NE2	1:D:87:GLU:OE1	2.35	0.60
1:A:73:MET:CE	1:B:73:MET:CE	2.78	0.60
1:C:66:ASP:CG	1:C:90:ARG:HD3	2.27	0.60
1:D:68:THR:HA	1:D:92:CYS:O	2.03	0.59
1:D:12:VAL:HG21	1:D:78:ASP:HB2	1.82	0.59
1:D:123:CYS:O	1:D:125:ASN:N	2.35	0.59
1:A:132:ILE:CD1	1:A:157:ILE:HG12	2.32	0.59
1:C:31:LEU:HD23	1:C:49:TYR:HA	1.85	0.59
1:B:55:GLY:O	1:B:57:LEU:CD1	2.35	0.59
1:B:155:GLU:CD	1:B:155:GLU:H	2.11	0.58
1:D:38:ARG:N	1:D:64:ALA:O	2.35	0.58
1:D:46:GLN:HA	1:D:46:GLN:OE1	2.04	0.58
1:D:103:GLU:O	1:D:104:ARG:C	2.45	0.58
1:D:4:TRP:O	1:D:5:LEU:C	2.47	0.58
1:B:99:ASP:OD2	1:B:127:THR:OG1	2.20	0.57
1:C:22:PRO:HB2	1:C:83:LEU:CD2	2.34	0.57
1:A:84:GLN:HB2	1:A:85:TYR:CE2	2.39	0.57
1:C:99:ASP:O	1:C:103:GLU:HG2	2.05	0.57
1:C:55:GLY:O	1:C:57:LEU:CD1	2.50	0.57
1:B:1:PHE:C	1:B:3:GLY:N	2.62	0.57
1:A:83:LEU:O	1:A:110:ASN:ND2	2.28	0.57
1:B:106:SER:HB2	1:B:133:ALA:O	2.05	0.57
1:C:80:MET:O	1:C:81:GLU:C	2.47	0.57
1:C:40:HIS:ND1	1:C:63:GLN:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:HE2	1:A:12:VAL:O	2.05	0.56
1:A:42:GLN:HE22	1:A:60:TYR:HE1	1.54	0.56
1:C:123:CYS:O	1:C:124:GLY:C	2.48	0.56
1:C:83:LEU:O	1:C:110:ASN:ND2	2.33	0.56
1:A:154:LYS:O	1:A:157:ILE:N	2.30	0.56
1:C:77:PHE:HB3	1:C:104:ARG:HD2	1.88	0.56
1:A:154:LYS:O	1:A:155:GLU:C	2.48	0.56
1:C:40:HIS:CE1	1:C:63:GLN:HB2	2.41	0.56
1:C:66:ASP:OD1	1:C:90:ARG:HD3	2.05	0.56
1:C:132:ILE:CD1	1:C:157:ILE:HG12	2.36	0.56
1:D:135:HIS:NE2	1:D:136:HIS:CE1	2.74	0.55
1:C:170:LEU:O	1:C:170:LEU:CG	2.52	0.55
1:C:1:PHE:O	1:C:1:PHE:CD2	2.58	0.55
1:B:68:THR:HA	1:B:92:CYS:O	2.07	0.55
1:D:40:HIS:CD2	1:D:63:GLN:HB2	2.41	0.55
1:C:77:PHE:CE1	1:C:101:CYS:HB3	2.42	0.54
1:C:80:MET:O	1:C:82:GLY:N	2.40	0.54
1:D:39:TYR:HE2	1:D:46:GLN:HE21	1.56	0.54
1:B:16:ARG:O	1:B:17:ILE:C	2.47	0.54
1:A:84:GLN:HB2	1:A:85:TYR:CD2	2.43	0.54
1:A:1:PHE:CD1	1:B:71:CYS:SG	3.01	0.54
1:A:40:HIS:NE2	1:A:85:TYR:HB3	2.23	0.54
1:B:84:GLN:HB2	1:B:85:TYR:CD2	2.43	0.54
1:D:39:TYR:O	1:D:40:HIS:C	2.51	0.54
1:C:132:ILE:HD11	1:C:157:ILE:HG12	1.89	0.53
1:A:135:HIS:NE2	1:A:136:HIS:CE1	2.77	0.53
1:C:29:TRP:CD1	1:C:33:CYS:HG	2.26	0.53
1:A:143:LEU:HD11	1:A:145:LEU:HD21	1.90	0.53
1:C:88:LYS:HA	1:C:117:GLU:O	2.09	0.53
1:A:154:LYS:O	1:A:156:LYS:N	2.41	0.53
1:B:22:PRO:HB2	1:B:83:LEU:HD23	1.90	0.53
