



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2017 – 11:02 AM EST

PDB ID : 2YVH
Title : Crystal structure of the operator-binding form of the multi-drug binding transcriptional repressor CgmR
Authors : Itou, H.; Shirakihara, Y.; Tanaka, I.
Deposited on : 2007-04-12
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

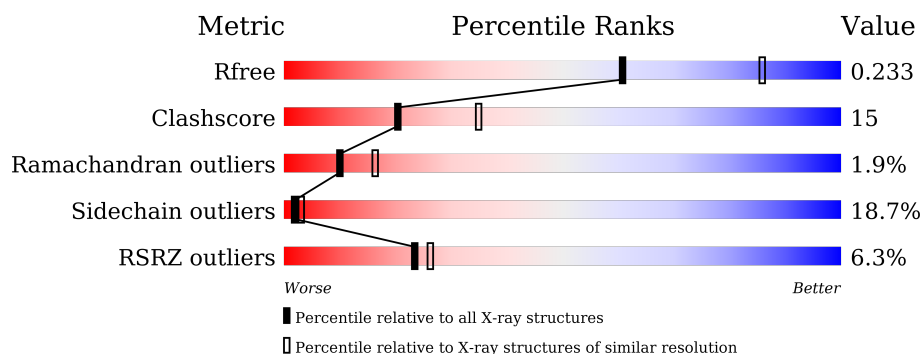
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	177	<div> <div>7%</div> <div>62%</div> <div>29%</div> <div>...</div> </div>
1	B	177	<div> <div>7%</div> <div>52%</div> <div>36%</div> <div>9%</div> <div>..</div> </div>
1	C	177	<div> <div>5%</div> <div>57%</div> <div>30%</div> <div>9%</div> <div>..</div> </div>
1	D	177	<div> <div>7%</div> <div>60%</div> <div>31%</div> <div>6%</div> <div>..</div> </div>
2	E	14	<div> <div>14%</div> <div>71%</div> <div>14%</div> </div>
2	G	14	<div> <div>14%</div> <div>64%</div> <div>21%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	14	 21% 29% 50%
3	H	14	 7% 64% 29%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6669 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 Transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	Se	0	0	0
			1379	877	234	265	3			
1	B	172	Total	C	N	O	Se	0	0	0
			1386	881	235	267	3			
1	C	171	Total	C	N	O	Se	0	0	0
			1379	877	234	265	3			
1	D	172	Total	C	N	O	Se	0	0	0
			1386	881	235	267	3			

- Molecule 2 is a DNA chain called 5'-D(*DTP*DAP*DAP*DCP*DTP*DGP*DTP*DAP*D CP*DCP*DGP*DAP*DCP*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	14	Total	C	N	O	P	0	0	0
			280	135	51	81	13			
2	G	14	Total	C	N	O	P	0	0	0
			280	135	51	81	13			

- Molecule 3 is a DNA chain called 5'-D(*DGP*DGP*DTP*DCP*DGP*DGP*DTP*DAP*D CP*DAP*DGP*DTP*DTP*DA)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			288	138	54	83	13			
3	H	14	Total	C	N	O	P	0	0	0
			288	138	54	83	13			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		

Continued on next page...

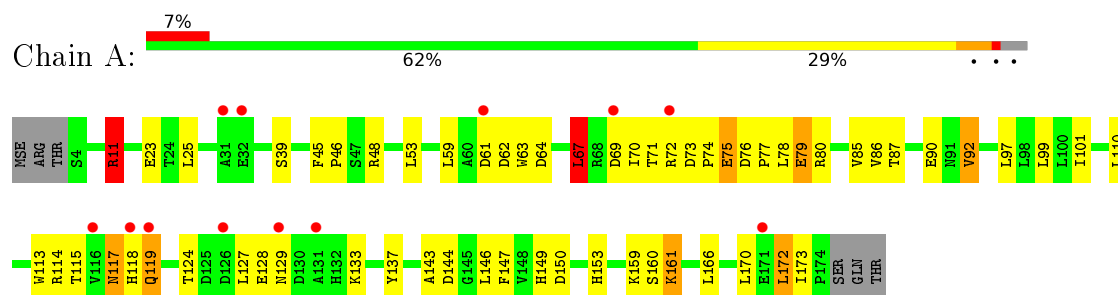
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	O	0	0
			1	1		
4	G	1	Total	O	0	0
			1	1		

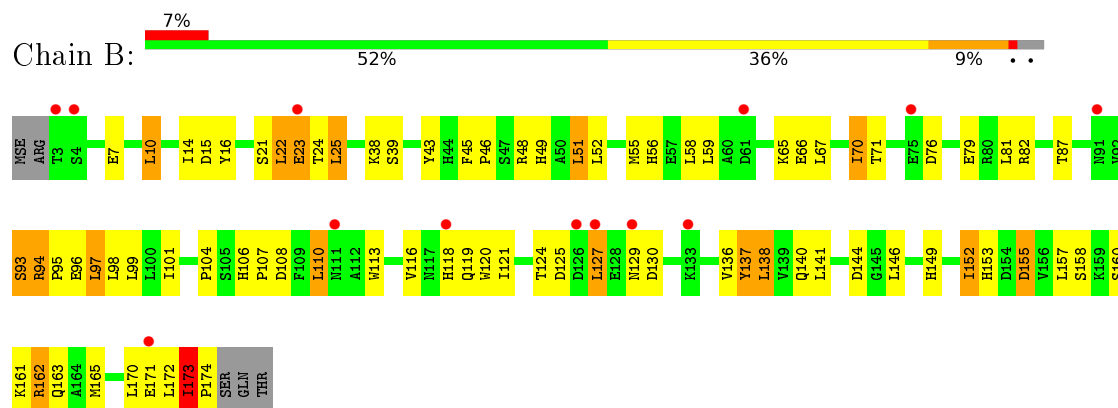
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

