



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:28 PM GMT

PDB ID : 3CVS  
Title : Crystal Structure of an AlkA Host/Guest Complex 8oxoGuanine:Adenine Base Pair  
Authors : Bowman, B.R.; Lee, S.; Wang, S.; Verdine, G.L.  
Deposited on : 2008-04-19  
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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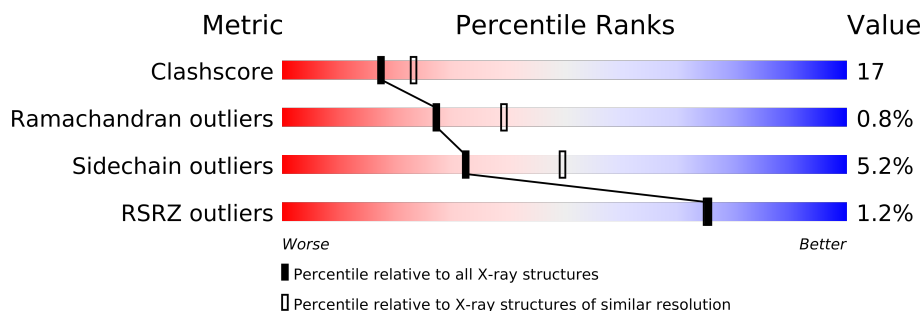
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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  $\geq 3$ , 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 10005 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\*DGP\*DAP\*(8OG)P\*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\*DAP\*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
			243	117	45	70	11			
3	H	12	Total	C	N	O	P	0	0	0
			243	117	45	70	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		

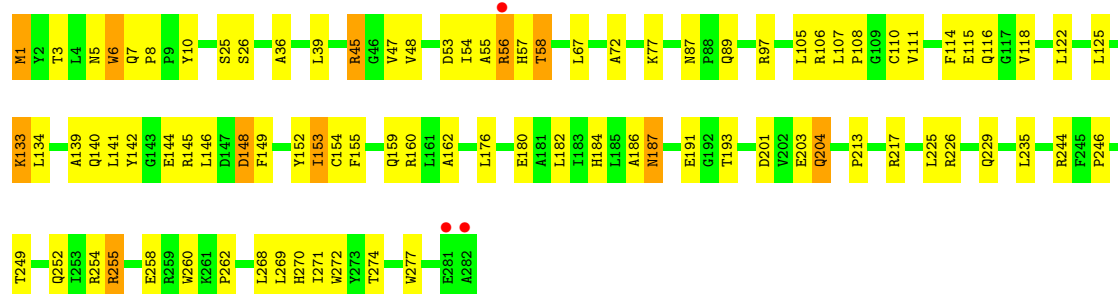
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	37	Total 37	O 37	0	0
4	C	40	Total 40	O 40	0	0
4	D	45	Total 45	O 45	0	0
4	E	1	Total 1	O 1	0	0
4	G	2	Total 2	O 2	0	0
4	H	3	Total 3	O 3	0	0

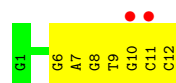


Chain D: 



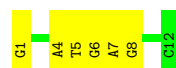
- Molecule 2: DNA (5'-D(\*DGP\*DAP\*DCP\*DAP\*DTP\*DGP\*DAP\*(8OG)P\*DTP\*DGP\*DCP\*DC)-3')

Chain E: 



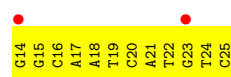
- Molecule 2: DNA (5'-D(\*DGP\*DAP\*DCP\*DAP\*DTP\*DGP\*DAP\*(8OG)P\*DTP\*DGP\*DCP\*DC)-3')

Chain G: 



- Molecule 3: DNA (5'-D(\*DGP\*DGP\*DCP\*DAP\*DAP\*DTP\*DCP\*DAP\*DTP\*DGP\*DTP\*D C)-3')

Chain F: 



- Molecule 3: DNA (5'-D(\*DGP\*DGP\*DCP\*DAP\*DAP\*DTP\*DCP\*DAP\*DTP\*DGP\*DTP\*D C)-3')

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.17Å 101.25Å 102.92Å 90.00° 94.19° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 31.85 – 2.39	Depositor EDS
% Data completeness (in resolution range)	93.3 (50.00-2.40) 92.9 (31.85-2.39)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.219 , 0.270 0.220 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	37.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 27.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 60149 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10005	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>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	0.38	0/2277	0.60	0/3104
1	B	0.38	0/2277	0.61	0/3104
1	C	0.37	0/2277	0.58	0/3104
1	D	0.39	0/2277	0.60	0/3104
2	E	0.64	0/249	0.97	0/380
2	G	0.46	0/249	0.81	0/380
3	F	0.70	0/272	0.94	0/418
3	H	0.44	0/272	0.70	0/418
All	All	0.40	0/10150	0.63	0/14012

There are no bond length outliers.