1:C:98:GLU:O	1:C:99:ASP:C	2.50	0.53
1:C:144:PHE:O	1:C:145:LEU:HD23	2.09	0.53
1:A:12:VAL:HG21	1:A:78:ASP:HB2	1.90	0.53
1:A:146:SER:CB	1:A:173:ASP:HB3	2.38	0.53
1:B:5:LEU:N	1:B:5:LEU:HD22	2.23	0.53
1:C:146:SER:O	1:C:147:ASP:C	2.50	0.53
1:B:74:SER:HA	1:B:77:PHE:CD2	2.44	0.53
1:C:92:CYS:HA	1:C:121:ILE:O	2.09	0.53
1:D:36:MET:HG2	1:D:47:LYS:HA	1.90	0.53
1:D:68:THR:HG23	1:D:92:CYS:SG	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PHE:HD1	1:A:171:LYS:HB3	1.75	0.52
1:D:40:HIS:HE2	1:D:85:TYR:HB2	1.75	0.52
1:A:159:GLN:NE2	1:A:162:LYS:HE3	2.23	0.52
1:D:62:ILE:HG22	1:D:86:VAL:HG22	1.92	0.52
1:C:144:PHE:CE1	1:C:146:SER:HB2	2.44	0.52
1:C:159:GLN:O	1:C:160:ALA:C	2.52	0.52
1:B:40:HIS:CE1	1:B:63:GLN:HB2	2.44	0.52
1:D:22:PRO:O	1:D:23:ASP:C	2.53	0.52
1:B:5:LEU:HD22	1:B:5:LEU:H	1.73	0.51
1:C:162:LYS:O	1:C:166:PRO:HA	2.10	0.51
1:A:1:PHE:CD2	1:A:1:PHE:C	2.87	0.51
1:B:15:ASP:OD2	1:C:14:HIS:HB2	2.11	0.51
1:C:66:ASP:OD1	1:C:66:ASP:C	2.53	0.51
1:A:78:ASP:OD2	1:A:104[B]:ARG:NH1	2.43	0.51
1:C:1:PHE:C	1:C:3:GLY:N	2.69	0.51
1:A:64:ALA:CB	1:A:88:LYS:HB2	2.41	0.51
1:A:32:ARG:HB3	1:A:49:TYR:CE1	2.46	0.50
1:A:153:GLU:HB2	1:A:156:LYS:CG	2.40	0.50
1:C:141:LYS:C	1:C:168:LEU:HD12	2.36	0.50
1:B:132:ILE:C	1:B:134:LEU:H	2.18	0.50
1:D:135:HIS:CD2	1:D:135:HIS:C	2.89	0.50
1:D:135:HIS:C	1:D:137:PHE:H	2.19	0.50
1:A:97:ILE:O	3:A:303:HOH:O	2.20	0.50
1:B:1:PHE:C	1:B:3:GLY:H	2.17	0.50
1:C:123:CYS:H	1:C:148:LEU:CD2	2.25	0.50
1:A:102:LEU:HD11	1:A:126:VAL:HG11	1.93	0.50
1:B:12:VAL:HG21	1:B:78:ASP:HB2	1.93	0.50
1:C:102:LEU:O	1:C:103:GLU:C	2.54	0.50
1:D:122:SER:HA	1:D:147:ASP:O	2.11	0.50
1:B:1:PHE:O	1:B:2:TRP:C	2.54	0.50
1:D:131:ILE:O	1:D:134:LEU:HB2	2.12	0.50
1:D:131:ILE:HG21	1:D:157:ILE:HD13	1.94	0.49
1:D:128:ASP:O	1:D:132:ILE:HG12	2.12	0.49
1:C:131:ILE:O	1:C:132:ILE:C	2.55	0.49
1:D:62:ILE:HG22	1:D:86:VAL:CG2	2.42	0.49
1:B:40:HIS:NE2	1:B:85:TYR:HB3	2.27	0.49
1:D:62:ILE:O	1:D:85:TYR:O	2.31	0.49
1:C:67:ALA:O	1:C:94:CYS:SG	2.71	0.48
1:D:40:HIS:NE2	1:D:85:TYR:HB2	2.28	0.48
1:C:46:GLN:OE1	1:C:46:GLN:HA	2.13	0.48
1:B:1:PHE:O	1:B:1:PHE:CD2	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:PHE:O	1:B:1:PHE:CD1	2.66	0.48
1:C:77:PHE:C	1:C:79:HIS:N	2.68	0.48
1:A:173:ASP:C	1:A:174:LEU:HD23	2.39	0.48
