Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 11:35 AM GMT

PDB ID : 3CVT

Title : Crystal Structure of an AlkA Host/Guest Complex 8oxoGuanine:Cytosine Base Pair

Authors : Bowman, B.R.; Lee, S.; Wang, S.; Verdine, G.L.

Deposited on : 2008-04-19

Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Clashscore		18
Ramachandran outliers		0.6%
Sidechain outliers		5.4%
RSRZ outliers		1.8%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
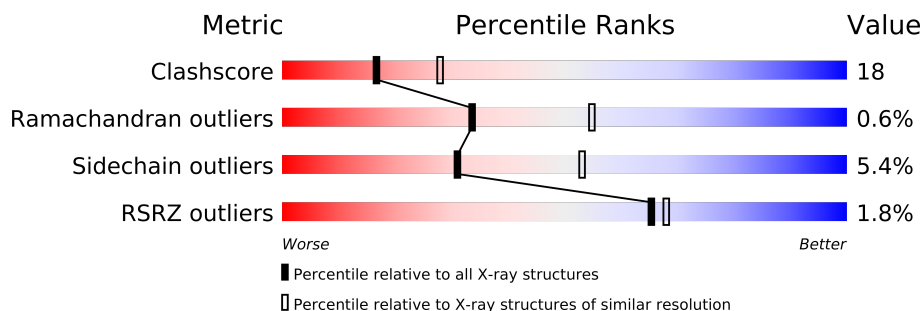
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	282	
1	B	282	
1	C	282	
1	D	282	
2	E	12	
2	G	12	
3	F	12	
3	H	12	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9863 atoms, of which 0 are hydrogen and 0 are deuterium.

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-3-methyladenine glycosylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			
1	B	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			
1	C	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			
1	D	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			

- Molecule 2 is a DNA chain called DNA (5'-D(*DGP*DAP*DCP*DAP*DTP*(8OG)P*DAP*DGP*DTP*DGP*DCP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	P	0	0	0
			246	117	48	70	11			
2	G	12	Total	C	N	O	P	0	0	0
			246	117	48	70	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			241	116	43	71	11			
3	H	12	Total	C	N	O	P	0	0	0
			241	116	43	71	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total 6	O 6	0	0
4	C	9	Total 9	O 9	0	0
4	D	8	Total 8	O 8	0	0

3 Residue-property plots ⓘ

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.
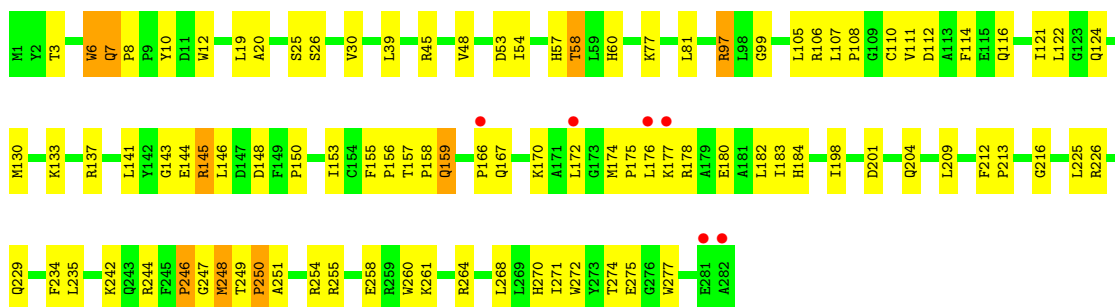
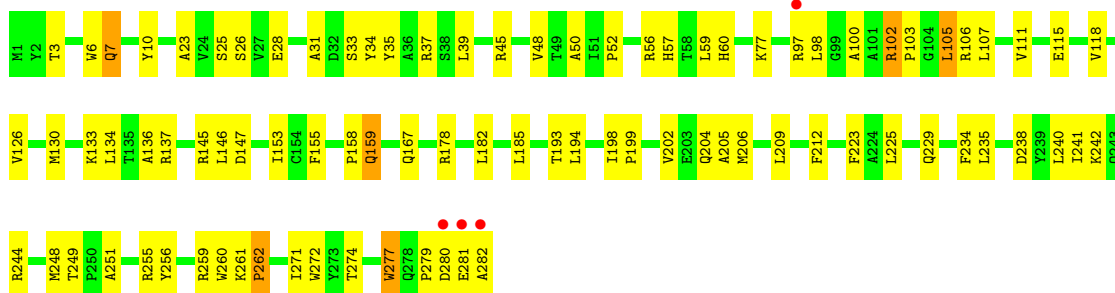- Molecule 1: DNA-3-methyladenine glycosylase 2

Chain A:
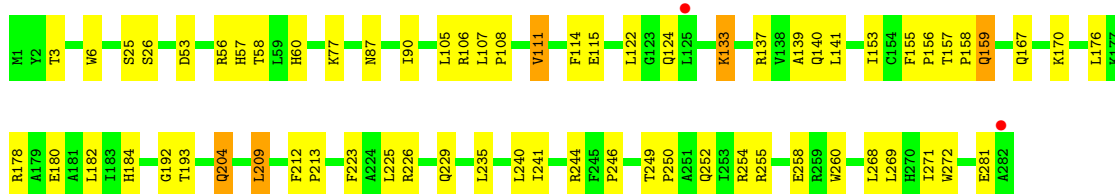
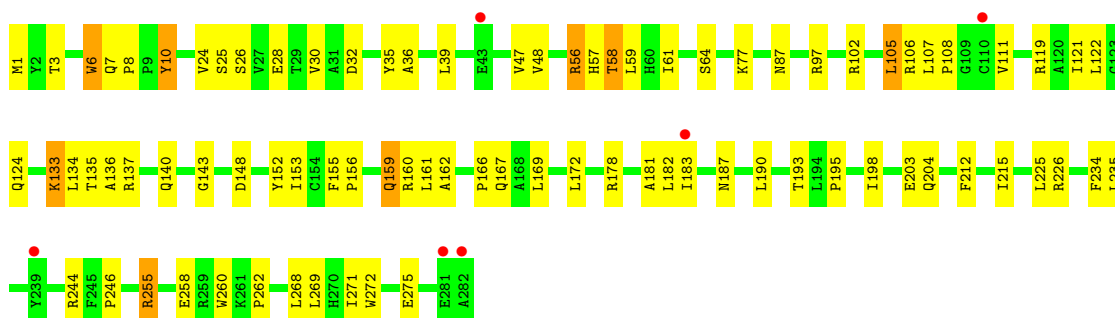- Molecule 1: DNA-3-methyladenine glycosylase 2

