



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:04 AM UTC

PDB ID : 7M5C / pdb_00007m5c
Title : Crystal Structure of human BAK in complex with WT BAK BH3 peptide
Authors : Singh, G.; Aggarwal, A.; Moldoveanu, T.
Deposited on : 2021-03-23
Resolution : 3.06 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
Mogul : 2022.3.0, CSD as543be (2022)
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

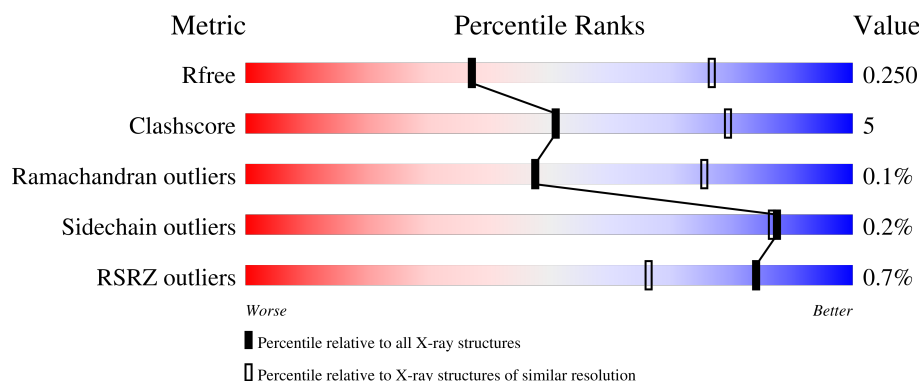
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	166	% 78% 13% 9%
1	C	166	76% 15% 9%
1	E	166	85% 10% 5%
1	G	166	% 76% 7% 16%
1	I	166	% 76% 11% 13%

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Mol	Chain	Length	Quality of chain
1	K	166	
1	M	166	
1	O	166	
1	Q	166	
1	S	166	
2	B	25	
2	D	25	
2	F	25	
2	H	25	
2	J	25	
2	L	25	
2	N	25	
2	P	25	
2	R	25	
2	T	25	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13528 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 Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1213	770	213	226	4			
1	C	151	Total	C	N	O	S	0	0	0
			1216	776	214	222	4			
1	E	157	Total	C	N	O	S	0	0	0
			1260	802	221	232	5			
1	G	139	Total	C	N	O	S	0	0	0
			1123	717	200	203	3			
1	I	145	Total	C	N	O	S	0	0	0
			1159	740	203	212	4			
1	K	147	Total	C	N	O	S	0	0	0
			1185	754	209	218	4			
1	M	149	Total	C	N	O	S	0	0	0
			1201	764	212	221	4			
1	O	151	Total	C	N	O	S	0	0	0
			1209	770	213	221	5			
1	Q	147	Total	C	N	O	S	0	1	0
			1199	766	210	219	4			
1	S	143	Total	C	N	O	S	0	0	0
			1140	728	204	204	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	SER	CYS	conflict	UNP Q16611
A	184	CYS	GLY	conflict	UNP Q16611
C	166	SER	CYS	conflict	UNP Q16611
C	184	CYS	GLY	conflict	UNP Q16611
E	166	SER	CYS	conflict	UNP Q16611
E	184	CYS	GLY	conflict	UNP Q16611
G	166	SER	CYS	conflict	UNP Q16611
G	184	CYS	GLY	conflict	UNP Q16611
I	166	SER	CYS	conflict	UNP Q16611

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Chain	Residue	Modelled	Actual	Comment	Reference
I	184	CYS	GLY	conflict	UNP Q16611
K	166	SER	CYS	conflict	UNP Q16611
K	184	CYS	GLY	conflict	UNP Q16611
M	166	SER	CYS	conflict	UNP Q16611
M	184	CYS	GLY	conflict	UNP Q16611
O	166	SER	CYS	conflict	UNP Q16611
O	184	CYS	GLY	conflict	UNP Q16611
Q	166	SER	CYS	conflict	UNP Q16611
Q	184	CYS	GLY	conflict	UNP Q16611
S	166	SER	CYS	conflict	UNP Q16611
S	184	CYS	GLY	conflict	UNP Q16611

- Molecule 2 is a protein called Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	22	Total	C	N	O	S	0	0	0
			164	99	31	33	1			
2	D	17	Total	C	N	O	S	0	0	0
			119	70	23	25	1			
2	F	24	Total	C	N	O	S	0	0	0
			175	104	36	33	2			
2	H	22	Total	C	N	O	S	0	0	0
			168	101	34	32	1			
2	J	20	Total	C	N	O	S	0	0	0
			149	87	32	29	1			
2	L	22	Total	C	N	O	S	0	0	0
			170	102	34	33	1			
2	N	19	Total	C	N	O	S	0	0	0
			151	92	31	27	1			
2	P	22	Total	C	N	O	S	0	0	0
			169	102	34	32	1			
2	R	19	Total	C	N	O	S	0	0	0
			149	90	31	27	1			
2	T	21	Total	C	N	O	S	0	0	0
			160	97	32	30	1			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	90	GLY	-	expression tag	UNP Q16611
B	91	GLY	-	expression tag	UNP Q16611
B	92	CYS	-	expression tag	UNP Q16611

