



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:45 AM UTC

PDB ID : 6WPA / pdb_00006wpa
Title : Structure of AvaR1 bound to DNA half-site
Authors : Kapoor, I.; Olivares, P.J.; Nair, S.K.
Deposited on : 2020-04-26
Resolution : 3.09 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

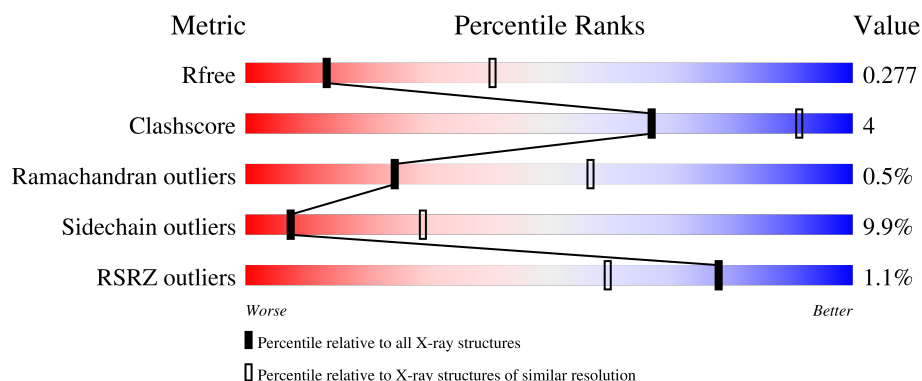
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	245	
1	B	245	
1	C	245	
1	D	245	
1	E	245	

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Mol	Chain	Length	Quality of chain
1	F	245	71%12%14%
1	G	245	74%11%14%
1	H	245	2%73%12%14%
2	M	28	61%36%
2	N	28	57%43%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14326 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 AvaR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1674	1054	303	312	5			
1	B	214	Total	C	N	O	S	0	0	0
			1661	1047	301	308	5			
1	C	212	Total	C	N	O	S	0	0	0
			1645	1038	296	306	5			
1	D	213	Total	C	N	O	S	0	0	0
			1660	1046	300	309	5			
1	E	212	Total	C	N	O	S	0	0	0
			1642	1035	296	306	5			
1	F	210	Total	C	N	O	S	0	0	0
			1632	1029	294	304	5			
1	G	210	Total	C	N	O	S	0	0	0
			1632	1029	294	304	5			
1	H	210	Total	C	N	O	S	0	0	0
			1632	1029	294	304	5			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	expression tag	UNP Q82H41
A	-8	SER	-	expression tag	UNP Q82H41
A	-7	GLU	-	expression tag	UNP Q82H41
A	-6	ASN	-	expression tag	UNP Q82H41
A	-5	LEU	-	expression tag	UNP Q82H41
A	-4	TYR	-	expression tag	UNP Q82H41
A	-3	PHE	-	expression tag	UNP Q82H41
A	-2	GLN	-	expression tag	UNP Q82H41
A	-1	SER	-	expression tag	UNP Q82H41
A	0	GLY	-	expression tag	UNP Q82H41
A	1	SER	-	expression tag	UNP Q82H41
B	-9	GLY	-	expression tag	UNP Q82H41
B	-8	SER	-	expression tag	UNP Q82H41

