



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:18 am BST

PDB ID : 3CW7  
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 : 2008-04-21  
Resolution : 2.30 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](mailto: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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

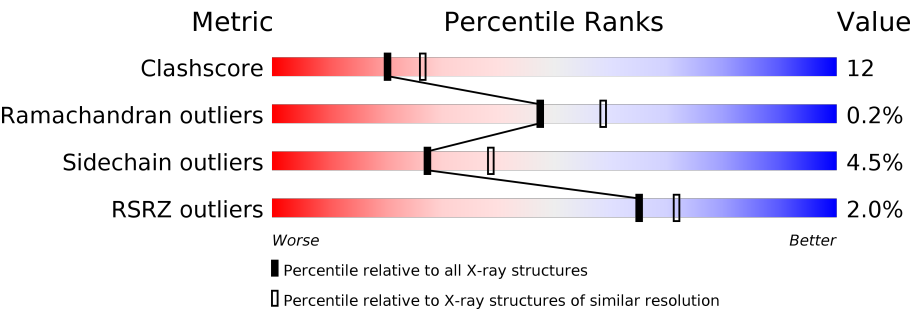
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	282	<div><div>2%</div><div>78%</div><div>20%</div><div>.</div></div>
1	B	282	<div><div>2%</div><div>76%</div><div>23%</div><div>.</div></div>
1	C	282	<div><div>2%</div><div>76%</div><div>23%</div><div>.</div></div>
1	D	282	<div><div>%</div><div>76%</div><div>22%</div><div>.</div></div>
2	E	12	<div><div>17%</div><div>58%</div><div>42%</div><div>.</div></div>
2	G	12	<div><div>67%</div><div>33%</div><div>.</div></div>
3	F	12	<div><div>17%</div><div>33%</div><div>50%</div><div>8%</div><div>8%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
3	H	12	 58% 42%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9861 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 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\*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	4	Total	O	0	0
			4	4		

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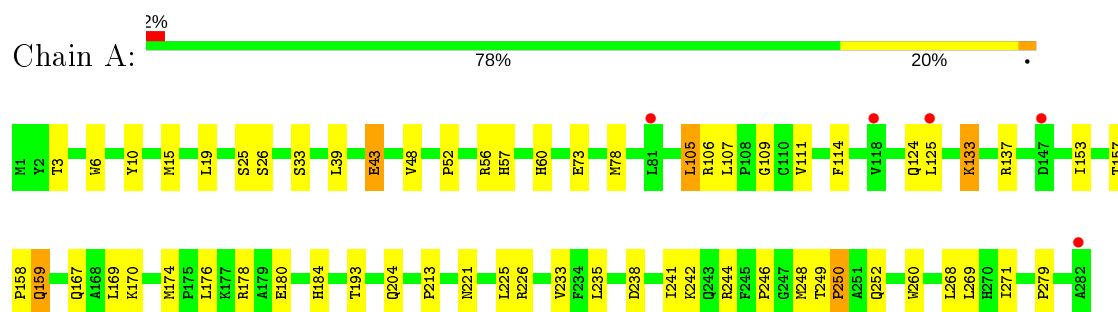
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total 6	O 6	0	0
4	C	7	Total 7	O 7	0	0
4	D	8	Total 8	O 8	0	0
4	E	1	Total 1	O 1	0	0
4	G	1	Total 1	O 1	0	0

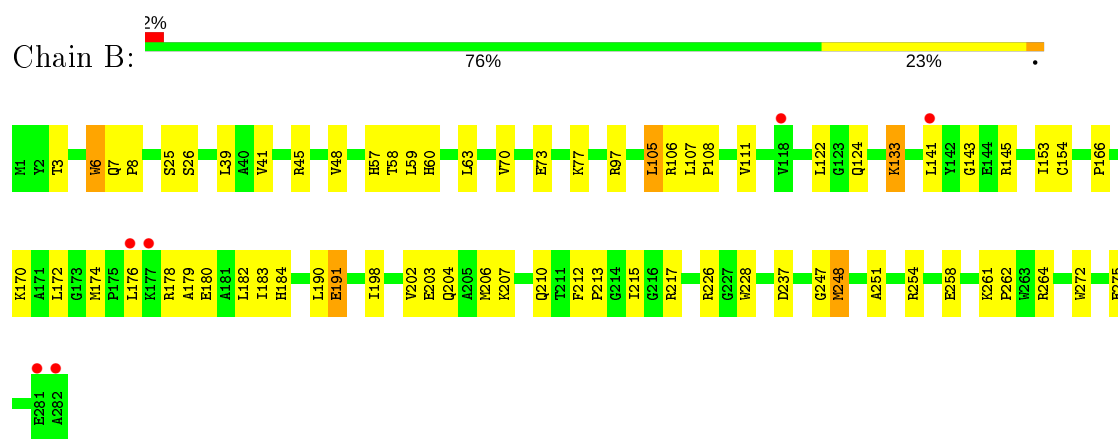
### 3 Residue-property plots [i](#)