Chain B:

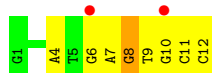- Molecule 1: DNA-3-methyladenine glycosylase 2

Chain C:

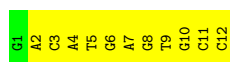- Molecule 1: DNA-3-methyladenine glycosylase 2

Chain D:

M1 Y2 T3 W6 Q7 P8 P9 Y10 V24 S25 S26 V27 E28 T29 V30 A31 D32 Y35 A36 L39 E43 V47 V48 R56 H57 T58 L59 H60 I61 S64 K77 N87 R97 R102 L105 R106 L107 P108 G109 C110 V111 R119 A120 I121 L122 G123

Q124 K133 L134 T135 A136 R137 Q140 G143 D148 Y152 I153 C154 F155 P156 Q159 R160 L161 A162 P166 Q167 A168 L169 L172 R178 A181 L182 I183 N187 L190 T193 L194 P195 I198 E203 Q204 F212 I215 L225 R226 F234 L235

Y239 R244 F245 P246 R255 E258 R259 W260 K261 P262 L268 L269 H270 I271 W272 E275 E281 A282

• Molecule 2: DNA (5'-D(*DGP*DAP*DCP*DAP*DTP*(8OG)P*DAP*DGP*DTP*DGP*DCP*DC)-3')

Chain E:

G1 A4 T5 G6 A7 G8 T9 G10 C11 C12

• Molecule 2: DNA (5'-D(*DGP*DAP*DCP*DAP*DTP*(8OG)P*DAP*DGP*DTP*DGP*DCP*DC)-3')

Chain G:

G1 A2 C3 A4 T5 G6 A7 G8 T9 G10 C11 C12

• Molecule 3: DNA (5'-D(*DGP*DGP*DCP*DAP*DCP*DTP*DCP*DAP*DTP*DGP*DTP*DC)-3')

Chain F:

G14 G15 C16 A17 C18 T19 C20 A21 T22 G23 T24 C25

• Molecule 3: DNA (5'-D(*DGP*DGP*DCP*DAP*DCP*DTP*DCP*DAP*DTP*DGP*DTP*DC)-3')

Chain H:

G14 C20 A21 T22 G23 T24 C25
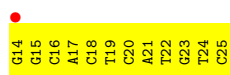
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.41Å 101.23Å 103.03Å 90.00° 94.28° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 45.81 – 2.49	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-2.50) 93.1 (45.81-2.49)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.274 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	48.3	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 28.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 52630 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9863	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
8OG

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	0.39	0/2277	0.61	0/3104
1	B	0.40	0/2277	0.63	0/3104
1	C	0.38	0/2277	0.59	0/3104
1	D	0.40	0/2277	0.61	0/3104
2	E	0.73	1/249 (0.4%)	0.93	0/380
2	G	0.48	0/249	0.74	0/380
3	F	0.63	0/269	0.94	0/413
3	H	0.47	0/269	0.74	0/413
All	All	0.42	1/10144 (0.0%)	0.64	0/14002

