WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 01:42 am GMT

PDB ID	:	1QMV
Title	:	thioredoxin peroxidase B from red blood cells
Authors	:	Isupov, M.N.; Littlechild, J.A.; Lebedev, A.A.; Errington, N.; Vagin, A.A.; Schroder, E.
Deposited on	:	1999-10-07
Resolution	:	1.70 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.70 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.
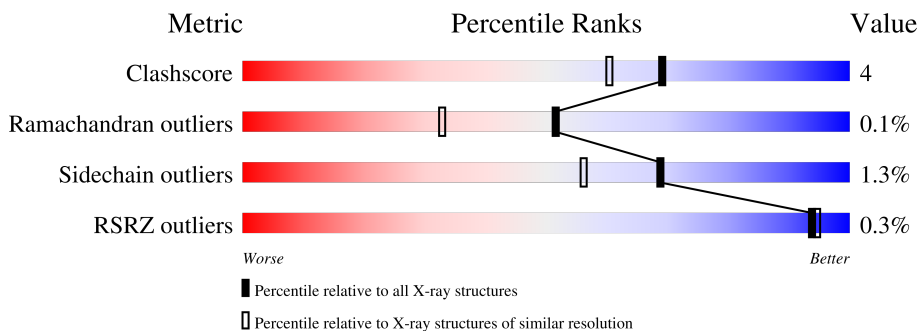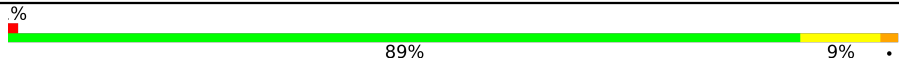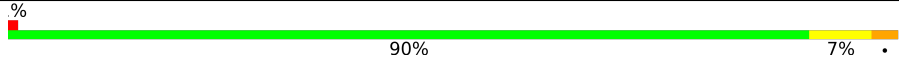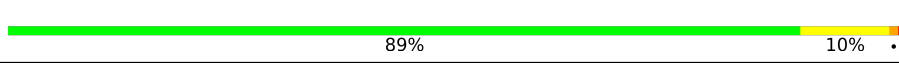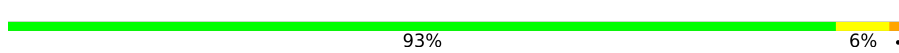
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	197	88% / 10% ••
1	B	197	92% / 6% •
1	C	197	88% / 11% ••
1	D	197	87% / 10% •
1	E	197	92% / 6% •
1	F	197	89% / 11%

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	197	89% 9%
1	H	197	90% 7%
1	I	197	89% 10%
1	J	197	93% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	NCB	A	2	-	X	-	-
1	NCB	B	2	X	-	-	-
1	NCB	D	2	X	-	-	-
1	NCB	E	2	X	X	-	-
1	NCB	F	2	X	-	-	-
1	NCB	G	2	X	-	-	-
1	NCB	H	2	-	X	-	-
1	NCB	I	2	X	-	-	-
1	NCB	J	2	X	X	-	-

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 17634 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 PEROXIREDOXIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1544	987	261	293	3			
1	B	197	Total	C	N	O	S	0	0	0
			1544	987	261	293	3			
1	C	197	Total	C	N	O	S	0	0	0
			1544	987	261	293	3			
1	D	197	Total	C	N	O	S	0	0	0
			1544	987	261	293	3			
1	E	197	Total	C	N	O	S	0	0	0
			1544	987	261	293	3			
1	F	197	Total	C	N	O	S	0	0	0
			1544	987	261	293	3			
1	G	197	Total	C	N	O	S	0	0	0
			1544	987	261	293	3			
1	H	197	Total	C	N	O	S	0	0	0
			1544	987	261	293	3			
1	I	197	Total	C	N	O	S	0	0	0
			1544	987	261	293	3			
1	J	197	Total	C	N	O	S	0	0	0
			1544	987	261	293	3			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	206	Total	O	0	0
			206	206		
2	B	204	Total	O	0	0
			204	204		
2	C	250	Total	O	0	0
			250	250		
2	D	228	Total	O	0	0
			228	228		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	254	Total 254	O 254	0	0
2	F	226	Total 226	O 226	0	0
2	G	184	Total 184	O 184	0	0
2	H	216	Total 216	O 216	0	0
2	I	183	Total 183	O 183	0	0
2	J	243	Total 243	O 243	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: PEROXIREDOXIN-2