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

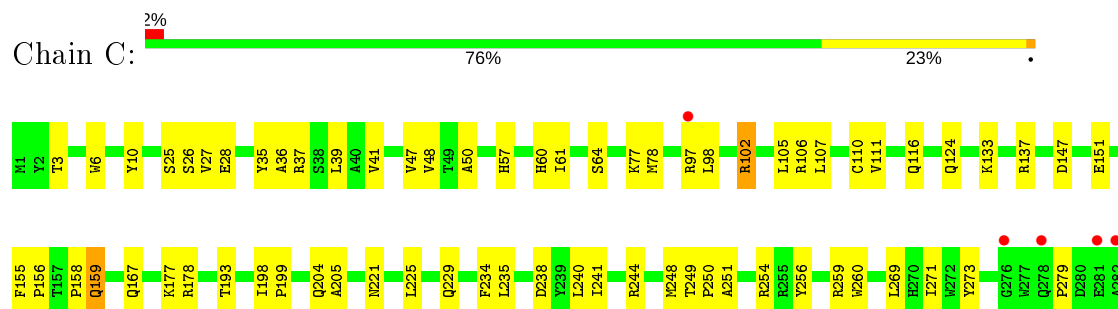
- Molecule 1: DNA-3-methyladenine glycosylase 2



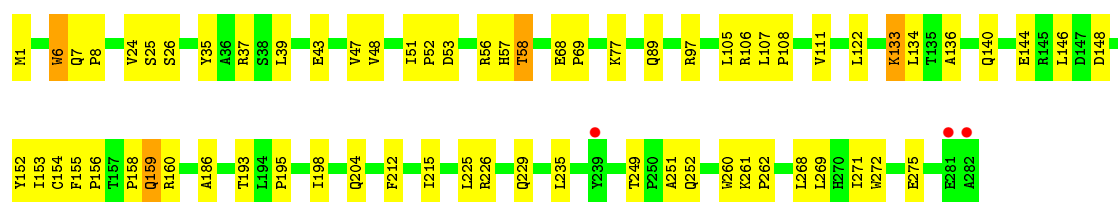
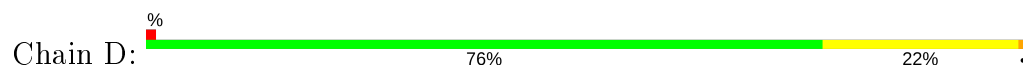
- Molecule 1: DNA-3-methyladenine glycosylase 2



- Molecule 1: DNA-3-methyladenine glycosylase 2



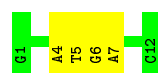
- Molecule 1: DNA-3-methyladenine glycosylase 2



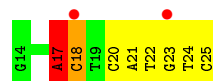
- Molecule 2: DNA (5'-D(\*DGP\*DAP\*DCP\*DAP\*DTP\*DGP\*DAP\*(8OG)P\*DTP\*DGP\*DCP\*DC)-3')



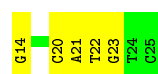
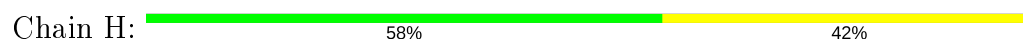
- Molecule 2: DNA (5'-D(\*DGP\*DAP\*DCP\*DAP\*DTP\*DGP\*DAP\*(8OG)P\*DTP\*DGP\*DCP\*DC)-3')



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.52Å 101.59Å 103.28Å 90.00° 94.23° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 29.50 – 2.31	Depositor EDS
% Data completeness (in resolution range)	87.9 (50.00-2.30) 88.8 (29.50-2.31)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 2.31Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.260 0.218 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.7	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9861	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.36	0/2277	0.58	0/3104
1	B	0.37	0/2277	0.59	0/3104
1	C	0.38	0/2277	0.57	0/3104
1	D	0.40	0/2277	0.59	0/3104
2	E	0.26	0/249	0.60	0/380
2	G	0.54	0/249	0.73	0/380
3	F	0.60	0/269	1.48	7/413 (1.7%)
3	H	0.51	0/269	0.73	0/413
All	All	0.39	0/10144	0.64	7/14002 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	18	DC	O5'-P-OP1	-18.43	88.58	110.70
3	F	17	DA	O3'-P-O5'	-7.51	89.74	104.00
3	F	18	DC	C5'-C4'-O4'	7.15	122.89	109.30
3	F	17	DA	OP1-P-O3'	6.25	118.96	105.20
3	F	17	DA	P-O3'-C3'	5.54	126.34	119.70
3	F	18	DC	O5'-P-OP2	5.13	116.86	110.70
3	F	18	DC	P-O5'-C5'	-5.03	112.85	120.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	17	DA	Sidechain

