



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:20 PM UTC

PDB ID : 4Q2J / pdb_00004q2j
Title : A novel structure-based mechanism for DNA-binding of SATB1
Authors : Wang, Z.; Long, J.; Yang, X.; Shen, Y.
Deposited on : 2014-04-08
Resolution : 2.60 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

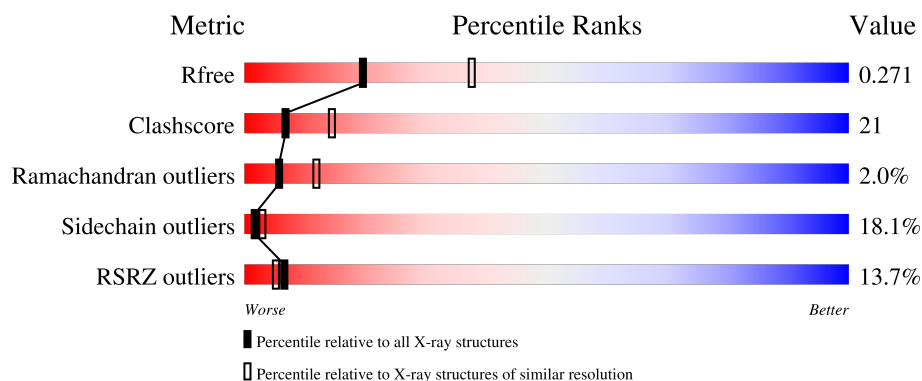
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	180	11% 49% 36% 9% 6%
1	B	180	6% 34% 13% 5% 48%
1	C	180	8% 29% 17% • • 49%
1	D	180	14% 48% 38% 8% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4034 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 DNA-binding protein SATB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1316	839	222	245	10			
1	B	94	Total	C	N	O	S	0	0	0
			720	464	117	134	5			
1	C	92	Total	C	N	O	S	0	0	0
			702	454	115	128	5			
1	D	169	Total	C	N	O	S	0	0	0
			1283	818	215	240	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	GLY	-	expression tag	UNP Q60611
A	68	PRO	-	expression tag	UNP Q60611
A	69	GLY	-	expression tag	UNP Q60611
A	70	SER	-	expression tag	UNP Q60611
B	67	GLY	-	expression tag	UNP Q60611
B	68	PRO	-	expression tag	UNP Q60611
B	69	GLY	-	expression tag	UNP Q60611
B	70	SER	-	expression tag	UNP Q60611
C	67	GLY	-	expression tag	UNP Q60611
C	68	PRO	-	expression tag	UNP Q60611
C	69	GLY	-	expression tag	UNP Q60611
C	70	SER	-	expression tag	UNP Q60611
D	67	GLY	-	expression tag	UNP Q60611
D	68	PRO	-	expression tag	UNP Q60611
D	69	GLY	-	expression tag	UNP Q60611
D	70	SER	-	expression tag	UNP Q60611

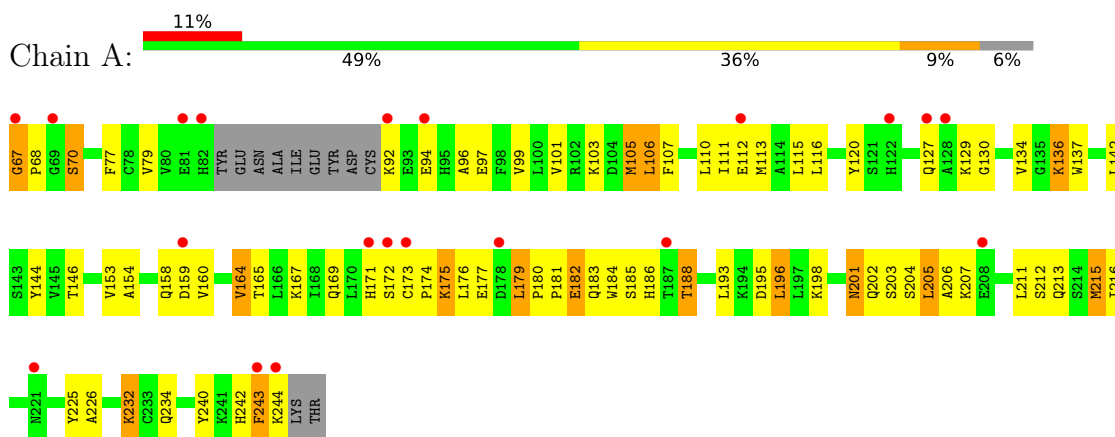
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	O 4	0	0
2	B	4	Total 4	O 4	0	0
2	C	1	Total 1	O 1	0	0
2	D	4	Total 4	O 4	0	0