Chain A:
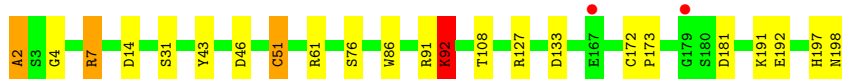
- Molecule 1: PEROXIREDOXIN-2

Chain B:
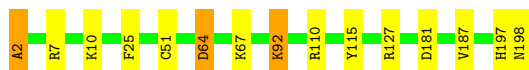
- Molecule 1: PEROXIREDOXIN-2

Chain C:
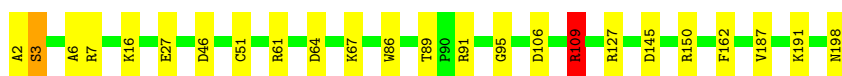
- Molecule 1: PEROXIREDOXIN-2

Chain D:
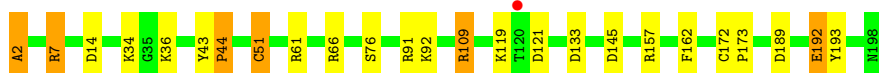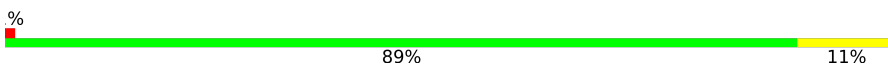
- Molecule 1: PEROXIREDOXIN-2

Chain E:
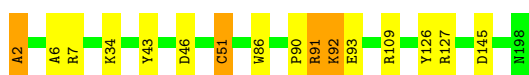
- Molecule 1: PEROXIREDOXIN-2

Chain F:

A2 F15 K16 K29 L30 S31 D32 Y33 K34 D46 C51 R61 R66 W86 R91 R109 D133 G169 C172 P173 K177 I183 E192 Y193 N198

• Molecule 1: PEROXIREDOXIN-2

Chain G:

89%　　　　　　9%

A2 R7 D32 Y43 P44 C51 R61 S76 R91 K92 N100 R109 G116 R150 Y164 E167 C172 P173 K177 T182 E192 S195 K196 H197 N198

• Molecule 1: PEROXIREDOXIN-2

Chain H:

90%　　　　　　7%

A2 R7 K26 Y43 D46 C51 R61 W86 L96 N100 R109 R127 V152 C172 P173 D181 D189 E192 H197 N198

• Molecule 1: PEROXIREDOXIN-2

Chain I:

89%　　　　　　10%

A2 Y43 C51 R61 S76 K92 L96 L99 N100 V107 T108 R109 R127 D145 V152 T165 E170 D181 D189 E192 Y193 H197 N198

• Molecule 1: PEROXIREDOXIN-2

Chain J:

93%　　　　　　6%

A2 R7 K26 K36 Y43 C51 P52 E63 E71 V75 L104 D181 K196 H197 N198

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.88Å　　107.03Å　　119.50Å 90.00°　　110.87°　　90.00°	Depositor
Resolution (Å)	20.00　–　1.70 19.99　–　1.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-1.70) 99.6 (19.99-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192　,　　　0.256 0.179　,　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.750	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 69.8	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	17634	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CSD, NCB

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	0.59	1/1564 (0.1%)	1.38	12/2119 (0.6%)
1	B	0.52	0/1564	1.14	5/2119 (0.2%)
1	C	0.57	0/1564	1.22	10/2119 (0.5%)
1	D	0.57	0/1564	1.27	14/2119 (0.7%)
1	E	0.59	0/1564	1.19	7/2119 (0.3%)
1	F	0.59	0/1564	1.20	5/2119 (0.2%)
1	G	0.53	0/1564	1.19	8/2119 (0.4%)
1	H	0.58	0/1564	1.18	8/2119 (0.4%)
1	I	0.53	0/1564	1.12	6/2119 (0.3%)
1	J	0.52	0/1564	1.13	1/2119 (0.0%)
All	All	0.56	1/15640 (0.0%)	1.20	76/21190 (0.4%)

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	B	1	0
1	D	1	0
1	E	1	0
1	F	1	0
1	G	1	0
1	I	1	0
1	J	1	0
All	All	7	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	ARG	CD-NE	-6.13	1.36	1.46