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	64	0
1	B	2215	0	2209	87	0
1	C	2215	0	2209	66	0
1	D	2215	0	2209	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	246	0	136	16	0
2	G	246	0	136	16	0
3	F	243	0	137	19	0
3	H	243	0	137	3	0
4	A	39	0	0	6	0
4	B	37	0	0	2	0
4	C	40	0	0	1	0
4	D	45	0	0	6	0
4	E	1	0	0	0	0
4	G	2	0	0	0	0
4	H	3	0	0	1	0
All	All	10005	0	9382	335	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 17.

All (335) 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'	1.19	1.16
2:G:5:DT:H2''	2:G:6:DG:H5''	1.09	1.07
2:G:5:DT:C2'	2:G:6:DG:H5''	1.85	1.05
2:G:4:DA:H2''	2:G:5:DT:H5''	1.47	0.96
1:A:124:GLN:NE2	1:A:178:ARG:HH11	1.65	0.92
1:A:124:GLN:HE21	1:A:178:ARG:HH11	0.99	0.92
1:D:56:ARG:HH21	1:D:57:HIS:CE1	1.89	0.90
1:C:97:ARG:HD2	1:C:98:LEU:N	1.86	0.90
2:G:5:DT:H2''	2:G:6:DG:C5'	2.00	0.88
2:G:4:DA:C2'	2:G:5:DT:H5''	2.04	0.87
1:B:174:MET:HB2	1:B:178:ARG:HG2	1.55	0.87
1:B:124:GLN:HB3	3:F:14:DG:H5'	1.55	0.87
1:A:124:GLN:HE21	1:A:178:ARG:NH1	1.74	0.86
1:A:3:THR:HG22	1:A:60:HIS:HD2	1.41	0.84
1:A:77:LYS:HB3	1:A:111:VAL:HG23	1.63	0.80
1:C:97:ARG:HD2	1:C:98:LEU:H	1.41	0.80
2:E:8:8OG:C2'	2:E:9:DT:H5''	2.12	0.80
1:B:124:GLN:NE2	1:B:178:ARG:HH12	1.81	0.78
1:B:143:GLY:HA3	1:B:153:ILE:HD11	1.65	0.78
2:E:8:8OG:H2'	2:E:9:DT:H5''	1.64	0.78
3:H:21:DA:C2'	3:H:22:DT:H5'	2.11	0.77
1:B:145:ARG:HH11	1:B:145:ARG:HG2	1.49	0.77
3:F:14:DG:H4'	3:F:15:DG:H5'	1.67	0.77
1:B:124:GLN:HE21	1:B:178:ARG:HH12	1.33	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:15:MET:HE2	1:A:19:LEU:HG	1.67	0.77
1:B:39:LEU:HD22	1:B:48:VAL:HG21	1.67	0.76
1:C:158:PRO:HD2	1:C:159:GLN:NE2	2.02	0.75
1:D:39:LEU:HD22	1:D:48:VAL:HG21	1.65	0.75
1:A:235:LEU:HD22	1:A:268:LEU:HD21	1.69	0.74
2:G:7:DA:H2''	2:G:8:8OG:H5'	1.68	0.74
3:F:18:DA:H2''	3:F:19:DT:O5'	1.88	0.74
1:B:77:LYS:HB3	1:B:111:VAL:HG23	1.71	0.73
1:D:254:ARG:HD2	4:H:98:HOH:O	1.88	0.73
1:B:130:MET:HG2	1:B:133:LYS:HE3	1.71	0.72
1:D:110:CYS:HB3	1:D:116:GLN:HE21	1.53	0.72
3:H:21:DA:H2''	3:H:22:DT:C5'	2.10	0.71
1:B:203:GLU:HG3	4:B:303:HOH:O	1.89	0.71
2:G:4:DA:C3'	2:G:5:DT:H5''	2.19	0.71
2:E:8:8OG:C3'	2:E:9:DT:H5''	2.21	0.71
1:D:8:PRO:HG2	1:D:57:HIS:CE1	2.25	0.71
1:D:108:PRO:O	1:D:226:ARG:HD2	1.91	0.71
2:E:8:8OG:OP1	2:E:8:8OG:H4'	1.91	0.71
1:C:133:LYS:HE3	1:C:137:ARG:NH2	2.06	0.70
1:D:77:LYS:HB3	1:D:111:VAL:HG23	1.74	0.70
1:B:184:HIS:CD2	1:B:213:PRO:HD2	2.27	0.70
1:C:158:PRO:HD2	1:C:159:GLN:HE21	1.55	0.70
2:G:7:DA:H2''	2:G:8:8OG:C5'	2.22	0.69
1:B:3:THR:HG22	1:B:60:HIS:HD2	1.59	0.68
1:C:235:LEU:HB3	1:C:238:ASP:HB2	1.76	0.68
1:B:261:LYS:HG2	1:B:264:ARG:CZ	2.24	0.68
3:F:21:DA:H1'	3:F:22:DT:H5''	1.76	0.67
1:A:249:THR:OG1	1:A:252:GLN:HG3	1.95	0.67
1:B:26:SER:HB3	1:B:153:ILE:HG22	1.75	0.67
1:D:134:LEU:HD23	1:D:134:LEU:C	2.15	0.67
1:C:251:ALA:HB3	2:G:7:DA:OP1	1.95	0.67
1:B:77:LYS:HB3	1:B:111:VAL:CG2	2.25	0.67
1:C:33:SER:O	1:C:52:PRO:HD2	1.95	0.66
1:D:45:ARG:HA	1:D:67:LEU:HD21	1.76	0.66
1:D:255:ARG:O	1:D:258:GLU:HG3	1.95	0.66
1:D:26:SER:HB3	1:D:153:ILE:CG2	2.25	0.66