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLU	-	expression tag	UNP Q82H41
B	-6	ASN	-	expression tag	UNP Q82H41
B	-5	LEU	-	expression tag	UNP Q82H41
B	-4	TYR	-	expression tag	UNP Q82H41
B	-3	PHE	-	expression tag	UNP Q82H41
B	-2	GLN	-	expression tag	UNP Q82H41
B	-1	SER	-	expression tag	UNP Q82H41
B	0	GLY	-	expression tag	UNP Q82H41
B	1	SER	-	expression tag	UNP Q82H41
C	-9	GLY	-	expression tag	UNP Q82H41
C	-8	SER	-	expression tag	UNP Q82H41
C	-7	GLU	-	expression tag	UNP Q82H41
C	-6	ASN	-	expression tag	UNP Q82H41
C	-5	LEU	-	expression tag	UNP Q82H41
C	-4	TYR	-	expression tag	UNP Q82H41
C	-3	PHE	-	expression tag	UNP Q82H41
C	-2	GLN	-	expression tag	UNP Q82H41
C	-1	SER	-	expression tag	UNP Q82H41
C	0	GLY	-	expression tag	UNP Q82H41
C	1	SER	-	expression tag	UNP Q82H41
D	-9	GLY	-	expression tag	UNP Q82H41
D	-8	SER	-	expression tag	UNP Q82H41
D	-7	GLU	-	expression tag	UNP Q82H41
D	-6	ASN	-	expression tag	UNP Q82H41
D	-5	LEU	-	expression tag	UNP Q82H41
D	-4	TYR	-	expression tag	UNP Q82H41
D	-3	PHE	-	expression tag	UNP Q82H41
D	-2	GLN	-	expression tag	UNP Q82H41
D	-1	SER	-	expression tag	UNP Q82H41
D	0	GLY	-	expression tag	UNP Q82H41
D	1	SER	-	expression tag	UNP Q82H41
E	-9	GLY	-	expression tag	UNP Q82H41
E	-8	SER	-	expression tag	UNP Q82H41
E	-7	GLU	-	expression tag	UNP Q82H41
E	-6	ASN	-	expression tag	UNP Q82H41
E	-5	LEU	-	expression tag	UNP Q82H41
E	-4	TYR	-	expression tag	UNP Q82H41
E	-3	PHE	-	expression tag	UNP Q82H41
E	-2	GLN	-	expression tag	UNP Q82H41
E	-1	SER	-	expression tag	UNP Q82H41
E	0	GLY	-	expression tag	UNP Q82H41
E	1	SER	-	expression tag	UNP Q82H41

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	GLY	-	expression tag	UNP Q82H41
F	-8	SER	-	expression tag	UNP Q82H41
F	-7	GLU	-	expression tag	UNP Q82H41
F	-6	ASN	-	expression tag	UNP Q82H41
F	-5	LEU	-	expression tag	UNP Q82H41
F	-4	TYR	-	expression tag	UNP Q82H41
F	-3	PHE	-	expression tag	UNP Q82H41
F	-2	GLN	-	expression tag	UNP Q82H41
F	-1	SER	-	expression tag	UNP Q82H41
F	0	GLY	-	expression tag	UNP Q82H41
F	1	SER	-	expression tag	UNP Q82H41
G	-9	GLY	-	expression tag	UNP Q82H41
G	-8	SER	-	expression tag	UNP Q82H41
G	-7	GLU	-	expression tag	UNP Q82H41
G	-6	ASN	-	expression tag	UNP Q82H41
G	-5	LEU	-	expression tag	UNP Q82H41
G	-4	TYR	-	expression tag	UNP Q82H41
G	-3	PHE	-	expression tag	UNP Q82H41
G	-2	GLN	-	expression tag	UNP Q82H41
G	-1	SER	-	expression tag	UNP Q82H41
G	0	GLY	-	expression tag	UNP Q82H41
G	1	SER	-	expression tag	UNP Q82H41
H	-9	GLY	-	expression tag	UNP Q82H41
H	-8	SER	-	expression tag	UNP Q82H41
H	-7	GLU	-	expression tag	UNP Q82H41
H	-6	ASN	-	expression tag	UNP Q82H41
H	-5	LEU	-	expression tag	UNP Q82H41
H	-4	TYR	-	expression tag	UNP Q82H41
H	-3	PHE	-	expression tag	UNP Q82H41
H	-2	GLN	-	expression tag	UNP Q82H41
H	-1	SER	-	expression tag	UNP Q82H41
H	0	GLY	-	expression tag	UNP Q82H41
H	1	SER	-	expression tag	UNP Q82H41