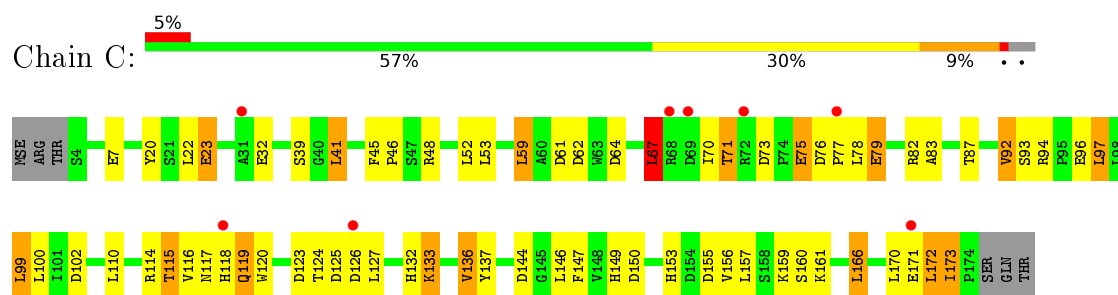
• Molecule 1: Transcriptional regulator



• Molecule 1: Transcriptional regulator

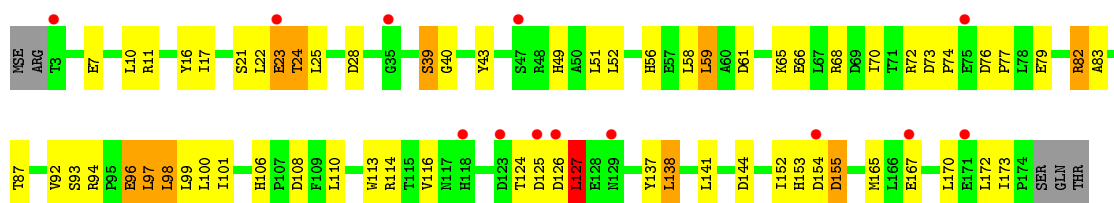


• Molecule 1: Transcriptional regulator



• Molecule 1: Transcriptional regulator





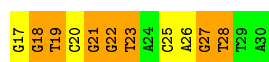
- Molecule 2: 5'-D(*DTP*DAP*DAP*DCP*DTP*DGP*DTP*DAP*DCP*DCP*DGP*DAP*D CP*DC)-3'



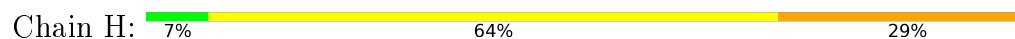
- Molecule 2: 5'-D(*DTP*DAP*DAP*DCP*DTP*DGP*DTP*DAP*DCP*DCP*DGP*DAP*D CP*DC)-3'



- Molecule 3: 5'-D(*DGP*DGP*DTP*DCP*DGP*DGP*DTP*DAP*DCP*DAP*DGP*DTP*D TP*DA)-3'



- Molecule 3: 5'-D(*DGP*DGP*DTP*DCP*DGP*DGP*DTP*DAP*DCP*DAP*DGP*DTP*D TP*DA)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	39.01Å 80.09Å 87.06Å 108.98° 102.25° 96.14°	Depositor
Resolution (Å)	10.00 – 2.50 9.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (10.00-2.50) 86.4 (9.99-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.259 0.235 , 0.233	Depositor DCC
R_{free} test set	1619 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 55.9	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	6669	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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	0.92	2/1406 (0.1%)	1.00	3/1909 (0.2%)
1	B	0.83	0/1413	0.91	1/1919 (0.1%)
1	C	0.86	0/1406	0.93	5/1909 (0.3%)
1	D	0.82	0/1413	0.94	4/1919 (0.2%)
2	E	1.64	1/313 (0.3%)	2.35	20/480 (4.2%)
2	G	1.61	3/313 (1.0%)	2.53	23/480 (4.8%)
3	F	1.56	1/323 (0.3%)	2.70	26/498 (5.2%)
3	H	1.59	2/323 (0.6%)	2.72	32/498 (6.4%)
All	All	1.03	9/6910 (0.1%)	1.44	114/9612 (1.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	GLU	CG-CD	8.44	1.64	1.51
2	G	12	DC	C1'-N1	6.39	1.57	1.49
2	G	10	DA	C3'-O3'	-6.19	1.35	1.44
2	G	12	DC	C3'-O3'	-6.13	1.35	1.44
2	E	11	DC	C3'-O3'	-6.11	1.36	1.44
1	A	23	GLU	CB-CG	5.60	1.62	1.52
3	H	19	DT	N1-C6	5.38	1.42	1.38
3	H	17	DG	C6-N1	5.21	1.43	1.39
3	F	17	DG	N7-C5	5.06	1.42	1.39