1:A:140:GLN:HE21	1:A:140:GLN:HA	1.61	0.65
1:A:6:TRP:CZ2	1:A:57:HIS:HA	2.30	0.65
1:B:238:ASP:HB3	1:B:241:ILE:HB	1.77	0.65
2:G:7:DA:H2'	2:G:8:8OG:N2	2.11	0.65
1:B:261:LYS:HE2	1:B:264:ARG:NH1	2.12	0.65
1:D:139:ALA:O	1:D:153:ILE:HD11	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:124:GLN:NE2	1:B:178:ARG:NH1	2.44	0.64
1:A:133:LYS:HD2	1:A:137:ARG:NH1	2.11	0.64
1:C:260:TRP:CH2	1:C:271:ILE:HD11	2.32	0.64
1:C:102:ARG:NH1	1:C:273:TYR:HB3	2.11	0.64
4:A:319:HOH:O	1:D:191:GLU:HB2	1.97	0.64
3:F:14:DG:H4'	3:F:15:DG:C5'	2.28	0.64
1:C:248:MET:HE1	1:C:279:PRO:HG3	1.80	0.62
1:A:133:LYS:HD2	1:A:137:ARG:HH11	1.65	0.62
3:F:21:DA:C2'	3:F:22:DT:H5''	2.30	0.62
1:B:8:PRO:HG2	1:B:57:HIS:CE1	2.35	0.62
1:B:124:GLN:HB3	3:F:14:DG:C5'	2.28	0.61
2:E:8:8OG:H2'	2:E:9:DT:O4'	1.99	0.61
2:G:5:DT:C3'	2:G:6:DG:H5''	2.30	0.61
1:C:248:MET:CE	1:C:279:PRO:HG3	2.31	0.61
3:F:23:DG:H2''	3:F:24:DT:OP2	2.00	0.61
1:D:39:LEU:CD2	1:D:48:VAL:HG21	2.31	0.61
1:D:25:SER:O	1:D:26:SER:HB2	2.01	0.61
1:D:107:LEU:CD1	1:D:269:LEU:HD11	2.32	0.60
1:B:251:ALA:HB2	2:E:6:DG:H3'	1.83	0.60
1:A:231:LYS:NZ	4:A:301:HOH:O	2.34	0.60
1:B:6:TRP:C	1:B:6:TRP:CD1	2.75	0.60
1:C:107:LEU:HD11	1:C:225:LEU:HD21	1.82	0.60
1:A:105:LEU:HD13	1:A:106:ARG:N	2.17	0.60
1:D:225:LEU:HD23	1:D:226:ARG:HG2	1.83	0.60
1:B:157:THR:HB	1:B:159:GLN:HE21	1.65	0.59
1:B:166:PRO:HG3	1:B:183:ILE:CD1	2.32	0.59
1:C:1:MET:N	1:C:60:HIS:CE1	2.70	0.59
1:D:77:LYS:HE3	1:D:111:VAL:O	2.02	0.59
2:E:11:DC:C2	2:E:12:DC:C5	2.91	0.58
1:D:77:LYS:HB3	1:D:111:VAL:CG2	2.33	0.58
1:B:261:LYS:HE2	1:B:264:ARG:CZ	2.33	0.58
1:D:203:GLU:CD	1:D:203:GLU:H	2.06	0.58
1:B:145:ARG:HG2	1:B:145:ARG:NH1	2.18	0.58
1:C:107:LEU:HD11	1:C:225:LEU:CD2	2.34	0.58
1:D:56:ARG:NH2	1:D:57:HIS:CE1	2.66	0.58
1:D:146:LEU:HB3	1:D:148:ASP:OD1	2.04	0.58
1:A:244:ARG:C	1:A:246:PRO:HD3	2.24	0.58
1:B:130:MET:HA	1:B:133:LYS:HG2	1.86	0.58
1:B:3:THR:HG22	1:B:60:HIS:CD2	2.39	0.58
3:F:21:DA:H2''	3:F:22:DT:H5''	1.84	0.58
1:B:234:PHE:C	1:B:235:LEU:HD12	2.24	0.58
1:C:254:ARG:HH11	1:C:254:ARG:HG3	1.69	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:110:CYS:HB3	1:A:116:GLN:HE21	1.69	0.57
1:A:3:THR:CG2	1:A:60:HIS:HD2	2.13	0.57
1:A:184:HIS:CD2	1:A:213:PRO:HD2	2.39	0.57
1:B:143:GLY:CA	1:B:153:ILE:HD11	2.34	0.57
1:D:107:LEU:HD11	1:D:225:LEU:HD21	1.86	0.57
1:D:145:ARG:HD2	4:D:297:HOH:O	2.04	0.57
1:B:141:LEU:HD23	1:B:172:LEU:HD11	1.87	0.57
3:F:24:DT:H2''	3:F:25:DC:C5'	2.35	0.57
1:D:47:VAL:HG21	1:D:152:TYR:CD2	2.39	0.57
1:A:41:VAL:HB	1:A:70:VAL:HG21	1.87	0.57
1:D:162:ALA:HB1	1:D:187:ASN:ND2	2.21	0.56
1:D:105:LEU:HD13	1:D:106:ARG:N	2.21	0.56
1:B:241:ILE:HD11	1:B:268:LEU:HD12	1.87	0.56
2:E:11:DC:H2''	2:E:12:DC:C5	2.41	0.56
1:B:167:GLN:NE2	1:B:170:LYS:HD3	2.20	0.56
1:D:36:ALA:HA	1:D:48:VAL:O	2.07	0.55
1:D:148:ASP:HB2	1:D:149:PHE:CD2	2.42	0.54
1:D:235:LEU:HD13	1:D:268:LEU:HD22	1.90	0.54
1:C:254:ARG:NH1	1:C:254:ARG:HG3	2.21	0.54
1:B:141:LEU:HD22	1:B:172:LEU:HD21	1.89	0.54
1:B:176:LEU:O	1:B:180:GLU:HG3	2.08	0.54
1:D:6:TRP:CD1	1:D:6:TRP:C	2.80	0.54