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	8	DG	N9-C4	5.12	1.42	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2215	0	2209	50	0
1	B	2215	0	2209	90	0
1	C	2215	0	2209	70	0
1	D	2215	0	2209	68	0
2	E	246	0	136	22	0
2	G	246	0	136	25	0
3	F	241	0	137	25	0
3	H	241	0	137	6	0
4	A	6	0	0	0	0
4	B	6	0	0	0	0
4	C	9	0	0	0	0
4	D	8	0	0	0	0
All	All	9863	0	9382	343	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (343) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:H:21:DA:H2"	3:H:22:DT:H5'	1.21	1.19
1:D:121:ILE:HA	1:D:124:GLN:HE21	0.99	1.15
1:B:77:LYS:HB3	1:B:111:VAL:HG23	1.35	1.07
2:G:5:DT:H1'	2:G:6:8OG:H5'	1.32	1.06
2:E:8:DG:H4'	2:E:9:DT:OP1	1.67	0.95
1:D:121:ILE:HA	1:D:124:GLN:NE2	1.82	0.93
2:G:5:DT:C1'	2:G:6:8OG:H5'	1.99	0.92
2:G:2:DA:H2"	2:G:3:DC:H5'	1.51	0.92
1:D:77:LYS:HB3	1:D:111:VAL:HG23	1.57	0.86
3:H:21:DA:H2"	3:H:22:DT:C5'	2.06	0.85
1:C:97:ARG:HD2	1:C:98:LEU:N	1.91	0.84
1:B:39:LEU:HD22	1:B:48:VAL:HG21	1.60	0.84
1:C:249:THR:HB	2:G:7:DA:H5'	1.60	0.82
1:B:174:MET:HB2	1:B:178:ARG:HG2	1.61	0.82
1:A:124:GLN:HE21	1:A:178:ARG:HH11	1.28	0.81
1:D:39:LEU:HD22	1:D:48:VAL:HG21	1.62	0.80
1:B:167:GLN:NE2	1:B:170:LYS:HD3	1.98	0.79
1:B:143:GLY:HA3	1:B:153:ILE:HD11	1.63	0.79
1:D:77:LYS:HD3	1:D:111:VAL:HG22	1.67	0.77
1:B:53:ASP:HB3	1:B:58:THR:HG22	1.67	0.77
1:B:145:ARG:HH11	1:B:145:ARG:HG2	1.47	0.76
3:H:21:DA:C2'	3:H:22:DT:H5'	2.10	0.76
2:G:5:DT:C2'	2:G:6:8OG:H5'	2.15	0.76
1:A:235:LEU:HD22	1:A:268:LEU:HD21	1.68	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:124:GLN:HE21	1:A:178:ARG:NH1	1.85	0.75
1:C:107:LEU:HD11	1:C:225:LEU:HD21	1.70	0.74
1:D:121:ILE:CA	1:D:124:GLN:HE21	1.91	0.73
1:A:124:GLN:NE2	1:A:178:ARG:HH11	1.86	0.72
1:C:158:PRO:HD2	1:C:159:GLN:HE21	1.55	0.72
1:B:184:HIS:CD2	1:B:213:PRO:HD2	2.24	0.72
2:G:11:DC:H2"	2:G:12:DC:O5'	1.90	0.72
1:C:238:ASP:HB3	1:C:241:ILE:HB	1.72	0.72
1:A:107:LEU:HD11	1:A:225:LEU:HD21	1.72	0.71
1:B:141:LEU:HD22	1:B:172:LEU:HD21	1.70	0.71
1:C:158:PRO:HD2	1:C:159:GLN:NE2	2.06	0.71
2:G:5:DT:H2"	2:G:6:8OG:H5'	1.73	0.70
1:C:97:ARG:HH12	1:C:277:TRP:HE1	1.38	0.70
1:B:122:LEU:HD21	1:B:182:LEU:HD11	1.73	0.70
1:C:260:TRP:CH2	1:C:271:ILE:HD11	2.29	0.68
3:F:21:DA:C2'	3:F:22:DT:H5"	2.23	0.68
1:D:225:LEU:HD23	1:D:226:ARG:HG2	1.76	0.68
1:C:107:LEU:HD11	1:C:225:LEU:CD2	2.25	0.67
1:C:249:THR:CB	2:G:7:DA:H5'	2.24	0.66
3:F:18:DC:H2"	3:F:19:DT:O5'	1.95	0.66
1:C:261:LYS:HG3	1:C:262:PRO:HA	1.77	0.66
2:G:4:DA:H2'	2:G:5:DT:H72	1.77	0.65
3:F:21:DA:H1'	3:F:22:DT:H5"	1.78	0.65
3:F:21:DA:H2"	3:F:22:DT:H5"	1.76	0.65
2:E:7:DA:C6	2:E:8:DG:O6	2.49	0.65
3:F:14:DG:H4'	3:F:15:DG:H5'	1.79	0.65
1:B:124:GLN:HB3	3:F:14:DG:H5'	1.78	0.65
1:D:39:LEU:CD2	1:D:48:VAL:HG21	2.27	0.65
1:B:121:ILE:O	1:B:124:GLN:HG3	1.97	0.64
2:G:5:DT:H1'	2:G:6:8OG:C5'	2.18	0.64
2:E:11:DC:H2"	2:E:12:DC:C5	2.33	0.64
1:B:26:SER:HB3	1:B:153:ILE:HG22	1.79	0.64
1:B:124:GLN:NE2	1:B:178:ARG:HH12	1.94	0.64
1:C:238:ASP:O	1:C:242:LYS:HG3	1.98	0.64
1:B:261:LYS:HG2	1:B:264:ARG:CZ	2.29	0.63
1:B:261:LYS:HE2	1:B:264:ARG:NH1	2.13	0.63
1:B:8:PRO:HG2	1:B:57:HIS:CE1	2.33	0.63
2:G:5:DT:H2"	2:G:6:8OG:H2"	1.81	0.62
1:B:97:ARG:HG3	1:B:97:ARG:HH21	1.64	0.62