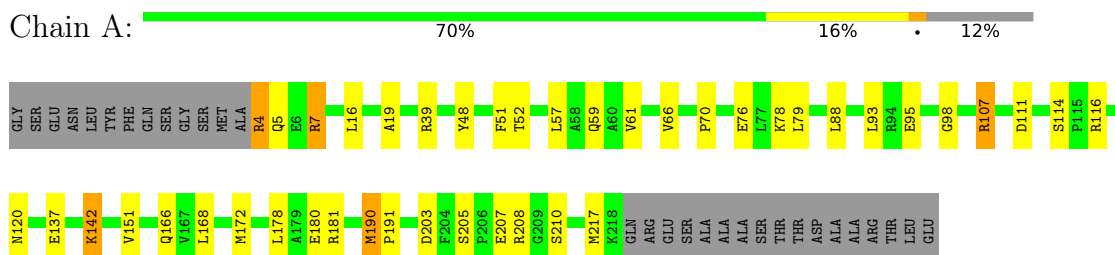
- Molecule 2 is a DNA chain called PAL2-1-5'-GC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	28	Total	C	N	O	P	0	0	0
			574	274	104	168	28			
2	N	28	Total	C	N	O	P	0	0	0
			574	274	104	168	28			

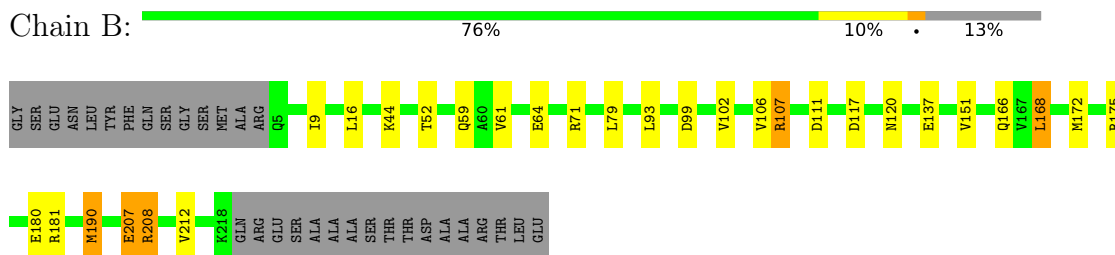
3 Residue-property plots [i](#)

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.