## 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	2215	0	2209	51	0
1	B	2215	0	2209	62	0
1	C	2215	0	2209	54	0
1	D	2215	0	2209	46	0
2	E	246	0	136	8	0
2	G	246	0	136	12	0
3	F	241	0	137	7	0
3	H	241	0	137	13	0
4	A	4	0	0	0	0
4	B	6	0	0	1	0
4	C	7	0	0	0	0
4	D	8	0	0	1	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
All	All	9861	0	9382	239	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 12.

All (239) 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)
3:H:21:DA:H2''	3:H:22:DT:H5'	1.27	1.13
2:G:4:DA:H2''	2:G:5:DT:H5''	1.26	1.09
1:C:177:LYS:NZ	3:H:14:DG:H21	1.48	1.09
1:C:177:LYS:HZ3	3:H:14:DG:H21	1.08	0.98
2:G:4:DA:C2'	2:G:5:DT:H5''	1.97	0.95
2:G:5:DT:H2''	2:G:6:DG:H5'	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LYS:NZ	3:H:14:DG:N2	2.22	0.88
1:D:133:LYS:HA	1:D:133:LYS:HE2	1.56	0.88
1:B:39:LEU:HD11	1:B:111:VAL:HG11	1.59	0.83
3:H:21:DA:H2''	3:H:22:DT:C5'	2.06	0.83
1:C:39:LEU:HD22	1:C:48:VAL:HG21	1.61	0.82
1:C:177:LYS:HZ3	3:H:14:DG:N2	1.79	0.80
1:A:124:GLN:HE21	1:A:178:ARG:HH11	1.29	0.80
1:B:143:GLY:HA3	1:B:153:ILE:HD11	1.65	0.79
1:B:145:ARG:HH11	1:B:145:ARG:HG2	1.48	0.78
2:G:4:DA:H2''	2:G:5:DT:C5'	2.11	0.78
1:A:43:GLU:CD	1:A:43:GLU:H	1.86	0.76
1:C:97:ARG:HD2	1:C:98:LEU:H	1.51	0.75
1:A:26:SER:HB3	1:A:153:ILE:HG22	1.69	0.75
1:A:124:GLN:HE21	1:A:178:ARG:NH1	1.83	0.74
1:B:261:LYS:HG3	1:B:264:ARG:NH2	2.03	0.74
2:G:5:DT:H2''	2:G:6:DG:C5'	2.17	0.74
3:F:21:DA:H1'	3:F:22:DT:H5''	1.71	0.73
1:A:124:GLN:NE2	1:A:178:ARG:HH11	1.86	0.72
1:B:8:PRO:HG2	1:B:57:HIS:CE1	2.26	0.70
3:F:24:DT:H2''	3:F:25:DC:O5'	1.92	0.69
1:B:39:LEU:CD1	1:B:111:VAL:HG11	2.21	0.69
1:B:210:GLN:O	4:B:288:HOH:O	2.10	0.68
1:B:124:GLN:HE21	1:B:178:ARG:NH1	1.90	0.68
1:B:39:LEU:HD22	1:B:48:VAL:HG21	1.75	0.68
1:C:158:PRO:HD2	1:C:159:GLN:NE2	2.10	0.67
1:A:56:ARG:HB2	1:A:56:ARG:HH21	1.59	0.67
1:A:167:GLN:NE2	1:A:170:LYS:HD3	2.09	0.66
1:C:97:ARG:HD2	1:C:98:LEU:N	2.09	0.66
1:B:184:HIS:CD2	1:B:213:PRO:HD2	2.31	0.66
1:A:25:SER:O	1:A:26:SER:HB2	1.96	0.66
1:D:77:LYS:HD3	1:D:111:VAL:HG22	1.78	0.65
1:B:6:TRP:HZ3	1:B:58:THR:O	1.78	0.64
1:D:122:LEU:HD13	1:D:134:LEU:HD22	1.80	0.64
1:B:39:LEU:HD11	1:B:111:VAL:CG1	2.27	0.64
1:A:107:LEU:HD12	1:A:269:LEU:HD11	1.79	0.64