1:D:119:GLU:C	1:D:120:ILE:HG13	2.38	0.48
1:A:153:GLU:HB2	1:A:156:LYS:HG3	1.94	0.48
1:C:74:SER:HB3	1:C:101:CYS:SG	2.54	0.48
1:B:127:THR:HA	1:B:150:GLY:O	2.13	0.48
1:D:13:ASP:O	1:D:16:ARG:HB3	2.14	0.48
1:B:152:LYS:HD3	1:B:152:LYS:HA	1.68	0.48
1:B:170:LEU:HG	1:B:170:LEU:O	2.14	0.48
1:A:1:PHE:O	1:A:3:GLY:N	2.47	0.48
1:C:74:SER:O	1:C:104:ARG:NH1	2.47	0.48
1:C:132:ILE:C	1:C:134:LEU:H	2.22	0.48
1:B:73:MET:HG3	1:B:75:ILE:HG12	1.96	0.47
1:C:156:LYS:O	1:C:159:GLN:HB2	2.14	0.47
1:C:163:THR:OG1	1:C:164:SER:N	2.47	0.47
1:D:77:PHE:CE1	1:D:105:LEU:HD11	2.49	0.47
1:B:84:GLN:HB2	1:B:85:TYR:CE2	2.49	0.47
1:A:132:ILE:C	1:A:134:LEU:H	2.22	0.47
1:D:89:ILE:O	1:D:118:MET:HA	2.15	0.47
1:A:128:ASP:OD1	1:A:151:VAL:HA	2.14	0.47
1:B:112:GLN:HA	1:B:137:PHE:HD1	1.79	0.47
1:C:52:LEU:CD2	1:C:53:PRO:HD2	2.44	0.47
1:C:74:SER:O	1:C:104:ARG:CZ	2.62	0.47
1:C:144:PHE:C	1:C:145:LEU:HD23	2.40	0.47
1:C:77:PHE:HB2	1:C:104:ARG:CD	2.43	0.47
1:D:98:GLU:O	1:D:99:ASP:C	2.58	0.47
1:D:143:LEU:HD11	1:D:145:LEU:CD2	2.43	0.47
1:A:105:LEU:C	1:A:107:GLN:H	2.22	0.47
1:C:141:LYS:O	1:C:168:LEU:HD12	2.15	0.47
1:D:31:LEU:N	1:D:31:LEU:CD1	2.78	0.47
1:B:13:ASP:C	1:B:13:ASP:OD2	2.58	0.47
1:C:61:LYS:HB3	1:C:85:TYR:HD2	1.79	0.47
1:C:132:ILE:C	1:C:134:LEU:N	2.72	0.47
1:C:135:HIS:C	1:C:137:PHE:N	2.72	0.47
1:C:135:HIS:C	1:C:137:PHE:H	2.23	0.47
1:A:118:MET:O	1:A:143:LEU:HA	2.15	0.46
1:B:131:ILE:HG21	1:B:157:ILE:HD13	1.96	0.46
1:A:112:GLN:HA	1:A:137:PHE:HD1	1.81	0.46
1:B:42:GLN:OE1	1:B:44:ARG:NH2	2.49	0.46
1:B:15:ASP:O	1:B:16:ARG:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:SER:HA	1:B:147:ASP:O	2.16	0.46
1:C:24:ARG:HH12	1:C:54:THR:HG22	1.80	0.46
1:C:68:THR:HA	1:C:92:CYS:O	2.15	0.46
1:D:148:LEU:HD23	1:D:148:LEU:HA	1.64	0.46
1:C:52:LEU:HD23	1:C:53:PRO:HD2	1.98	0.46
1:D:101:CYS:O	1:D:105:LEU:HD12	2.16	0.46
1:C:39:TYR:HE1	1:C:62:ILE:HG13	1.81	0.45
1:D:84:GLN:HB2	1:D:85:TYR:CE2	2.52	0.45
1:A:20:VAL:CG2	1:A:24:ARG:HG2	2.46	0.45
1:B:132:ILE:C	1:B:134:LEU:N	2.72	0.45
1:D:40:HIS:HA	1:D:63:GLN:OE1	2.16	0.45
1:C:87:GLU:HG2	1:C:116:LEU:CD1	2.46	0.45
1:C:171:LYS:O	1:C:172:LEU:HD23	2.17	0.45
1:D:159:GLN:O	1:D:162:LYS:HB3	2.17	0.45
1:B:42:GLN:OE1	1:B:44:ARG:CZ	2.65	0.45
1:A:39:TYR:O	1:A:40:HIS:C	2.58	0.45