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	ARG	CG-CD-NE	23.61	161.38	111.80
1	A	61	ARG	CD-NE-CZ	14.57	144.00	123.60
1	G	109	ARG	NE-CZ-NH1	10.66	125.63	120.30
1	A	127	ARG	NE-CZ-NH2	-9.83	115.39	120.30
1	A	7	ARG	CD-NE-CZ	9.24	136.54	123.60
1	A	7	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	C	109	ARG	CD-NE-CZ	8.63	135.68	123.60
1	D	91	ARG	NE-CZ-NH1	-8.60	116.00	120.30
1	I	109	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	H	7	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	G	61	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	C	61	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	I	109	ARG	CD-NE-CZ	7.75	134.46	123.60
1	D	61	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	D	66	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	G	109	ARG	CD-NE-CZ	7.55	134.17	123.60
1	D	109	ARG	CD-NE-CZ	7.46	134.05	123.60
1	E	91	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	H	109	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	C	150	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	D	66	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	D	7	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	F	91	ARG	CD-NE-CZ	7.06	133.49	123.60
1	A	61	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	E	145	ASP	CB-CG-OD1	6.73	124.36	118.30
1	E	127	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	61	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	115	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	F	133	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	192	GLU	CA-CB-CG	6.48	127.66	113.40
1	H	61	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	92	LYS	CG-CD-CE	6.25	130.66	111.90
1	D	145	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	E	126	TYR	CB-CG-CD1	-6.10	117.34	121.00
1	H	127	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	G	150	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	61	ARG	CD-NE-CZ	5.98	131.97	123.60
1	C	127	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	G	61	ARG	CD-NE-CZ	5.87	131.82	123.60
1	D	145	ASP	CB-CG-OD1	5.83	123.55	118.30
1	I	145	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	106	ASP	CB-CG-OD1	5.79	123.51	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	TYR	CB-CG-CD2	5.72	124.44	121.00
1	G	109	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	192	GLU	CA-CB-CG	5.66	125.84	113.40
1	H	7	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	F	192	GLU	CA-CB-CG	5.58	125.67	113.40
1	I	145	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	D	14	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	64	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	D	133	ASP	CB-CG-OD1	5.47	123.22	118.30
1	H	127	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	133	ASP	CB-CG-OD1	5.45	123.20	118.30
1	I	127	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	127	ARG	CG-CD-NE	-5.42	100.41	111.80
1	E	91	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	C	91	ARG	CD-NE-CZ	5.36	131.10	123.60
1	A	127	ARG	CG-CD-NE	-5.35	100.56	111.80
1	H	127	ARG	CG-CD-NE	-5.34	100.59	111.80
1	G	76	SER	N-CA-CB	5.33	118.50	110.50
1	C	145	ASP	CB-CG-OD1	5.33	123.09	118.30
1	F	61	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	3	SER	CA-C-O	-5.29	108.99	120.10
1	D	157	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	E	145	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	I	127	ARG	CG-CD-NE	-5.16	100.97	111.80
1	F	66	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	H	7	ARG	CD-NE-CZ	5.13	130.78	123.60
1	E	127	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	D	162	PHE	CB-CG-CD1	-5.11	117.23	120.80
1	G	32	ASP	CB-CG-OD1	5.09	122.88	118.30
1	C	162	PHE	CB-CG-CD1	-5.06	117.26	120.80
1	B	25	PHE	CB-CG-CD1	5.05	124.34	120.80
1	J	197	HIS	CA-CB-CG	-5.01	105.08	113.60
1	A	14	ASP	CB-CG-OD1	5.00	122.81	118.30
1	B	110	ARG	NE-CZ-NH2	-5.00	117.80	120.30

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	2	NCB	CA
1	D	2	NCB	CA
1	E	2	NCB	CA
1	F	2	NCB	CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
1	G	2	NCB	CA
1	I	2	NCB	CA
1	J	2	NCB	CA

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	1544	0	1525	19	0
1	B	1544	0	1525	10	0
1	C	1544	0	1524	9	0
1	D	1544	0	1523	9	0
1	E	1544	0	1525	13	0
1	F	1544	0	1525	11	0
1	G	1544	0	1524	12	0
1	H	1544	0	1524	13	0
1	I	1544	0	1525	13	0
1	J	1544	0	1524	11	0
2	A	206	0	0	5	0
2	B	204	0	0	1	0
2	C	250	0	0	1	0
2	D	228	0	0	3	0
2	E	254	0	0	0	0
2	F	226	0	0	3	0
2	G	184	0	0	1	0
2	H	216	0	0	3	0
2	I	183	0	0	1	0
2	J	243	0	0	4	0
All	All	17634	0	15244	113	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 4.