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	17	DG	O4'-C1'-N9	20.55	122.39	108.00
3	F	25	DC	O4'-C1'-N1	14.43	118.10	108.00
3	H	21	DG	O4'-C1'-N9	14.16	117.91	108.00
3	F	21	DG	O4'-C1'-N9	12.47	116.73	108.00
3	H	18	DG	O4'-C4'-C3'	-12.32	98.61	106.00
3	H	25	DC	O4'-C1'-N1	11.93	116.35	108.00
3	H	21	DG	O5'-P-OP1	-11.53	95.33	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	DT	P-O3'-C3'	10.28	132.04	119.70
1	A	67	LEU	CA-CB-CG	10.13	138.60	115.30
3	F	18	DG	C5'-C4'-O4'	-10.02	90.26	109.30
3	H	21	DG	C5'-C4'-C3'	-9.95	96.20	114.10
2	G	15	DC	O4'-C1'-N1	-9.87	101.09	108.00
2	G	15	DC	O4'-C1'-C2'	-9.84	98.03	105.90
2	G	5	DA	O4'-C1'-N9	9.58	114.71	108.00
3	H	23	DT	P-O3'-C3'	9.57	131.18	119.70
2	E	9	DT	C4-C5-C7	9.53	124.72	119.00
2	G	6	DC	O4'-C4'-C3'	-9.40	100.36	106.00
3	H	19	DT	O4'-C1'-N1	-9.27	101.51	108.00
3	H	18	DG	P-O5'-C5'	9.22	135.65	120.90
2	G	11	DC	O4'-C1'-N1	9.05	114.33	108.00
2	G	12	DC	P-O3'-C3'	9.04	130.55	119.70
3	F	17	DG	C8-N9-C4	-8.94	102.82	106.40
3	F	18	DG	O4'-C4'-C3'	-8.75	100.75	106.00
3	H	23	DT	N3-C4-O4	8.51	125.01	119.90
3	H	19	DT	O4'-C4'-C3'	-8.10	101.14	106.00
2	G	16	DC	N3-C4-C5	7.85	125.04	121.90
3	F	19	DT	O4'-C1'-N1	-7.70	102.61	108.00
2	E	3	DT	O4'-C1'-N1	7.50	113.25	108.00
3	H	18	DG	C5'-C4'-O4'	-7.44	95.17	109.30
3	H	23	DT	C5-C4-O4	-7.36	119.75	124.90
3	H	19	DT	N3-C2-O2	-7.34	117.90	122.30
2	E	14	DA	P-O3'-C3'	7.29	128.45	119.70
1	C	67	LEU	CA-CB-CG	7.16	131.77	115.30
3	H	27	DG	P-O3'-C3'	7.12	128.25	119.70
3	H	29	DT	P-O3'-C3'	7.10	128.22	119.70
2	E	8	DG	P-O3'-C3'	7.04	128.15	119.70
3	F	22	DG	O5'-P-OP2	-6.99	99.41	105.70
3	F	20	DC	OP2-P-O3'	6.97	120.53	105.20
1	A	11	ARG	NE-CZ-NH2	-6.95	116.83	120.30
3	H	18	DG	N1-C6-O6	-6.95	115.73	119.90
2	G	3	DT	O4'-C1'-N1	6.79	112.76	108.00
3	F	23	DT	O4'-C1'-N1	6.79	112.75	108.00
1	D	127	LEU	CA-CB-CG	6.75	130.82	115.30
3	F	27	DG	O4'-C1'-N9	6.74	112.72	108.00
2	E	14	DA	C2-N3-C4	6.70	113.95	110.60
3	H	26	DA	O5'-P-OP2	-6.70	99.67	105.70
2	E	9	DT	C6-C5-C7	-6.68	118.89	122.90
3	F	17	DG	N9-C4-C5	6.68	108.07	105.40
2	G	12	DC	O4'-C1'-N1	6.60	112.62	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	12	DC	C6-N1-C2	-6.59	117.67	120.30
3	H	21	DG	OP1-P-OP2	6.59	129.48	119.60
3	F	25	DC	C1'-O4'-C4'	-6.57	103.53	110.10
3	F	18	DG	O4'-C1'-N9	-6.52	103.44	108.00
3	H	18	DG	C5-C6-N1	6.47	114.73	111.50
2	E	11	DC	O4'-C1'-C2'	6.46	111.07	105.90
3	F	19	DT	P-O3'-C3'	6.43	127.42	119.70