1:A:132:ILE:C	1:A:134:LEU:N	2.73	0.45
1:C:23:ASP:O	1:C:27:SER:OG	2.35	0.45
1:C:149:PRO:C	1:C:151:VAL:H	2.25	0.45
1:D:74:SER:O	1:D:76:GLY:N	2.50	0.45
1:B:1:PHE:C	1:B:1:PHE:CD2	2.89	0.45
1:B:118:MET:HE2	1:B:120:ILE:HD11	1.98	0.45
1:A:68:THR:HA	1:A:92:CYS:O	2.16	0.44
1:C:55:GLY:O	1:C:57:LEU:N	2.51	0.44
1:C:100:GLY:O	1:C:103:GLU:HB2	2.17	0.44
1:D:66:ASP:CG	1:D:90:ARG:HD3	2.42	0.44
1:D:99:ASP:OD2	1:D:127:THR:OG1	2.31	0.44
1:C:17:ILE:O	1:C:21:GLY:N	2.50	0.44
1:A:74:SER:C	1:A:76:GLY:N	2.75	0.44
1:A:20:VAL:HG21	1:A:24:ARG:HG2	2.00	0.44
1:C:138:ARG:HA	1:C:165:LEU:HD21	2.00	0.44
1:C:144:PHE:C	1:C:144:PHE:CD1	2.96	0.44
1:D:31:LEU:HD23	1:D:48:ASP:C	2.43	0.44
1:A:77:PHE:HB2	1:A:104[A]:ARG:HD2	1.98	0.44
1:B:154:LYS:O	1:B:155:GLU:C	2.60	0.44
1:A:1:PHE:O	1:A:2:TRP:C	2.61	0.44
1:B:155:GLU:OE2	1:B:155:GLU:N	2.41	0.44
1:C:63:GLN:NE2	1:C:87:GLU:OE1	2.50	0.44
1:D:154:LYS:O	1:D:158:VAL:HG23	2.17	0.44
1:C:103:GLU:HG2	1:C:103:GLU:H	1.71	0.43
1:D:74:SER:C	1:D:76:GLY:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD21	1:A:172:LEU:HD21	1.99	0.43
1:C:144:PHE:HA	1:C:171:LYS:O	2.17	0.43
1:D:162:LYS:O	1:D:166:PRO:HA	2.18	0.43
1:A:92:CYS:HB2	1:A:121:ILE:HB	2.00	0.43
1:B:38:ARG:HH11	1:B:38:ARG:HG2	1.82	0.43
1:D:30:LEU:O	1:D:31:LEU:C	2.60	0.43
1:D:31:LEU:HD12	1:D:31:LEU:H	1.82	0.43
1:B:170:LEU:HD21	1:B:172:LEU:HD21	2.01	0.43
1:A:108:LEU:O	1:A:112:GLN:HG3	2.19	0.43
1:C:1:PHE:C	1:C:3:GLY:H	2.27	0.42
1:C:62:ILE:HG22	1:C:86:VAL:HG22	2.01	0.42
1:D:86:VAL:HG12	1:D:115:MET:SD	2.59	0.42
1:D:93:LYS:HB2	1:D:93:LYS:HE3	1.82	0.42
1:D:154:LYS:O	1:D:157:ILE:HB	2.19	0.42
1:B:140:LEU:HD23	1:B:168:LEU:CD1	2.50	0.42
1:A:15:ASP:OD2	1:D:14:HIS:HB2	2.19	0.42
1:D:31:LEU:CD1	1:D:31:LEU:H	2.31	0.42
1:D:38:ARG:HG2	1:D:38:ARG:HH11	1.84	0.42
1:D:135:HIS:C	1:D:137:PHE:N	2.77	0.42
1:A:74:SER:C	1:A:76:GLY:H	2.27	0.42
1:D:126:VAL:CG1	1:D:127:THR:N	2.79	0.42
1:D:128:ASP:OD1	1:D:152:LYS:N	2.46	0.42
1:A:1:PHE:O	1:A:1:PHE:CD1	2.71	0.42
1:A:159:GLN:O	1:A:163:THR:HG23	2.20	0.42
1:A:4:TRP:O	1:A:5:LEU:C	2.63	0.42
1:D:13:ASP:CG	1:D:16:ARG:HB2	2.45	0.42
1:D:103:GLU:HG2	1:D:103:GLU:H	1.62	0.42
1:A:131:ILE:O	1:A:132:ILE:C	2.58	0.42
1:A:1:PHE:O	1:A:1:PHE:CD2	2.73	0.41
1:B:74:SER:O	1:B:75:ILE:C	2.61	0.41