All (113) 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:92:LYS:H	1:A:92:LYS:HD2	1.14	1.11
1:J:2:NCB:HB1	1:J:7:ARG:HD3	1.52	0.92
1:A:92:LYS:HD3	2:A:2050:HOH:O	1.77	0.84
1:A:92:LYS:HD2	1:A:92:LYS:N	1.98	0.76
1:B:92:LYS:H	1:B:92:LYS:HE2	1.49	0.75
1:I:92:LYS:H	1:I:92:LYS:HE2	1.50	0.75
1:F:16:LYS:HB3	1:F:29:LYS:HG2	1.70	0.71
1:F:16:LYS:CB	1:F:29:LYS:HG2	2.20	0.71
1:B:2:NCB:HA	1:B:7:ARG:HD3	1.72	0.71
1:F:29:LYS:O	1:F:32:ASP:HB2	1.93	0.69
1:H:189:ASP:O	1:H:192:GLU:HG2	1.94	0.67
1:C:109:ARG:NH1	1:H:109:ARG:HD3	2.11	0.65
1:E:92:LYS:H	1:E:92:LYS:CD	2.08	0.65
1:A:92:LYS:H	1:A:92:LYS:CD	1.96	0.63
1:E:2:NCB:HA	1:E:6:ALA:O	1.98	0.63
1:C:64:ASP:HA	1:C:67:LYS:HE2	1.80	0.62
1:I:92:LYS:H	1:I:92:LYS:CE	2.14	0.61
1:D:36:LYS:HE3	2:D:2045:HOH:O	2.01	0.61
1:D:189:ASP:O	1:D:192:GLU:HG2	2.01	0.61
1:B:92:LYS:H	1:B:92:LYS:CE	2.15	0.59
1:E:90:PRO:HG2	1:E:93:GLU:OE2	2.02	0.59
1:G:116:GLY:O	1:H:2:NCB:HB2	2.02	0.59
1:G:192:GLU:O	1:G:196:LYS:HG3	2.02	0.59
1:G:92:LYS:HE2	1:G:92:LYS:H	1.68	0.58
1:E:91:ARG:N	1:E:92:LYS:HE3	2.18	0.58
1:H:61:ARG:HG3	1:H:152:VAL:HG11	1.87	0.57
1:A:91:ARG:H	1:A:92:LYS:NZ	2.03	0.57
1:H:26:LYS:HD2	2:H:2046:HOH:O	2.05	0.56
1:E:92:LYS:H	1:E:92:LYS:CE	2.19	0.55
1:A:198:ASN:HB3	1:B:92:LYS:HD3	1.90	0.54
1:J:43:TYR:HB2	1:J:51:CSD:OD1	2.08	0.53
1:I:192:GLU:HG3	1:I:193:TYR:N	2.24	0.53
1:D:2:NCB:HB2	2:D:2001:HOH:O	2.09	0.53
1:E:2:NCB:HB3	1:E:7:ARG:NH1	2.25	0.52
1:G:91:ARG:N	1:G:92:LYS:HE2	2.25	0.52
1:A:2:NCB:HB1	1:A:7:ARG:HG2	1.91	0.51
1:E:92:LYS:HE2	2:F:2223:HOH:O	2.10	0.51
1:B:64:ASP:HA	1:B:67:LYS:HE2	1.92	0.51
1:I:92:LYS:H	1:I:92:LYS:CD	2.22	0.51
1:A:91:ARG:H	1:A:92:LYS:HZ2	1.60	0.50
1:D:34:LYS:HD2	2:D:2049:HOH:O	2.12	0.50
1:J:71:GLU:HB3	2:J:2110:HOH:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ARG:NH1	2:F:2133:HOH:O	2.45	0.49
1:C:198:ASN:OXT	1:D:92:LYS:HE2	2.11	0.49
1:A:4:GLY:HA2	2:A:2002:HOH:O	2.11	0.49
1:A:191:LYS:HE3	2:A:2189:HOH:O	2.13	0.49
1:A:108:THR:HG23	2:A:2119:HOH:O	2.13	0.49
1:F:16:LYS:HB2	1:F:29:LYS:HG2	1.93	0.49
1:H:109:ARG:NH1	2:H:2130:HOH:O	2.46	0.49
1:H:43:TYR:HB2	1:H:51:CSD:OD1	2.12	0.49
1:I:96:LEU:HD13	1:I:99:LEU:HD11	1.94	0.48
1:G:92:LYS:H	1:G:92:LYS:CD	2.26	0.48
1:A:46:ASP:HA	1:A:86:TRP:CZ3	2.49	0.48
1:B:7:ARG:CB	1:B:10:LYS:HD2	2.44	0.48
1:E:91:ARG:H	1:E:92:LYS:HE3	1.79	0.48
1:J:181:ASP:OD2	1:J:196:LYS:HE3	2.14	0.47
1:G:164:TYR:CE2	1:G:182:THR:HG21	2.50	0.47
1:C:187:VAL:O	1:C:191:LYS:HE2	2.15	0.47
1:G:177:LYS:HE3	2:G:2163:HOH:O	2.13	0.47
1:A:43:TYR:HB2	1:A:51:CSD:OD1	2.15	0.47
1:B:187:VAL:HG23	2:B:2196:HOH:O	2.15	0.47
1:J:2:NCB:CB	1:J:7:ARG:HD3	2.33	0.47
1:G:44:PRO:HD2	1:G:51:CSD:OD1	2.16	0.46
1:I:61:ARG:HG3	1:I:152:VAL:HG11	1.96	0.46
1:A:92:LYS:HG3	1:B:198:ASN:HB2	1.97	0.46
1:F:109:ARG:HD3	1:I:109:ARG:NH1	2.31	0.46
1:H:7:ARG:HD2	2:H:2004:HOH:O	2.15	0.45
1:C:187:VAL:HG23	2:C:2231:HOH:O	2.15	0.45
1:H:181:ASP:OD2	1:H:197:HIS:NE2	2.41	0.45
1:I:181:ASP:OD2	1:I:197:HIS:NE2	2.47	0.45
1:A:2:NCB:HA	2:A:2001:HOH:O	2.17	0.45
1:J:36:LYS:HE3	2:J:2111:HOH:O	2.17	0.45
1:A:181:ASP:OD2	1:A:197:HIS:NE2	2.49	0.44
1:C:46:ASP:HA	1:C:86:TRP:CZ3	2.52	0.44
1:E:92:LYS:H	1:E:92:LYS:HE3	1.82	0.44
1:C:16:LYS:HE2	1:C:27:GLU:CD	2.37	0.44
1:E:46:ASP:HA	1:E:86:TRP:CZ3	2.53	0.44
1:H:86:TRP:CE3	1:H:96:LEU:HD11	2.53	0.44
1:H:172:CYS:HA	1:H:173:PRO:HD3	1.89	0.44
1:E:2:NCB:O3	1:E:2:NCB:HB1	2.17	0.44
1:I:43:TYR:CZ	1:I:76:SER:HB3	2.53	0.44
1:G:92:LYS:H	1:G:92:LYS:CE	2.29	0.43
1:G:2:NCB:HA	1:G:7:ARG:HD3	2.00	0.43