3:F:23:DG:H2"	3:F:24:DT:OP2	1.98	0.62
1:A:249:THR:OG1	1:A:252:GLN:HG3	1.99	0.62
1:D:25:SER:O	1:D:26:SER:HB2	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:158:PRO:HD2	1:B:159:GLN:NE2	2.15	0.62
1:D:122:LEU:HD13	1:D:134:LEU:HD22	1.81	0.62
1:C:39:LEU:HD11	1:C:111:VAL:HG21	1.81	0.62
1:A:184:HIS:CD2	1:A:213:PRO:HD2	2.34	0.62
1:B:124:GLN:HE21	3:F:14:DG:H5'	1.65	0.62
1:C:134:LEU:HA	1:C:137:ARG:NH1	2.15	0.62
1:D:26:SER:HB3	1:D:153:ILE:HG22	1.82	0.62
1:B:6:TRP:C	1:B:6:TRP:CD1	2.73	0.61
2:G:8:DG:H2'	2:G:9:DT:H71	1.81	0.61
2:G:2:DA:C2'	2:G:3:DC:H5'	2.27	0.61
1:D:108:PRO:O	1:D:226:ARG:HD2	2.00	0.61
1:D:235:LEU:HD13	1:D:268:LEU:HD22	1.83	0.61
1:A:140:GLN:HE21	1:A:140:GLN:HA	1.66	0.61
2:G:10:DG:H2"	2:G:11:DC:H5"	1.84	0.60
1:D:134:LEU:HD23	1:D:134:LEU:C	2.20	0.60
1:A:157:THR:HB	1:A:159:GLN:HE21	1.66	0.60
1:B:167:GLN:HE22	1:B:170:LYS:HD3	1.66	0.60
1:A:133:LYS:HD2	1:A:137:ARG:HH11	1.67	0.60
3:F:14:DG:H4'	3:F:15:DG:C5'	2.32	0.60
2:G:7:DA:H2"	2:G:8:DG:H5'	1.84	0.59
1:D:8:PRO:HG2	1:D:57:HIS:CE1	2.37	0.59
1:C:248:MET:CE	1:C:279:PRO:HG3	2.33	0.59
1:B:145:ARG:HD2	1:B:150:PRO:HA	1.83	0.59
1:D:28:GLU:CD	1:D:119:ARG:HH22	2.06	0.59
2:E:8:DG:OP2	2:E:8:DG:H2'	2.03	0.59
1:D:203:GLU:CD	1:D:203:GLU:H	2.05	0.58
1:B:177:LYS:HA	1:B:180:GLU:HG3	1.86	0.58
3:F:21:DA:H2"	3:F:22:DT:C5'	2.32	0.58
1:A:107:LEU:CD1	1:A:269:LEU:HD11	2.32	0.58
1:D:166:PRO:HG3	1:D:183:ILE:HD12	1.84	0.58
1:B:166:PRO:HG3	1:B:183:ILE:CD1	2.34	0.58
1:D:77:LYS:HB3	1:D:111:VAL:CG2	2.31	0.58
1:B:261:LYS:HE2	1:B:264:ARG:CZ	2.33	0.58
3:F:15:DG:H2"	3:F:16:DC:O5'	2.04	0.58
1:C:133:LYS:HE3	1:C:137:ARG:NH2	2.19	0.57
2:E:8:DG:C1'	2:E:9:DT:H5"	2.33	0.57
1:A:107:LEU:HD12	1:A:269:LEU:HD11	1.87	0.57
1:B:124:GLN:HB2	1:B:178:ARG:NH1	2.19	0.57
2:G:7:DA:H2"	2:G:8:DG:C5'	2.34	0.57
1:A:158:PRO:HD2	1:A:159:GLN:NE2	2.20	0.57
1:A:244:ARG:C	1:A:246:PRO:HD3	2.25	0.57
3:F:24:DT:H2"	3:F:25:DC:C5'	2.35	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:244:ARG:C	1:D:246:PRO:HD3	2.26	0.56
1:B:157:THR:OG1	1:B:159:GLN:HG2	2.05	0.56
1:D:162:ALA:HB1	1:D:187:ASN:ND2	2.19	0.56
1:C:235:LEU:HB3	1:C:238:ASP:HB2	1.86	0.56
1:D:235:LEU:HD13	1:D:268:LEU:CD2	2.35	0.56
1:C:202:VAL:O	1:C:206:MET:HG3	2.06	0.56
1:B:255:ARG:HH11	1:B:255:ARG:HG2	1.70	0.56
1:B:108:PRO:O	1:B:226:ARG:HD2	2.06	0.56
2:E:6:8OG:H2'	2:E:7:DA:OP2	2.06	0.56
1:C:248:MET:HE1	1:C:279:PRO:HG3	1.87	0.56
1:A:105:LEU:HD13	1:A:106:ARG:N	2.21	0.56
1:B:145:ARG:HG2	1:B:145:ARG:NH1	2.20	0.56
1:D:159:GLN:HB3	1:D:190:LEU:HD21	1.87	0.56
1:A:260:TRP:CH2	1:A:271:ILE:HD11	2.41	0.56
2:E:11:DC:C2'	2:E:12:DC:H5	2.18	0.55
1:D:24:VAL:HG11	1:D:135:THR:HG22	1.87	0.55
1:C:25:SER:O	1:C:26:SER:HB2	2.06	0.55
1:B:143:GLY:CA	1:B:153:ILE:HD11	2.34	0.55
2:E:7:DA:C2	2:E:8:DG:C6	2.95	0.54
1:C:26:SER:O	1:C:153:ILE:HG22	2.07	0.54
1:A:107:LEU:HD11	1:A:225:LEU:CD2	2.36	0.54
3:F:17:DA:H1'	3:F:18:DC:H5'	1.89	0.54
1:D:47:VAL:HG21	1:D:152:TYR:CD2	2.43	0.54
1:B:6:TRP:CZ3	1:B:58:THR:O	2.61	0.54
1:B:6:TRP:HZ3	1:B:58:THR:O	1.90	0.54
1:C:10:TYR:CD2	1:C:106:ARG:NH1	2.76	0.54
1:A:25:SER:O	1:A:26:SER:HB2	2.08	0.54
3:F:21:DA:C1'	3:F:22:DT:H5"	2.38	0.53
1:B:133:LYS:O	1:B:137:ARG:HG3	2.08	0.53