1:B:107:LEU:HD23	1:B:107:LEU:C	2.28	0.54
1:C:110:CYS:CB	1:C:116:GLN:HE21	2.21	0.54
1:A:187:ASN:O	1:A:191:GLU:HG3	2.07	0.54
1:C:10:TYR:HB2	4:C:317:HOH:O	2.07	0.54
1:B:251:ALA:HB3	2:E:7:DA:OP1	2.07	0.54
1:C:159:GLN:NE2	1:C:159:GLN:H	2.06	0.54
1:A:68:GLU:HG3	4:D:307:HOH:O	2.08	0.54
3:F:19:DT:OP1	3:F:19:DT:H4'	2.08	0.54
1:B:6:TRP:HZ3	1:B:58:THR:O	1.91	0.54
1:A:15:MET:CE	1:A:19:LEU:HG	2.37	0.53
1:B:108:PRO:O	1:B:226:ARG:HD2	2.09	0.53
1:C:225:LEU:O	1:C:229:GLN:HA	2.08	0.53
1:D:235:LEU:HD13	1:D:268:LEU:CD2	2.38	0.53
3:F:24:DT:H2''	3:F:25:DC:O5'	2.08	0.53
1:C:6:TRP:CZ2	1:C:57:HIS:HA	2.43	0.53
1:D:107:LEU:HD13	1:D:269:LEU:HD11	1.90	0.53
1:A:39:LEU:HD23	1:A:48:VAL:HG21	1.90	0.53
1:A:248:MET:HE2	1:A:279:PRO:HG3	1.89	0.53
1:B:159:GLN:NE2	1:B:159:GLN:H	2.06	0.53
1:D:141:LEU:HD23	1:D:142:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:249:THR:HB	2:G:7:DA:H5'	1.91	0.53
1:B:124:GLN:HB2	1:B:178:ARG:NH1	2.24	0.53
1:B:145:ARG:HD2	1:B:150:PRO:HA	1.90	0.53
1:C:102:ARG:HH11	1:C:273:TYR:HB3	1.75	0.52
1:D:225:LEU:O	1:D:229:GLN:HA	2.09	0.52
3:F:21:DA:H2''	3:F:22:DT:C5'	2.38	0.52
1:A:7:GLN:NE2	1:A:89:GLN:HE21	2.07	0.52
1:C:53:ASP:OD2	1:C:56:ARG:HB2	2.10	0.52
3:F:21:DA:C1'	3:F:22:DT:H5''	2.40	0.52
1:D:146:LEU:HD21	1:D:154:CYS:SG	2.50	0.52
1:A:167:GLN:NE2	1:A:170:LYS:HD3	2.25	0.52
1:A:235:LEU:HB3	1:A:238:ASP:HB2	1.92	0.51
1:A:248:MET:CE	1:A:279:PRO:HG3	2.39	0.51
2:E:11:DC:N1	2:E:12:DC:H5	2.09	0.51
1:D:107:LEU:HD11	1:D:225:LEU:CD2	2.41	0.51
1:D:260:TRP:CH2	1:D:271:ILE:HD11	2.45	0.51
1:A:158:PRO:HD2	1:A:159:GLN:HE21	1.75	0.51
1:B:25:SER:O	1:B:26:SER:HB2	2.11	0.51
1:B:159:GLN:HA	1:B:190:LEU:HD11	1.93	0.51
1:C:157:THR:OG1	1:C:159:GLN:HG2	2.11	0.50
1:C:1:MET:HG2	1:C:62:ASN:HA	1.92	0.50
1:C:249:THR:OG1	1:C:252:GLN:HG3	2.10	0.50
1:C:97:ARG:NH1	1:C:98:LEU:HB2	2.26	0.50
3:F:15:DG:H2''	3:F:16:DC:O5'	2.12	0.50
1:D:122:LEU:HD13	1:D:134:LEU:CD2	2.41	0.50
1:D:148:ASP:HB2	1:D:149:PHE:HD2	1.76	0.50
1:B:187:ASN:O	1:B:191:GLU:HG2	2.12	0.50
1:C:1:MET:HG3	1:C:2:TYR:H	1.77	0.50
1:C:193:THR:CG2	1:C:193:THR:O	2.60	0.50
1:A:25:SER:O	1:A:26:SER:HB2	2.12	0.50
3:F:24:DT:H2''	3:F:25:DC:H5''	1.93	0.49
1:D:274:THR:HG22	1:D:277:TRP:HB2	1.94	0.49
1:B:121:ILE:O	1:B:124:GLN:HG3	2.12	0.49
1:D:110:CYS:CB	1:D:116:GLN:HE21	2.21	0.49
1:B:261:LYS:HE2	1:B:264:ARG:NH2	2.27	0.49
1:D:54:ILE:O	1:D:55:ALA:C	2.50	0.49
1:D:57:HIS:CD2	1:D:57:HIS:N	2.80	0.49
1:D:7:GLN:NE2	1:D:87:ASN:HA	2.27	0.49
1:B:166:PRO:HG3	1:B:183:ILE:HD12	1.95	0.49
1:B:77:LYS:HD3	1:B:111:VAL:HG22	1.94	0.49
1:B:167:GLN:HE21	1:B:170:LYS:HD3	1.78	0.48
1:B:175:PRO:HD2	1:B:178:ARG:HB2	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:9:DT:H2'	2:E:10:DG:C8	2.48	0.48
1:D:122:LEU:HD22	1:D:134:LEU:HD21	1.95	0.48
1:D:201:ASP:CG	1:D:204:GLN:HB2	2.34	0.48
1:C:105:LEU:HD13	1:C:106:ARG:N	2.28	0.48
1:C:110:CYS:HB2	1:C:116:GLN:HE21	1.78	0.48
1:A:6:TRP:CZ3	1:A:58:THR:O	2.67	0.48
1:C:215:ILE:HG23	1:C:219:THR:HB	1.96	0.48
1:A:229:GLN:O	1:A:231:LYS:HE2	2.14	0.48
1:A:231:LYS:HE3	4:A:290:HOH:O	2.12	0.48