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Chain	Residue	Modelled	Actual	Comment	Reference
D	90	GLY	-	expression tag	UNP Q16611
D	91	GLY	-	expression tag	UNP Q16611
D	92	CYS	-	expression tag	UNP Q16611
F	90	GLY	-	expression tag	UNP Q16611
F	91	GLY	-	expression tag	UNP Q16611
F	92	CYS	-	expression tag	UNP Q16611
H	90	GLY	-	expression tag	UNP Q16611
H	91	GLY	-	expression tag	UNP Q16611
H	92	CYS	-	expression tag	UNP Q16611
J	90	GLY	-	expression tag	UNP Q16611
J	91	GLY	-	expression tag	UNP Q16611
J	92	CYS	-	expression tag	UNP Q16611
L	90	GLY	-	expression tag	UNP Q16611
L	91	GLY	-	expression tag	UNP Q16611
L	92	CYS	-	expression tag	UNP Q16611
N	90	GLY	-	expression tag	UNP Q16611
N	91	GLY	-	expression tag	UNP Q16611
N	92	CYS	-	expression tag	UNP Q16611
P	90	GLY	-	expression tag	UNP Q16611
P	91	GLY	-	expression tag	UNP Q16611
P	92	CYS	-	expression tag	UNP Q16611
R	90	GLY	-	expression tag	UNP Q16611
R	91	GLY	-	expression tag	UNP Q16611
R	92	CYS	-	expression tag	UNP Q16611
T	90	GLY	-	expression tag	UNP Q16611
T	91	GLY	-	expression tag	UNP Q16611
T	92	CYS	-	expression tag	UNP Q16611

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu 1 1	0	0
3	C	1	Total Cu 1 1	0	0
3	E	1	Total Cu 1 1	0	0
3	G	1	Total Cu 1 1	0	0
3	I	1	Total Cu 1 1	0	0
3	M	1	Total Cu 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	1	Total	Cu	0	0
			1	1		
3	Q	1	Total	Cu	0	0
			1	1		
3	S	1	Total	Cu	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

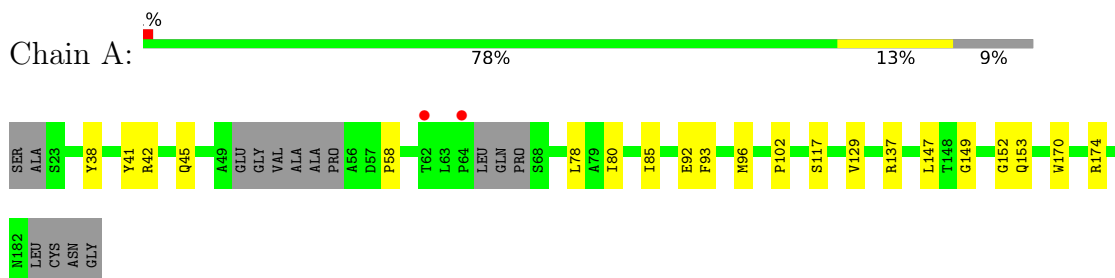


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		
4	T	1	Total	O	S	0	0
			5	4	1		

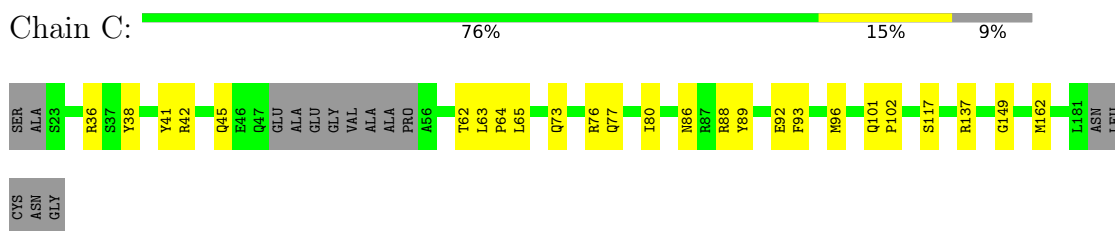
3 Residue-property plots [i](#)

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.