1:A:108:PRO:O	1:A:226:ARG:HD2	2.09	0.53
1:B:260:TRP:CH2	1:B:271:ILE:HD11	2.42	0.53
1:C:234:PHE:O	1:C:235:LEU:HD12	2.09	0.53
1:D:166:PRO:HG3	1:D:183:ILE:CD1	2.38	0.53
1:B:145:ARG:NE	1:B:150:PRO:O	2.41	0.52
1:C:251:ALA:HB3	2:G:7:DA:OP1	2.08	0.52
3:F:19:DT:OP1	3:F:19:DT:H4'	2.09	0.52
1:C:6:TRP:CZ2	1:C:57:HIS:HA	2.44	0.52
1:B:274:THR:HG22	1:B:277:TRP:HB2	1.92	0.52
1:B:25:SER:O	1:B:26:SER:HB2	2.09	0.52
1:B:107:LEU:HD23	1:B:107:LEU:C	2.30	0.52
1:B:159:GLN:CD	1:B:159:GLN:H	2.14	0.52
1:A:133:LYS:HD2	1:A:137:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:137:ARG:O	1:D:140:GLN:HB3	2.09	0.52
1:C:133:LYS:HE3	1:C:137:ARG:HH22	1.75	0.51
1:C:126:VAL:HB	1:C:130:MET:HB3	1.92	0.51
2:G:5:DT:H2"	2:G:6:8OG:C5'	2.41	0.51
1:B:261:LYS:HE2	1:B:264:ARG:NH2	2.25	0.51
3:F:24:DT:H2"	3:F:25:DC:H5"	1.92	0.51
1:B:77:LYS:HD3	1:B:111:VAL:HG22	1.93	0.51
2:E:11:DC:C2	2:E:12:DC:C5	2.99	0.51
1:C:100:ALA:O	1:C:103:PRO:HD3	2.11	0.51
1:D:10:TYR:CD2	1:D:106:ARG:NH1	2.79	0.51
3:F:24:DT:H2"	3:F:25:DC:O5'	2.11	0.51
1:C:97:ARG:HD2	1:C:98:LEU:H	1.75	0.50
1:B:254:ARG:O	1:B:258:GLU:HG3	2.11	0.50
1:B:159:GLN:NE2	1:B:159:GLN:H	2.09	0.50
1:D:105:LEU:HD13	1:D:106:ARG:N	2.26	0.50
1:D:30:VAL:HG22	1:D:35:TYR:CD1	2.47	0.50
2:E:9:DT:H2"	2:E:10:DG:O5'	2.11	0.50
2:E:11:DC:H2"	2:E:12:DC:C6	2.47	0.50
1:A:87:ASN:HB3	1:A:90:ILE:HD12	1.92	0.50
1:C:10:TYR:CE2	1:C:106:ARG:HG3	2.46	0.50
1:B:110:CYS:HB3	1:B:116:GLN:HE21	1.77	0.50
1:B:45:ARG:HG3	1:B:45:ARG:HH11	1.77	0.50
1:C:39:LEU:HD22	1:C:48:VAL:HG21	1.92	0.50
1:D:24:VAL:CG1	1:D:135:THR:HG22	2.42	0.50
1:B:251:ALA:HB3	2:E:7:DA:OP1	2.12	0.50
1:B:124:GLN:NE2	3:F:14:DG:H5'	2.26	0.50
1:D:143:GLY:HA3	1:D:153:ILE:HD11	1.93	0.50
1:B:234:PHE:C	1:B:235:LEU:HD12	2.31	0.50
2:E:8:DG:O4'	2:E:9:DT:H5"	2.11	0.50
1:D:133:LYS:HA	1:D:133:LYS:HE2	1.94	0.49
1:A:167:GLN:NE2	1:A:170:LYS:HD3	2.27	0.49
1:D:36:ALA:HA	1:D:48:VAL:O	2.11	0.49
1:B:176:LEU:O	1:B:180:GLU:HG2	2.13	0.49
1:B:158:PRO:HD2	1:B:159:GLN:HE21	1.77	0.49
1:C:193:THR:O	1:C:193:THR:HG22	2.13	0.49
1:B:130:MET:HA	1:B:133:LYS:CE	2.43	0.49
1:D:166:PRO:O	1:D:169:LEU:N	2.46	0.48
1:D:244:ARG:O	1:D:246:PRO:HD3	2.13	0.48
1:C:107:LEU:CD1	1:C:225:LEU:HD21	2.43	0.48
2:E:8:DG:H1'	2:E:9:DT:H5"	1.95	0.48
1:A:25:SER:O	1:A:26:SER:CB	2.61	0.48
1:D:133:LYS:HA	1:D:133:LYS:CE	2.43	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:159:GLN:NE2	1:C:159:GLN:H	2.12	0.48
1:A:225:LEU:O	1:A:229:GLN:HA	2.14	0.48
1:C:45:ARG:HB3	1:C:146:LEU:CD2	2.44	0.48
1:C:77:LYS:HB3	1:C:111:VAL:CG2	2.44	0.48
1:D:255:ARG:O	1:D:258:GLU:HG3	2.13	0.48
1:C:249:THR:CG2	2:G:7:DA:H5'	2.44	0.47
1:A:141:LEU:O	1:A:141:LEU:HD12	2.14	0.47
1:B:97:ARG:NH2	1:B:97:ARG:HG3	2.29	0.47
1:B:3:THR:HG22	1:B:60:HIS:CD2	2.50	0.47
1:C:77:LYS:HB3	1:C:111:VAL:HG23	1.96	0.47
1:B:166:PRO:HG3	1:B:183:ILE:HD12	1.95	0.47
1:B:235:LEU:HD13	1:B:268:LEU:HD22	1.96	0.47
1:D:107:LEU:CD1	1:D:269:LEU:HD11	2.44	0.47
1:C:134:LEU:HA	1:C:137:ARG:HH12	1.80	0.47
1:B:242:LYS:NZ	1:B:250:PRO:HG3	2.30	0.47
3:H:20:DC:H2"	3:H:21:DA:O5'	2.14	0.47
1:A:122:LEU:HD21	1:A:182:LEU:HD11	1.96	0.47
2:E:11:DC:N1	2:E:12:DC:H5	2.13	0.47
1:B:45:ARG:HB3	1:B:146:LEU:CD2	2.45	0.47