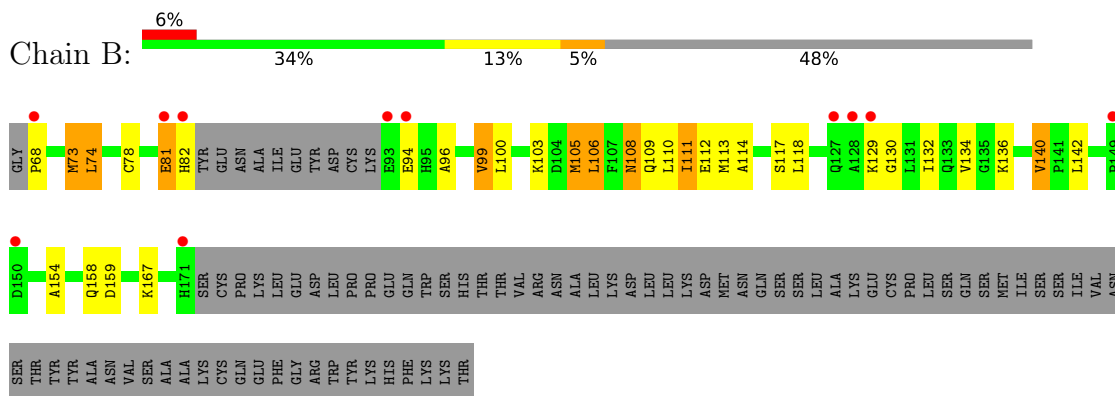
3 Residue-property plots [i](#)

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.

