



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:29 AM GMT

PDB ID : 3FSQ  
Title : MutY adenine glycosylase bound to a transition state analog (1N) paired with d(8-oxoG) in duplexed DNA  
Authors : O'Shea, V.L.; Horvath, M.P.; David, S.S.  
Deposited on : 2009-01-11  
Resolution : 2.30 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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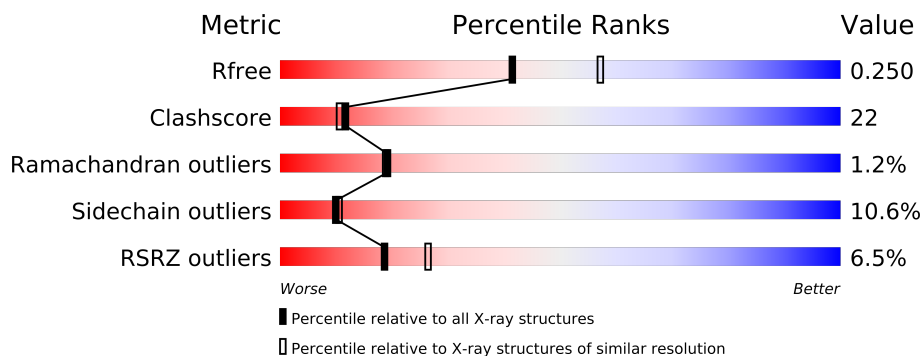
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. 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	369	
2	B	11	
3	C	11	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3335 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 A/G-specific adenine glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	2	0
			2768	1775	477	505	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P83847
A	-1	SER	-	EXPRESSION TAG	UNP P83847
A	0	HIS	-	EXPRESSION TAG	UNP P83847
A	144	ASP	ASN	SEE REMARK 999	UNP P83847

- Molecule 2 is a DNA chain called 5'-D(\*AP\*AP\*GP\*AP\*CP\*(8OG)P\*TP\*GP\*GP\*AP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			228	108	48	62	10			

- Molecule 3 is a DNA chain called 5'-D(\*T\*GP\*TP\*CP\*CP\*AP\*(NRI)P\*GP\*TP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	P	0	0	0
			193	92	31	60	10			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

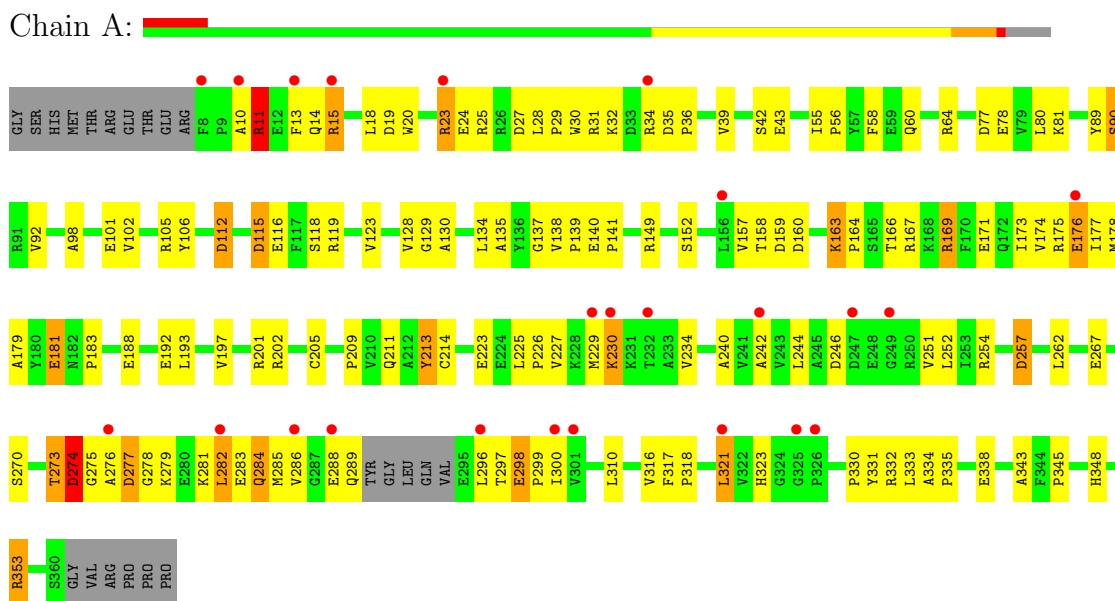
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	96	Total	O	0	0
			96	96		
6	B	22	Total	O	0	1
			23	23		
6	C	18	Total	O	0	0
			18	18		