1:B:258:GLU:O	1:B:261:LYS:HG3	2.14	0.47
1:B:201:ASP:OD2	1:B:204:GLN:HB2	2.15	0.46
1:A:204:GLN:NE2	1:A:204:GLN:C	2.68	0.46
1:C:256:TYR:O	1:C:259:ARG:HG2	2.15	0.46
1:A:26:SER:HB3	1:A:153:ILE:HG22	1.96	0.46
1:C:50:ALA:HB1	1:C:59:LEU:HD11	1.97	0.46
1:C:3:THR:HG22	1:C:60:HIS:CD2	2.51	0.46
1:C:240:LEU:HD11	1:C:244:ARG:NH1	2.30	0.46
1:D:6:TRP:CD1	1:D:6:TRP:C	2.88	0.46
2:E:11:DC:C2'	2:E:12:DC:C5	2.95	0.46
1:A:159:GLN:NE2	1:A:159:GLN:H	2.14	0.46
1:B:249:THR:O	1:B:251:ALA:N	2.49	0.46
1:A:26:SER:CB	1:A:153:ILE:HG22	2.46	0.46
1:D:178:ARG:O	1:D:181:ALA:HB3	2.16	0.46
1:D:6:TRP:CZ3	1:D:58:THR:O	2.69	0.46
1:D:260:TRP:CH2	1:D:271:ILE:HD11	2.51	0.45
3:H:24:DT:H2"	3:H:25:DC:C6	2.52	0.45
2:E:6:8OG:H2"	2:E:6:8OG:O8	2.16	0.45
1:C:118:VAL:HG13	1:C:182:LEU:HD22	1.99	0.45
1:D:198:ILE:HG23	1:D:198:ILE:O	2.16	0.45
1:C:225:LEU:O	1:C:229:GLN:HA	2.16	0.45
1:C:6:TRP:C	1:C:6:TRP:CD1	2.90	0.45
1:B:144:GLU:HA	1:B:144:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:53:ASP:OD1	1:A:56:ARG:NH1	2.48	0.45
1:A:225:LEU:C	1:A:225:LEU:HD23	2.36	0.45
1:D:134:LEU:CD2	1:D:134:LEU:C	2.85	0.45
1:D:102:ARG:HB3	1:D:102:ARG:HE	1.64	0.45
2:E:6:8OG:N2	3:F:20:DC:N3	2.57	0.45
1:C:240:LEU:HD11	1:C:244:ARG:CZ	2.47	0.45
2:E:8:DG:H1'	2:E:9:DT:C5'	2.47	0.45
2:E:9:DT:C4	2:E:10:DG:C6	3.05	0.45
1:D:234:PHE:C	1:D:235:LEU:HD12	2.36	0.45
1:A:115:GLU:HG3	1:A:155:PHE:CZ	2.52	0.45
1:C:274:THR:HG22	1:C:277:TRP:H	1.81	0.44
1:A:241:ILE:HD11	1:A:268:LEU:HD12	2.00	0.44
1:A:209:LEU:O	1:A:212:PHE:HB2	2.17	0.44
3:F:14:DG:H4'	3:F:15:DG:O5'	2.18	0.44
1:C:106:ARG:HA	1:C:106:ARG:HD3	1.73	0.44
1:B:130:MET:HA	1:B:133:LYS:HE2	1.99	0.44
1:A:6:TRP:C	1:A:6:TRP:CD1	2.91	0.44
1:B:12:TRP:CD1	1:B:54:ILE:HD11	2.52	0.44
1:A:254:ARG:O	1:A:258:GLU:HG3	2.17	0.44
2:G:10:DG:C2'	2:G:11:DC:H5"	2.46	0.44
1:D:155:PHE:CD2	1:D:156:PRO:HD2	2.52	0.44
1:B:99:GLY:HA2	1:B:270:HIS:CD2	2.53	0.44
2:E:4:DA:N6	3:F:21:DA:H61	2.15	0.44
1:C:133:LYS:O	1:C:136:ALA:HB3	2.17	0.44
1:C:6:TRP:CD1	1:C:7:GLN:N	2.86	0.44
2:G:11:DC:H5'	2:G:11:DC:H6	1.83	0.44
1:A:140:GLN:NE2	1:A:140:GLN:HA	2.31	0.44
1:B:170:LYS:HG3	1:B:174:MET:O	2.17	0.44
1:C:39:LEU:HB2	1:C:48:VAL:HG23	2.00	0.44
1:B:244:ARG:C	1:B:246:PRO:HD3	2.38	0.44
1:B:155:PHE:CD2	1:B:156:PRO:HD2	2.52	0.44
1:A:3:THR:HG22	1:A:60:HIS:CD2	2.53	0.43
1:B:7:GLN:H	1:B:7:GLN:HG2	1.65	0.43
1:B:225:LEU:O	1:B:229:GLN:HA	2.18	0.43
1:C:115:GLU:HG3	1:C:155:PHE:CZ	2.54	0.43
1:D:121:ILE:HG23	1:D:124:GLN:NE2	2.34	0.43
1:A:209:LEU:HD11	1:A:223:PHE:CD2	2.53	0.43
1:C:23:ALA:HA	1:C:28:GLU:OE2	2.18	0.43
1:B:247:GLY:O	1:B:248:MET:O	2.36	0.43
1:D:39:LEU:HD11	1:D:111:VAL:HG21	2.01	0.43
1:A:115:GLU:HG3	1:A:155:PHE:CE2	2.53	0.43
1:B:261:LYS:HG2	1:B:264:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:45:ARG:NH1	1:B:45:ARG:HG3	2.34	0.43
1:C:199:PRO:HG3	1:C:205:ALA:CB	2.48	0.43
2:G:8:DG:H2"	2:G:9:DT:O5'	2.19	0.43
1:B:216:GLY:HA3	3:F:15:DG:OP2	2.18	0.43
1:B:275:GLU:C	1:B:277:TRP:H	2.22	0.43
1:A:139:ALA:HA	1:A:156:PRO:CG	2.49	0.43
1:C:280:ASP:O	1:C:282:ALA:N	2.51	0.42
1:D:107:LEU:HD11	1:D:225:LEU:HD21	2.02	0.42
1:D:28:GLU:OE2	1:D:119:ARG:NH2	2.50	0.42
1:D:56:ARG:HE	1:D:56:ARG:HA	1.83	0.42