3	F	27	DG	P-O3'-C3'	6.39	127.37	119.70
2	G	10	DA	N1-C2-N3	-6.36	126.12	129.30
2	G	10	DA	P-O3'-C3'	6.33	127.30	119.70
3	H	19	DT	C5-C6-N1	-6.32	119.91	123.70
3	F	17	DG	N7-C8-N9	6.27	116.24	113.10
3	F	26	DA	P-O3'-C3'	6.15	127.08	119.70
3	F	23	DT	P-O3'-C3'	6.09	127.01	119.70
3	F	22	DG	N1-C6-O6	-6.02	116.29	119.90
3	H	25	DC	N3-C4-N4	-6.01	113.79	118.00
2	E	11	DC	O5'-P-OP1	-6.01	100.29	105.70
3	H	23	DT	OP1-P-OP2	6.00	128.59	119.60
3	H	17	DG	O4'-C1'-N9	5.95	112.16	108.00
1	D	94	ARG	NE-CZ-NH1	-5.94	117.33	120.30
3	H	22	DG	C4'-C3'-C2'	5.93	108.43	103.10
2	E	10	DA	O4'-C1'-C2'	-5.92	101.16	105.90
3	H	24	DA	O4'-C1'-N9	5.88	112.12	108.00
2	E	10	DA	O5'-P-OP1	-5.81	100.47	105.70
3	F	18	DG	N1-C6-O6	-5.80	116.42	119.90
2	E	16	DC	N3-C4-N4	-5.76	113.97	118.00
2	G	12	DC	C5-C4-N4	5.75	124.22	120.20
1	B	127	LEU	CA-CB-CG	5.69	128.39	115.30
2	E	13	DG	C5-C6-N1	5.64	114.32	111.50
2	E	13	DG	N1-C6-O6	-5.64	116.52	119.90
2	G	8	DG	C5-C6-O6	-5.62	125.22	128.60
2	E	5	DA	O4'-C1'-N9	5.56	111.89	108.00
3	H	21	DG	N3-C2-N2	-5.53	116.03	119.90
2	E	16	DC	C5-C4-N4	5.50	124.05	120.20
2	G	13	DG	N1-C6-O6	-5.46	116.63	119.90
3	F	17	DG	C5-C6-O6	5.44	131.86	128.60
3	F	19	DT	C6-N1-C2	-5.43	118.58	121.30
1	C	67	LEU	CB-CG-CD1	-5.40	101.82	111.00
3	H	17	DG	C6-N1-C2	-5.39	121.86	125.10
2	G	12	DC	C5-C6-N1	5.37	123.69	121.00
2	G	12	DC	OP2-P-O3'	5.36	116.99	105.20
1	D	98	LEU	CA-CB-CG	5.36	127.62	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	LEU	CB-CG-CD1	-5.32	101.96	111.00
3	H	19	DT	N3-C4-O4	-5.32	116.71	119.90
2	E	16	DC	C2-N3-C4	5.32	122.56	119.90
3	H	25	DC	N1-C2-O2	5.30	122.08	118.90
2	G	11	DC	N3-C4-C5	-5.29	119.78	121.90
1	C	48	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	E	15	DC	O4'-C1'-C2'	-5.29	101.67	105.90
3	F	21	DG	O4'-C1'-C2'	-5.28	101.67	105.90
1	D	61	ASP	CB-CG-OD1	5.26	123.03	118.30
3	H	18	DG	O5'-P-OP2	-5.22	101.00	105.70
2	G	16	DC	N3-C4-N4	-5.18	114.38	118.00
2	G	16	DC	C6-N1-C2	5.17	122.37	120.30
3	F	20	DC	P-O3'-C3'	5.16	125.89	119.70
2	E	13	DG	C2-N3-C4	5.16	114.48	111.90
3	H	19	DT	N1-C2-O2	5.15	127.22	123.10
2	E	10	DA	N1-C2-N3	-5.11	126.75	129.30
3	F	28	DT	P-O3'-C3'	5.06	125.78	119.70
3	H	26	DA	O4'-C1'-N9	5.06	111.54	108.00
1	C	97	LEU	CA-CB-CG	5.06	126.93	115.30
2	G	8	DG	P-O3'-C3'	5.03	125.74	119.70
2	E	16	DC	O4'-C1'-N1	-5.03	104.48	108.00
2	G	7	DT	C6-C5-C7	-5.02	119.89	122.90
1	C	62	ASP	CB-CG-OD2	5.02	122.81	118.30