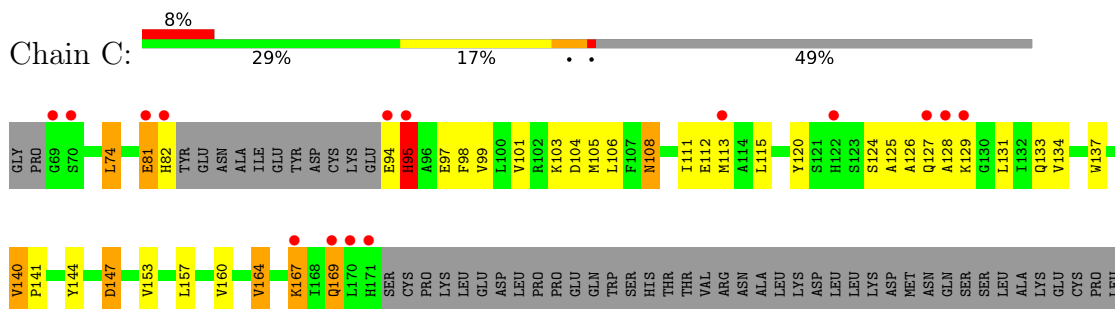
• Molecule 1: DNA-binding protein SATB1



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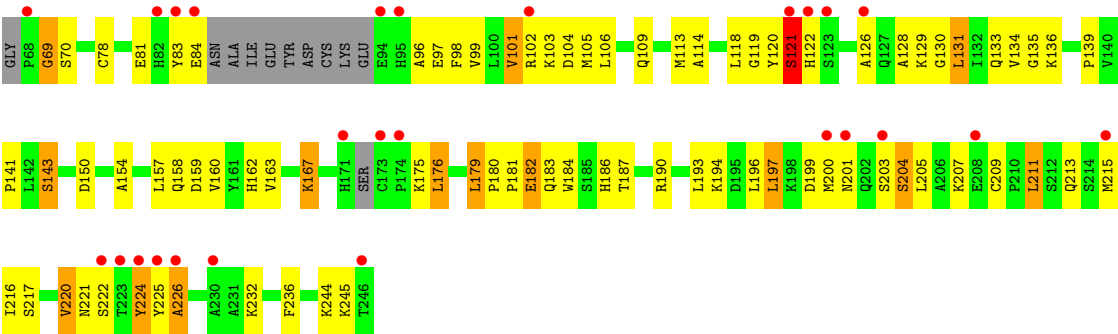


• Molecule 1: DNA-binding protein SATB1



SER	GLN	SER	MET	ILE	SER	SER	ILE	VAL	ASN	SER	THR	TYR	ALA	ASN	VAL	SER	ALA	ALA	LYS	CYS	GLN	GLU	PHE	GLY	ARG	TRP	TYR	LYS	HIS	PHE	LYS	LYS	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 1: DNA-binding protein SATB1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.98Å 91.97Å 100.24Å 90.00° 128.97° 90.00°	Depositor
Resolution (Å)	42.47 – 2.60 42.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.8 (42.47-2.60) 90.6 (42.47-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.228 , 0.271 0.230 , 0.271	Depositor DCC
R_{free} test set	1394 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4034	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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	0.57	0/1346	0.93	2/1826 (0.1%)
1	B	0.65	0/734	1.02	2/998 (0.2%)
1	C	0.56	0/716	1.03	4/974 (0.4%)
1	D	0.53	0/1308	0.91	1/1775 (0.1%)
All	All	0.57	0/4104	0.96	9/5573 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	GLN	N-CA-C	-11.30	98.80	112.59
1	A	67	GLY	CA-C-N	7.44	129.13	119.84
1	A	67	GLY	C-N-CA	7.44	129.13	119.84
1	B	68	PRO	N-CA-CB	7.04	110.75	103.00
1	B	140	VAL	N-CA-C	6.62	114.62	109.19
1	C	111	ILE	CB-CA-C	-5.48	104.96	111.81
1	D	160	VAL	N-CA-C	5.38	118.06	112.90
1	C	140	VAL	CA-C-N	-5.08	114.49	119.92
1	C	140	VAL	C-N-CA	-5.08	114.49	119.92