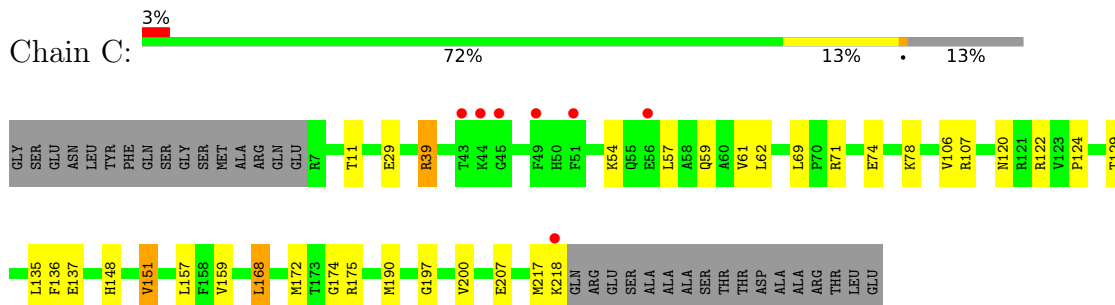
- Molecule 1: AvaR1



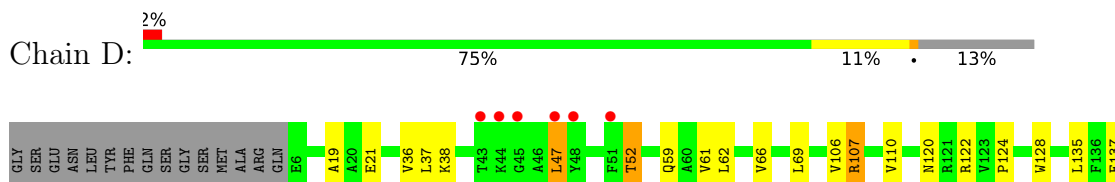
- Molecule 1: AvaR1

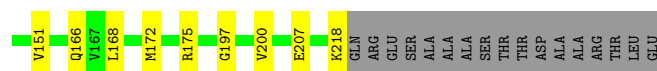


- Molecule 1: AvaR1

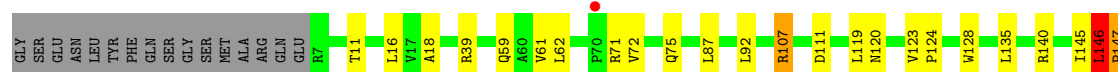


- Molecule 1: AvaR1

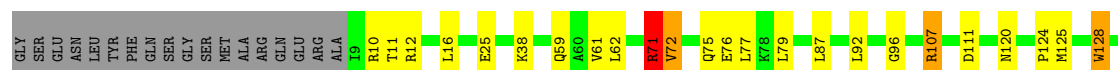




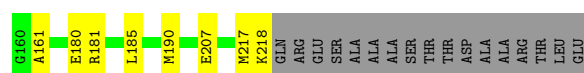
- Molecule 1: AvaR1



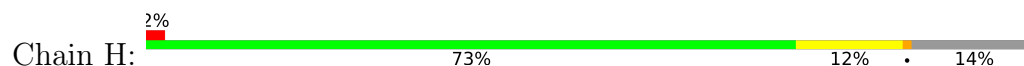
- Molecule 1: AvaR1



- Molecule 1: AvaR1



- Molecule 1: AvaR1

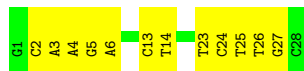


- Molecule 2: PAL2-1-5'-GC



- Molecule 2: PAL2-1-5'-GC

Chain N:  57% 43%



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	130.52Å 130.52Å 180.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.09 25.00 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-3.09) 100.0 (25.00-3.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.210 , 0.265 0.214 , 0.277	Depositor DCC
R_{free} test set	2801 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	98.3	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 104.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14326	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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	0.55	0/1702	1.07	3/2303 (0.1%)
1	B	0.54	0/1689	1.07	0/2286
1	C	0.54	0/1673	1.05	0/2265
1	D	0.54	0/1688	1.05	0/2284
1	E	0.53	0/1670	1.08	4/2261 (0.2%)
1	F	0.54	0/1660	1.09	1/2247 (0.0%)
1	G	0.56	0/1660	1.11	0/2247
1	H	0.56	0/1660	1.10	0/2247
2	M	0.32	0/643	0.90	2/990 (0.2%)
2	N	0.32	0/643	0.89	1/990 (0.1%)
All	All	0.53	0/14688	1.06	11/20120 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	GLN	N-CA-C	8.64	121.48	111.11
2	N	23	DT	C2'-C3'-O3'	7.03	122.05	111.50
2	M	23	DT	C2'-C3'-O3'	6.25	120.87	111.50
1	E	205	SER	N-CA-C	5.63	116.07	109.60
1	A	4	ARG	CA-C-N	5.20	127.56	120.54
1	A	4	ARG	C-N-CA	5.20	127.56	120.54
1	F	128	TRP	CA-CB-CG	5.13	123.35	113.60
1	E	128	TRP	CA-CB-CG	5.12	123.32	113.60
1	E	146	LEU	CA-C-N	5.11	126.22	119.84
1	E	146	LEU	C-N-CA	5.11	126.22	119.84
2	M	5	DG	C4'-C3'-O3'	5.06	117.58	110.00