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	1379	0	1363	37	0
1	B	1386	0	1370	63	0
1	C	1379	0	1363	46	0
1	D	1386	0	1370	50	0
2	E	280	0	159	4	0
2	G	280	0	159	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	288	0	160	4	0
3	H	288	0	160	5	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	G	1	0	0	0	0
All	All	6669	0	6104	186	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 15.

All (186) 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:173:ILE:HG23	1:B:174:PRO:CD	1.72	1.19
1:B:173:ILE:CG2	1:B:174:PRO:HD3	1.78	1.10
1:C:71:THR:HG22	1:C:83:ALA:HB2	1.27	1.10
1:B:16:TYR:OH	1:B:24:THR:HG22	1.58	1.01
1:B:56:HIS:HD2	1:B:113:TRP:HE1	1.08	0.92
1:D:56:HIS:HD2	1:D:113:TRP:HE1	1.17	0.92
1:C:71:THR:CG2	1:C:83:ALA:HB2	2.01	0.89
1:A:144:ASP:OD2	1:B:153:HIS:HE1	1.55	0.89
1:B:93:SER:H	1:B:96:GLU:HG3	1.38	0.88
1:C:92:VAL:HG13	1:C:147:PHE:CE1	2.11	0.86
1:A:144:ASP:OD2	1:B:153:HIS:CE1	2.27	0.86
1:D:21:SER:OG	1:D:23:GLU:OE1	1.94	0.85
1:B:173:ILE:HG23	1:B:174:PRO:HD3	0.90	0.83
1:C:172:LEU:HD11	1:D:138:LEU:HD11	1.59	0.81
1:D:92:VAL:HA	1:D:96:GLU:OE1	1.79	0.81
1:B:51:LEU:O	1:B:55:MSE:HG3	1.81	0.80
1:A:172:LEU:HD11	1:B:138:LEU:HD11	1.63	0.80
1:D:21:SER:CB	1:D:23:GLU:OE1	2.28	0.80
2:E:11:DC:H2''	2:E:12:DC:H5'	1.63	0.79
1:A:25:LEU:O	1:A:48:ARG:NH2	2.13	0.78
3:F:22:DG:H2'	3:F:23:DT:H71	1.65	0.78
1:B:106:HIS:HD2	1:B:108:ASP:H	1.31	0.77
3:F:21:DG:H2''	3:F:22:DG:H5''	1.66	0.76
1:C:71:THR:HG22	1:C:83:ALA:CB	2.13	0.76
1:B:173:ILE:O	1:B:174:PRO:C	2.21	0.76
1:A:92:VAL:HG13	1:A:147:PHE:CE1	2.21	0.75
1:D:56:HIS:CD2	1:D:113:TRP:HE1	2.05	0.74
1:B:21:SER:OG	1:B:23:GLU:OE1	2.05	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:HIS:CD2	1:B:113:TRP:HE1	1.99	0.73
1:D:97:LEU:HD22	1:D:101:ILE:HD12	1.69	0.73
1:C:149:HIS:HD2	1:C:150:ASP:OD1	1.72	0.72
1:B:23:GLU:CD	1:B:23:GLU:H	1.93	0.72
1:B:146:LEU:O	1:B:162:ARG:NH1	2.25	0.70
1:B:38:LYS:NZ	3:H:22:DG:N7	2.40	0.70
1:D:23:GLU:CD	1:D:23:GLU:H	1.95	0.69
1:A:73:ASP:OD1	1:A:75:GLU:HB3	1.93	0.68
1:C:71:THR:CG2	1:C:83:ALA:CB	2.72	0.68
1:C:92:VAL:HG22	1:C:96:GLU:HG2	1.76	0.67
1:B:97:LEU:HD22	1:B:101:ILE:HD12	1.75	0.66
1:D:66:GLU:OE2	1:D:66:GLU:HA	1.96	0.66
1:A:127:LEU:HD21	1:B:165:MSE:SE	2.46	0.66
1:D:11:ARG:CZ	1:D:58:LEU:HD21	2.27	0.65
3:H:25:DC:H2"	3:H:26:DA:C8	2.31	0.65
1:D:21:SER:HB2	1:D:23:GLU:OE1	1.95	0.65
1:D:154:ASP:O	1:D:155:ASP:HB2	1.97	0.64
1:A:149:HIS:HE1	1:B:137:TYR:OH	1.80	0.64
1:C:127:LEU:HD21	1:D:165:MSE:SE	2.48	0.64
1:D:106:HIS:HD2	1:D:108:ASP:H	1.45	0.64
1:C:161:LYS:HD3	1:D:127:LEU:HD22	1.79	0.63
1:C:153:HIS:HE1	1:D:144:ASP:OD1	1.81	0.62
1:B:16:TYR:OH	1:B:24:THR:CG2	2.42	0.62
1:C:153:HIS:CE1	1:D:144:ASP:OD1	2.53	0.62
1:D:59:LEU:HG	1:D:96:GLU:OE2	1.99	0.61
1:B:173:ILE:CG2	1:B:174:PRO:CD	2.55	0.60
1:B:93:SER:N	1:B:96:GLU:HG3	2.14	0.60
1:B:56:HIS:HD2	1:B:113:TRP:NE1	1.89	0.60
1:D:97:LEU:HD22	1:D:101:ILE:CD1	2.32	0.59
1:A:74:PRO:O	1:A:80:ARG:NH1	2.36	0.59
1:B:23:GLU:CD	1:B:23:GLU:N	2.55	0.59