### 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: A/G-specific adenine glycosylase



- Molecule 2: 5'-D(\*AP\*AP\*GP\*AP\*CP\*(8OG)P\*TP\*GP\*GP\*AP\*C)-3'



- Molecule 3: 5'-D(\*T\*GP\*TP\*CP\*CP\*AP\*(NRI)P\*GP\*TP\*CP\*T)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.79Å 86.52Å 140.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.34 – 2.30 41.34 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (41.34-2.30) 96.7 (41.34-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.224 , 0.249 0.225 , 0.250	Depositor DCC
$R_{free}$ test set	978 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 21064 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3335	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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, NRI, CA, SF4

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	0.34	0/2839	0.51	0/3863
2	B	0.65	0/230	1.34	4/351 (1.1%)
3	C	0.69	0/201	1.41	1/305 (0.3%)
All	All	0.40	0/3270	0.71	5/4519 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	DT	C1'-O4'-C4'	-7.50	102.60	110.10
3	C	16	DC	O4'-C1'-N1	6.59	112.61	108.00
2	B	5	DC	O4'-C1'-N1	6.10	112.27	108.00
2	B	2	DA	O4'-C1'-N9	5.57	111.90	108.00
2	B	5	DC	C1'-O4'-C4'	-5.38	104.72	110.10

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	2768	0	2686	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	228	0	124	4	0
3	C	193	0	112	1	0
4	A	8	0	0	2	0
5	A	1	0	0	0	0
6	A	96	0	0	8	0
6	B	23	0	0	1	0
6	C	18	0	0	0	0
All	All	3335	0	2922	134	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 22.

