Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2026 – 12:14 PM EST

PDB ID	:	11JI / pdb_000011ji
Title	:	Human MUTYH adenine glycosylase bound to DNA containing a transition state analog (1N) paired with d(8-oxo-G) and full Zn coordination
Authors	:	Trasvina-Arenas, C.H.; David, S.S.; Hashemian, M.; Fisher, A.J.; Malek, M.
Deposited on	:	2026-02-26
Resolution	:	1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

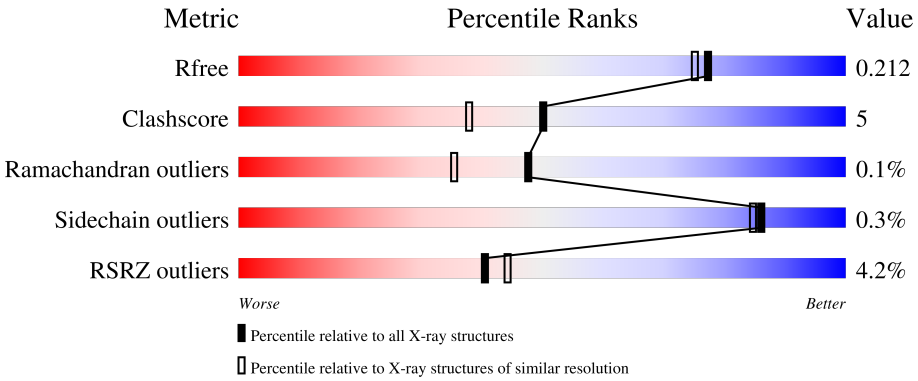
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	459	3% 78% 10% 12%
1	D	459	4% 81% 7% 11%
2	B	11	55% 45%
2	E	11	64% 36%
3	C	11	9% 64% 36%

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Mol	Chain	Length	Quality of chain
3	F	11	45% 55%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GOL	D	603	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 14398 atoms, of which 6362 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 Isoform Alpha-1 of Adenine DNA glycosylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	406	Total	C	H	N	O	S	0	8	0
			6154	2002	2975	573	584	20			
1	D	407	Total	C	H	N	O	S	0	4	0
			6082	2010	2889	575	592	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLY	-	expression tag	UNP Q9UIF7
A	62	HIS	-	expression tag	UNP Q9UIF7
A	63	MET	-	expression tag	UNP Q9UIF7
A	64	ALA	-	expression tag	UNP Q9UIF7
A	65	CYS	-	expression tag	UNP Q9UIF7
A	66	ASP	-	expression tag	UNP Q9UIF7
D	61	GLY	-	expression tag	UNP Q9UIF7
D	62	HIS	-	expression tag	UNP Q9UIF7
D	63	MET	-	expression tag	UNP Q9UIF7
D	64	ALA	-	expression tag	UNP Q9UIF7
D	65	CYS	-	expression tag	UNP Q9UIF7
D	66	ASP	-	expression tag	UNP Q9UIF7

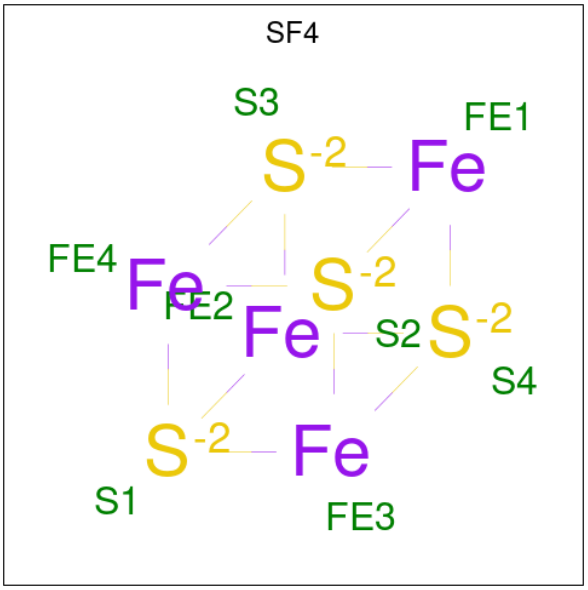
- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	11	Total	C	H	N	O	P	0	0	0
			352	108	124	48	62	10			
2	E	11	Total	C	H	N	O	P	0	0	0
			352	108	124	48	62	10			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	11	Total C H N O P 323 102 113 33 65 10	0	0	0
3	F	11	Total C H N O P 323 102 113 33 65 10	0	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 16 8 8	0	1
4	D	1	Total Fe S 8 4 4	0	0