1:A:92:VAL:CG1	1:A:147:PHE:CD1	2.87	0.57
1:A:124:THR:HG21	1:B:155:ASP:OD2	2.04	0.57
2:G:4:DA:OP2	2:G:4:DA:H8	1.87	0.56
1:C:83:ALA:O	1:C:87:THR:HG23	2.04	0.56
1:A:76:ASP:HB2	1:A:77:PRO:HD2	1.87	0.56
1:D:106:HIS:CD2	1:D:108:ASP:H	2.23	0.56
1:D:93:SER:H	1:D:96:GLU:HG3	1.70	0.56
1:A:127:LEU:H	1:B:161:LYS:HZ1	1.53	0.55
1:C:123:ASP:OD2	1:C:133:LYS:HE3	2.05	0.55
1:C:149:HIS:HE1	1:D:137:TYR:OH	1.90	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:VAL:CG1	1:A:147:PHE:CE1	2.89	0.55
1:C:114:ARG:HE	1:C:118:HIS:CD2	2.24	0.55
1:A:76:ASP:O	1:A:80:ARG:HG3	2.08	0.54
1:A:153:HIS:HE1	1:B:140:GLN:HE21	1.56	0.54
1:B:22:LEU:HD21	1:B:52:LEU:HD11	1.89	0.54
1:D:93:SER:N	1:D:96:GLU:HG3	2.23	0.54
1:C:67:LEU:HD21	1:C:120:TRP:CD1	2.43	0.53
1:B:71:THR:HG23	1:B:79:GLU:HG3	1.90	0.53
2:E:10:DA:H2''	2:E:11:DC:H5''	1.91	0.53
1:C:132:HIS:O	1:C:136:VAL:HG12	2.08	0.53
1:D:79:GLU:OE2	1:D:79:GLU:HA	2.09	0.53
1:B:116:VAL:HA	1:B:120:TRP:HD1	1.74	0.53
1:B:49:HIS:HE1	1:B:108:ASP:OD2	1.91	0.52
1:B:66:GLU:OE1	1:B:70:ILE:HD12	2.09	0.52
1:B:10:LEU:O	1:B:14:ILE:HD12	2.09	0.52
3:H:22:DG:OP1	3:H:22:DG:H4'	2.09	0.52
1:A:161:LYS:HD2	1:B:124:THR:OG1	2.10	0.51
3:F:18:DG:H2''	3:F:19:DT:H5'	1.93	0.51
1:C:20:TYR:O	1:C:94:ARG:NH1	2.43	0.51
1:D:116:VAL:O	1:D:116:VAL:HG22	2.09	0.51
1:B:76:ASP:HB3	1:B:79:GLU:HB3	1.91	0.51
1:A:113:TRP:O	1:A:117:ASN:HB2	2.11	0.50
1:A:128:GLU:HB3	1:A:129:ASN:ND2	2.26	0.50
1:C:144:ASP:OD2	1:D:153:HIS:HE1	1.94	0.50
1:B:158:SER:OG	1:B:161:LYS:HG3	2.11	0.50
1:C:123:ASP:HB2	1:C:125:ASP:OD1	2.12	0.50
2:G:4:DA:OP2	2:G:4:DA:C8	2.64	0.49
1:B:170:LEU:O	1:B:173:ILE:HB	2.13	0.49
1:D:17:ILE:HG21	1:D:22:LEU:HD23	1.95	0.49
1:D:23:GLU:CD	1:D:23:GLU:N	2.66	0.49
1:D:167:GLU:OE2	1:D:167:GLU:HA	2.12	0.49
1:A:85:VAL:HG22	1:A:143:ALA:HB2	1.94	0.48
1:C:150:ASP:HB3	1:C:156:VAL:HG22	1.96	0.48
1:C:64:ASP:OD1	1:C:64:ASP:C	2.52	0.48
1:C:73:ASP:OD1	1:C:75:GLU:HB3	2.13	0.48
1:A:115:THR:O	1:A:119:GLN:HB3	2.13	0.48
1:C:100:LEU:HD13	1:D:152:ILE:HG13	1.96	0.47
1:A:67:LEU:HB2	1:A:87:THR:HG21	1.96	0.47
1:D:106:HIS:HD2	1:D:108:ASP:N	2.11	0.47
1:B:81:LEU:HD22	1:B:136:VAL:HG13	1.96	0.47
1:C:22:LEU:HD11	1:C:99:LEU:HD12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TRP:O	1:A:67:LEU:HB3	2.15	0.46
1:B:97:LEU:HD22	1:B:101:ILE:CD1	2.43	0.46
1:C:92:VAL:HG22	1:C:96:GLU:CG	2.45	0.46
1:B:94:ARG:O	1:B:95:PRO:C	2.53	0.46
1:C:76:ASP:OD1	1:C:79:GLU:HB2	2.16	0.46
1:B:82:ARG:HG3	1:B:170:LEU:HD22	1.98	0.46
1:B:106:HIS:CD2	1:B:108:ASP:H	2.21	0.46
1:D:39:SER:HB3	2:E:7:DT:C7	2.46	0.46
1:D:49:HIS:HE1	1:D:108:ASP:OD2	1.99	0.46
1:C:67:LEU:HA	1:C:70:ILE:HG22	1.98	0.46
1:C:118:HIS:O	1:C:119:GLN:HB2	2.15	0.46
1:C:149:HIS:CD2	1:C:157:LEU:HG	2.51	0.46
1:A:124:THR:O	1:B:161:LYS:HE3	2.17	0.45
1:C:59:LEU:HD12	1:C:59:LEU:HA	1.83	0.45
1:D:83:ALA:O	1:D:87:THR:HG23	2.17	0.45
2:E:11:DC:H2''	2:E:12:DC:C5'	2.42	0.45
1:A:149:HIS:CE1	1:B:137:TYR:OH	2.67	0.45
1:D:116:VAL:O	1:D:116:VAL:CG2	2.65	0.45