1:A:56:ARG:HB2	1:A:56:ARG:NH2	2.12	0.64
1:C:249:THR:CB	2:G:7:DA:H5'	2.27	0.64
1:C:249:THR:HG21	2:G:7:DA:H5'	1.80	0.64
1:B:48:VAL:HG22	1:B:63:LEU:CD2	2.27	0.64
1:A:249:THR:OG1	1:A:252:GLN:HG3	1.98	0.63
1:D:235:LEU:HD13	1:D:268:LEU:HD22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:GLY:CA	1:B:153:ILE:HD11	2.27	0.63
1:D:146:LEU:HD21	1:D:154:CYS:SG	2.39	0.62
1:C:107:LEU:HD11	1:C:225:LEU:HD21	1.81	0.62
1:C:177:LYS:HZ1	3:H:14:DG:N2	1.93	0.62
1:C:133:LYS:NZ	1:C:137:ARG:HH22	1.98	0.62
1:C:159:GLN:NE2	1:C:159:GLN:H	1.98	0.62
1:C:260:TRP:CH2	1:C:271:ILE:HD11	2.34	0.61
1:B:204:GLN:HE22	1:B:207:LYS:HE2	1.65	0.61
3:H:21:DA:C2'	3:H:22:DT:H5'	2.17	0.61
1:B:261:LYS:HG2	1:B:262:PRO:HA	1.81	0.61
1:D:53:ASP:HB3	1:D:58:THR:HG22	1.82	0.60
1:A:158:PRO:HD2	1:A:159:GLN:NE2	2.16	0.60
1:C:27:VAL:HG12	1:C:28:GLU:HG3	1.82	0.60
3:F:17:DA:H2''	3:F:18:DC:C6	2.36	0.60
1:A:133:LYS:HD2	1:A:137:ARG:HH11	1.67	0.60
1:A:184:HIS:CD2	1:A:213:PRO:HD2	2.36	0.60
1:D:134:LEU:HD23	1:D:134:LEU:C	2.22	0.60
1:C:3:THR:HG22	1:C:60:HIS:ND1	2.15	0.60
2:E:7:DA:H2''	2:E:8:8OG:H5'	1.82	0.60
1:C:249:THR:HB	2:G:7:DA:H5'	1.84	0.59
1:C:249:THR:CG2	2:G:7:DA:H5'	2.32	0.59
1:B:97:ARG:NH2	1:B:97:ARG:HB2	2.17	0.59
1:C:254:ARG:HH11	1:C:254:ARG:HG3	1.66	0.59
1:B:251:ALA:HB2	2:E:6:DG:H3'	1.85	0.59
1:D:25:SER:O	1:D:26:SER:HB2	2.02	0.59
1:D:235:LEU:HD13	1:D:268:LEU:CD2	2.32	0.59
2:G:4:DA:C3'	2:G:5:DT:H5''	2.27	0.58
1:C:177:LYS:HZ1	3:H:14:DG:H21	1.39	0.58
1:B:166:PRO:HG3	1:B:183:ILE:HD12	1.84	0.58
1:D:133:LYS:HA	1:D:133:LYS:CE	2.30	0.58
1:B:261:LYS:HG3	1:B:264:ARG:HH21	1.69	0.58
1:A:15:MET:HE2	1:A:19:LEU:HG	1.85	0.58
1:B:77:LYS:HD3	1:B:111:VAL:HG13	1.86	0.57
1:B:107:LEU:HD23	1:B:107:LEU:C	2.25	0.57
1:C:256:TYR:O	1:C:259:ARG:HG2	2.04	0.57
1:C:133:LYS:HZ2	1:C:137:ARG:HH22	1.51	0.57
1:A:56:ARG:HH21	1:A:56:ARG:CB	2.18	0.57
1:B:6:TRP:CZ3	1:B:58:THR:O	2.57	0.57
1:B:179:ALA:O	1:B:183:ILE:HG13	2.05	0.56
1:B:25:SER:O	1:B:26:SER:HB2	2.05	0.56
1:D:260:TRP:CH2	1:D:271:ILE:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:8:8OG:O8	2:E:8:8OG:H2''	2.07	0.55
1:A:107:LEU:HD11	1:A:225:LEU:HD21	1.87	0.55
1:A:43:GLU:CD	1:A:43:GLU:N	2.59	0.55