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	1674	0	1692	18	0
1	B	1661	0	1680	10	0
1	C	1645	0	1665	12	0
1	D	1660	0	1682	11	0
1	E	1642	0	1656	10	0
1	F	1632	0	1649	12	0
1	G	1632	0	1649	8	0
1	H	1632	0	1649	12	0
2	M	574	0	317	8	0
2	N	574	0	317	9	0
All	All	14326	0	13956	104	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 (104) 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)
2:N:24:DC:H2''	2:N:25:DT:H5'	1.58	0.85
2:N:5:DG:H2'	2:N:6:DA:C8	2.13	0.82
1:D:59:GLN:HE22	1:D:120:ASN:H	1.28	0.79
1:B:168:LEU:HD23	1:F:125:MET:HE3	1.66	0.76
2:M:24:DC:H2''	2:M:25:DT:H5'	1.67	0.75
1:C:39:ARG:HH11	1:C:39:ARG:HG3	1.53	0.74
1:F:62:LEU:HD22	1:F:124:PRO:HG3	1.71	0.73
1:H:161:ALA:HB1	1:H:185:LEU:HD11	1.70	0.72
1:B:59:GLN:HE22	1:B:120:ASN:H	1.37	0.70
1:A:7:ARG:HH11	1:A:7:ARG:HG2	1.58	0.69
2:M:16:DG:H1'	2:M:17:DT:H5'	1.74	0.69
1:D:62:LEU:HD22	1:D:124:PRO:HG3	1.75	0.67
1:E:62:LEU:HD22	1:E:124:PRO:HG3	1.76	0.66
1:A:4:ARG:CB	1:A:7:ARG:HH12	2.09	0.66
1:G:161:ALA:HB1	1:G:185:LEU:HD11	1.78	0.64
1:F:76:GLU:HG2	1:F:77:LEU:HD12	1.82	0.61
1:A:7:ARG:HH11	1:A:7:ARG:CG	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LEU:HD22	1:C:124:PRO:HG3	1.81	0.61
1:A:59:GLN:HE22	1:A:120:ASN:H	1.47	0.61
1:F:146:LEU:HB2	1:F:147:PRO:HD2	1.83	0.60
2:M:5:DG:H2''	2:M:6:DA:O5'	2.01	0.59
1:E:161:ALA:HB1	1:E:185:LEU:HD11	1.84	0.57
1:E:59:GLN:HE22	1:E:120:ASN:H	1.53	0.57
2:M:5:DG:H2'	2:M:6:DA:C8	2.40	0.57
1:E:59:GLN:NE2	1:E:120:ASN:H	2.02	0.57
1:G:137:GLU:HG3	1:G:151:VAL:HG11	1.87	0.57
1:H:39:ARG:CG	1:H:39:ARG:HH11	2.18	0.57
1:G:69:LEU:HD13	1:G:71:ARG:HH12	1.70	0.56
1:D:166:GLN:NE2	1:D:175:ARG:HH21	2.03	0.55
1:H:39:ARG:HH11	1:H:39:ARG:HG3	1.73	0.54
1:E:140:ARG:HD3	1:E:145:ILE:HD11	1.90	0.53
1:D:197:GLY:HA2	1:D:200:VAL:HG22	1.90	0.52
1:D:52:THR:OG1	1:E:11:THR:HB	2.09	0.52
1:F:59:GLN:HE22	1:F:120:ASN:H	1.57	0.52
1:F:87:LEU:HD21	1:F:183:ALA:HB2	1.92	0.52
1:F:107:ARG:HD2	1:F:111:ASP:OD2	2.10	0.52
1:F:59:GLN:NE2	1:F:120:ASN:H	2.09	0.51
2:N:3:DA:H2''	2:N:4:DA:H5''	1.93	0.51
1:B:107:ARG:HD2	1:B:111:ASP:OD2	2.11	0.50
2:M:26:DT:H2''	2:M:27:DG:C8	2.47	0.50
1:H:133:GLN:HG3	1:H:151:VAL:HG12	1.92	0.50
1:C:59:GLN:HE22	1:C:120:ASN:H	1.59	0.50
1:G:99:ASP:HB3	1:G:102:VAL:HG22	1.93	0.50
1:D:172:MET:HE1	1:H:126:GLN:HG2	1.94	0.49
1:B:99:ASP:HB3	1:B:102:VAL:HG22	1.93	0.49
2:M:5:DG:C2'	2:M:6:DA:C8	2.96	0.48
1:H:137:GLU:HG3	1:H:151:VAL:HG11	1.95	0.48
1:B:166:GLN:HE21	1:B:175:ARG:HE	1.62	0.48
1:A:210:SER:HB2	1:B:207:GLU:HB3	1.96	0.48
2:N:26:DT:H2''	2:N:27:DG:C8	2.48	0.47
1:G:133:GLN:HG3	1:G:151:VAL:HG12	1.96	0.47
1:C:174:GLY:O	1:C:175:ARG:HB2	2.14	0.47
1:A:93:LEU:HD13	1:A:166:GLN:HG3	1.96	0.47