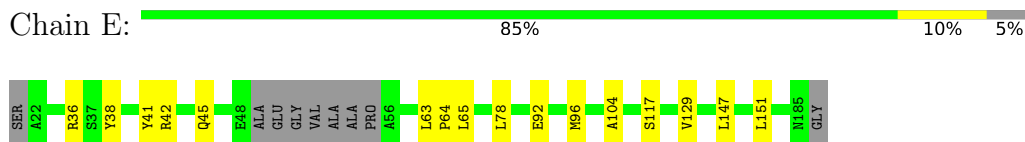
- Molecule 1: Bcl-2 homologous antagonist/killer



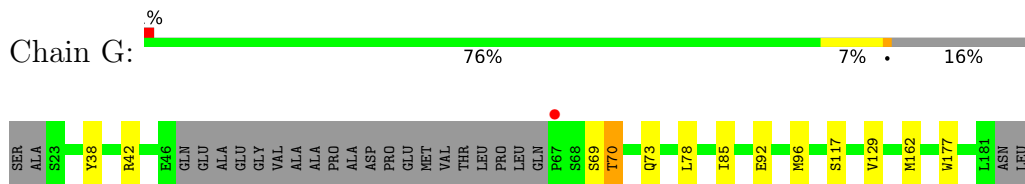
- Molecule 1: Bcl-2 homologous antagonist/killer



- Molecule 1: Bcl-2 homologous antagonist/killer

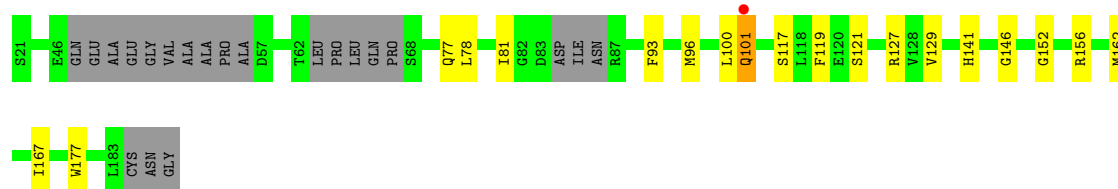


- Molecule 1: Bcl-2 homologous antagonist/killer

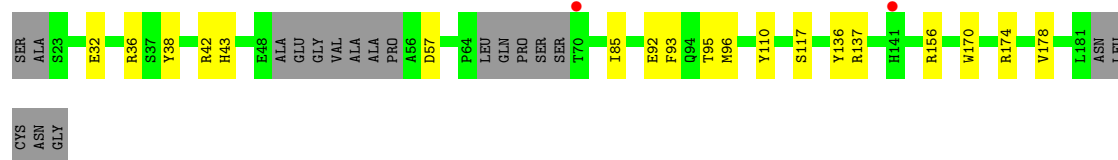
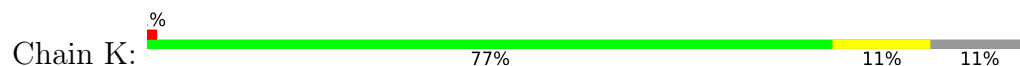


- Molecule 1: Bcl-2 homologous antagonist/killer

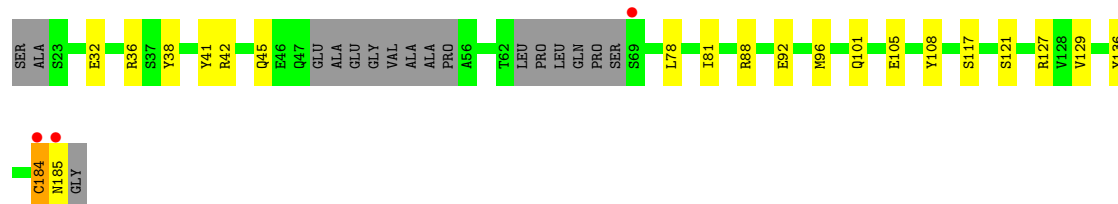
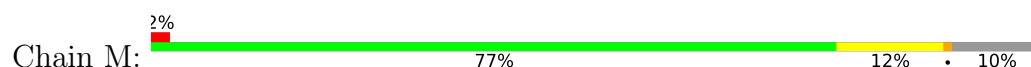




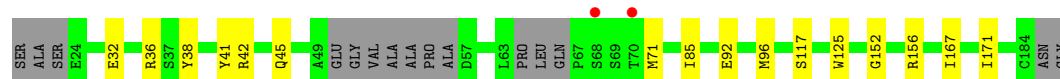
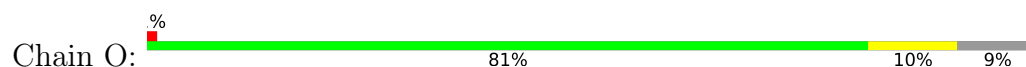
- Molecule 1: Bcl-2 homologous antagonist/killer



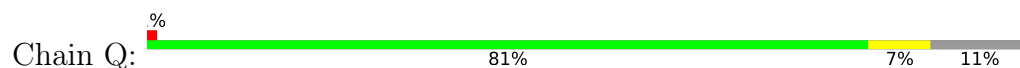
- Molecule 1: Bcl-2 homologous antagonist/killer



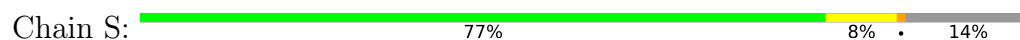
- Molecule 1: Bcl-2 homologous antagonist/killer



- Molecule 1: Bcl-2 homologous antagonist/killer



- Molecule 1: Bcl-2 homologous antagonist/killer



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain B:  68% 20% 12%



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain D:  44% 24% 32%



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain F:  88% 8% .