1:C:254:ARG:NH1	1:C:254:ARG:HG3	2.22	0.55
1:A:124:GLN:O	1:A:125:LEU:HB3	2.07	0.54
1:B:122:LEU:HD21	1:B:182:LEU:HD11	1.88	0.54
1:B:124:GLN:NE2	1:B:178:ARG:HH11	2.05	0.54
1:B:6:TRP:C	1:B:6:TRP:CD1	2.80	0.54
1:C:25:SER:O	1:C:26:SER:HB2	2.08	0.54
1:C:251:ALA:HB3	2:G:7:DA:OP1	2.08	0.54
1:C:238:ASP:HB3	1:C:241:ILE:HB	1.91	0.53
1:B:105:LEU:HD13	1:B:106:ARG:N	2.24	0.53
1:D:107:LEU:CD1	1:D:269:LEU:HD11	2.38	0.53
1:B:39:LEU:CD2	1:B:48:VAL:HG21	2.39	0.53
1:A:244:ARG:C	1:A:246:PRO:HD3	2.29	0.52
1:A:114:PHE:CD2	1:A:158:PRO:HG3	2.45	0.52
1:A:6:TRP:CZ2	1:A:57:HIS:HA	2.44	0.52
1:C:159:GLN:HE21	1:C:159:GLN:H	1.58	0.52
1:A:241:ILE:HD11	1:A:268:LEU:HD12	1.91	0.52
1:B:261:LYS:HE2	1:B:264:ARG:NH2	2.24	0.52
1:C:248:MET:HE1	1:C:279:PRO:HG3	1.91	0.52
1:C:41:VAL:HG22	1:C:77:LYS:HE3	1.91	0.51
1:C:107:LEU:HD11	1:C:225:LEU:CD2	2.39	0.51
1:D:107:LEU:HD13	1:D:269:LEU:HD11	1.91	0.51
3:F:23:DG:H2''	3:F:24:DT:OP2	2.10	0.51
1:D:225:LEU:O	1:D:229:GLN:HA	2.11	0.51
2:E:7:DA:C2'	2:E:8:8OG:H5'	2.40	0.51
1:B:124:GLN:NE2	1:B:178:ARG:NH1	2.58	0.51
1:C:158:PRO:HD2	1:C:159:GLN:HE21	1.75	0.51
1:B:45:ARG:HD3	1:B:154:CYS:SG	2.50	0.51
1:B:176:LEU:O	1:B:180:GLU:HG3	2.11	0.50
1:B:108:PRO:O	1:B:226:ARG:HD2	2.11	0.50
1:A:157:THR:HB	1:A:159:GLN:HE21	1.77	0.50
1:A:3:THR:HG22	1:A:60:HIS:CD2	2.46	0.50
1:D:108:PRO:O	1:D:226:ARG:HD2	2.12	0.50
1:B:145:ARG:HG2	1:B:145:ARG:NH1	2.17	0.50
1:B:247:GLY:O	1:B:248:MET:O	2.30	0.50
1:D:158:PRO:O	1:D:186:ALA:HB1	2.12	0.50
1:A:248:MET:CE	1:A:279:PRO:HG3	2.42	0.50
1:A:33:SER:O	1:A:52:PRO:HD2	2.11	0.49
1:D:8:PRO:HG2	1:D:57:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD11	1:A:225:LEU:CD2	2.42	0.49
1:B:26:SER:HB3	1:B:153:ILE:HG22	1.94	0.49
1:D:212:PHE:HB2	1:D:215:ILE:HD12	1.94	0.49
3:F:24:DT:H1'	3:F:25:DC:OP1	2.13	0.49
1:C:248:MET:CE	1:C:279:PRO:HG3	2.43	0.48
1:A:167:GLN:HE22	1:A:170:LYS:HD3	1.75	0.48
1:A:248:MET:HE2	1:A:279:PRO:HG3	1.94	0.48
1:A:242:LYS:HZ1	1:A:250:PRO:HG3	1.77	0.48
1:C:155:PHE:CD2	1:C:156:PRO:HD2	2.48	0.48
1:B:170:LYS:HG3	1:B:174:MET:O	2.12	0.48
1:C:6:TRP:CZ2	1:C:57:HIS:HA	2.48	0.48
1:D:226:ARG:NH2	4:D:284:HOH:O	2.47	0.48
1:C:240:LEU:HD11	1:C:244:ARG:NH1	2.29	0.47
1:A:25:SER:O	1:A:26:SER:CB	2.63	0.47