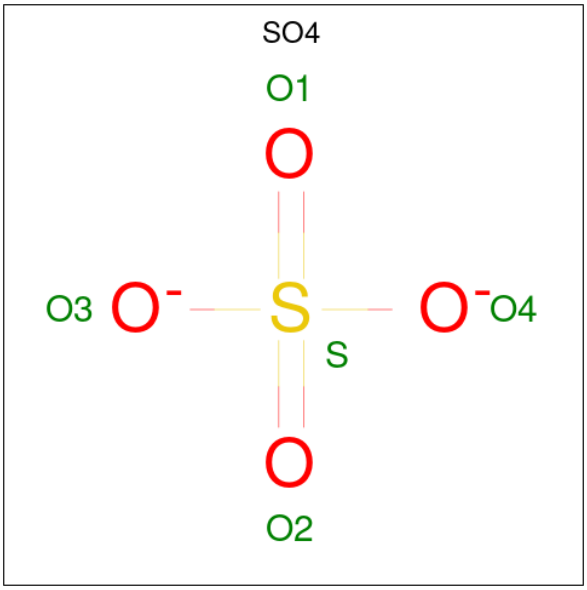
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	D	1	Total Zn 1 1	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

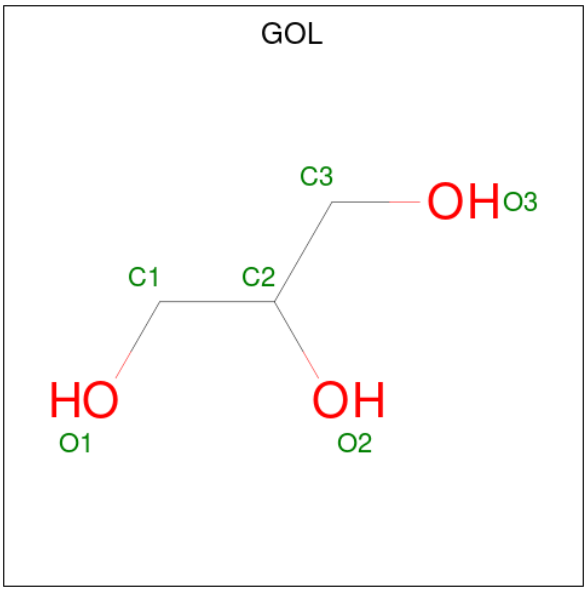
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Na 1 1	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C H O 14 3 8 3	0	0
8	D	1	Total C H O 14 3 8 3	0	0
8	D	1	Total C H O 14 3 8 3	0	0

- Molecule 9 is water.

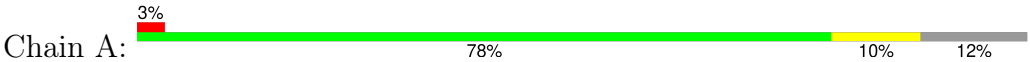
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	293	Total O 293 293	0	0
9	B	22	Total O 22 22	0	0
9	C	26	Total O 26 26	0	0
9	D	321	Total O 321 321	0	0
9	E	30	Total O 30 30	0	0
9	F	26	Total O 26 26	0	0