1:D:37:LEU:HD13	1:D:47:LEU:HD12	1.96	0.47
1:A:137:GLU:HG3	1:A:151:VAL:HG21	1.97	0.47
1:F:71:ARG:HB3	1:F:72:VAL:H	1.58	0.47
1:E:107:ARG:HD2	1:E:111:ASP:OD2	2.15	0.47
1:B:137:GLU:HG3	1:B:151:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:HD2	1:A:111:ASP:OD2	2.14	0.46
1:C:129:THR:HA	1:C:159:VAL:HG21	1.98	0.46
1:H:39:ARG:HG3	1:H:39:ARG:NH1	2.30	0.46
1:F:180:GLU:O	1:F:184:ASP:HB2	2.15	0.46
1:H:144:GLU:HA	1:H:198:ILE:HD13	1.97	0.46
1:C:39:ARG:HG3	1:C:39:ARG:NH1	2.26	0.46
1:C:136:PHE:HB3	1:C:151:VAL:HG22	1.98	0.45
1:A:190:MET:N	1:A:191:PRO:HD2	2.31	0.45
2:N:2:DC:H2''	2:N:3:DA:N7	2.31	0.45
1:A:78:LYS:HD3	1:A:142:LYS:HD3	1.99	0.45
2:N:4:DA:H2''	2:N:5:DG:O5'	2.17	0.45
2:M:24:DC:H2''	2:M:25:DT:C5'	2.44	0.44
1:C:197:GLY:HA2	1:C:200:VAL:HG22	1.99	0.44
1:D:19:ALA:HA	1:D:36:VAL:HG22	1.99	0.44
1:B:93:LEU:HD21	1:B:106:VAL:HG21	1.99	0.44
2:N:4:DA:H2''	2:N:5:DG:O4'	2.17	0.44
1:A:205:SER:HB2	1:A:207:GLU:HG2	1.99	0.43
2:M:2:DC:H2''	2:M:3:DA:N7	2.32	0.43
1:E:180:GLU:O	1:E:184:ASP:HB2	2.19	0.43
1:A:203:ASP:HB3	1:A:208:ARG:HD2	2.00	0.43
1:A:19:ALA:HB2	1:A:57:LEU:HD22	2.00	0.43
1:A:48:TYR:HA	1:A:51:PHE:O	2.18	0.43
1:H:109:THR:HA	1:H:121:ARG:HG2	2.02	0.42
1:H:166:GLN:HE21	1:H:175:ARG:HE	1.66	0.42
1:C:54:LYS:HA	1:C:57:LEU:HD12	2.01	0.42
1:C:172:MET:HE1	1:G:126:GLN:HG2	2.02	0.42
1:A:70:PRO:HB2	1:A:88:LEU:HD21	2.01	0.42
1:B:79:LEU:HD22	1:B:190:MET:HE2	2.02	0.42
1:B:208:ARG:O	1:B:212:VAL:HG23	2.20	0.41
1:C:137:GLU:HG3	1:C:151:VAL:HG11	2.00	0.41
1:F:79:LEU:HD21	1:F:145:ILE:HD11	2.02	0.41
1:A:114:SER:C	1:A:116:ARG:H	2.29	0.41
1:G:79:LEU:HG	1:G:144:GLU:HG3	2.01	0.41
2:N:24:DC:H2''	2:N:25:DT:C5'	2.39	0.41
1:D:107:ARG:NH1	1:H:113:GLY:H	2.19	0.41
1:E:18:ALA:HB1	1:E:39:ARG:HB3	2.02	0.41
1:E:146:LEU:HB2	1:E:147:PRO:HD2	2.03	0.41
2:N:13:DC:H2'	2:N:14:DT:C6	2.56	0.40
1:F:207:GLU:O	1:F:211:ARG:HG3	2.21	0.40
1:H:70:PRO:HB2	1:H:216:ALA:HB1	2.03	0.40
1:A:79:LEU:HD22	1:A:190:MET:HE2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:LEU:HD22	1:C:172:MET:HG2	2.03	0.40
1:D:59:GLN:HE22	1:D:120:ASN:N	2.06	0.40
1:D:66:VAL:HG22	1:D:128:TRP:HE3	1.85	0.40
1:G:128:TRP:HD1	1:G:159:VAL:HG13	1.86	0.40
1:A:166:GLN:HA	1:A:178:LEU:HD13	2.02	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	213/245 (87%)	201 (94%)	10 (5%)	2 (1%)	14	44
1	B	212/245 (86%)	205 (97%)	7 (3%)	0	100	100
1	C	210/245 (86%)	201 (96%)	7 (3%)	2 (1%)	12	41
1	D	211/245 (86%)	201 (95%)	10 (5%)	0	100	100
1	E	210/245 (86%)	200 (95%)	9 (4%)	1 (0%)	24	57
1	F	208/245 (85%)	198 (95%)	7 (3%)	3 (1%)	9	34
1	G	208/245 (85%)	193 (93%)	15 (7%)	0	100	100
1	H	208/245 (85%)	196 (94%)	11 (5%)	1 (0%)	24	57
All	All	1680/1960 (86%)	1595 (95%)	76 (4%)	9 (0%)	24	57