1:C:1:PHE:CD2	1:C:1:PHE:C	2.93	0.41
1:C:148:LEU:O	1:C:149:PRO:C	2.63	0.41
1:D:144:PHE:O	1:D:145:LEU:HD23	2.20	0.41
1:B:118:MET:O	1:B:143:LEU:HA	2.19	0.41
1:C:37:VAL:HG22	1:C:46:GLN:HB2	2.01	0.41
1:C:154:LYS:O	1:C:157:ILE:N	2.53	0.41
1:A:29:TRP:HB2	1:A:79:HIS:CE1	2.54	0.41
1:C:142:TYR:CD2	1:C:142:TYR:C	2.98	0.41
1:D:4:TRP:O	1:D:7:ALA:N	2.48	0.41
1:C:1:PHE:O	1:C:1:PHE:CD1	2.71	0.41
1:C:144:PHE:CD1	1:C:145:LEU:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LYS:HB3	1:C:153:GLU:OE1	2.20	0.41
1:D:132:ILE:C	1:D:134:LEU:H	2.28	0.41
1:D:13:ASP:OD2	1:D:13:ASP:C	2.64	0.41
1:A:73:MET:HG3	1:A:75:ILE:HG12	2.03	0.41
1:C:149:PRO:C	1:C:151:VAL:N	2.78	0.41
1:D:61:LYS:HG3	1:D:85:TYR:CD2	2.56	0.41
1:D:142:TYR:HA	1:D:169:GLU:O	2.20	0.41
1:C:77:PHE:C	1:C:79:HIS:H	2.28	0.41
1:C:99:ASP:OD1	1:C:130:GLY:HA3	2.20	0.41
1:C:131:ILE:HG21	1:C:157:ILE:HD13	2.02	0.41
1:D:5:LEU:CD2	1:D:5:LEU:N	2.75	0.41
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.75	0.41
1:C:77:PHE:O	1:C:78:ASP:C	2.62	0.41
1:C:90:ARG:NH1	1:C:119:GLU:CD	2.79	0.41
1:D:39:TYR:CD1	1:D:61:LYS:O	2.67	0.41
1:C:116:LEU:C	1:C:140:LEU:HD12	2.46	0.41
1:D:1:PHE:O	1:D:2:TRP:C	2.62	0.41
1:D:22:PRO:O	1:D:26:ALA:N	2.45	0.41
1:A:24:ARG:NH2	1:A:54:THR:HG22	2.36	0.41
1:A:155:GLU:H	1:A:155:GLU:CD	2.30	0.40
1:C:149:PRO:O	1:C:151:VAL:N	2.54	0.40
1:D:121:ILE:O	1:D:122:SER:HB2	2.22	0.40
1:A:16:ARG:O	1:A:17:ILE:C	2.61	0.40
1:A:161:PHE:O	1:A:162:LYS:C	2.65	0.40
1:C:29:TRP:CE3	1:C:79:HIS:CB	3.04	0.40
1:A:52:LEU:HA	1:A:53:PRO:HD2	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	174/176 (99%)	146 (84%)	21 (12%)	7 (4%)	2	9
1	B	173/176 (98%)	154 (89%)	13 (8%)	6 (4%)	3	12
1	C	173/176 (98%)	137 (79%)	29 (17%)	7 (4%)	2	9
1	D	173/176 (98%)	135 (78%)	29 (17%)	9 (5%)	1	5
All	All	693/704 (98%)	572 (82%)	92 (13%)	29 (4%)	2	9

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	B	2	TRP
1	B	131	ILE
1	C	2	TRP
1	C	56	PRO
1	D	2	TRP
1	D	56	PRO
1	A	154	LYS
1	A	155	GLU
1	B	75	ILE
1	B	106	SER
1	C	81	GLU
1	C	124	GLY
1	C	136	HIS
1	D	112	GLN
1	D	124	GLY
1	A	56	PRO
1	A	106	SER
1	B	56	PRO
1	D	40	HIS
1	A	3	GLY
1	A	17	ILE
1	D	136	HIS
1	C	131	ILE
1	D	3	GLY
1	D	75	ILE
1	B	17	ILE
1	C	55	GLY