1:C:92:VAL:CG1	1:C:147:PHE:CD1	3.00	0.45
1:D:96:GLU:HG2	1:D:96:GLU:H	1.31	0.45
1:C:73:ASP:N	1:C:79:GLU:OE2	2.50	0.45
1:D:16:TYR:OH	1:D:24:THR:HG23	2.17	0.45
3:F:27:DG:H2''	3:F:28:DT:OP2	2.17	0.45
1:B:138:LEU:CD1	1:B:172:LEU:HD21	2.47	0.44
1:C:92:VAL:HG13	1:C:147:PHE:CD1	2.49	0.44
1:B:43:TYR:CE1	2:G:5:DA:H2'	2.52	0.44
3:H:19:DT:H1'	3:H:20:DC:H5'	1.99	0.44
1:B:58:LEU:C	1:B:58:LEU:HD23	2.38	0.44
1:C:23:GLU:HB2	1:D:23:GLU:HB3	1.99	0.44
1:A:149:HIS:HD2	1:A:150:ASP:OD1	2.01	0.44
2:G:12:DC:H2''	2:G:13:DG:C8	2.53	0.44
1:A:76:ASP:OD1	1:A:79:GLU:HB2	2.17	0.44
1:D:106:HIS:CD2	1:D:108:ASP:HB2	2.53	0.44
1:C:149:HIS:CE1	1:D:137:TYR:OH	2.70	0.44
1:A:64:ASP:OD1	1:A:64:ASP:C	2.55	0.44
2:G:4:DA:C2	3:H:30:DA:C2	3.05	0.44
1:B:152:ILE:HA	1:B:152:ILE:HD12	1.82	0.43
1:A:45:PHE:HA	1:A:46:PRO:HD3	1.79	0.43
1:D:170:LEU:O	1:D:173:ILE:HG13	2.19	0.43
1:C:76:ASP:HA	1:C:77:PRO:HD2	1.82	0.43
1:A:11:ARG:NH2	1:A:62:ASP:OD1	2.23	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLN:NE2	1:B:163:GLN:HA	2.34	0.43
1:C:41:LEU:HA	1:C:41:LEU:HD12	1.75	0.43
1:A:117:ASN:HD22	1:A:117:ASN:HA	1.66	0.42
1:B:25:LEU:O	1:B:48:ARG:NH2	2.52	0.42
1:C:39:SER:HB2	2:G:12:DC:C5	2.54	0.42
1:D:76:ASP:HA	1:D:77:PRO:HD2	1.77	0.42
1:D:96:GLU:O	1:D:100:LEU:HG	2.20	0.42
1:A:137:TYR:OH	1:B:149:HIS:NE2	2.38	0.42
1:C:45:PHE:HA	1:C:46:PRO:HD3	1.78	0.42
1:D:58:LEU:O	1:D:58:LEU:HD23	2.19	0.42
1:D:138:LEU:HD12	1:D:172:LEU:HD21	2.01	0.42
1:A:86:VAL:O	1:A:90:GLU:HG2	2.20	0.42
1:D:40:GLY:O	1:D:43:TYR:HB3	2.19	0.42
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.92	0.42
1:C:39:SER:HB2	2:G:12:DC:C6	2.55	0.41
1:C:115:THR:HG22	1:C:116:VAL:N	2.36	0.41
1:B:10:LEU:HD13	1:B:45:PHE:CZ	2.56	0.41
1:B:110:LEU:HA	1:B:110:LEU:HD12	1.87	0.41
1:C:76:ASP:OD1	1:C:76:ASP:N	2.53	0.41
1:B:49:HIS:CE1	1:B:108:ASP:OD2	2.72	0.41
1:D:93:SER:H	1:D:96:GLU:CG	2.32	0.41
1:B:104:PRO:HA	1:B:110:LEU:HD13	2.02	0.41
1:B:67:LEU:HD13	1:B:120:TRP:CD2	2.55	0.41
1:C:166:LEU:HD22	1:C:170:LEU:HG	2.01	0.41
1:A:153:HIS:CE1	1:B:144:ASP:OD1	2.73	0.41
1:B:45:PHE:HA	1:B:46:PRO:HD2	1.85	0.41
1:D:73:ASP:HA	1:D:74:PRO:HD3	1.72	0.41
1:D:72:ARG:NH2	1:D:82:ARG:CZ	2.84	0.40
1:B:163:GLN:HE21	1:B:163:GLN:HA	1.87	0.40
1:A:73:ASP:CG	1:A:73:ASP:O	2.59	0.40
1:B:149:HIS:CE1	1:B:157:LEU:HG	2.56	0.40
1:D:100:LEU:HA	1:D:100:LEU:HD23	1.84	0.40
1:A:153:HIS:CE1	1:B:140:GLN:HE21	2.39	0.40
1:B:10:LEU:CD1	1:B:45:PHE:CZ	3.04	0.40
1:C:171:GLU:O	1:C:173:ILE:N	2.55	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	169/177 (96%)	147 (87%)	20 (12%)	2 (1%)	16	29
1	B	170/177 (96%)	151 (89%)	16 (9%)	3 (2%)	11	18
1	C	169/177 (96%)	149 (88%)	13 (8%)	7 (4%)	3	4
1	D	170/177 (96%)	158 (93%)	11 (6%)	1 (1%)	30	50
All	All	678/708 (96%)	605 (89%)	60 (9%)	13 (2%)	10	16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	B	173	ILE
1	C	172	LEU
1	D	155	ASP
1	B	155	ASP
1	C	75	GLU
1	C	119	GLN
1	C	117	ASN
1	B	130	ASP
1	C	32	GLU
1	C	126	ASP
1	C	155	ASP
1	A	75	GLU