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:165:THR:HG22	1:I:170:GLU:O	2.18	0.43
1:E:43:TYR:HB2	1:E:51:CSD:OD1	2.18	0.43
1:F:183:ILE:HG12	1:F:193:TYR:CG	2.54	0.43
1:F:177:LYS:HD2	2:F:2092:HOH:O	2.19	0.42
1:I:92:LYS:NZ	2:J:2239:HOH:O	2.51	0.42
1:J:2:NCB:HB2	2:J:2001:HOH:O	2.19	0.42
1:J:181:ASP:OD2	1:J:197:HIS:NE2	2.48	0.42
1:B:181:ASP:OD2	1:B:197:HIS:NE2	2.51	0.42
1:C:89:THR:O	1:C:95:GLY:HA3	2.19	0.42
1:J:51:CSD:HB3	1:J:52:PRO:CD	2.49	0.42
1:C:6:ALA:O	1:C:7:ARG:HG3	2.20	0.42
1:G:43:TYR:HB2	1:G:51:CSD:OD1	2.19	0.42
1:J:51:CSD:HB3	1:J:52:PRO:HD3	2.01	0.42
1:A:43:TYR:CZ	1:A:76:SER:HB3	2.54	0.42
1:E:92:LYS:H	1:E:92:LYS:HD2	1.81	0.42
1:H:46:ASP:HA	1:H:86:TRP:CZ3	2.54	0.42
1:F:172:CYS:HA	1:F:173:PRO:HD3	1.92	0.42
1:F:46:ASP:HA	1:F:86:TRP:CZ3	2.55	0.41
1:H:7:ARG:HG2	1:H:7:ARG:HH11	1.85	0.41
1:D:119:LYS:HG2	1:D:121:ASP:OD1	2.21	0.41
1:A:172:CYS:HA	1:A:173:PRO:HD3	1.97	0.41
1:J:75:VAL:HB	1:J:104:LEU:HB2	2.03	0.41
1:D:44:PRO:HD2	1:D:51:CSD:OD1	2.19	0.41
1:D:43:TYR:CZ	1:D:76:SER:HB3	2.56	0.41
1:I:107:VAL:HG23	2:I:2110:HOH:O	2.21	0.41
1:I:189:ASP:O	1:I:192:GLU:HG2	2.21	0.41
1:A:92:LYS:HG3	1:B:198:ASN:CB	2.51	0.41
1:G:172:CYS:HA	1:G:173:PRO:HD3	1.97	0.41
1:F:15:PHE:CE2	1:F:30:LEU:HB2	2.56	0.40
1:D:172:CYS:HA	1:D:173:PRO:HD3	1.96	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	194/197 (98%)	190 (98%)	4 (2%)	0	100	100
1	B	194/197 (98%)	189 (97%)	5 (3%)	0	100	100
1	C	194/197 (98%)	189 (97%)	5 (3%)	0	100	100
1	D	194/197 (98%)	190 (98%)	3 (2%)	1 (0%)	29	13
1	E	194/197 (98%)	190 (98%)	4 (2%)	0	100	100
1	F	194/197 (98%)	190 (98%)	4 (2%)	0	100	100
1	G	194/197 (98%)	188 (97%)	6 (3%)	0	100	100
1	H	194/197 (98%)	190 (98%)	4 (2%)	0	100	100
1	I	194/197 (98%)	190 (98%)	4 (2%)	0	100	100
1	J	194/197 (98%)	188 (97%)	6 (3%)	0	100	100
All	All	1940/1970 (98%)	1894 (98%)	45 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	44	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	164/164 (100%)	162 (99%)	2 (1%)	71	59
1	B	164/164 (100%)	163 (99%)	1 (1%)	86	80
1	C	164/164 (100%)	162 (99%)	2 (1%)	71	59
1	D	164/164 (100%)	162 (99%)	2 (1%)	71	59
1	E	164/164 (100%)	161 (98%)	3 (2%)	59	43
1	F	164/164 (100%)	163 (99%)	1 (1%)	86	80
1	G	164/164 (100%)	160 (98%)	4 (2%)	49	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	H	164/164 (100%)	163 (99%)	1 (1%)	86	80	
1	I	164/164 (100%)	161 (98%)	3 (2%)	59	43	
1	J	164/164 (100%)	162 (99%)	2 (1%)	71	59	
All	All	1640/1640 (100%)	1619 (99%)	21 (1%)	69	56	