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	1316	0	1306	62	0
1	B	720	0	716	28	0
1	C	702	0	704	33	0
1	D	1283	0	1264	54	0
2	A	4	0	0	0	0
2	B	4	0	0	1	0
2	C	1	0	0	0	0
2	D	4	0	0	0	0
All	All	4034	0	3990	171	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 21.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:SER:HA	1:A:213:GLN:HE21	1.22	1.04
1:A:243:PHE:HA	1:A:244:LYS:C	1.86	0.98
1:B:105:MET:HE1	1:B:113:MET:HB2	1.52	0.91
1:A:212:SER:O	1:A:216:ILE:HG13	1.74	0.87
1:C:105:MET:SD	1:C:113:MET:HG3	2.19	0.82
1:A:154:ALA:O	1:A:158:GLN:HB2	1.78	0.82
1:D:133:GLN:HB2	1:D:139:PRO:HB3	1.62	0.81
1:C:108:ASN:H	1:C:108:ASN:HD22	1.27	0.80
1:D:225:TYR:HA	1:D:226:ALA:HB3	1.62	0.80
1:A:103:LYS:HG2	1:A:154:ALA:HB2	1.63	0.79
1:D:167:LYS:HB2	1:D:167:LYS:NZ	1.97	0.79
1:C:108:ASN:H	1:C:108:ASN:ND2	1.80	0.79
1:C:129:LYS:HE3	1:C:169:GLN:HB3	1.64	0.79
1:D:216:ILE:O	1:D:220:VAL:HG23	1.83	0.77
1:A:185:SER:H	1:A:188:THR:HG23	1.48	0.76
1:D:175:LYS:NZ	1:D:175:LYS:HB2	2.01	0.74
1:A:182:GLU:HA	1:A:234:GLN:HE21	1.52	0.74
1:A:185:SER:H	1:A:188:THR:CG2	2.02	0.73
1:D:69:GLY:HA2	1:D:103:LYS:NZ	2.03	0.72
1:B:105:MET:SD	1:B:113:MET:HG3	2.29	0.72
1:A:203:SER:CA	1:A:213:GLN:HE21	2.03	0.70
1:D:179:LEU:HD22	1:D:183:GLN:HB2	1.73	0.70
1:A:179:LEU:HD23	1:A:180:PRO:HD2	1.73	0.70
1:C:81:GLU:O	1:C:82:HIS:HB2	1.92	0.69
1:B:114:ALA:O	1:B:118:LEU:HB2	1.92	0.69
1:A:105:MET:SD	1:A:113:MET:HG3	2.33	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:GLU:O	1:C:95:HIS:HB2	1.92	0.68
1:C:120:TYR:HB3	1:C:124:SER:OG	1.94	0.68
1:A:206:ALA:CB	1:A:213:GLN:HG3	2.24	0.67
1:C:112:GLU:HA	1:C:125:ALA:HB1	1.75	0.67
1:A:175:LYS:NZ	1:A:175:LYS:HB2	2.11	0.65
1:B:81:GLU:HG2	1:B:82:HIS:H	1.62	0.65
1:A:101:VAL:HB	1:A:105:MET:HE1	1.78	0.64
1:D:167:LYS:HB2	1:D:167:LYS:HZ2	1.62	0.64
1:D:225:TYR:CA	1:D:226:ALA:HB3	2.26	0.64
1:D:175:LYS:HB2	1:D:175:LYS:HZ3	1.63	0.64
1:B:105:MET:SD	1:B:113:MET:CG	2.86	0.64
1:C:115:LEU:HD12	1:C:125:ALA:HB2	1.79	0.64
1:A:103:LYS:CG	1:A:154:ALA:HB2	2.28	0.63
1:A:172:SER:CB	1:A:173:CYS:HA	2.29	0.63
1:A:105:MET:SD	1:A:113:MET:CG	2.89	0.60
1:A:172:SER:CB	1:A:173:CYS:CA	2.80	0.59
1:C:167:LYS:HB3	1:C:167:LYS:NZ	2.18	0.59
1:D:187:THR:HG22	1:D:190:ARG:NH2	2.18	0.58
1:D:205:LEU:HD23	1:D:205:LEU:O	2.03	0.58
1:A:195:ASP:HA	1:A:198:LYS:HE3	1.85	0.58
1:C:131:LEU:HD23	1:C:141:PRO:HA	1.85	0.58
1:A:181:PRO:HA	1:A:184:TRP:CD1	2.39	0.58
1:A:79:VAL:HG23	1:A:165:THR:CG2	2.34	0.58
1:D:221:ASN:O	1:D:222:SER:HB2	2.03	0.57
1:A:177:GLU:HG3	1:A:240:TYR:HE2	1.69	0.57
1:A:203:SER:HA	1:A:213:GLN:NE2	2.05	0.57
1:D:224:TYR:N	1:D:225:TYR:HA	2.19	0.57
1:A:185:SER:N	1:A:188:THR:HG23	2.20	0.56
1:B:99:VAL:HG23	1:B:117:SER:OG	2.06	0.56
1:A:105:MET:HG3	1:A:106:LEU:N	2.19	0.55