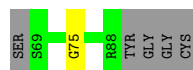
- Molecule 2: Bcl-2 homologous antagonist/killer

Chain H:  72% 16% 12%



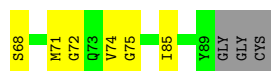
- Molecule 2: Bcl-2 homologous antagonist/killer

Chain J:  76% . 20%



- Molecule 2: Bcl-2 homologous antagonist/killer

Chain L:  64% 24% 12%



- Molecule 2: Bcl-2 homologous antagonist/killer

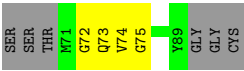
Chain N:  60% 16% 24%



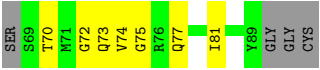
- Molecule 2: Bcl-2 homologous antagonist/killer



• Molecule 2: Bcl-2 homologous antagonist/killer



• Molecule 2: Bcl-2 homologous antagonist/killer



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.39Å 132.22Å 89.38Å 90.00° 119.20° 90.00°	Depositor
Resolution (Å)	29.34 – 3.06 29.34 – 3.06	Depositor EDS
% Data completeness (in resolution range)	90.8 (29.34-3.06) 90.7 (29.34-3.06)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.05Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.213 , 0.249 0.214 , 0.250	Depositor DCC
R_{free} test set	2029 reflections (5.95%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h-l 0.000 for -h-l,k,h 0.014 for -h-l,-k,l 0.019 for h,-k,-h-l 0.030 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13528	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: SO4, CU

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	0.21	0/1240	0.44	0/1676
1	C	0.19	0/1245	0.46	0/1683
1	E	0.16	0/1290	0.44	0/1746
1	G	0.44	3/1150 (0.3%)	0.46	0/1551
1	I	0.18	0/1183	0.76	2/1595 (0.1%)
1	K	0.16	0/1213	0.41	0/1640
1	M	0.18	0/1228	0.47	1/1661 (0.1%)
1	O	0.43	2/1235 (0.2%)	0.43	0/1669
1	Q	0.18	0/1231	0.43	0/1664
1	S	0.40	3/1168 (0.3%)	0.61	2/1577 (0.1%)
2	B	0.22	0/164	0.46	0/219
2	D	0.21	0/117	0.50	0/155
2	F	0.19	0/175	0.36	0/231
2	H	0.18	0/168	0.38	0/224
2	J	0.13	0/148	0.32	0/196
2	L	0.16	0/170	0.35	0/226
2	N	0.15	0/151	0.37	0/200
2	P	0.22	0/169	0.55	0/224
2	R	0.21	0/149	0.44	0/198
2	T	0.20	0/160	0.43	0/213
All	All	0.27	8/13754 (0.1%)	0.49	5/18548 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	71	MET	C-O	-6.59	1.14	1.23
1	G	70	THR	CA-C	-5.70	1.45	1.52
1	G	70	THR	C-O	-5.53	1.17	1.24
1	S	106	ASN	N-CA	-5.36	1.39	1.46
1	G	69	SER	C-O	-5.20	1.17	1.24
1	O	71	MET	CA-C	-5.10	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	102	PRO	C-O	-5.10	1.17	1.24
1	S	106	ASN	C-O	-5.01	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	101	GLN	CA-C-N	17.13	137.52	118.85
1	I	101	GLN	C-N-CA	17.13	137.52	118.85
1	S	106	ASN	N-CA-C	-14.45	91.69	114.09
1	S	106	ASN	CB-CA-C	7.04	121.14	109.80
1	M	184	CYS	N-CA-CB	-5.51	107.89	114.17

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1213	0	1137	18	0
1	C	1216	0	1149	23	0
1	E	1260	0	1195	10	0
1	G	1123	0	1054	12	0
1	I	1159	0	1089	10	0
1	K	1185	0	1106	15	0
1	M	1201	0	1132	17	0
1	O	1209	0	1121	9	0
1	Q	1199	0	1130	10	0
1	S	1140	0	1060	11	0
2	B	164	0	159	6	0
2	D	119	0	104	5	0
2	F	175	0	166	2	0
2	H	168	0	162	4	0
2	J	149	0	142	1	0
2	L	170	0	170	6	0
2	N	151	0	153	4	0
2	P	169	0	169	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	149	0	143	5	0
2	T	160	0	156	5	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
3	Q	1	0	0	0	0
3	S	1	0	0	0	0
4	A	5	0	0	0	0
4	G	5	0	0	0	0
4	H	10	0	0	0	0
4	M	10	0	0	0	0
4	P	5	0	0	0	0
4	T	5	0	0	0	0
All	All	13528	0	12697	135	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 5.