1:C:1:MET:H1	1:C:60:HIS:CE1	2.30	0.48
1:C:45:ARG:HB3	1:C:146:LEU:CD2	2.44	0.48
1:D:107:LEU:HD12	1:D:269:LEU:HD11	1.96	0.48
1:B:6:TRP:CZ3	1:B:58:THR:O	2.66	0.48
1:B:158:PRO:HD2	1:B:159:GLN:NE2	2.28	0.47
1:D:6:TRP:CZ3	1:D:58:THR:O	2.67	0.47
2:G:7:DA:H2'	2:G:8:8OG:C2	2.44	0.47
2:E:7:DA:H2"	2:E:8:8OG:H5"	1.96	0.47
1:C:198:ILE:O	1:C:198:ILE:HG23	2.14	0.47
1:A:54:ILE:HD12	4:A:313:HOH:O	2.13	0.47
1:C:25:SER:O	1:C:26:SER:HB2	2.14	0.47
2:E:8:8OG:H2'	2:E:9:DT:C5'	2.42	0.47
1:C:145:ARG:HG3	1:C:145:ARG:HH11	1.79	0.47
1:A:77:LYS:HD3	1:A:111:VAL:HG22	1.96	0.47
1:B:238:ASP:O	1:B:242:LYS:HG3	2.14	0.47
1:D:53:ASP:HB3	1:D:58:THR:HG22	1.97	0.47
1:A:224:ALA:O	1:A:228:TRP:HB2	2.15	0.47
1:C:209:LEU:HD11	1:C:223:PHE:CD2	2.50	0.47
1:A:15:MET:HE1	1:A:108:PRO:HB3	1.95	0.47
1:C:195:PRO:HB2	1:C:228:TRP:CZ2	2.50	0.47
2:E:11:DC:C2'	2:E:12:DC:H5	2.28	0.46
1:A:6:TRP:C	1:A:6:TRP:CD1	2.89	0.46
1:D:5:ASN:HB2	4:D:307:HOH:O	2.15	0.46
1:B:249:THR:O	1:B:252:GLN:N	2.49	0.46
1:A:274:THR:CG2	1:A:277:TRP:HB2	2.45	0.46
1:A:114:PHE:CD2	1:A:158:PRO:HG3	2.50	0.46
1:B:168:ALA:O	1:B:171:ALA:HB3	2.16	0.46
1:D:118:VAL:HG13	1:D:182:LEU:HD22	1.96	0.45
1:B:243:GLN:O	1:B:246:PRO:HD3	2.15	0.45
1:B:48:VAL:HG22	1:B:63:LEU:CD2	2.46	0.45
1:B:159:GLN:CD	1:B:159:GLN:H	2.18	0.45
1:D:176:LEU:O	1:D:180:GLU:HG3	2.15	0.45
2:G:6:DG:H2"	2:G:7:DA:C8	2.51	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:134:LEU:HD23	1:D:134:LEU:O	2.17	0.45
2:G:7:DA:H2"	2:G:8:8OG:H5"	1.98	0.45
1:B:145:ARG:CD	1:B:150:PRO:O	2.64	0.45
1:C:257:ALA:HA	1:C:260:TRP:CE3	2.51	0.45
1:C:1:MET:H1	1:C:60:HIS:HE1	1.64	0.45
2:E:11:DC:H2"	2:E:12:DC:C6	2.52	0.45
1:A:242:LYS:HG2	4:A:288:HOH:O	2.16	0.45
1:B:261:LYS:HE2	1:B:264:ARG:HH12	1.82	0.45
1:B:225:LEU:O	1:B:229:GLN:HA	2.17	0.45
1:B:133:LYS:O	1:B:137:ARG:HG3	2.17	0.44
1:C:47:VAL:H	1:C:64:SER:HB3	1.82	0.44
1:C:39:LEU:HD22	1:C:48:VAL:HG21	1.99	0.44
1:A:87:ASN:HB3	1:A:90:ILE:HD12	1.99	0.44
1:B:250:PRO:O	1:B:254:ARG:HB2	2.16	0.44
1:C:14:TRP:HZ3	1:C:106:ARG:O	2.00	0.44
1:D:270:HIS:HE1	4:D:283:HOH:O	2.01	0.44
1:C:276:GLY:O	1:C:277:TRP:O	2.36	0.44
1:B:114:PHE:CD2	1:B:158:PRO:HG3	2.53	0.44
1:C:1:MET:H2	1:C:60:HIS:CE1	2.34	0.44
1:A:114:PHE:CE1	1:A:186:ALA:HA	2.52	0.44
1:A:23:ALA:HA	1:A:28:GLU:OE2	2.18	0.44
1:C:249:THR:HB	1:C:250:PRO:HD2	1.99	0.44
1:C:6:TRP:C	1:C:6:TRP:CD1	2.90	0.44
1:A:249:THR:HB	3:F:20:DC:H5'	2.00	0.44
1:D:249:THR:OG1	1:D:252:GLN:HG3	2.18	0.44
1:A:3:THR:HG22	1:A:60:HIS:CD2	2.33	0.43
1:B:254:ARG:HH11	1:B:254:ARG:HG3	1.83	0.43
1:C:114:PHE:CE1	1:C:186:ALA:HA	2.53	0.43
1:A:209:LEU:HD11	1:A:223:PHE:CD2	2.53	0.43
1:B:255:ARG:HH11	1:B:255:ARG:HG2	1.82	0.43
1:D:114:PHE:CE1	1:D:186:ALA:HA	2.53	0.43
1:D:55:ALA:O	1:D:56:ARG:HD2	2.17	0.43
1:D:122:LEU:HD13	1:D:134:LEU:HD22	2.00	0.43
1:B:7:GLN:HG3	1:B:86:CYS:O	2.18	0.43
1:A:76:ALA:HA	1:D:72:ALA:HB1	1.99	0.43
1:B:7:GLN:HA	1:B:8:PRO:HD3	1.91	0.43
1:D:1:MET:N	4:D:326:HOH:O	2.50	0.43
3:F:17:DA:H1'	3:F:18:DA:H5'	2.01	0.43
1:A:140:GLN:NE2	1:A:140:GLN:HA	2.29	0.43