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	147	PRO
1	H	95	GLU
1	F	96	GLY
1	A	98	GLY
1	C	217	MET

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Mol	Chain	Res	Type
1	F	71	ARG
1	C	74	GLU
1	A	66	VAL
1	E	147	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	175/198 (88%)	160 (91%)	15 (9%)	10	34
1	B	173/198 (87%)	157 (91%)	16 (9%)	8	31
1	C	172/198 (87%)	154 (90%)	18 (10%)	6	26
1	D	174/198 (88%)	158 (91%)	16 (9%)	8	31
1	E	171/198 (86%)	153 (90%)	18 (10%)	6	26
1	F	171/198 (86%)	151 (88%)	20 (12%)	5	22
1	G	171/198 (86%)	155 (91%)	16 (9%)	8	31
1	H	171/198 (86%)	153 (90%)	18 (10%)	6	26
All	All	1378/1584 (87%)	1241 (90%)	137 (10%)	7	29

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	16	LEU
1	A	39	ARG
1	A	52	THR
1	A	61	VAL
1	A	76	GLU
1	A	95	GLU
1	A	107	ARG
1	A	142	LYS
1	A	168	LEU
1	A	172	MET

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Mol	Chain	Res	Type
1	A	180	GLU
1	A	181	ARG
1	A	190	MET
1	A	217	MET
1	B	9	ILE
1	B	16	LEU
1	B	44	LYS
1	B	52	THR
1	B	61	VAL
1	B	64	GLU
1	B	71	ARG
1	B	107	ARG
1	B	117	ASP
1	B	168	LEU
1	B	172	MET
1	B	180	GLU
1	B	181	ARG
1	B	190	MET
1	B	207	GLU
1	B	208	ARG
1	C	11	THR
1	C	29	GLU
1	C	39	ARG
1	C	61	VAL
1	C	69	LEU
1	C	71	ARG
1	C	78	LYS
1	C	106	VAL
1	C	107	ARG
1	C	122	ARG
1	C	135	LEU
1	C	148	HIS
1	C	151	VAL
1	C	157	LEU
1	C	168	LEU
1	C	190	MET
1	C	207	GLU
1	C	218	LYS
1	D	21	GLU
1	D	38	LYS
1	D	47	LEU
1	D	52	THR

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Mol	Chain	Res	Type
1	D	61	VAL
1	D	69	LEU
1	D	106	VAL
1	D	107	ARG
1	D	110	VAL
1	D	122	ARG
1	D	135	LEU
1	D	137	GLU
1	D	151	VAL
1	D	168	LEU
1	D	207	GLU
1	D	218	LYS
1	E	16	LEU
1	E	61	VAL
1	E	71	ARG
1	E	72	VAL
1	E	75	GLN
1	E	87	LEU
1	E	92	LEU
1	E	107	ARG
1	E	119	LEU
1	E	123	VAL
1	E	135	LEU
1	E	146	LEU
1	E	163	THR
1	E	168	LEU
1	E	184	ASP
1	E	189	LEU
1	E	199	LEU
1	E	200	VAL
1	F	10	ARG
1	F	11	THR
1	F	12	ARG
1	F	16	LEU
1	F	25	GLU
1	F	38	LYS
1	F	61	VAL
1	F	71	ARG
1	F	72	VAL
1	F	75	GLN
1	F	92	LEU
1	F	107	ARG