All (135) 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:Q:62:THR:O	1:Q:63:LEU:HD22	1.76	0.83
1:A:80:ILE:HG23	1:K:178:VAL:HG23	1.65	0.78
1:M:32:GLU:OE1	1:M:36:ARG:NH2	2.20	0.75
1:I:117:SER:HB2	2:J:75:GLY:HA3	1.68	0.74
1:K:117:SER:HB2	2:L:75:GLY:HA3	1.71	0.72
1:O:117:SER:HB2	2:P:75:GLY:HA3	1.72	0.72
1:A:117:SER:HB2	2:B:75:GLY:HA3	1.73	0.71
1:E:117:SER:HB2	2:F:75:GLY:HA3	1.73	0.70
1:G:117:SER:HB2	2:H:75:GLY:HA3	1.72	0.70
1:Q:117:SER:HB2	2:R:75:GLY:HA3	1.75	0.69
1:S:38:TYR:OH	1:S:42:ARG:NH1	2.27	0.68
1:M:117:SER:HB2	2:N:75:GLY:HA3	1.77	0.67
1:I:152:GLY:O	1:I:156:ARG:HG2	1.95	0.66
1:K:38:TYR:OH	1:K:42:ARG:NH1	2.30	0.65
1:C:93:PHE:HB3	1:C:137:ARG:NH1	2.12	0.65
1:S:117:SER:HB2	2:T:75:GLY:HA3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:SER:HB2	2:D:75:GLY:HA3	1.81	0.62
1:C:137:ARG:HH11	1:C:137:ARG:HG3	1.66	0.61
1:M:101:GLN:NE2	1:M:105:GLU:HB3	2.17	0.60
1:M:81:ILE:HG22	1:M:185:ASN:HA	1.83	0.60
1:K:32:GLU:OE1	1:K:36:ARG:NH2	2.35	0.59
1:M:38:TYR:OH	1:M:42:ARG:NH1	2.35	0.59
1:E:38:TYR:OH	1:E:42:ARG:NH1	2.35	0.59
1:G:38:TYR:OH	1:G:42:ARG:NH1	2.37	0.58
1:M:101:GLN:HE21	1:M:105:GLU:HB3	1.67	0.58
1:A:149:GLY:O	1:C:36:ARG:NH2	2.36	0.58
1:C:38:TYR:OH	1:C:42:ARG:NH1	2.37	0.57
1:O:32:GLU:OE1	1:O:36:ARG:NH2	2.37	0.56
1:Q:38:TYR:OH	1:Q:42:ARG:NH1	2.37	0.56
1:A:85:ILE:HG13	2:B:85:ILE:HG12	1.87	0.56
1:A:93:PHE:HB3	1:A:137:ARG:HD2	1.88	0.56
1:I:121:SER:OG	1:I:127:ARG:NH1	2.33	0.56
1:O:152:GLY:O	1:O:156:ARG:HD3	2.05	0.56
1:G:92:GLU:O	1:G:96:MET:HG3	2.05	0.55
1:Q:36:ARG:NH1	1:Q:63:LEU:HD11	2.22	0.55
1:E:63:LEU:HD11	1:E:151:LEU:HD21	1.88	0.54
1:O:38:TYR:OH	1:O:42:ARG:NH1	2.40	0.54
1:A:92:GLU:HG2	2:B:77:GLN:HE21	1.72	0.54
1:C:92:GLU:O	1:C:96:MET:HG3	2.08	0.54
1:K:32:GLU:OE2	1:K:156:ARG:NH2	2.41	0.53
1:C:93:PHE:HB3	1:C:137:ARG:HH12	1.72	0.53
1:S:92:GLU:O	1:S:96:MET:HG3	2.09	0.53
1:Q:36:ARG:HH11	1:Q:63:LEU:HD11	1.74	0.53
1:K:92:GLU:O	1:K:96:MET:HG3	2.10	0.52
1:S:117:SER:OG	2:T:72:GLY:HA2	2.09	0.52
1:A:38:TYR:OH	1:A:42:ARG:NH1	2.44	0.51
1:M:41:TYR:O	1:M:45:GLN:HG2	2.11	0.51
1:K:93:PHE:HB3	1:K:137:ARG:HD3	1.93	0.51
1:A:153:GLN:OE1	1:C:62:THR:HB	2.11	0.50
1:M:88:ARG:NH2	2:N:84:ASP:OD2	2.44	0.50
1:O:41:TYR:O	1:O:45:GLN:HG2	2.12	0.50
1:M:121:SER:OG	1:M:127:ARG:NH1	2.41	0.50
1:G:78:LEU:HD22	1:G:129:VAL:HG22	1.94	0.50
1:A:170:TRP:O	1:A:174:ARG:HG2	2.12	0.49
1:E:41:TYR:O	1:E:45:GLN:HG2	2.12	0.49
1:E:117:SER:OG	2:F:72:GLY:HA2	2.12	0.49
1:M:92:GLU:O	1:M:96:MET:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:41:TYR:O	1:S:45:GLN:HG2	2.12	0.49
1:C:63:LEU:HG	1:C:65:LEU:HG	1.95	0.49
1:C:89:TYR:OH	2:D:84:ASP:OD2	2.30	0.49
2:R:73:GLN:HG2	2:R:74:VAL:N	2.27	0.48
1:C:88:ARG:HG3	1:C:89:TYR:CD1	2.48	0.48
1:I:78:LEU:HD22	1:I:129:VAL:HG22	1.96	0.48
2:T:77:GLN:O	2:T:81:ILE:HG22	2.13	0.48
1:Q:117:SER:OG	2:R:72:GLY:HA2	2.14	0.48
1:C:41:TYR:O	1:C:45:GLN:HG2	2.13	0.47
1:S:96:MET:HG2	2:T:74:VAL:HG13	1.96	0.47
1:A:58:PRO:HB3	1:I:146:GLY:HA3	1.96	0.47
1:E:36:ARG:HD3	1:E:63:LEU:HD22	1.95	0.47
1:C:101:GLN:HG3	1:C:102:PRO:HD2	1.97	0.47
1:I:100:LEU:HD23	1:I:141:HIS:HD2	1.79	0.47
1:Q:96:MET:HG3	2:R:74:VAL:HG11	1.96	0.47
1:M:78:LEU:HD22	1:M:129:VAL:HG22	1.97	0.47
2:T:70:THR:HG22	2:T:73:GLN:CD	2.40	0.47
1:M:96:MET:HG2	2:N:74:VAL:HG13	1.97	0.46
1:K:85:ILE:HG13	2:L:85:ILE:HG12	1.98	0.46
1:A:78:LEU:HD22	1:A:129:VAL:HG22	1.96	0.46
1:G:70:THR:O	1:G:70:THR:HG22	2.15	0.46
1:E:78:LEU:HD22	1:E:129:VAL:HG22	1.96	0.45