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	92	LYS
1	B	92	LYS
1	C	3	SER
1	C	109	ARG
1	D	7	ARG
1	D	109	ARG
1	E	34	LYS
1	E	92	LYS
1	E	109	ARG
1	F	34	LYS
1	G	92	LYS
1	G	100	ASN
1	G	109	ARG
1	G	167	GLU
1	H	100	ASN
1	I	92	LYS
1	I	100	ASN
1	I	109	ARG
1	J	26	LYS
1	J	63	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	160	GLN
1	G	100	ASN
1	H	100	ASN
1	I	100	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

20 non-standard protein/DNA/RNA residues are modelled in this entry.

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	#$|Z| > 2$
1	CSD	H	51	1	3,7,8	1.14	0	1,8,10	4.96	1 (100%)
1	NCB	G	2	1	6,7,8	1.33	1 (16%)	5,8,10	4.48	3 (60%)
1	NCB	E	2	1	6,7,8	1.26	1 (16%)	5,8,10	3.71	4 (80%)
1	NCB	C	2	1	6,7,8	1.73	2 (33%)	5,8,10	4.51	4 (80%)
1	NCB	A	2	1	6,7,8	1.82	3 (50%)	5,8,10	5.76	4 (80%)
1	CSD	A	51	1	3,7,8	1.32	0	1,8,10	3.64	1 (100%)
1	CSD	E	51	1	3,7,8	1.09	0	1,8,10	4.67	1 (100%)
1	CSD	B	51	1	3,7,8	0.83	0	1,8,10	3.81	1 (100%)
1	CSD	D	51	1	3,7,8	1.93	1 (33%)	1,8,10	3.79	1 (100%)
1	CSD	C	51	1	3,7,8	0.83	0	1,8,10	3.92	1 (100%)
1	NCB	I	2	1	6,7,8	1.29	1 (16%)	5,8,10	3.81	3 (60%)
1	CSD	I	51	1	3,7,8	1.24	0	1,8,10	4.19	1 (100%)
1	CSD	J	51	1	3,7,8	2.28	1 (33%)	1,8,10	2.33	1 (100%)
1	CSD	F	51	1	3,7,8	0.90	0	1,8,10	6.24	1 (100%)
1	NCB	B	2	1	6,7,8	1.17	1 (16%)	5,8,10	3.42	4 (80%)
1	NCB	H	2	1	6,7,8	2.10	3 (50%)	5,8,10	6.48	5 (100%)
1	NCB	J	2	1	6,7,8	1.71	2 (33%)	5,8,10	6.54	3 (60%)
1	NCB	F	2	1	6,7,8	1.60	1 (16%)	5,8,10	5.73	3 (60%)
1	CSD	G	51	1	3,7,8	1.40	1 (33%)	1,8,10	4.71	1 (100%)
1	NCB	D	2	1	6,7,8	1.45	1 (16%)	5,8,10	6.56	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	H	51	1	-	0/2/6/8	-
1	NCB	G	2	1	1/1/2/4	3/4/6/8	-
1	NCB	E	2	1	1/1/2/4	4/4/6/8	-
1	NCB	C	2	1	-	2/4/6/8	-
1	NCB	A	2	1	-	2/4/6/8	-
1	CSD	A	51	1	-	0/2/6/8	-
1	CSD	E	51	1	-	0/2/6/8	-
1	CSD	B	51	1	-	0/2/6/8	-
1	CSD	D	51	1	-	0/2/6/8	-
1	CSD	C	51	1	-	0/2/6/8	-
1	NCB	I	2	1	1/1/2/4	3/4/6/8	-
1	CSD	I	51	1	-	0/2/6/8	-
1	CSD	J	51	1	-	0/2/6/8	-
1	CSD	F	51	1	-	0/2/6/8	-
1	NCB	B	2	1	1/1/2/4	3/4/6/8	-
1	NCB	H	2	1	-	2/4/6/8	-
1	NCB	J	2	1	1/1/2/4	4/4/6/8	-
1	NCB	F	2	1	1/1/2/4	4/4/6/8	-
1	CSD	G	51	1	-	0/2/6/8	-
1	NCB	D	2	1	1/1/2/4	4/4/6/8	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	51	CSD	CB-SG	3.66	1.99	1.79
1	H	2	NCB	CA-N	-3.54	1.42	1.46
1	F	2	NCB	O3-C3	3.06	1.29	1.24
1	D	51	CSD	CB-SG	3.06	1.96	1.79
1	H	2	NCB	O-C	2.99	1.31	1.19
1	C	2	NCB	O-C	2.90	1.31	1.19
1	J	2	NCB	CA-N	-2.84	1.43	1.46
1	C	2	NCB	CA-N	-2.74	1.43	1.46
1	A	2	NCB	CA-N	-2.73	1.43	1.46
1	A	2	NCB	O3-C3	2.40	1.28	1.24
1	A	2	NCB	O-C	2.33	1.29	1.19
1	I	2	NCB	O-C	2.28	1.29	1.19
1	H	2	NCB	O3-C3	2.18	1.27	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2	NCB	O3-C3	2.15	1.27	1.24
1	B	2	NCB	O-C	2.13	1.28	1.19
1	J	2	NCB	O3-C3	2.10	1.27	1.24
1	G	51	CSD	CB-SG	2.08	1.90	1.79
1	D	2	NCB	O-C	2.08	1.28	1.19
1	G	2	NCB	O-C	2.06	1.28	1.19