1:A:136:LYS:NZ	1:B:159:ASP:OD2	2.37	0.55
1:B:108:ASN:C	1:B:108:ASN:HD22	2.14	0.55
1:C:94:GLU:O	1:C:95:HIS:CB	2.54	0.55
1:C:129:LYS:CE	1:C:169:GLN:HB3	2.34	0.55
1:C:167:LYS:HB3	1:C:167:LYS:HZ2	1.72	0.55
1:A:177:GLU:HG3	1:A:240:TYR:CE2	2.42	0.55
1:A:243:PHE:CA	1:A:244:LYS:C	2.72	0.55
1:B:113:MET:O	1:B:117:SER:HB3	2.06	0.55
1:C:140:VAL:HG23	1:C:141:PRO:O	2.07	0.55
1:D:245:LYS:O	1:D:245:LYS:HG3	2.06	0.55
1:C:112:GLU:HA	1:C:125:ALA:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:HB2	1:A:175:LYS:HZ3	1.72	0.54
1:C:141:PRO:HD2	1:C:144:TYR:CE1	2.43	0.54
1:A:160:VAL:O	1:A:164:VAL:HG13	2.08	0.54
1:B:103:LYS:HB3	1:B:154:ALA:HB2	1.89	0.54
1:D:159:ASP:O	1:D:162:HIS:HE1	1.91	0.54
1:D:217:SER:O	1:D:221:ASN:HB2	2.08	0.53
1:A:101:VAL:HB	1:A:105:MET:CE	2.37	0.53
1:A:96:ALA:O	1:A:97:GLU:HB2	2.08	0.52
1:A:67:GLY:N	1:A:68:PRO:HD2	2.25	0.52
1:A:105:MET:HE3	1:A:153:VAL:HG21	1.91	0.52
1:D:225:TYR:HA	1:D:226:ALA:CB	2.37	0.52
1:D:201:ASN:HB3	1:D:204:SER:OG	2.11	0.51
1:B:78:CYS:O	1:B:96:ALA:HA	2.10	0.51
1:D:101:VAL:HB	1:D:105:MET:HE2	1.91	0.51
1:D:114:ALA:O	1:D:118:LEU:HG	2.10	0.51
1:D:141:PRO:C	1:D:143:SER:H	2.17	0.51
1:D:167:LYS:HB2	1:D:167:LYS:HZ3	1.72	0.51
1:C:160:VAL:O	1:C:164:VAL:HG13	2.11	0.51
1:D:209:CYS:SG	1:D:211:LEU:HB2	2.51	0.51
1:D:105:MET:HE1	1:D:113:MET:HB2	1.93	0.50
1:D:215:MET:HE3	1:D:232:LYS:NZ	2.27	0.50
1:C:137:TRP:CD1	1:C:137:TRP:N	2.77	0.50
1:A:206:ALA:HB2	1:A:213:GLN:HG3	1.94	0.50
1:B:81:GLU:HA	1:B:94:GLU:OE1	2.11	0.50
1:A:181:PRO:HG2	1:A:182:GLU:OE2	2.12	0.50
1:D:159:ASP:O	1:D:162:HIS:CE1	2.65	0.50
1:A:204:SER:HA	1:A:207:LYS:HD2	1.93	0.50
1:C:141:PRO:HD2	1:C:144:TYR:CD1	2.47	0.49
1:A:215:MET:HE3	1:A:225:TYR:OH	2.12	0.49
1:C:108:ASN:HD22	1:C:108:ASN:N	2.01	0.49
1:C:133:GLN:HB3	1:C:167:LYS:HE2	1.95	0.49
1:B:105:MET:HG3	1:B:106:LEU:N	2.27	0.49
1:A:115:LEU:O	1:A:120:TYR:HB2	2.13	0.48
1:C:126:ALA:HB1	1:C:128:ALA:H	1.78	0.48
1:D:141:PRO:C	1:D:143:SER:N	2.71	0.48
1:A:112:GLU:OE2	1:A:116:LEU:HG	2.14	0.48
1:D:186:HIS:CD2	1:D:186:HIS:C	2.92	0.48
1:A:201:ASN:HB2	1:A:204:SER:OG	2.13	0.48
1:A:173:CYS:SG	1:A:174:PRO:HD2	2.54	0.47
1:C:153:VAL:O	1:C:157:LEU:HB2	2.14	0.47
1:D:126:ALA:C	1:D:128:ALA:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:GLU:HG3	1:D:98:PHE:N	2.30	0.47
1:D:162:HIS:CD2	1:D:163:VAL:HG13	2.49	0.47
1:A:67:GLY:N	1:A:68:PRO:CD	2.78	0.47
1:A:111:ILE:HD13	1:A:130:GLY:HA3	1.96	0.47
1:A:105:MET:CG	1:A:106:LEU:N	2.77	0.47
1:A:232:LYS:HB2	1:A:232:LYS:HE2	1.49	0.46
1:C:125:ALA:HA	1:C:126:ALA:HA	1.58	0.46
1:D:130:GLY:O	1:D:131:LEU:HD23	2.15	0.46
1:C:129:LYS:C	1:C:129:LYS:HD2	2.40	0.46
1:D:204:SER:O	1:D:207:LYS:HB2	2.14	0.46
1:B:81:GLU:CG	1:B:82:HIS:H	2.27	0.46