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Mol	Chain	Res	Type
1	F	128	TRP
1	F	134	SER
1	F	163	THR
1	F	168	LEU
1	F	180	GLU
1	F	184	ASP
1	F	199	LEU
1	F	200	VAL
1	G	12	ARG
1	G	16	LEU
1	G	25	GLU
1	G	39	ARG
1	G	61	VAL
1	G	69	LEU
1	G	89	LEU
1	G	91	HIS
1	G	107	ARG
1	G	132	THR
1	G	180	GLU
1	G	181	ARG
1	G	190	MET
1	G	207	GLU
1	G	217	MET
1	G	218	LYS
1	H	12	ARG
1	H	16	LEU
1	H	39	ARG
1	H	55	GLN
1	H	61	VAL
1	H	69	LEU
1	H	75	GLN
1	H	76	GLU
1	H	89	LEU
1	H	93	LEU
1	H	107	ARG
1	H	126	GLN
1	H	180	GLU
1	H	181	ARG
1	H	190	MET
1	H	198	ILE
1	H	207	GLU
1	H	217	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	59	GLN
1	A	75	GLN
1	A	81	GLN
1	A	112	GLN
1	B	55	GLN
1	B	59	GLN
1	B	75	GLN
1	B	81	GLN
1	B	112	GLN
1	B	166	GLN
1	C	59	GLN
1	C	75	GLN
1	C	166	GLN
1	D	59	GLN
1	D	166	GLN
1	E	13	GLN
1	E	59	GLN
1	E	126	GLN
1	E	166	GLN
1	F	59	GLN
1	F	126	GLN
1	F	166	GLN
1	G	59	GLN
1	G	65	GLN
1	G	118	HIS
1	G	120	ASN
1	H	126	GLN
1	H	133	GLN
1	H	148	HIS
1	H	166	GLN

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 [i](#)

There are no oligosaccharides 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	215/245 (87%)	-0.63	0	100	100	64, 94, 154, 175	0
1	B	214/245 (87%)	-0.57	0	100	100	64, 92, 152, 176	0
1	C	212/245 (86%)	-0.42	7 (3%)	49	29	78, 106, 168, 193	0
1	D	213/245 (86%)	-0.52	6 (2%)	55	34	75, 105, 163, 188	0
1	E	212/245 (86%)	-0.56	1 (0%)	87	73	69, 100, 157, 191	0
1	F	210/245 (85%)	-0.58	0	100	100	69, 100, 156, 186	0
1	G	210/245 (85%)	-0.41	1 (0%)	87	73	71, 110, 173, 196	0
1	H	210/245 (85%)	-0.31	4 (1%)	66	45	70, 111, 175, 201	0
2	M	28/28 (100%)	-1.15	0	100	100	72, 84, 96, 101	0
2	N	28/28 (100%)	-1.12	0	100	100	72, 85, 96, 97	0
All	All	1752/2016 (86%)	-0.52	19 (1%)	78	59	64, 101, 162, 201	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	120	ASN	4.0
1	D	43	THR	3.7
1	D	45	GLY	3.5
1	C	218	LYS	3.2
1	D	51	PHE	3.0
1	C	43	THR	2.9
1	C	49	PHE	2.8
1	C	56	GLU	2.7
1	C	51	PHE	2.7
1	H	96	GLY	2.7
1	C	44	LYS	2.6
1	D	44	LYS	2.6
1	C	45	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	48	TYR	2.3
1	G	70	PRO	2.2
1	H	52	THR	2.1
1	D	47	LEU	2.1
1	H	119	LEU	2.1
1	E	70	PRO	2.1

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.