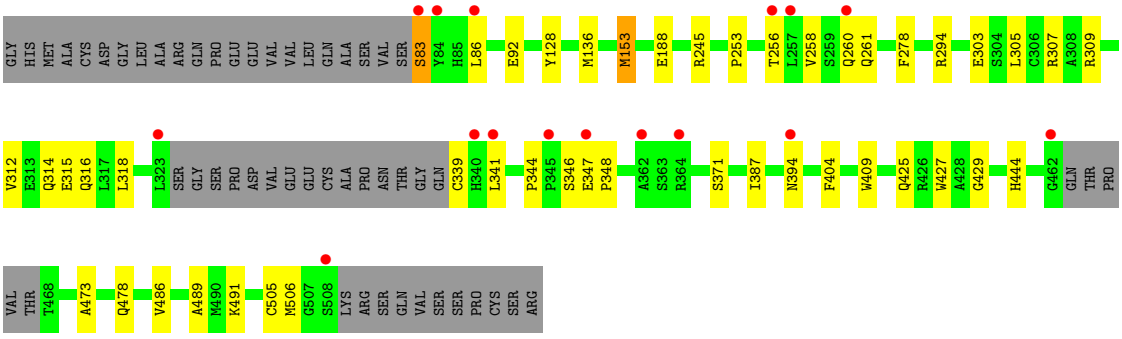
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Isoform Alpha-1 of Adenine DNA glycosylase

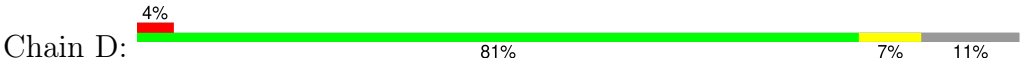
Chain A:

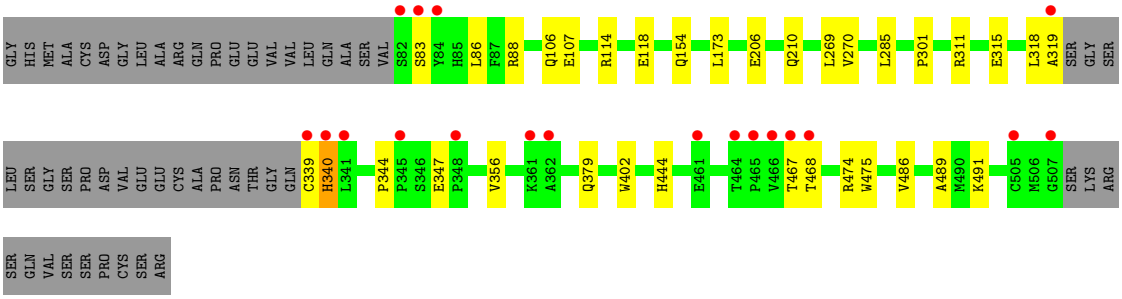




• Molecule 1: Isoform Alpha-1 of Adenine DNA glycosylase

Chain D:

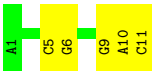




• Molecule 2: DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3')

Chain B:

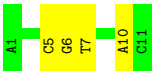




• Molecule 2: DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3')

Chain E:

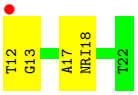




• Molecule 3: DNA (5'-D(*TP*GP*TP*CP*CP*AP*(NRI)P*GP*TP*CP*T)-3')

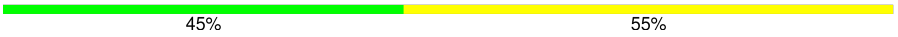
Chain C:





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

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.95Å 116.76Å 118.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.87 – 1.85 38.87 – 1.85	Depositor EDS
% Data completeness (in resolution range)	95.3 (38.87-1.85) 95.4 (38.87-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.170 , 0.212 0.170 , 0.212	Depositor DCC
R_{free} test set	4942 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 37.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.032 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14398	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NA, GOL, SF4, ZN, 8OG, NRI, SO4