All (134) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:240:ALA:HB1	1:A:282:LEU:HD11	1.32	1.05
1:A:10:ALA:C	1:A:14:GLN:HE21	1.64	0.98
1:A:14:GLN:O	1:A:18:LEU:HD12	1.71	0.90
1:A:10:ALA:O	1:A:14:GLN:NE2	2.08	0.86
1:A:118:SER:HB2	1:A:128:VAL:HG21	1.56	0.86
1:A:213:TYR:H	1:A:213:TYR:HD2	1.23	0.84
1:A:297:THR:HG22	1:A:298:GLU:N	1.93	0.83
1:A:105:ARG:HD3	1:A:106:TYR:CZ	2.16	0.80
1:A:115:ASP:O	1:A:119:ARG:HG3	1.83	0.79
1:A:284:GLN:HG3	1:A:285:MET:N	1.98	0.78
1:A:277:ASP:O	1:A:281:LYS:HG3	1.85	0.76
1:A:277:ASP:CG	1:A:281:LYS:HE3	2.06	0.75
1:A:176:GLU:HG2	1:A:177:ILE:HG23	1.68	0.74
1:A:10:ALA:C	1:A:14:GLN:NE2	2.41	0.74
1:A:116:GLU:HA	1:A:119:ARG:HD3	1.71	0.73
1:A:211:GLN:HA	4:A:400:SF4:S3	2.31	0.71
1:A:240:ALA:HB1	1:A:282:LEU:CD1	2.15	0.70
1:A:152:SER:O	1:A:225:LEU:HD13	1.92	0.69
1:A:279:LYS:O	1:A:283:GLU:HG3	1.93	0.69
1:A:284:GLN:HE21	1:A:284:GLN:C	1.95	0.68
1:A:227:VAL:HG22	6:A:488:HOH:O	1.92	0.68
1:A:267:GLU:OE1	6:A:459:HOH:O	2.11	0.68
1:A:134:LEU:HD21	1:A:188:GLU:HG3	1.76	0.67
1:A:15:ARG:NH1	1:A:19:ASP:OD2	2.22	0.66
1:A:273:THR:HG23	1:A:275:GLY:O	1.97	0.65
1:A:213:TYR:CD2	1:A:213:TYR:N	2.63	0.64
1:A:274:ASP:CG	1:A:275:GLY:N	2.50	0.64
1:A:299:PRO:HG3	1:A:317:PHE:CE1	2.33	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:183:PRO:HD2	6:A:508:HOH:O	1.98	0.63
1:A:118:SER:HB2	1:A:128:VAL:CG2	2.29	0.62
1:A:174:VAL:O	1:A:178:MET:HB2	1.99	0.62
1:A:90:SER:HB3	6:B:436:HOH:O	2.01	0.61
1:A:274:ASP:CG	1:A:275:GLY:H	2.04	0.61
1:A:278:GLY:O	1:A:282:LEU:HD12	2.00	0.61
1:A:14:GLN:O	1:A:18:LEU:CD1	2.48	0.61
1:A:89:TYR:O	1:A:92:VAL:HG12	2.01	0.60
1:A:193:LEU:HD12	1:A:197:VAL:HB	1.83	0.59
1:A:298:GLU:CD	1:A:299:PRO:HD2	2.23	0.59
1:A:25:ARG:NH1	6:A:535:HOH:O	2.35	0.59
1:A:262:LEU:HD22	1:A:345:PRO:HB3	1.85	0.59
1:A:149:ARG:HG3	1:A:226:PRO:HD3	1.86	0.58
1:A:240:ALA:CB	1:A:282:LEU:HD11	2.21	0.58
1:A:28:LEU:HB2	1:A:31:ARG:HG3	1.84	0.58
1:A:267:GLU:HB2	1:A:348:HIS:CE1	2.40	0.57
1:A:141:PRO:HB3	1:A:174:VAL:HG11	1.87	0.57
1:A:115:ASP:O	1:A:119:ARG:CG	2.51	0.57
2:B:9:DG:C8	2:B:9:DG:H5'	2.38	0.56
1:A:137:GLY:O	1:A:183:PRO:HG2	2.04	0.56
1:A:284:GLN:C	1:A:284:GLN:NE2	2.60	0.56
1:A:273:THR:HG22	1:A:274:ASP:N	2.21	0.56
1:A:171:GLU:O	1:A:175:ARG:HG2	2.05	0.55
1:A:297:THR:HG22	1:A:298:GLU:H	1.70	0.55
1:A:284:GLN:CG	1:A:285:MET:N	2.69	0.54
1:A:160:ASP:HB3	1:A:163:LYS:HD3	1.89	0.54
1:A:115:ASP:O	1:A:119:ARG:CD	2.56	0.54
1:A:276:ALA:O	1:A:277:ASP:CB	2.56	0.54
1:A:323:HIS:HE1	1:A:333:LEU:HD22	1.73	0.54
1:A:254:ARG:NH2	1:A:270:SER:H	2.06	0.53
1:A:284:GLN:HE21	1:A:285:MET:HA	1.75	0.52
1:A:246:ASP:OD1	1:A:246:ASP:C	2.49	0.51
1:A:240:ALA:O	1:A:270:SER:HA	2.11	0.51
1:A:252:LEU:HD11	1:A:331:TYR:HB3	1.93	0.51
1:A:141:PRO:HB3	1:A:174:VAL:CG1	2.41	0.51
1:A:181:GLU:H	1:A:181:GLU:CD	2.13	0.50
1:A:299:PRO:HD3	1:A:317:PHE:CE1	2.46	0.50
1:A:205:CYS:O	1:A:211:GLN:HB2	2.12	0.49
1:A:160:ASP:HA	1:A:227:VAL:HG23	1.94	0.49
1:A:234:VAL:HB	1:A:310:LEU:HA	1.94	0.49