1:B:195:PRO:HB2	1:B:228:TRP:CZ2	2.54	0.43
1:B:209:LEU:O	1:B:212:PHE:HB2	2.18	0.42
1:C:151:GLU:HG2	1:C:152:TYR:N	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:61:ILE:HD12	1:C:78:MET:HG3	2.01	0.42
1:B:98:LEU:HD22	1:B:260:TRP:CE2	2.54	0.42
3:F:14:DG:O4'	3:F:14:DG:N3	2.53	0.42
1:C:110:CYS:HB3	1:C:116:GLN:HE21	1.84	0.42
1:B:143:GLY:HA3	1:B:153:ILE:CD1	2.41	0.42
1:C:51:ILE:HB	1:C:60:HIS:HB3	2.02	0.42
1:A:7:GLN:NE2	1:A:89:GLN:NE2	2.68	0.42
1:D:176:LEU:N	4:D:305:HOH:O	2.52	0.42
1:B:46:GLY:HA3	1:B:64:SER:OG	2.19	0.42
1:A:181:ALA:HB2	1:A:214:GLY:HA3	2.01	0.42
1:C:155:PHE:CD2	1:C:156:PRO:HD2	2.54	0.42
1:B:174:MET:HB2	1:B:178:ARG:CG	2.39	0.42
1:C:51:ILE:HD12	1:C:60:HIS:HD2	1.84	0.42
1:C:51:ILE:HD12	1:C:60:HIS:CD2	2.54	0.42
1:C:20:ALA:HA	1:C:30:VAL:HG21	2.00	0.42
1:B:18:PHE:CD1	1:B:18:PHE:C	2.94	0.42
1:A:43:GLU:HG3	1:A:43:GLU:H	1.48	0.42
1:B:105:LEU:HD13	1:B:106:ARG:N	2.34	0.41
1:A:151:GLU:N	1:A:151:GLU:OE1	2.42	0.41
1:B:261:LYS:HG2	1:B:264:ARG:NE	2.35	0.41
1:A:68:GLU:HB3	1:A:69:PRO:HD3	2.02	0.41
1:A:158:PRO:HD2	1:A:159:GLN:NE2	2.35	0.41
1:D:149:PHE:CD2	1:D:149:PHE:N	2.88	0.41
1:B:122:LEU:HD23	1:B:122:LEU:HA	1.86	0.41
1:D:184:HIS:CD2	1:D:213:PRO:HD2	2.55	0.41
1:A:105:LEU:O	1:A:106:ARG:HD3	2.20	0.41
1:C:39:LEU:CD2	1:C:48:VAL:HG21	2.51	0.41
1:A:254:ARG:HD3	1:A:254:ARG:HA	1.81	0.41
1:D:56:ARG:NH2	1:D:57:HIS:NE2	2.68	0.41
1:D:201:ASP:OD2	1:D:204:GLN:HB2	2.21	0.41
1:C:145:ARG:NH1	1:C:145:ARG:HG3	2.36	0.41
1:D:125:LEU:HD13	2:G:1:DG:C8	2.55	0.41
1:D:115:GLU:HG3	1:D:155:PHE:CE1	2.55	0.41
1:D:274:THR:CG2	1:D:277:TRP:HB2	2.51	0.41
1:C:18:PHE:CE1	1:C:22:ARG:HD2	2.56	0.41
1:B:110:CYS:SG	1:B:227:GLY:HA2	2.60	0.41
1:A:6:TRP:HZ3	1:A:58:THR:O	2.02	0.41
1:A:245:PHE:N	1:A:246:PRO:HD3	2.36	0.41
1:B:192:GLY:HA2	4:B:301:HOH:O	2.19	0.41
1:B:99:GLY:HA2	1:B:270:HIS:CD2	2.56	0.41
1:B:235:LEU:HD13	1:B:268:LEU:HD22	2.03	0.41
1:A:122:LEU:HD21	1:A:182:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:209:LEU:HA	1:B:209:LEU:HD23	1.88	0.40
1:A:254:ARG:HD2	4:A:320:HOH:O	2.21	0.40
1:A:107:LEU:HD11	1:A:225:LEU:HD21	2.03	0.40
1:B:275:GLU:C	1:B:277:TRP:H	2.24	0.40
1:A:141:LEU:O	1:A:141:LEU:HD12	2.22	0.40
1:C:199:PRO:HG3	1:C:205:ALA:CB	2.52	0.40
1:A:241:ILE:HD11	1:A:268:LEU:CD1	2.51	0.40
1:D:217:ARG:NH1	1:D:254:ARG:HH22	2.18	0.40
2:E:11:DC:C2'	2:E:12:DC:C5	3.02	0.40
1:B:106:ARG:O	1:B:108:PRO:HD3	2.21	0.40
1:C:144:GLU:HB3	1:C:154:CYS:HB2	2.04	0.40
1:D:244:ARG:C	1:D:246:PRO:HD3	2.42	0.40
1:D:193:THR:O	1:D:193:THR:HG22	2.21	0.40
1:D:133:LYS:HA	1:D:133:LYS:HE2	2.02	0.40
1:C:50:ALA:HA	1:C:60:HIS:O	2.21	0.40
1:C:10:TYR:CE2	1:C:106:ARG:HG3	2.55	0.40
1:B:106:ARG:HD3	1:B:106:ARG:HA	1.80	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%)	272 (97%)	7 (2%)	1 (0%)	43	61
1	B	280/282 (99%)	264 (94%)	10 (4%)	6 (2%)	11	12
1	C	280/282 (99%)	264 (94%)	14 (5%)	2 (1%)	30	43
1	D	280/282 (99%)	264 (94%)	16 (6%)	0	100	100
All	All	1120/1128 (99%)	1064 (95%)	47 (4%)	9 (1%)	27	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	248	MET