1:B:73:MET:HE3	1:B:73:MET:HB3	1.84	0.46
1:B:73:MET:HE3	1:B:100:LEU:HB3	1.97	0.46
1:A:77:PHE:CZ	1:A:96:ALA:HB1	2.51	0.46
1:A:215:MET:HE2	1:A:225:TYR:HE2	1.81	0.46
1:D:211:LEU:HA	1:D:211:LEU:HD12	1.78	0.45
1:D:134:VAL:O	1:D:135:GLY:C	2.59	0.45
1:B:111:ILE:CD1	1:B:130:GLY:HA3	2.47	0.45
1:D:211:LEU:HD22	1:D:236:PHE:CD1	2.52	0.45
1:A:196:LEU:HB3	1:A:205:LEU:HD22	1.99	0.45
1:D:102:ARG:O	1:D:105:MET:HG2	2.17	0.45
1:D:78:CYS:O	1:D:96:ALA:HA	2.16	0.44
1:D:180:PRO:HA	1:D:181:PRO:HD3	1.92	0.44
1:A:92:LYS:HE3	1:A:92:LYS:HB2	1.80	0.44
1:A:136:LYS:HZ2	1:B:159:ASP:CG	2.22	0.44
1:B:111:ILE:HD11	1:B:130:GLY:HA3	1.98	0.44
1:D:200:MET:HE2	1:D:200:MET:HB3	1.78	0.44
1:D:181:PRO:O	1:D:184:TRP:HB2	2.17	0.44
1:D:103:LYS:HB2	1:D:154:ALA:HB2	1.99	0.43
1:A:137:TRP:CZ3	1:B:134:VAL:CG2	3.01	0.43
1:A:179:LEU:HD22	1:A:183:GLN:HB3	2.00	0.43
1:B:132:ILE:HG22	1:B:140:VAL:O	2.18	0.43
1:C:112:GLU:CD	1:C:113:MET:HE2	2.44	0.43
1:A:110:LEU:HD13	1:A:153:VAL:HG22	2.01	0.43
1:D:69:GLY:HA2	1:D:103:LYS:HZ1	1.80	0.43
1:A:144:TYR:CD1	1:A:144:TYR:N	2.86	0.43
1:B:105:MET:HE1	1:B:113:MET:CB	2.37	0.43
1:D:244:LYS:HD3	1:D:244:LYS:HA	1.88	0.43
1:C:147:ASP:OD2	1:C:147:ASP:N	2.52	0.42
1:C:97:GLU:HG3	1:C:98:PHE:N	2.34	0.42
1:D:120:TYR:O	1:D:121:SER:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LEU:HD12	1:D:197:LEU:HA	1.70	0.42
1:A:107:PHE:O	1:A:110:LEU:HB2	2.19	0.42
1:A:137:TRP:CZ3	1:B:134:VAL:HG21	2.55	0.42
1:B:109:GLN:NE2	1:B:112:GLU:OE2	2.52	0.42
1:B:129:LYS:HA	1:D:119:GLY:O	2.19	0.42
1:C:74:LEU:HD22	1:C:103:LYS:HG2	2.00	0.42
1:D:176:LEU:HA	1:D:176:LEU:HD12	1.73	0.42
1:B:74:LEU:HD21	1:B:158:GLN:HA	2.01	0.42
1:D:83:TYR:O	1:D:84:GLU:C	2.62	0.42
1:A:136:LYS:HB2	1:A:136:LYS:HE2	1.85	0.42
1:A:144:TYR:N	1:A:144:TYR:HD1	2.17	0.42
1:D:154:ALA:O	1:D:158:GLN:HB2	2.20	0.41
1:D:182:GLU:H	1:D:182:GLU:HG3	1.56	0.41
1:A:136:LYS:HD3	1:B:159:ASP:OD2	2.21	0.41
1:C:140:VAL:HB	1:C:144:TYR:HD1	1.85	0.41
1:D:97:GLU:HG3	1:D:98:PHE:H	1.85	0.41
1:A:182:GLU:H	1:A:182:GLU:HG2	1.52	0.41
1:A:186:HIS:CD2	1:A:226:ALA:HA	2.56	0.41
1:B:112:GLU:HB2	2:B:304:HOH:O	2.20	0.40
1:C:131:LEU:HB2	1:C:167:LYS:CG	2.51	0.40
1:C:74:LEU:HD12	1:C:74:LEU:HA	1.85	0.40
1:D:157:LEU:O	1:D:158:GLN:C	2.63	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	165/180 (92%)	150 (91%)	12 (7%)	3 (2%)	6	14
1	B	90/180 (50%)	82 (91%)	7 (8%)	1 (1%)	11	25
1	C	88/180 (49%)	79 (90%)	8 (9%)	1 (1%)	11	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	163/180 (91%)	146 (90%)	12 (7%)	5 (3%)	3	5
All	All	506/720 (70%)	457 (90%)	39 (8%)	10 (2%)	6	12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	95	HIS
1	A	176	LEU
1	A	242	HIS
1	B	142	LEU
1	D	69	GLY
1	D	70	SER
1	D	226	ALA
1	A	70	SER
1	D	121	SER
1	D	224	TYR