1:A:284:GLN:HE21	1:A:285:MET:CA	2.26	0.48
1:A:55:ILE:HB	1:A:56:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:112:ASP:N	1:A:112:ASP:OD1	2.46	0.48
1:A:257:ASP:N	1:A:257:ASP:OD1	2.43	0.48
1:A:181:GLU:OE2	1:A:181:GLU:N	2.47	0.48
1:A:34:ARG:NH1	1:A:134:LEU:O	2.45	0.47
1:A:284:GLN:HE21	1:A:285:MET:N	2.12	0.47
1:A:297:THR:HG21	6:A:478:HOH:O	2.15	0.47
1:A:297:THR:CG2	1:A:298:GLU:N	2.65	0.47
1:A:176:GLU:CG	1:A:177:ILE:HG23	2.41	0.47
1:A:164:PRO:HD2	6:A:471:HOH:O	2.14	0.46
1:A:64:ARG:HH21	1:A:78:GLU:CG	2.28	0.46
1:A:242:ALA:HB2	1:A:282:LEU:CD2	2.46	0.46
1:A:229:MET:O	1:A:230:LYS:O	2.34	0.46
1:A:167:ARG:NE	1:A:171:GLU:OE1	2.38	0.46
1:A:81:LYS:HA	1:A:343:ALA:HB2	1.96	0.46
1:A:98:ALA:O	1:A:102:VAL:HG23	2.15	0.46
1:A:31:ARG:HH22	1:A:192:GLU:CD	2.19	0.45
1:A:335:PRO:HG2	1:A:338:GLU:OE1	2.16	0.45
1:A:23:ARG:HG2	1:A:24:GLU:HG2	1.97	0.45
1:A:149:ARG:NH1	3:C:17:DA:OP1	2.48	0.45
1:A:214:CYS:HB2	4:A:400:SF4:S3	2.56	0.44
2:B:10:DA:H2''	2:B:11:DC:O5'	2.16	0.44
1:A:276:ALA:O	1:A:277:ASP:HB3	2.16	0.44
1:A:158:THR:O	1:A:227:VAL:HG21	2.17	0.44
1:A:42:SER:HB3	1:A:58:PHE:CE1	2.52	0.44
1:A:242:ALA:HB2	1:A:282:LEU:HD22	1.99	0.44
1:A:251:VAL:HG12	1:A:252:LEU:N	2.32	0.44
1:A:299:PRO:HA	1:A:316:VAL:O	2.18	0.44
1:A:64:ARG:NH2	1:A:78:GLU:CG	2.80	0.44
1:A:105:ARG:HD3	1:A:106:TYR:CE2	2.53	0.44
1:A:159:ASP:OD2	1:A:169:ARG:NH2	2.45	0.44
1:A:330:PRO:HD2	1:A:331:TYR:CD2	2.52	0.44
1:A:29:PRO:O	1:A:32:LYS:HD2	2.18	0.44
1:A:35:ASP:OD1	1:A:35:ASP:C	2.57	0.44
1:A:11:ARG:NH2	6:A:430:HOH:O	2.45	0.43
1:A:299:PRO:HD3	1:A:317:PHE:HE1	1.84	0.43
1:A:178:MET:HG2	1:A:179:ALA:N	2.33	0.43
1:A:30:TRP:HB3	1:A:58:PHE:CZ	2.53	0.43
1:A:129:GLY:HA3	1:A:141:PRO:O	2.18	0.43
1:A:43[B]:GLU:HG2	1:A:130:ALA:HB3	2.00	0.43
1:A:173:ILE:HG22	1:A:173:ILE:O	2.19	0.43
1:A:254:ARG:NH2	1:A:270:SER:O	2.51	0.42
1:A:244:LEU:O	1:A:251:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:334:ALA:HA	1:A:335:PRO:HD3	1.90	0.42
1:A:288:GLU:O	1:A:289:GLN:C	2.57	0.42
1:A:15:ARG:HD2	1:A:15:ARG:HA	1.19	0.42
1:A:166:THR:O	1:A:169:ARG:HB3	2.20	0.42
1:A:123:VAL:HG12	1:A:128:VAL:HG23	2.02	0.42
1:A:36:PRO:HG3	1:A:135:ALA:HB1	2.02	0.42
1:A:353:ARG:NH1	6:A:425:HOH:O	2.50	0.42
1:A:20:TRP:CG	1:A:209:PRO:HG3	2.55	0.42
1:A:60:GLN:O	1:A:64:ARG:HG3	2.19	0.42
1:A:157:VAL:HG13	1:A:169:ARG:NH1	2.35	0.42
1:A:211:GLN:O	1:A:211:GLN:HG2	2.18	0.42
1:A:138:VAL:HA	1:A:139:PRO:HD3	1.80	0.41
1:A:178:MET:HE2	1:A:178:MET:HB2	1.92	0.41
2:B:9:DG:H8	2:B:9:DG:H5'	1.82	0.41
1:A:267:GLU:HB2	1:A:348:HIS:ND1	2.36	0.41
1:A:13:PHE:HB2	1:A:213:TYR:CE1	2.56	0.40
1:A:297:THR:HB	1:A:318:PRO:O	2.20	0.40
1:A:298:GLU:OE1	1:A:299:PRO:HD2	2.20	0.40
1:A:39:VAL:O	1:A:43[A]:GLU:HG2	2.21	0.40
2:B:1:DA:H5'	2:B:1:DA:C8	2.57	0.40
1:A:300:ILE:HG23	1:A:318:PRO:HD3	2.03	0.40
1:A:244:LEU:HB3	1:A:321:LEU:HD23	2.02	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	346/369 (94%)	307 (89%)	35 (10%)	4 (1%)	19 19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	LYS