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	0.47	1/3259 (0.0%)	0.61	1/4442 (0.0%)
1	D	0.48	0/3268	0.61	0/4455
2	B	1.29	0/230	1.21	1/351 (0.3%)
2	E	1.46	0/230	1.22	2/351 (0.6%)
3	C	1.37	1/220 (0.5%)	1.23	0/335
3	F	1.37	1/220 (0.5%)	1.19	0/335
All	All	0.65	3/7427 (0.0%)	0.72	4/10269 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	MET	SD-CE	-7.09	1.61	1.79
3	C	17	DA	C3'-C2'	6.90	1.57	1.52
3	F	17	DA	C3'-O3'	5.96	1.51	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	5	DC	O4'-C1'-N1	8.06	113.65	108.00
2	B	5	DC	O4'-C1'-N1	7.49	113.24	108.00
1	A	136	MET	N-CA-CB	-6.44	100.30	110.22
2	E	7	DT	C1'-O4'-C4'	-5.58	104.52	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3179	2975	3089	31	0
1	D	3193	2889	3115	31	0
2	B	228	124	124	4	0
2	E	228	124	124	1	0
3	C	210	113	125	3	0
3	F	210	113	125	4	0
4	A	16	0	0	2	0
4	D	8	0	0	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
7	A	20	0	0	0	0
7	D	5	0	0	0	0
8	A	6	8	8	0	0
8	D	12	16	16	1	0
9	A	293	0	0	6	0
9	B	22	0	0	2	0
9	C	26	0	0	0	0
9	D	321	0	0	6	0
9	E	30	0	0	1	0
9	F	26	0	0	3	0
All	All	8036	6362	6726	74	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 5.