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	147/159 (92%)	118 (80%)	29 (20%)	1	2
1	B	79/159 (50%)	68 (86%)	11 (14%)	3	7
1	C	77/159 (48%)	64 (83%)	13 (17%)	2	4
1	D	140/159 (88%)	113 (81%)	27 (19%)	1	2
All	All	443/636 (70%)	363 (82%)	80 (18%)	2	3

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	SER
1	A	94	GLU
1	A	99	VAL
1	A	105	MET

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Mol	Chain	Res	Type
1	A	106	LEU
1	A	127	GLN
1	A	129	LYS
1	A	134	VAL
1	A	136	LYS
1	A	142	LEU
1	A	146	THR
1	A	159	ASP
1	A	164	VAL
1	A	167	LYS
1	A	169	GLN
1	A	171	HIS
1	A	175	LYS
1	A	179	LEU
1	A	182	GLU
1	A	188	THR
1	A	193	LEU
1	A	196	LEU
1	A	201	ASN
1	A	202	GLN
1	A	205	LEU
1	A	211	LEU
1	A	215	MET
1	A	232	LYS
1	A	243	PHE
1	B	73	MET
1	B	74	LEU
1	B	81	GLU
1	B	99	VAL
1	B	105	MET
1	B	106	LEU
1	B	108	ASN
1	B	110	LEU
1	B	111	ILE
1	B	136	LYS
1	B	167	LYS
1	C	74	LEU
1	C	81	GLU
1	C	95	HIS
1	C	99	VAL
1	C	101	VAL
1	C	104	ASP