1:Q:78:LEU:HD22	1:Q:129:VAL:HG22	1.98	0.45
1:A:96:MET:HG3	2:B:74:VAL:HG11	1.97	0.45
1:C:36:ARG:NH1	1:C:64:PRO:HG3	2.31	0.45
1:E:92:GLU:O	1:E:96:MET:HG3	2.16	0.45
2:D:78:LEU:HA	2:D:81:ILE:HG23	1.98	0.45
1:E:63:LEU:C	1:E:65:LEU:H	2.24	0.45
1:S:162:MET:HE1	1:S:177:TRP:CZ2	2.52	0.45
1:K:117:SER:OG	2:L:72:GLY:HA2	2.17	0.45
1:G:162:MET:HE1	1:G:177:TRP:CZ2	2.52	0.44
2:P:88:ARG:O	2:P:89:TYR:HB2	2.16	0.44
1:Q:162:MET:HE1	1:Q:177:TRP:CZ2	2.52	0.44
1:O:92:GLU:O	1:O:96:MET:HG3	2.17	0.44
1:C:76:ARG:O	1:C:80:ILE:HD12	2.18	0.44
1:K:110:TYR:HA	2:L:71:MET:SD	2.57	0.44
1:A:147:LEU:HD12	1:C:149:GLY:HA2	1.99	0.44
1:O:117:SER:OG	2:P:72:GLY:HA2	2.17	0.44
1:S:78:LEU:HD22	1:S:129:VAL:HG22	2.00	0.44
1:C:96:MET:HG2	2:D:74:VAL:HG13	1.99	0.43
1:K:96:MET:HG2	2:L:74:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TYR:O	1:A:45:GLN:HG2	2.18	0.43
2:B:77:GLN:HA	2:B:77:GLN:OE1	2.19	0.43
1:O:85:ILE:HG13	2:P:85:ILE:HG12	2.01	0.43
2:D:81:ILE:O	2:D:85:ILE:HG13	2.19	0.42
1:M:42:ARG:HG2	1:M:136:TYR:CE2	2.54	0.42
2:H:88:ARG:HD3	2:H:88:ARG:HA	1.84	0.42
1:I:119:PHE:CD1	1:I:167:ILE:HD11	2.54	0.42
1:C:42:ARG:NH2	1:C:86:ASN:OD1	2.52	0.42
1:I:93:PHE:O	1:I:96:MET:HG2	2.20	0.42
1:A:152:GLY:HA3	1:C:64:PRO:HB2	2.02	0.42
1:S:106:ASN:O	1:S:107:ALA:C	2.61	0.42
1:E:104:ALA:HB3	1:E:147:LEU:HD22	2.02	0.42
1:O:125:TRP:CH2	1:O:171:ILE:HG12	2.54	0.42
1:A:102:PRO:HD3	1:M:108:TYR:CZ	2.55	0.42
2:B:88:ARG:HA	2:B:88:ARG:HD2	1.81	0.42
1:G:162:MET:HE2	1:G:162:MET:HB3	1.87	0.42
1:K:43:HIS:CE1	1:K:57:ASP:H	2.38	0.42
1:C:80:ILE:HG23	1:G:70:THR:OG1	2.20	0.41
1:K:170:TRP:O	1:K:174:ARG:HG2	2.20	0.41
1:C:73:GLN:HG2	1:C:76:ARG:HH12	1.84	0.41
1:G:117:SER:OG	2:H:72:GLY:HA2	2.20	0.41
1:M:81:ILE:HD11	1:M:129:VAL:HG21	2.03	0.41
1:C:77:GLN:HA	1:G:73:GLN:NE2	2.35	0.41
1:G:96:MET:HE1	2:H:78:LEU:HD21	2.01	0.41
1:K:95:THR:HG21	2:L:68:SER:HB2	2.01	0.41
1:I:162:MET:HE1	1:I:177:TRP:CZ2	2.56	0.41
2:N:80:ILE:HD13	2:N:80:ILE:HA	1.87	0.41
1:Q:96:MET:HG3	2:R:74:VAL:CG1	2.51	0.40
1:S:162:MET:HE2	1:S:162:MET:HB3	1.87	0.40
1:A:93:PHE:HD1	1:A:96:MET:HE1	1.85	0.40
1:A:102:PRO:HD3	1:M:108:TYR:CE1	2.57	0.40
1:S:162:MET:HE1	1:S:177:TRP:HZ2	1.85	0.40
1:M:184:CYS:O	1:M:185:ASN:CB	2.68	0.40
1:G:85:ILE:HD13	1:G:85:ILE:HA	1.92	0.40
1:C:162:MET:HE2	1:C:162:MET:HB3	1.93	0.40
1:I:77:GLN:O	1:I:81:ILE:HG13	2.22	0.40
1:K:42:ARG:HG2	1:K:136:TYR: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	145/166 (87%)	143 (99%)	2 (1%)	0	100	100
1	C	147/166 (89%)	145 (99%)	2 (1%)	0	100	100
1	E	153/166 (92%)	149 (97%)	3 (2%)	1 (1%)	18	45
1	G	135/166 (81%)	132 (98%)	3 (2%)	0	100	100
1	I	137/166 (82%)	135 (98%)	1 (1%)	1 (1%)	18	45
1	K	141/166 (85%)	139 (99%)	2 (1%)	0	100	100
1	M	143/166 (86%)	139 (97%)	4 (3%)	0	100	100
1	O	145/166 (87%)	142 (98%)	3 (2%)	0	100	100
1	Q	142/166 (86%)	140 (99%)	2 (1%)	0	100	100
1	S	137/166 (82%)	133 (97%)	4 (3%)	0	100	100
2	B	20/25 (80%)	20 (100%)	0	0	100	100
2	D	15/25 (60%)	14 (93%)	1 (7%)	0	100	100
2	F	22/25 (88%)	22 (100%)	0	0	100	100
2	H	20/25 (80%)	20 (100%)	0	0	100	100
2	J	18/25 (72%)	18 (100%)	0	0	100	100
2	L	20/25 (80%)	20 (100%)	0	0	100	100
2	N	17/25 (68%)	17 (100%)	0	0	100	100
2	P	20/25 (80%)	19 (95%)	1 (5%)	0	100	100
2	R	17/25 (68%)	17 (100%)	0	0	100	100
2	T	19/25 (76%)	19 (100%)	0	0	100	100
All	All	1613/1910 (84%)	1583 (98%)	28 (2%)	2 (0%)	48	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	101	GLN