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	2	NCB	CB-CA-N	13.26	124.34	109.61
1	D	2	NCB	CB-CA-N	13.08	124.14	109.61
1	F	2	NCB	CB-CA-N	11.56	122.45	109.61
1	H	2	NCB	CB-CA-N	10.07	120.80	109.61
1	A	2	NCB	CB-CA-N	8.92	119.52	109.61
1	C	2	NCB	CB-CA-N	8.63	119.20	109.61
1	G	2	NCB	CB-CA-N	8.63	119.20	109.61
1	A	2	NCB	N2-C3-N	7.74	134.11	116.77
1	H	2	NCB	N2-C3-N	7.37	133.28	116.77
1	I	2	NCB	CB-CA-N	7.06	117.45	109.61
1	F	51	CSD	OD1-SG-CB	-6.24	93.66	105.54
1	D	2	NCB	N2-C3-N	5.27	128.58	116.77
1	E	2	NCB	CB-CA-N	5.16	115.34	109.61
1	H	51	CSD	OD1-SG-CB	-4.96	96.11	105.54
1	J	2	NCB	N2-C3-N	4.87	127.68	116.77
1	H	2	NCB	O3-C3-N2	-4.83	114.92	123.22
1	B	2	NCB	N2-C3-N	4.78	127.48	116.77
1	G	51	CSD	OD1-SG-CB	-4.71	96.57	105.54
1	E	51	CSD	OD1-SG-CB	-4.67	96.64	105.54
1	H	2	NCB	CA-N-C3	4.61	130.19	121.15
1	A	2	NCB	O3-C3-N	-4.54	106.69	121.45
1	I	51	CSD	OD1-SG-CB	-4.19	97.57	105.54
1	B	2	NCB	O3-C3-N	-4.17	107.91	121.45
1	E	2	NCB	O3-C3-N	-4.14	107.98	121.45
1	C	2	NCB	N2-C3-N	4.09	125.94	116.77
1	F	2	NCB	N2-C3-N	4.09	125.94	116.77
1	C	51	CSD	OD1-SG-CB	-3.92	98.08	105.54
1	B	51	CSD	OD1-SG-CB	-3.81	98.29	105.54
1	D	2	NCB	O3-C3-N	-3.80	109.10	121.45
1	D	51	CSD	OD1-SG-CB	-3.79	98.32	105.54
1	F	2	NCB	O3-C3-N	-3.68	109.49	121.45
1	A	51	CSD	OD1-SG-CB	-3.64	98.61	105.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	2	NCB	N2-C3-N	3.60	124.83	116.77
1	E	2	NCB	N2-C3-N	3.58	124.80	116.77
1	G	2	NCB	N2-C3-N	3.50	124.60	116.77
1	H	2	NCB	O3-C3-N	-3.14	111.25	121.45
1	I	2	NCB	O3-C3-N	-3.14	111.25	121.45
1	E	2	NCB	CA-N-C3	-3.12	115.03	121.15
1	G	2	NCB	O3-C3-N	-3.09	111.42	121.45
1	J	2	NCB	O3-C3-N	-3.02	111.63	121.45
1	B	2	NCB	CA-N-C3	-2.97	115.32	121.15
1	B	2	NCB	CB-CA-N	2.94	112.88	109.61
1	C	2	NCB	O3-C3-N2	-2.40	119.09	123.22
1	A	2	NCB	O3-C3-N2	-2.34	119.20	123.22
1	J	51	CSD	OD1-SG-CB	-2.33	101.09	105.54
1	C	2	NCB	O3-C3-N	-2.09	114.68	121.45

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	2	NCB	CA
1	D	2	NCB	CA
1	E	2	NCB	CA
1	F	2	NCB	CA
1	G	2	NCB	CA
1	I	2	NCB	CA
1	J	2	NCB	CA