All (74) 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)
1:D:83:SER:HB3	1:D:88:ARG:HG3	1.42	0.99
1:A:314:GLN:OE1	9:A:701:HOH:O	1.89	0.90
3:F:22:DT:OP2	9:F:101:HOH:O	1.92	0.86
3:C:12:DT:H4'	3:C:13:DG:O5'	1.82	0.79
1:D:344:PRO:HG2	1:D:347:GLU:HG2	1.64	0.79
8:D:603:GOL:O2	9:D:701:HOH:O	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:SER:CB	1:D:88:ARG:HG3	2.17	0.75
3:F:13:DG:N3	9:F:103:HOH:O	2.18	0.74
1:A:188:GLU:OE1	9:A:702:HOH:O	2.05	0.74
1:A:505:CYS:SG	9:A:955:HOH:O	2.44	0.74
1:D:83:SER:HB3	1:D:88:ARG:CG	2.15	0.74
2:E:10:DA:OP1	9:E:101:HOH:O	2.06	0.73
1:D:154:GLN:NE2	9:D:704:HOH:O	2.20	0.73
3:F:15:DC:OP1	9:F:102:HOH:O	2.07	0.72
1:A:92:GLU:HG3	1:A:305:LEU:HD22	1.72	0.71
2:B:11:DC:O2	9:B:101:HOH:O	2.08	0.70
1:A:83:SER:HB3	1:A:86[A]:LEU:O	1.92	0.69
1:D:118:GLU:OE2	9:D:702:HOH:O	2.12	0.66
1:D:106:GLN:NE2	1:D:107:GLU:OE2	2.28	0.64
1:A:83:SER:HB3	1:A:86[B]:LEU:O	1.98	0.63
1:D:467:THR:HG22	1:D:468:THR:N	2.13	0.63
1:D:347:GLU:O	1:D:347:GLU:HG3	1.98	0.63
1:A:256:THR:O	1:A:260:GLN:HG3	2.02	0.60
1:A:294:ARG:NH2	9:A:709:HOH:O	2.34	0.59
1:A:394:ASN:ND2	9:A:710:HOH:O	2.35	0.58
1:A:478:GLN:HB2	1:A:506:MET:HE3	1.86	0.56
1:D:467:THR:HG22	1:D:468:THR:H	1.70	0.56
1:D:467:THR:C	1:D:468:THR:HG23	2.31	0.55
3:C:12:DT:H2"	3:C:13:DG:OP2	2.09	0.53
1:D:311:ARG:O	1:D:315:GLU:HG3	2.09	0.53
1:A:444:HIS:CD2	1:A:489:ALA:HB2	2.44	0.53
1:A:128:TYR:CE2	1:A:153:MET:HE1	2.44	0.52
1:D:339:CYS:O	1:D:340:HIS:CB	2.58	0.52
1:D:340:HIS:O	9:D:703:HOH:O	2.19	0.52
1:D:318:LEU:O	1:D:319:ALA:HB3	2.10	0.51
1:D:467:THR:CG2	1:D:468:THR:H	2.25	0.50
2:B:11:DC:HO3'	3:F:12:DT:H3	1.59	0.49
1:A:486[B]:VAL:CG2	1:A:491:LYS:HE3	2.42	0.49
1:A:303:GLU:HG3	1:A:309:ARG:HG2	1.95	0.49
1:A:86[A]:LEU:HB2	9:A:711:HOH:O	2.12	0.48
1:D:467:THR:CG2	1:D:468:THR:N	2.75	0.48
1:A:344:PRO:HG2	1:A:347:GLU:CB	2.43	0.47
1:A:245:ARG:HD3	4:A:601[B]:SF4:S1	2.54	0.47
1:D:173:LEU:HD23	1:D:173:LEU:O	2.15	0.47
1:D:486:VAL:CG2	1:D:491:LYS:HE3	2.45	0.46
1:D:444:HIS:CD2	1:D:489:ALA:HB2	2.51	0.46
1:D:86:LEU:HB2	1:D:88:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:PRO:HA	1:A:258:VAL:HG11	1.97	0.46
1:A:427:TRP:CE3	1:A:473:ALA:HB2	2.51	0.45
1:A:315:GLU:HA	1:A:318:LEU:HG	1.99	0.45
1:D:206:GLU:HG3	9:D:1002:HOH:O	2.16	0.45
1:D:210:GLN:OE1	9:D:705:HOH:O	2.21	0.45
1:A:83:SER:CB	1:A:86[A]:LEU:O	2.63	0.45
1:D:356:VAL:HG12	1:D:356:VAL:O	2.17	0.44
1:A:83:SER:HB2	1:A:307:ARG:NH2	2.33	0.44
1:D:285:LEU:HD11	1:D:301:PRO:HD2	1.99	0.44
1:A:371:SER:OG	1:A:409:TRP:HB3	2.18	0.44
1:D:402:TRP:CZ3	1:D:474:ARG:HG3	2.52	0.43
1:A:261:GLN:HG2	1:A:341:LEU:HD11	2.01	0.43
1:A:425:GLN:HG2	1:A:429:GLY:O	2.19	0.42
2:B:11:DC:H1'	9:B:101:HOH:O	2.18	0.42
1:A:86[B]:LEU:HD21	1:A:261:GLN:OE1	2.18	0.42
1:D:114:ARG:O	1:D:118:GLU:HG3	2.18	0.42
1:D:344:PRO:HD2	1:D:347:GLU:HG3	2.02	0.41
1:A:387:ILE:HD12	1:A:404:PHE:HE1	1.85	0.41
3:C:12:DT:H6	3:C:12:DT:O5'	2.04	0.41
1:D:269:LEU:O	1:D:270:VAL:C	2.63	0.41
1:A:303:GLU:HA	4:A:601[A]:SF4:S2	2.60	0.41
1:A:312:VAL:O	1:A:316:GLN:HG3	2.21	0.41
1:A:346:SER:C	1:A:348:PRO:HD3	2.46	0.40
1:D:379:GLN:HG2	1:D:475:TRP:CZ3	2.56	0.40
1:A:278:PHE:CD1	1:A:278:PHE:C	3.00	0.40
1:D:344:PRO:HD2	1:D:347:GLU:CG	2.50	0.40
2:B:9:DG:H2"	2:B:10:DA:C5'	2.51	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	408/459 (89%)	399 (98%)	9 (2%)	0	100 100
1	D	407/459 (89%)	399 (98%)	7 (2%)	1 (0%)	43 31
All	All	815/918 (89%)	798 (98%)	16 (2%)	1 (0%)	48 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	340	HIS