5.3.2 Protein sidechains [i](#)

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	152/154 (99%)	125 (82%)	27 (18%)	2	3
1	B	153/154 (99%)	120 (78%)	33 (22%)	1	2
1	C	152/154 (99%)	124 (82%)	28 (18%)	2	3
1	D	153/154 (99%)	127 (83%)	26 (17%)	2	4
All	All	610/616 (99%)	496 (81%)	114 (19%)	2	3

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	39	SER
1	A	53	LEU
1	A	59	LEU
1	A	61	ASP
1	A	67	LEU
1	A	69	ASP
1	A	70	ILE
1	A	71	THR
1	A	72	ARG
1	A	78	LEU
1	A	79	GLU
1	A	92	VAL
1	A	97	LEU
1	A	99	LEU
1	A	101	ILE
1	A	110	LEU
1	A	114	ARG
1	A	117	ASN
1	A	118	HIS
1	A	133	LYS
1	A	146	LEU
1	A	159	LYS
1	A	160	SER
1	A	161	LYS
1	A	166	LEU
1	A	173	ILE
1	B	7	GLU
1	B	10	LEU
1	B	15	ASP
1	B	22	LEU
1	B	23	GLU
1	B	25	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	39	SER
1	B	51	LEU
1	B	59	LEU
1	B	65	LYS
1	B	70	ILE
1	B	87	THR
1	B	93	SER
1	B	94	ARG
1	B	97	LEU
1	B	98	LEU
1	B	99	LEU
1	B	107	PRO
1	B	110	LEU
1	B	118	HIS
1	B	119	GLN
1	B	121	ILE
1	B	125	ASP
1	B	127	LEU
1	B	129	ASN
1	B	137	TYR
1	B	138	LEU
1	B	141	LEU
1	B	152	ILE
1	B	160	SER
1	B	162	ARG
1	B	171	GLU
1	B	173	ILE
1	C	7	GLU
1	C	23	GLU
1	C	41	LEU
1	C	52	LEU
1	C	53	LEU
1	C	59	LEU
1	C	61	ASP
1	C	67	LEU
1	C	71	THR
1	C	78	LEU
1	C	79	GLU
1	C	82	ARG
1	C	92	VAL
1	C	93	SER
1	C	97	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	99	LEU
1	C	102	ASP
1	C	110	LEU
1	C	115	THR
1	C	124	THR
1	C	133	LYS
1	C	136	VAL
1	C	137	TYR
1	C	146	LEU
1	C	159	LYS
1	C	160	SER
1	C	166	LEU
1	C	173	ILE
1	D	7	GLU
1	D	10	LEU
1	D	23	GLU
1	D	24	THR
1	D	25	LEU
1	D	28	ASP
1	D	39	SER
1	D	51	LEU
1	D	52	LEU
1	D	59	LEU
1	D	65	LYS
1	D	68	ARG
1	D	70	ILE
1	D	82	ARG
1	D	96	GLU
1	D	97	LEU
1	D	98	LEU
1	D	99	LEU
1	D	110	LEU
1	D	114	ARG
1	D	124	THR
1	D	125	ASP
1	D	126	ASP
1	D	127	LEU
1	D	138	LEU
1	D	141	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	129	ASN
1	A	132	HIS
1	A	149	HIS
1	A	153	HIS
1	B	49	HIS
1	B	56	HIS
1	B	106	HIS
1	B	117	ASN
1	B	153	HIS
1	B	163	GLN
1	C	117	ASN
1	C	118	HIS
1	C	119	GLN
1	C	132	HIS
1	C	149	HIS
1	C	153	HIS
1	D	49	HIS
1	D	56	HIS
1	D	106	HIS
1	D	117	ASN
1	D	153	HIS

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	168/177 (94%)	0.34	12 (7%) 19 21	32, 49, 78, 84	0
1	B	169/177 (95%)	0.35	13 (7%) 16 18	35, 53, 76, 85	0
1	C	168/177 (94%)	0.35	8 (4%) 34 39	32, 48, 78, 84	0
1	D	169/177 (95%)	0.46	13 (7%) 16 18	33, 51, 75, 84	0
2	E	14/14 (100%)	-0.40	0 100 100	35, 50, 67, 84	0
2	G	14/14 (100%)	-0.37	0 100 100	33, 46, 73, 85	0
3	F	14/14 (100%)	-0.30	0 100 100	27, 51, 89, 91	0
3	H	14/14 (100%)	-0.05	0 100 100	27, 48, 90, 97	0
All	All	730/764 (95%)	0.32	46 (6%) 23 26	27, 51, 79, 97	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	THR	5.1
1	D	3	THR	5.0
1	D	126	ASP	4.9
1	B	23	GLU	4.4
1	D	118	HIS	4.3
1	D	125	ASP	4.1
1	B	129	ASN	4.1
1	D	75	GLU	3.9
1	C	77	PRO	3.7
1	C	126	ASP	3.7
1	D	129	ASN	3.5
1	A	69	ASP	3.5
1	C	118	HIS	3.4
1	B	171	GLU	3.4
1	C	171	GLU	3.4
1	D	123	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	171	GLU	3.2
1	C	69	ASP	3.2
1	A	61	ASP	3.1
1	A	72	ARG	3.0
1	A	171	GLU	2.9
1	B	4	SER	2.8
1	A	118	HIS	2.8
1	C	72	ARG	2.8
1	C	31	ALA	2.7
1	D	47	SER	2.7
1	B	75	GLU	2.5
1	A	116	VAL	2.5
1	B	111	ASN	2.5
1	D	167	GLU	2.5
1	B	133	LYS	2.5
1	D	23	GLU	2.5
1	D	154	ASP	2.3
1	B	91	ASN	2.3
1	B	127	LEU	2.3
1	B	118	HIS	2.3
1	A	119	GLN	2.2
1	A	129	ASN	2.2
1	B	126	ASP	2.2
1	C	68	ARG	2.2
1	A	126	ASP	2.2
1	B	61	ASP	2.2
1	D	35	GLY	2.1
1	A	31	ALA	2.1
1	A	131	ALA	2.0
1	A	32	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.