1:C:10:TYR:CE2	1:C:106:ARG:HG3	2.49	0.47
1:A:169:LEU:HB3	1:A:174:MET:HE3	1.97	0.47
1:A:242:LYS:NZ	1:A:250:PRO:HG3	2.30	0.47
1:C:198:ILE:O	1:C:198:ILE:HG23	2.15	0.47
1:D:47:VAL:HG21	1:D:152:TYR:CD2	2.50	0.47
2:E:7:DA:H1'	2:E:8:8OG:H5'	1.96	0.47
1:B:206:MET:O	1:B:210:GLN:HG3	2.14	0.46
1:D:77:LYS:HB3	1:D:111:VAL:HG23	1.97	0.46
1:D:122:LEU:HD13	1:D:134:LEU:CD2	2.45	0.46
1:B:217:ARG:NE	1:B:237:ASP:OD2	2.48	0.46
1:B:204:GLN:NE2	1:B:207:LYS:HE2	2.30	0.46
1:C:36:ALA:HA	1:C:48:VAL:O	2.16	0.46
1:D:26:SER:HB3	1:D:153:ILE:HG22	1.97	0.46
1:A:39:LEU:HD13	1:A:111:VAL:HG21	1.97	0.46
1:B:77:LYS:HB3	1:B:111:VAL:HG13	1.98	0.46
1:C:133:LYS:NZ	1:C:137:ARG:NH2	2.63	0.46
1:D:39:LEU:CD2	1:D:48:VAL:HG21	2.45	0.46
1:D:6:TRP:CZ3	1:D:58:THR:O	2.69	0.46
1:A:221:ASN:HB3	1:A:235:LEU:CD1	2.45	0.45
1:B:254:ARG:HH11	1:B:254:ARG:HG3	1.80	0.45
1:C:225:LEU:O	1:C:229:GLN:HA	2.16	0.45
1:A:238:ASP:HB3	1:A:241:ILE:HB	1.96	0.45
1:C:110:CYS:CB	1:C:116:GLN:HE21	2.30	0.45
1:A:15:MET:CE	1:A:19:LEU:HG	2.45	0.45
1:B:190:LEU:HD23	1:B:190:LEU:HA	1.85	0.45
1:B:191:GLU:HG3	1:B:191:GLU:H	1.62	0.45
1:A:6:TRP:C	1:A:6:TRP:CD1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:GLY:HA3	1:B:153:ILE:CD1	2.42	0.45
1:D:261:LYS:HG3	1:D:262:PRO:HA	1.99	0.44
1:B:48:VAL:HG22	1:B:63:LEU:HD23	1.98	0.44
3:H:20:DC:H2''	3:H:21:DA:O5'	2.17	0.44
1:B:41:VAL:HB	1:B:70:VAL:HG21	1.99	0.44
1:B:166:PRO:HG3	1:B:183:ILE:CD1	2.46	0.44
1:D:155:PHE:CD2	1:D:156:PRO:HD2	2.52	0.44
2:E:9:DT:H2''	2:E:10:DG:OP2	2.18	0.44
1:B:124:GLN:HE21	1:B:178:ARG:HH11	1.58	0.43
1:B:141:LEU:HD22	1:B:172:LEU:HD21	1.99	0.43
1:C:61:ILE:HD12	1:C:78:MET:HG3	1.99	0.43
1:D:105:LEU:HD13	1:D:106:ARG:N	2.33	0.43
3:F:20:DC:H2''	3:F:21:DA:O5'	2.18	0.43
1:B:111:VAL:HG12	1:B:111:VAL:O	2.17	0.43
1:B:198:ILE:HB	1:B:228:TRP:HB3	2.00	0.43
1:C:241:ILE:HA	1:C:241:ILE:HD13	1.83	0.43
1:D:193:THR:O	1:D:195:PRO:HD3	2.18	0.43
1:D:106:ARG:HA	1:D:106:ARG:HD3	1.89	0.43
3:H:21:DA:H2'	3:H:22:DT:H71	2.01	0.43
1:B:58:THR:CG2	1:B:59:LEU:N	2.81	0.43
1:A:26:SER:HB3	1:A:153:ILE:CG2	2.44	0.43
2:G:4:DA:C2'	2:G:5:DT:C5'	2.84	0.43
1:A:105:LEU:HD13	1:A:106:ARG:N	2.34	0.43
1:A:260:TRP:CH2	1:A:271:ILE:HD11	2.54	0.43
1:D:39:LEU:HD23	1:D:48:VAL:HG21	2.00	0.43