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Mol	Chain	Res	Type
1	C	277	TRP
1	B	65	ALA
1	C	281	GLU
1	B	246	PRO
1	B	275	GLU
1	B	250	PRO
1	B	276	GLY
1	A	126	VAL

### 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%)	215 (97%)	7 (3%)	51	72
1	B	222/222 (100%)	214 (96%)	8 (4%)	47	68
1	C	222/222 (100%)	212 (96%)	10 (4%)	38	57
1	D	222/222 (100%)	201 (90%)	21 (10%)	12	18
All	All	888/888 (100%)	842 (95%)	46 (5%)	32	49

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	73	GLU
1	A	133	LYS
1	A	140	GLN
1	A	159	GLN
1	A	204	GLN
1	A	254	ARG
1	B	6	TRP
1	B	7	GLN
1	B	58	THR
1	B	105	LEU
1	B	144	GLU
1	B	159	GLN
1	B	246	PRO

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Mol	Chain	Res	Type
1	B	255	ARG
1	C	7	GLN
1	C	102	ARG
1	C	111	VAL
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	272	TRP
1	D	1	MET
1	D	3	THR
1	D	6	TRP
1	D	10	TYR
1	D	45	ARG
1	D	56	ARG
1	D	58	THR
1	D	89	GLN
1	D	97	ARG
1	D	133	LYS
1	D	140	GLN
1	D	144	GLU
1	D	148	ASP
1	D	153	ILE
1	D	159	GLN
1	D	160	ARG
1	D	187	ASN
1	D	204	GLN
1	D	255	ARG
1	D	262	PRO
1	D	272	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	89	GLN
1	A	116	GLN
1	A	124	GLN
1	A	140	GLN
1	A	159	GLN