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Mol	Chain	Res	Type
1	C	106	LEU
1	C	108	ASN
1	C	134	VAL
1	C	147	ASP
1	C	164	VAL
1	C	167	LYS
1	C	169	GLN
1	D	81	GLU
1	D	99	VAL
1	D	101	VAL
1	D	104	ASP
1	D	106	LEU
1	D	109	GLN
1	D	121	SER
1	D	122	HIS
1	D	129	LYS
1	D	131	LEU
1	D	136	LYS
1	D	143	SER
1	D	150	ASP
1	D	167	LYS
1	D	176	LEU
1	D	179	LEU
1	D	182	GLU
1	D	193	LEU
1	D	194	LYS
1	D	196	LEU
1	D	197	LEU
1	D	199	ASP
1	D	203	SER
1	D	204	SER
1	D	211	LEU
1	D	213	GLN
1	D	220	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	127	GLN
1	A	169	GLN
1	A	186	HIS

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Mol	Chain	Res	Type
1	A	213	GLN
1	A	234	GLN
1	B	82	HIS
1	B	95	HIS
1	B	108	ASN
1	B	127	GLN
1	B	133	GLN
1	B	138	ASN
1	B	169	GLN
1	C	108	ASN
1	C	109	GLN
1	C	162	HIS
1	C	169	GLN
1	D	162	HIS
1	D	169	GLN
1	D	183	GLN
1	D	186	HIS
1	D	234	GLN
1	D	242	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 ⓘ

There are no ligands in this entry.

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 ⓘ

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	169/180 (93%)	0.87	20 (11%) 9 7	39, 67, 89, 103	0
1	B	94/180 (52%)	0.61	11 (11%) 9 7	40, 58, 94, 109	0
1	C	92/180 (51%)	0.97	15 (16%) 4 3	53, 67, 87, 95	0
1	D	169/180 (93%)	1.05	26 (15%) 5 4	47, 72, 95, 106	0
All	All	524/720 (72%)	0.90	72 (13%) 6 5	39, 67, 92, 109	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	HIS	6.2
1	A	243	PHE	5.3
1	C	69	GLY	5.2
1	D	82	HIS	4.8
1	C	171	HIS	4.7
1	D	171	HIS	4.5
1	A	69	GLY	4.2
1	A	67	GLY	4.2
1	D	208	GLU	3.9
1	C	129	LYS	3.8
1	C	82	HIS	3.8
1	C	94	GLU	3.6
1	D	174	PRO	3.5
1	A	128	ALA	3.3
1	C	113	MET	3.3
1	D	223	THR	3.3
1	A	82	HIS	3.3
1	B	127	GLN	3.1
1	D	83	TYR	3.1
1	A	112	GLU	3.1
1	C	81	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	169	GLN	3.0
1	D	84	GLU	3.0
1	D	94	GLU	3.0
1	D	246	THR	3.0
1	A	208	GLU	2.9
1	C	70	SER	2.9
1	D	95	HIS	2.9
1	D	102	ARG	2.9
1	D	222	SER	2.8
1	A	92	LYS	2.7
1	D	122	HIS	2.7
1	D	226	ALA	2.7
1	C	128	ALA	2.7
1	B	93	GLU	2.7
1	C	95	HIS	2.6
1	D	68	PRO	2.6
1	D	173	CYS	2.5
1	D	203	SER	2.5
1	A	221	ASN	2.5
1	D	121	SER	2.4
1	C	127	GLN	2.4
1	B	128	ALA	2.4
1	A	173	CYS	2.3
1	A	171	HIS	2.3
1	C	167	LYS	2.3
1	A	178	ASP	2.3
1	A	81	GLU	2.3
1	B	81	GLU	2.3
1	A	244	LYS	2.2
1	B	68	PRO	2.2
1	A	159	ASP	2.2
1	B	82	HIS	2.2
1	B	150	ASP	2.2
1	B	129	LYS	2.2
1	D	126	ALA	2.2
1	A	187	THR	2.2
1	C	122	HIS	2.2
1	A	94	GLU	2.2
1	B	94	GLU	2.2
1	B	149	PRO	2.2
1	D	201	ASN	2.2
1	D	123	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	230	ALA	2.1
1	A	127	GLN	2.1
1	C	170	LEU	2.1
1	D	224	TYR	2.1
1	A	172	SER	2.1
1	D	215	MET	2.1
1	D	225	TYR	2.0
1	D	200	MET	2.0
1	A	122	HIS	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.