1:D:7:GLN:HA	1:D:8:PRO:HD3	1.85	0.43
1:C:124:GLN:HE21	1:C:178:ARG:HH11	1.67	0.42
1:A:221:ASN:HB3	1:A:235:LEU:HD12	2.01	0.42
1:C:221:ASN:HB3	1:C:235:LEU:CD1	2.49	0.42
1:A:109:GLY:O	1:A:226:ARG:NH1	2.52	0.42
1:C:105:LEU:HD11	1:C:269:LEU:HB3	2.01	0.42
1:A:15:MET:HE2	1:A:15:MET:O	2.18	0.42
1:D:134:LEU:HD23	1:D:134:LEU:O	2.19	0.42
3:H:22:DT:H2''	3:H:23:DG:C8	2.54	0.42
1:B:212:PHE:CB	1:B:215:ILE:HD12	2.50	0.42
1:D:24:VAL:CG1	1:D:136:ALA:HA	2.50	0.42
1:D:251:ALA:HB3	3:H:20:DC:OP1	2.19	0.42
1:D:77:LYS:HB3	1:D:111:VAL:CG2	2.49	0.42
1:A:176:LEU:HG	1:A:180:GLU:OE2	2.20	0.42
1:A:48:VAL:HG11	1:A:78:MET:CE	2.50	0.42
1:C:102:ARG:NH1	1:C:273:TYR:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:O	1:B:77:LYS:HG3	2.19	0.42
1:C:35:TYR:OH	1:C:37:ARG:HD2	2.20	0.42
1:A:26:SER:CB	1:A:153:ILE:HG22	2.47	0.41
1:D:158:PRO:HD2	1:D:159:GLN:HE21	1.86	0.41
1:D:198:ILE:HG23	1:D:198:ILE:O	2.20	0.41
1:D:51:ILE:HA	1:D:52:PRO:HD2	1.95	0.41
1:B:3:THR:HG22	1:B:60:HIS:CD2	2.55	0.41
1:C:193:THR:CG2	1:C:193:THR:O	2.69	0.41
1:D:68:GLU:HB2	1:D:69:PRO:HD3	2.03	0.41
1:C:234:PHE:O	1:C:235:LEU:HD12	2.20	0.41
1:D:134:LEU:C	1:D:134:LEU:CD2	2.86	0.41
1:A:225:LEU:HD23	1:A:225:LEU:C	2.41	0.41
1:C:50:ALA:HA	1:C:61:ILE:HD13	2.03	0.41
1:B:251:ALA:CB	2:E:6:DG:H3'	2.51	0.41
1:D:6:TRP:CD1	1:D:6:TRP:C	2.94	0.41
1:D:35:TYR:HE2	1:D:37:ARG:HG2	1.86	0.41
2:E:8:8OG:H1'	2:E:9:DT:C6	2.55	0.41
1:C:199:PRO:HG3	1:C:205:ALA:CB	2.51	0.40
1:D:249:THR:OG1	1:D:252:GLN:HG3	2.21	0.40
1:A:159:GLN:NE2	1:A:159:GLN:H	2.19	0.40
1:C:47:VAL:H	1:C:64:SER:HB3	1.87	0.40
1:B:133:LYS:N	1:B:133:LYS:HE3	2.36	0.40
1:D:160:ARG:HH11	1:D:160:ARG:HG3	1.86	0.40
1:B:77:LYS:HD3	1:B:111:VAL:CG1	2.51	0.40
1:D:25:SER:O	1:D:26:SER:CB	2.68	0.40
1:A:193:THR:CG2	1:A:193:THR:O	2.70	0.40
1:B:202:VAL:O	1:B:206:MET:HG3	2.22	0.40
3:F:23:DG:C8	3:F:24:DT:H73	2.57	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	280/282 (99%)	269 (96%)	11 (4%)	0	100	100
1	B	280/282 (99%)	266 (95%)	12 (4%)	2 (1%)	22	26
1	C	280/282 (99%)	265 (95%)	15 (5%)	0	100	100
1	D	280/282 (99%)	269 (96%)	11 (4%)	0	100	100
All	All	1120/1128 (99%)	1069 (95%)	49 (4%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	248	MET
1	B	275	GLU