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Mol	Chain	Res	Type
1	A	167	GLN
1	A	204	GLN
1	A	221	ASN
1	A	243	GLN
1	B	7	GLN
1	B	60	HIS
1	B	116	GLN
1	B	124	GLN
1	B	159	GLN
1	B	167	GLN
1	B	184	HIS
1	B	187	ASN
1	B	221	ASN
1	B	270	HIS
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	167	GLN
1	C	221	ASN
1	D	5	ASN
1	D	7	GLN
1	D	57	HIS
1	D	116	GLN
1	D	124	GLN
1	D	184	HIS
1	D	187	ASN
1	D	270	HIS

### 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	8	3,2	23,25,26	0.75	1 (4%)	27,37,40	1.89	6 (22%)
2	8OG	G	8	3,2	23,25,26	0.76	1 (4%)	27,37,40	1.73	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	8	3,2	-	0/6/21/22	0/1/3/3
2	8OG	G	8	3,2	-	1/6/21/22	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	8	8OG	P-OP1	2.25	1.49	1.46
2	E	8	8OG	P-OP1	2.14	1.49	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	8OG	C4-C5-N7	5.66	110.87	106.14
2	G	8	8OG	C4-C5-N7	5.64	110.86	106.14
2	E	8	8OG	C8-N9-C1'	3.80	127.28	125.17
2	G	8	8OG	C8-N7-C5	-3.64	103.79	107.48
2	E	8	8OG	C8-N7-C5	-3.63	103.80	107.48
2	E	8	8OG	C6-N1-C2	3.26	125.20	119.51
2	G	8	8OG	C6-N1-C2	3.22	125.14	119.51
2	E	8	8OG	C2'-C1'-N9	-3.11	112.64	115.79
2	G	8	8OG	C2-N3-C4	-2.34	111.81	115.09
2	G	8	8OG	C8-N9-C1'	2.29	126.44	125.17
2	E	8	8OG	C2-N3-C4	-2.28	111.89	115.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	8	8OG	OP2-P-O5'-C5'

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	282/282 (100%)	-0.24	0 100 100	20, 40, 70, 99	0
1	B	282/282 (100%)	-0.19	4 (1%) 72 71	22, 42, 78, 128	0
1	C	282/282 (100%)	-0.22	3 (1%) 77 77	19, 42, 79, 132	0
1	D	282/282 (100%)	-0.19	3 (1%) 77 77	24, 40, 69, 141	0
2	E	12/12 (100%)	1.13	2 (16%) 2 2	55, 107, 123, 132	0
2	G	12/12 (100%)	-0.32	0 100 100	42, 65, 80, 84	0
3	F	12/12 (100%)	1.20	2 (16%) 2 2	71, 105, 120, 124	0
3	H	12/12 (100%)	-0.15	0 100 100	37, 60, 75, 79	0
All	All	1176/1176 (100%)	-0.18	14 (1%) 75 75	19, 42, 82, 141	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	282	ALA	8.2
1	C	282	ALA	5.8
1	C	281	GLU	4.3
1	D	56	ARG	3.5
1	B	282	ALA	3.5
1	C	60	HIS	3.4
1	B	281	GLU	3.4
1	D	281	GLU	3.3
2	E	10	DG	2.8
3	F	14	DG	2.8
1	B	247	GLY	2.4
2	E	11	DC	2.3
3	F	23	DG	2.2
1	B	177	LYS	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	8OG	E	8	23/24	0.24	1.08	101,103,106,112	0
2	8OG	G	8	23/24	0.13	-0.70	62,64,70,73	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.