1	D	53	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	152/157 (97%)	132 (87%)	20 (13%)	4	13
1	B	151/157 (96%)	137 (91%)	14 (9%)	8	27
1	C	147/157 (94%)	128 (87%)	19 (13%)	4	13
1	D	149/157 (95%)	128 (86%)	21 (14%)	3	11
All	All	599/628 (95%)	525 (88%)	74 (12%)	4	15

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PHE
1	A	2	TRP
1	A	5	LEU
1	A	6	ASN
1	A	11	LYS
1	A	38	ARG
1	A	51	HIS
1	A	59	LYS
1	A	63	GLN
1	A	81	GLU
1	A	83	LEU
1	A	92	CYS
1	A	98	GLU
1	A	126	VAL
1	A	153	GLU
1	A	156	LYS
1	A	159	GLN
1	A	163	THR
1	A	168	LEU
1	A	170	LEU
1	B	2	TRP
1	B	6	ASN
1	B	59	LYS
1	B	75	ILE

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Mol	Chain	Res	Type
1	B	97	ILE
1	B	98	GLU
1	B	103	GLU
1	B	106	SER
1	B	141	LYS
1	B	146	SER
1	B	159	GLN
1	B	162	LYS
1	B	170	LEU
1	B	172	LEU
1	C	2	TRP
1	C	11	LYS
1	C	15	ASP
1	C	24	ARG
1	C	27	SER
1	C	59	LYS
1	C	83	LEU
1	C	97	ILE
1	C	98	GLU
1	C	119	GLU
1	C	125	ASN
1	C	127	THR
1	C	138	ARG
1	C	141	LYS
1	C	152	LYS
1	C	158	VAL
1	C	163	THR
1	C	170	LEU
1	C	174	LEU
1	D	2	TRP
1	D	5	LEU
1	D	15	ASP
1	D	37	VAL
1	D	59	LYS
1	D	73	MET
1	D	75	ILE
1	D	86	VAL
1	D	97	ILE
1	D	98	GLU
1	D	118	MET
1	D	119	GLU
1	D	131	ILE

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Mol	Chain	Res	Type
1	D	141	LYS
1	D	146	SER
1	D	153	GLU
1	D	154	LYS
1	D	158	VAL
1	D	159	GLN
1	D	170	LEU
1	D	172	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	136	HIS
1	B	79	HIS
1	B	107	GLN
1	B	112	GLN
1	B	136	HIS
1	C	51	HIS
1	C	112	GLN
1	C	136	HIS
1	D	14	HIS
1	D	107	GLN
1	D	112	GLN
1	D	136	HIS

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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	175/176 (99%)	-0.11	0 100 100	32, 67, 84, 100	1 (0%)
1	B	175/176 (99%)	-0.16	1 (0%) 85 81	49, 67, 84, 100	0
1	C	175/176 (99%)	-0.13	0 100 100	50, 70, 86, 100	0
1	D	175/176 (99%)	-0.00	0 100 100	50, 71, 86, 100	0
All	All	700/704 (99%)	-0.10	1 (0%) 92 90	32, 69, 86, 100	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	LEU	2.7

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	D	301	1/1	0.48	0.27	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	C	301	1/1	0.82	0.21	76,76,76,76	0
2	MG	B	301	1/1	0.82	0.07	57,57,57,57	0
2	MG	A	301	1/1	0.83	0.11	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.