### 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%)	30	43
1	B	222/222 (100%)	214 (96%)	8 (4%)	35	49
1	C	222/222 (100%)	214 (96%)	8 (4%)	35	49
1	D	222/222 (100%)	207 (93%)	15 (7%)	16	21
All	All	888/888 (100%)	848 (96%)	40 (4%)	27	39

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	TYR
1	A	43	GLU
1	A	73	GLU
1	A	105	LEU
1	A	133	LYS
1	A	159	GLN
1	A	204	GLN
1	A	233	VAL
1	A	250	PRO

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Mol	Chain	Res	Type
1	B	6	TRP
1	B	7	GLN
1	B	105	LEU
1	B	133	LYS
1	B	191	GLU
1	B	203	GLU
1	B	258	GLU
1	B	272	TRP
1	C	102	ARG
1	C	111	VAL
1	C	147	ASP
1	C	151	GLU
1	C	159	GLN
1	C	167	GLN
1	C	204	GLN
1	C	250	PRO
1	D	1	MET
1	D	6	TRP
1	D	43	GLU
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	159	GLN
1	D	204	GLN
1	D	272	TRP
1	D	275	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) 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

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Mol	Chain	Res	Type
1	A	221	ASN
1	A	243	GLN
1	B	7	GLN
1	B	57	HIS
1	B	60	HIS
1	B	116	GLN
1	B	124	GLN
1	B	140	GLN
1	B	159	GLN
1	B	167	GLN
1	B	184	HIS
1	B	204	GLN
1	B	221	ASN
1	B	243	GLN
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	184	HIS
1	C	221	ASN
1	D	5	ASN
1	D	116	GLN
1	D	124	GLN
1	D	140	GLN
1	D	159	GLN
1	D	184	HIS
1	D	187	ASN
1	D	221	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	18,25,26	1.29	2 (11%)	21,37,40	2.58	4 (19%)
2	8OG	G	8	3,2	18,25,26	1.30	2 (11%)	21,37,40	2.61	6 (28%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	8	8OG	C6-N1	3.93	1.39	1.33
2	G	8	8OG	C6-N1	3.79	1.39	1.33
2	E	8	8OG	C8-N7	-3.16	1.30	1.34
2	G	8	8OG	C8-N7	-3.03	1.30	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	8OG	C5-C6-N1	-8.72	111.50	123.43
2	G	8	8OG	C5-C6-N1	-8.62	111.64	123.43
2	G	8	8OG	C6-N1-C2	5.88	125.27	115.93
2	E	8	8OG	C6-N1-C2	5.85	125.23	115.93
2	E	8	8OG	C2-N3-C4	-3.14	111.77	115.36
2	G	8	8OG	C2-N3-C4	-2.98	111.95	115.36
2	G	8	8OG	N3-C2-N1	-2.52	123.86	127.22
2	G	8	8OG	C6-C5-C4	-2.42	118.49	120.80
2	E	8	8OG	N3-C2-N1	-2.40	124.02	127.22
2	G	8	8OG	O4'-C4'-C5'	2.12	116.36	109.37

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	8	8OG	O4'-C4'-C5'-O5'
2	G	8	8OG	O4'-C4'-C5'-O5'
2	G	8	8OG	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	8	8OG	5	0

## 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, 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%)	-0.03	5 (1%) 68 74	35, 55, 86, 114	0
1	B	282/282 (100%)	0.12	6 (2%) 63 70	35, 53, 89, 143	0
1	C	282/282 (100%)	-0.03	5 (1%) 68 74	35, 54, 94, 175	0
1	D	282/282 (100%)	0.09	3 (1%) 80 85	35, 54, 84, 155	0
2	E	11/12 (91%)	0.53	2 (18%) 1 1	61, 113, 145, 146	0
2	G	11/12 (91%)	-0.05	0 100 100	54, 78, 94, 105	0
3	F	12/12 (100%)	1.08	2 (16%) 1 2	77, 122, 146, 147	0
3	H	12/12 (100%)	-0.22	0 100 100	47, 69, 91, 109	0
All	All	1174/1176 (99%)	0.05	23 (1%) 65 71	35, 55, 96, 175	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	282	ALA	9.9
1	D	282	ALA	7.0
1	C	281	GLU	5.2
1	B	282	ALA	5.0
1	D	281	GLU	4.6
1	B	176	LEU	4.2
3	F	18	DC	4.2
1	B	281	GLU	3.5
1	D	239	TYR	3.0
1	B	118	VAL	2.7
1	B	177	LYS	2.7
1	C	278	GLN	2.4
3	F	23	DG	2.4
1	A	282	ALA	2.4
1	A	81	LEU	2.3
1	A	125	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	10	DG	2.2
1	C	276	GLY	2.2
1	A	147	ASP	2.2
2	E	11	DC	2.1
1	C	97	ARG	2.1
1	B	141	LEU	2.1
1	A	118	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	8OG	E	8	23/24	0.77	0.25	76,83,88,90	0
2	8OG	G	8	23/24	0.94	0.15	76,83,88,90	0

## 6.3 Carbohydrates [i](#)

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.