1:A:193:THR:O	1:A:193:THR:CG2	2.67	0.42
1:B:209:LEU:O	1:B:212:PHE:HB2	2.18	0.42
3:F:14:DG:O4'	3:F:14:DG:N3	2.53	0.42
1:C:35:TYR:OH	1:C:37:ARG:HD2	2.18	0.42
1:D:161:LEU:O	1:D:161:LEU:HD23	2.19	0.42
1:C:209:LEU:O	1:C:212:PHE:HB2	2.19	0.42
1:B:19:LEU:HD21	1:B:81:LEU:HD11	2.01	0.42
1:C:39:LEU:HD11	1:C:111:VAL:CG2	2.49	0.42
1:C:33:SER:O	1:C:52:PRO:HD2	2.18	0.42
1:A:176:LEU:HG	1:A:180:GLU:OE2	2.20	0.42
1:D:59:LEU:CD2	1:D:61:ILE:HD11	2.49	0.42
2:G:5:DT:C4'	2:G:6:8OG:OP1	2.67	0.42
2:G:4:DA:H2'	2:G:5:DT:C7	2.46	0.42
1:D:7:GLN:NE2	1:D:87:ASN:HA	2.34	0.42
1:C:31:ALA:HB3	1:C:34:TYR:CD1	2.54	0.42
1:C:198:ILE:O	1:C:198:ILE:HG23	2.19	0.42
1:D:182:LEU:O	1:D:183:ILE:C	2.56	0.42
1:C:97:ARG:NH1	1:C:277:TRP:HE1	2.13	0.41
1:C:193:THR:CG2	1:C:193:THR:O	2.68	0.41
2:G:8:DG:H8	2:G:8:DG:H5'	1.86	0.41
1:B:177:LYS:HA	1:B:180:GLU:CG	2.49	0.41
1:C:209:LEU:HD11	1:C:223:PHE:CD2	2.55	0.41
1:D:193:THR:O	1:D:193:THR:HG22	2.20	0.41
1:A:77:LYS:HB3	1:A:111:VAL:HG22	2.02	0.41
1:D:212:PHE:CB	1:D:215:ILE:HD12	2.50	0.41
1:B:261:LYS:HE2	1:B:264:ARG:HH12	1.83	0.41
1:D:137:ARG:NH1	1:D:172:LEU:O	2.53	0.41
1:D:106:ARG:HA	1:D:106:ARG:HD3	1.82	0.41
1:B:12:TRP:HD1	1:B:54:ILE:HD11	1.85	0.41
1:B:112:ASP:OD2	1:B:114:PHE:HB3	2.21	0.41
2:E:4:DA:N6	3:F:21:DA:N6	2.68	0.41
3:F:23:DG:H2"	3:F:24:DT:H71	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:162:ALA:HB1	1:D:187:ASN:HD21	1.85	0.41
1:D:24:VAL:CG1	1:D:136:ALA:HA	2.50	0.41
1:C:56:ARG:O	1:C:57:HIS:C	2.59	0.41
1:C:39:LEU:CD1	1:C:111:VAL:HG21	2.49	0.41
1:D:10:TYR:CE2	1:D:106:ARG:HG3	2.55	0.41
1:B:124:GLN:NE2	1:B:178:ARG:NH1	2.67	0.41
1:A:192:GLY:O	1:D:195:PRO:HG3	2.21	0.41
1:C:6:TRP:HD1	1:C:7:GLN:C	2.24	0.41
1:B:198:ILE:O	1:B:198:ILE:HG23	2.21	0.41
1:A:107:LEU:HD13	1:A:269:LEU:HD11	2.00	0.40
1:B:10:TYR:CE2	1:B:106:ARG:HG3	2.56	0.40
1:B:20:ALA:HB2	1:B:30:VAL:HG11	2.03	0.40
1:B:143:GLY:HA3	1:B:153:ILE:CD1	2.43	0.40
1:D:58:THR:HG23	1:D:59:LEU:N	2.36	0.40
1:B:209:LEU:HD23	1:B:209:LEU:HA	1.90	0.40
1:D:148:ASP:OD1	1:D:148:ASP:N	2.54	0.40
1:A:240:LEU:HD23	1:A:272:TRP:CD1	2.56	0.40
1:C:185:LEU:HD11	1:C:194:LEU:HD22	2.04	0.40
3:H:21:DA:H4'	3:H:21:DA:OP1	2.21	0.40
1:D:107:LEU:HD11	1:D:225:LEU:CD2	2.52	0.40
1:A:114:PHE:CD2	1:A:158:PRO:HG3	2.56	0.40
1:B:77:LYS:HD3	1:B:111:VAL:CG2	2.52	0.40
1:A:58:THR:HG22	1:A:60:HIS:CD2	2.57	0.40
1:B:39:LEU:HD22	1:B:48:VAL:CG2	2.39	0.40
1:C:102:ARG:O	1:C:105:LEU:HB2	2.21	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	280/282 (99%)	268 (96%)	12 (4%)	0	100	100
1	B	280/282 (99%)	257 (92%)	19 (7%)	4 (1%)	16	27
1	C	280/282 (99%)	262 (94%)	16 (6%)	2 (1%)	30	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	280/282 (99%)	255 (91%)	24 (9%)	1 (0%)	43	66
All	All	1120/1128 (99%)	1042 (93%)	71 (6%)	7 (1%)	33	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	248	MET
1	C	277	TRP
1	C	281	GLU
1	D	64	SER
1	B	250	PRO
1	B	175	PRO
1	B	246	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	222/222 (100%)	213 (96%)	9 (4%)	41	67
1	B	222/222 (100%)	213 (96%)	9 (4%)	41	67
1	C	222/222 (100%)	210 (95%)	12 (5%)	31	53
1	D	222/222 (100%)	204 (92%)	18 (8%)	17	30
All	All	888/888 (100%)	840 (95%)	48 (5%)	31	53