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Mol	Chain	Res	Type
1	E	64	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	123/136 (90%)	123 (100%)	0	100	100
1	C	125/136 (92%)	125 (100%)	0	100	100
1	E	130/136 (96%)	130 (100%)	0	100	100
1	G	112/136 (82%)	112 (100%)	0	100	100
1	I	116/136 (85%)	116 (100%)	0	100	100
1	K	118/136 (87%)	118 (100%)	0	100	100
1	M	121/136 (89%)	121 (100%)	0	100	100
1	O	118/136 (87%)	117 (99%)	1 (1%)	73	79
1	Q	122/136 (90%)	120 (98%)	2 (2%)	55	72
1	S	111/136 (82%)	110 (99%)	1 (1%)	70	78
2	B	17/19 (90%)	17 (100%)	0	100	100
2	D	10/19 (53%)	10 (100%)	0	100	100
2	F	15/19 (79%)	15 (100%)	0	100	100
2	H	16/19 (84%)	16 (100%)	0	100	100
2	J	14/19 (74%)	14 (100%)	0	100	100
2	L	18/19 (95%)	18 (100%)	0	100	100
2	N	15/19 (79%)	15 (100%)	0	100	100
2	P	18/19 (95%)	18 (100%)	0	100	100
2	R	13/19 (68%)	13 (100%)	0	100	100
2	T	15/19 (79%)	15 (100%)	0	100	100
All	All	1347/1550 (87%)	1343 (100%)	4 (0%)	87	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	167	ILE
1	Q	108[A]	TYR
1	Q	108[B]	TYR
1	S	103	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	94	GLN
1	A	165	HIS
2	B	86	ASN
1	C	26	GLN
1	C	29	GLN
1	C	94	GLN
1	C	144	GLN
1	G	26	GLN
1	G	45	GLN
1	G	73	GLN
1	G	77	GLN
2	H	86	ASN
1	I	44	GLN
1	I	77	GLN
1	I	165	HIS
1	K	26	GLN
1	K	77	GLN
1	M	44	GLN
1	M	47	GLN
1	M	101	GLN
1	O	44	GLN
1	Q	44	GLN
1	Q	165	HIS
1	S	26	GLN
1	S	44	GLN
1	S	86	ASN
1	S	165	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	H	101	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	A	202	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	H	102	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	T	101	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	M	202	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	G	202	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	P	101	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	M	203	-	4,4,4	0.25	0	6,6,6	0.09	0