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Mol	Chain	Res	Type
1	A	277	ASP
1	A	11	ARG
1	A	274	ASP

### 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	286/315 (91%)	256 (90%)	30 (10%)	10	11

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	15	ARG
1	A	23	ARG
1	A	27	ASP
1	A	77	ASP
1	A	80	LEU
1	A	90	SER
1	A	101	GLU
1	A	112	ASP
1	A	115	ASP
1	A	140	GLU
1	A	163	LYS
1	A	169	ARG
1	A	176	GLU
1	A	181	GLU
1	A	201	ARG
1	A	202	ARG
1	A	213	TYR
1	A	223	GLU
1	A	257	ASP
1	A	273	THR
1	A	274	ASP
1	A	282	LEU
1	A	284	GLN
1	A	286	VAL

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Mol	Chain	Res	Type
1	A	296	LEU
1	A	298	GLU
1	A	321	LEU
1	A	332	ARG
1	A	353	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	94	ASN
1	A	182	ASN
1	A	211	GLN
1	A	284	GLN
1	A	323	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	B	6	2	23,25,26	2.04	6 (26%)	27,37,40	1.67	5 (18%)
3	NRI	C	18	3	11,11,12	2.07	2 (18%)	13,14,17	1.53	4 (30%)

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	B	6	2	-	0/6/21/22	0/1/3/3
3	NRI	C	18	3	-	0/5/15/16	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	8OG	C2-N2	5.48	1.40	1.32
3	C	18	NRI	C4'-C3'	5.33	1.61	1.53
2	B	6	8OG	C4-N9	3.50	1.42	1.37
2	B	6	8OG	C8-N9	3.33	1.44	1.36
2	B	6	8OG	C2-N1	3.24	1.41	1.36
3	C	18	NRI	O3'-C3'	-2.60	1.37	1.43
2	B	6	8OG	C6-N1	2.43	1.41	1.37
2	B	6	8OG	C4-N3	2.36	1.39	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	8OG	C5-C4-N9	3.91	107.94	106.00
2	B	6	8OG	C4-C5-N7	3.43	109.01	106.14
2	B	6	8OG	N2-C2-N1	-3.41	114.10	117.86
2	B	6	8OG	N1-C2-N3	2.85	125.77	121.78
3	C	18	NRI	C4'-C6'-N1'	2.66	111.13	105.75
2	B	6	8OG	C8-N9-C1'	2.49	126.55	125.17
3	C	18	NRI	O3P-P-O5'	-2.44	105.71	113.42
3	C	18	NRI	C6'-C4'-C5'	2.39	115.67	112.66
3	C	18	NRI	C3'-C2'-N1'	2.11	108.96	105.22

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 ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
4	SF4	A	400	1	12,12,12	16.92	11 (91%)	0,24,24	0.00	-

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
4	SF4	A	400	1	-	0/0/48/48	0/0/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	SF4	S3-FE2	-37.95	2.07	2.33
4	A	400	SF4	S2-FE3	-26.80	2.15	2.33
4	A	400	SF4	S4-FE2	19.41	2.46	2.33
4	A	400	SF4	S4-FE3	17.46	2.45	2.33
4	A	400	SF4	S3-FE1	-14.88	2.23	2.33
4	A	400	SF4	S1-FE4	-13.32	2.24	2.33
4	A	400	SF4	S2-FE1	10.01	2.40	2.33
4	A	400	SF4	S1-FE3	-6.07	2.29	2.33
4	A	400	SF4	S3-FE4	-5.31	2.29	2.33
4	A	400	SF4	S4-FE1	-4.52	2.30	2.33
4	A	400	SF4	S2-FE4	-2.87	2.31	2.33

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	348/369 (94%)	0.51	24 (6%)	17 24	22, 54, 76, 98	3 (0%)
2	B	11/11 (100%)	-0.40	0	100 100	28, 36, 53, 64	0
3	C	10/11 (90%)	-0.24	0	100 100	24, 34, 55, 65	0
All	All	369/391 (94%)	0.46	24 (6%)	18 26	22, 53, 76, 98	3 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	MET	5.6
1	A	23	ARG	5.1
1	A	156	LEU	4.4
1	A	10	ALA	3.9
1	A	296	LEU	3.8
1	A	232	THR	3.7
1	A	230	LYS	3.3
1	A	326	PRO	3.2
1	A	8	PHE	3.1
1	A	286	VAL	3.1
1	A	247	ASP	3.0
1	A	15	ARG	3.0
1	A	282	LEU	2.7
1	A	300	ILE	2.7
1	A	301	VAL	2.7
1	A	34	ARG	2.5
1	A	13	PHE	2.5
1	A	249	GLY	2.5
1	A	321	LEU	2.3
1	A	288	GLU	2.2
1	A	325	GLY	2.2
1	A	276	ALA	2.1
1	A	176	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	242	ALA	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	B	6	23/24	0.15	0.46	20,28,35,43	0
3	NRI	C	18	11/12	0.14	-0.11	20,23,28,29	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
4	SF4	A	400	8/8	0.13	-0.69	46,49,54,58	3
5	CA	A	501	1/1	0.10	-2.62	42,42,42,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.