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	111	VAL
1	A	133	LYS
1	A	159	GLN
1	A	204	GLN
1	A	209	LEU
1	A	250	PRO
1	A	255	ARG

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Mol	Chain	Res	Type
1	A	281	GLU
1	B	6	TRP
1	B	7	GLN
1	B	58	THR
1	B	97	ARG
1	B	105	LEU
1	B	145	ARG
1	B	148	ASP
1	B	159	GLN
1	B	272	TRP
1	C	7	GLN
1	C	102	ARG
1	C	105	LEU
1	C	145	ARG
1	C	147	ASP
1	C	159	GLN
1	C	167	GLN
1	C	178	ARG
1	C	204	GLN
1	C	255	ARG
1	C	262	PRO
1	C	272	TRP
1	D	1	MET
1	D	3	THR
1	D	6	TRP
1	D	10	TYR
1	D	32	ASP
1	D	56	ARG
1	D	58	THR
1	D	97	ARG
1	D	105	LEU
1	D	133	LYS
1	D	159	GLN
1	D	160	ARG
1	D	167	GLN
1	D	204	GLN
1	D	255	ARG
1	D	262	PRO
1	D	272	TRP
1	D	275	GLU

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

Mol	Chain	Res	Type
1	A	60	HIS
1	A	124	GLN
1	A	140	GLN
1	A	159	GLN
1	A	167	GLN
1	A	184	HIS
1	A	204	GLN
1	A	221	ASN
1	B	7	GLN
1	B	116	GLN
1	B	124	GLN
1	B	159	GLN
1	B	167	GLN
1	B	184	HIS
1	B	221	ASN
1	C	60	HIS
1	C	89	GLN
1	C	116	GLN
1	C	124	GLN
1	C	140	GLN
1	C	159	GLN
1	C	184	HIS
1	C	187	ASN
1	C	221	ASN
1	D	5	ASN
1	D	7	GLN
1	D	116	GLN
1	D	124	GLN
1	D	140	GLN
1	D	187	ASN
1	D	221	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 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	#$|Z| > 2$
2	8OG	E	6	3,2	23,25,26	0.91	1 (4%)	27,37,40	2.08	5 (18%)
2	8OG	G	6	3,2	23,25,26	0.78	0	27,37,40	1.99	5 (18%)

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
2	8OG	E	6	3,2	-	0/6/21/22	0/1/3/3
2	8OG	G	6	3,2	-	0/6/21/22	0/1/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	6	8OG	P-OP1	2.63	1.49	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	6	8OG	C8-N9-C1'	6.81	128.95	125.17
2	E	6	8OG	C4-C5-N7	5.58	110.81	106.14
2	G	6	8OG	C4-C5-N7	5.51	110.74	106.14
2	G	6	8OG	C8-N9-C1'	5.27	128.10	125.17
2	G	6	8OG	C8-N7-C5	-3.78	103.65	107.48
2	E	6	8OG	C8-N7-C5	-3.70	103.73	107.48
2	G	6	8OG	C6-N1-C2	3.14	125.00	119.51
2	E	6	8OG	C6-N1-C2	3.11	124.94	119.51
2	E	6	8OG	C2-N3-C4	-2.29	111.88	115.09
2	G	6	8OG	C2-N3-C4	-2.23	111.95	115.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates 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	282/282 (100%)	-0.01	2 (0%)	84	86	29, 49, 81, 110	0
1	B	282/282 (100%)	0.10	6 (2%)	60	63	26, 51, 91, 141	0
1	C	282/282 (100%)	0.06	4 (1%)	72	74	28, 50, 94, 159	0
1	D	282/282 (100%)	0.17	6 (2%)	60	63	31, 50, 82, 168	0
2	E	12/12 (100%)	1.14	2 (16%)	2	2	64, 116, 154, 172	0
2	G	12/12 (100%)	-0.13	0	100	100	50, 73, 93, 101	0
3	F	12/12 (100%)	0.83	1 (8%)	11	10	92, 127, 145, 149	0
3	H	12/12 (100%)	-0.26	0	100	100	45, 67, 85, 97	0
All	All	1176/1176 (100%)	0.09	21 (1%)	65	68	26, 51, 94, 172	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	282	ALA	9.3
1	D	282	ALA	7.5
1	A	282	ALA	4.1
1	C	281	GLU	4.1
1	C	97	ARG	3.4
1	A	125	LEU	3.3
1	B	176	LEU	3.1
1	D	281	GLU	3.1
1	B	282	ALA	2.8
1	C	280	ASP	2.5
2	E	6	8OG	2.4
1	D	110	CYS	2.4
1	D	239	TYR	2.3
1	D	43	GLU	2.2
1	B	281	GLU	2.2
3	F	14	DG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	166	PRO	2.1
1	B	172	LEU	2.1
1	B	177	LYS	2.1
2	E	10	DG	2.1
1	D	183	ILE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	8OG	E	6	23/24	0.30	2.74	76,82,88,89	0
2	8OG	G	6	23/24	0.16	-0.40	76,82,88,89	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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.