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 [i](#)

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 ⓘ

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	151/166 (90%)	-0.24	2 (1%) 75 53	28, 48, 90, 113	0
1	C	151/166 (90%)	-0.36	0 100 100	31, 50, 81, 88	0
1	E	157/166 (94%)	-0.23	0 100 100	32, 50, 85, 108	0
1	G	139/166 (83%)	-0.24	1 (0%) 84 66	35, 55, 90, 108	0
1	I	145/166 (87%)	-0.20	1 (0%) 84 66	36, 55, 99, 129	0
1	K	147/166 (88%)	-0.25	2 (1%) 73 51	36, 54, 78, 118	0
1	M	149/166 (89%)	-0.18	3 (2%) 65 42	34, 57, 92, 115	0
1	O	151/166 (90%)	-0.23	2 (1%) 75 53	31, 54, 94, 115	0
1	Q	147/166 (88%)	-0.11	1 (0%) 84 66	28, 66, 97, 123	1 (0%)
1	S	143/166 (86%)	-0.02	0 100 100	50, 74, 109, 120	0
2	B	22/25 (88%)	-0.42	0 100 100	35, 46, 64, 79	0
2	D	17/25 (68%)	-0.22	0 100 100	50, 59, 78, 79	0
2	F	24/25 (96%)	-0.08	0 100 100	49, 60, 82, 92	0
2	H	22/25 (88%)	-0.30	0 100 100	34, 43, 70, 98	0
2	J	20/25 (80%)	-0.12	0 100 100	55, 68, 90, 93	0
2	L	22/25 (88%)	-0.21	0 100 100	38, 51, 69, 101	0
2	N	19/25 (76%)	0.03	0 100 100	58, 68, 103, 107	0
2	P	22/25 (88%)	-0.42	0 100 100	39, 47, 76, 118	0
2	R	19/25 (76%)	-0.02	0 100 100	58, 69, 99, 104	0
2	T	21/25 (84%)	-0.08	0 100 100	59, 73, 96, 106	0
All	All	1688/1910 (88%)	-0.21	12 (0%) 84 66	28, 57, 94, 129	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	67	PRO	3.8
1	M	184	CYS	3.8
1	I	101	GLN	3.5
1	O	70	THR	3.4
1	K	70	THR	3.0
1	Q	108[A]	TYR	2.9
1	O	68	SER	2.7
1	M	69	SER	2.1
1	K	141	HIS	2.1
1	M	185	ASN	2.0
1	A	64	PRO	2.0
1	A	62	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](#)

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
4	SO4	T	101	5/5	0.80	0.10	114,114,115,116	0
4	SO4	G	202	5/5	0.82	0.14	106,109,115,115	0
4	SO4	M	202	5/5	0.84	0.08	84,88,90,90	0
4	SO4	M	203	5/5	0.87	0.12	125,126,126,127	0
4	SO4	H	102	5/5	0.88	0.09	68,68,70,71	0
4	SO4	A	202	5/5	0.95	0.07	67,68,69,76	0
4	SO4	H	101	5/5	0.96	0.06	39,41,43,46	0
3	CU	C	201	1/1	0.98	0.03	60,60,60,60	0
3	CU	E	201	1/1	0.98	0.03	43,43,43,43	0
3	CU	G	201	1/1	0.98	0.02	49,49,49,49	0
3	CU	I	201	1/1	0.98	0.04	51,51,51,51	0
3	CU	M	201	1/1	0.98	0.03	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CU	O	201	1/1	0.98	0.03	69,69,69,69	0
3	CU	Q	201	1/1	0.98	0.03	54,54,54,54	0
3	CU	S	201	1/1	0.99	0.02	62,62,62,62	0
4	SO4	P	101	5/5	0.99	0.04	45,46,48,48	0
3	CU	A	201	1/1	0.99	0.06	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.