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2	NCB	O3-C3-N-CA
1	A	2	NCB	N2-C3-N-CA
1	B	2	NCB	CB-CA-N-C3
1	B	2	NCB	O3-C3-N-CA
1	B	2	NCB	N2-C3-N-CA
1	D	2	NCB	CB-CA-N-C3
1	D	2	NCB	O3-C3-N-CA
1	D	2	NCB	N2-C3-N-CA
1	E	2	NCB	CB-CA-N-C3
1	E	2	NCB	O3-C3-N-CA
1	E	2	NCB	N2-C3-N-CA
1	F	2	NCB	CB-CA-N-C3
1	F	2	NCB	O3-C3-N-CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	G	2	NCB	CB-CA-N-C3
1	G	2	NCB	O3-C3-N-CA
1	G	2	NCB	N2-C3-N-CA
1	I	2	NCB	CB-CA-N-C3
1	I	2	NCB	O3-C3-N-CA
1	I	2	NCB	N2-C3-N-CA
1	J	2	NCB	CB-CA-N-C3
1	J	2	NCB	O3-C3-N-CA
1	J	2	NCB	N2-C3-N-CA
1	F	2	NCB	N2-C3-N-CA
1	H	2	NCB	O3-C3-N-CA
1	D	2	NCB	C-CA-N-C3
1	E	2	NCB	C-CA-N-C3
1	F	2	NCB	C-CA-N-C3
1	J	2	NCB	C-CA-N-C3
1	C	2	NCB	O3-C3-N-CA
1	C	2	NCB	N2-C3-N-CA
1	H	2	NCB	N2-C3-N-CA

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	51	CSD	1	0
1	G	2	NCB	1	0
1	E	2	NCB	3	0
1	A	2	NCB	2	0
1	A	51	CSD	1	0
1	E	51	CSD	1	0
1	D	51	CSD	1	0
1	J	51	CSD	3	0
1	B	2	NCB	1	0
1	H	2	NCB	1	0
1	J	2	NCB	3	0
1	G	51	CSD	2	0
1	D	2	NCB	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides 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	195/197 (98%)	-0.20	2 (1%)	82	85	21, 30, 47, 54	0
1	B	195/197 (98%)	-0.26	0	100	100	21, 29, 46, 55	0
1	C	195/197 (98%)	-0.35	0	100	100	20, 27, 41, 50	0
1	D	195/197 (98%)	-0.36	1 (0%)	91	92	21, 27, 42, 52	0
1	E	195/197 (98%)	-0.44	0	100	100	21, 25, 38, 54	0
1	F	195/197 (98%)	-0.25	1 (0%)	91	92	20, 28, 45, 51	0
1	G	195/197 (98%)	0.00	1 (0%)	91	92	21, 34, 50, 60	0
1	H	195/197 (98%)	-0.29	1 (0%)	91	92	21, 28, 43, 56	0
1	I	195/197 (98%)	-0.22	0	100	100	21, 30, 47, 56	0
1	J	195/197 (98%)	-0.39	0	100	100	22, 28, 40, 50	0
All	All	1950/1970 (98%)	-0.28	6 (0%)	94	94	20, 29, 45, 60	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	169	GLY	2.5
1	G	195	SER	2.4
1	A	167	GLU	2.3
1	A	179	GLY	2.3
1	D	120	THR	2.2
1	H	198	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	NCB	C	2	8/9	0.67	0.23	40,45,53,65	0
1	NCB	G	2	8/9	0.81	0.17	41,45,53,59	0
1	NCB	F	2	8/9	0.84	0.12	32,34,39,40	0
1	NCB	H	2	8/9	0.86	0.19	27,42,50,60	0
1	NCB	D	2	8/9	0.87	0.12	29,38,43,45	0
1	NCB	B	2	8/9	0.89	0.14	35,47,55,57	0
1	NCB	A	2	8/9	0.89	0.11	28,40,44,47	0
1	NCB	I	2	8/9	0.89	0.14	38,49,56,57	0
1	NCB	E	2	8/9	0.93	0.12	32,42,44,50	0
1	NCB	J	2	8/9	0.93	0.10	29,39,43,48	0
1	CSD	G	51	8/9	0.96	0.08	23,24,27,30	0
1	CSD	F	51	8/9	0.97	0.06	20,23,23,24	0
1	CSD	H	51	8/9	0.97	0.07	23,24,25,27	0
1	CSD	A	51	8/9	0.98	0.05	21,22,24,26	0
1	CSD	D	51	8/9	0.98	0.06	21,23,24,24	0
1	CSD	C	51	8/9	0.98	0.06	21,22,26,26	0
1	CSD	I	51	8/9	0.98	0.06	20,22,23,24	0
1	CSD	E	51	8/9	0.98	0.05	21,22,23,24	0
1	CSD	J	51	8/9	0.98	0.05	24,26,28,31	0
1	CSD	B	51	8/9	0.99	0.05	22,24,26,28	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.