5.3.2 Protein sidechains (i)

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	333/380 (88%)	331 (99%)	2 (1%)	78 73
1	D	334/380 (88%)	334 (100%)	0	100 100
All	All	667/760 (88%)	665 (100%)	2 (0%)	86 85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	SER
1	A	339	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	138	GLN
1	A	187	GLN
1	A	394	ASN
1	A	435	HIS
1	A	482	HIS
1	D	435	HIS
1	D	482	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\| > 2$
3	NRI	C	18	3	7,11,12	4.15	4 (57%)	3,14,17	0.27	0
2	8OG	B	6	2	22,25,26	3.68	11 (50%)	26,37,40	1.70	7 (26%)
2	8OG	E	6	2	22,25,26	3.76	10 (45%)	26,37,40	2.03	7 (26%)
3	NRI	F	18	3	7,11,12	3.88	3 (42%)	3,14,17	0.77	0

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
3	NRI	C	18	3	-	0/3/15/16	0/1/1/1
2	8OG	B	6	2	-	1/7/21/22	0/3/3/3
2	8OG	E	6	2	-	1/7/21/22	0/3/3/3
3	NRI	F	18	3	-	0/3/15/16	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	18	NRI	O3'-C3'	-9.83	1.22	1.43
2	B	6	8OG	O3'-C3'	-9.41	1.23	1.43
3	F	18	NRI	O3'-C3'	-9.23	1.24	1.43
2	E	6	8OG	O3'-C3'	-8.84	1.24	1.43
2	E	6	8OG	O8-C8	7.94	1.37	1.23
2	E	6	8OG	O6-C6	7.19	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6	8OG	O6-C6	7.18	1.37	1.23
2	B	6	8OG	O8-C8	6.90	1.35	1.23
2	E	6	8OG	C4-N3	5.26	1.46	1.34
2	E	6	8OG	C5-N7	5.00	1.45	1.37
2	B	6	8OG	C4-N3	4.84	1.45	1.34
2	B	6	8OG	C5-N7	4.84	1.45	1.37
2	E	6	8OG	C4-N9	4.04	1.46	1.39
2	B	6	8OG	C2-N1	3.97	1.47	1.37
2	E	6	8OG	C2-N2	3.80	1.43	1.34
2	E	6	8OG	C2-N1	3.69	1.46	1.37
2	B	6	8OG	C2-N2	3.65	1.42	1.34
2	B	6	8OG	C4-N9	3.27	1.45	1.39
2	E	6	8OG	C8-N9	-2.79	1.35	1.40
3	F	18	NRI	C2'-N1'	2.70	1.55	1.46
2	B	6	8OG	C8-N9	-2.67	1.36	1.40
3	C	18	NRI	C2'-C3'	2.67	1.56	1.53
2	E	6	8OG	C5-C4	2.67	1.41	1.37
3	F	18	NRI	C5'-C4'	2.59	1.56	1.51
3	C	18	NRI	C5'-C4'	2.35	1.56	1.51
3	C	18	NRI	C2'-N1'	2.16	1.53	1.46
2	B	6	8OG	C8-N7	-2.08	1.34	1.38
2	B	6	8OG	C5-C4	2.05	1.40	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	6	8OG	C1'-N9-C4	-5.21	117.70	126.88
2	E	6	8OG	N9-C4-N3	4.93	132.29	126.13
2	B	6	8OG	C1'-N9-C4	-4.34	119.23	126.88
2	B	6	8OG	N9-C4-N3	3.89	131.00	126.13
2	E	6	8OG	C2-N3-C4	3.25	117.89	112.30
2	E	6	8OG	C6-C5-N7	2.84	137.05	131.54
2	E	6	8OG	C5-C6-N1	2.65	119.40	112.13
2	B	6	8OG	C2-N3-C4	2.47	116.56	112.30
2	B	6	8OG	O8-C8-N9	2.33	129.16	126.00
2	B	6	8OG	C6-C5-N7	2.24	135.89	131.54
2	E	6	8OG	C5-N7-C8	2.13	112.41	109.47
2	E	6	8OG	O6-C6-C5	-2.06	122.30	127.26
2	B	6	8OG	O6-C6-C5	-2.03	122.37	127.26
2	B	6	8OG	C2-N1-C6	-2.02	121.45	125.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	6	8OG	C4'-C5'-O5'-P
2	B	6	8OG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	D	601	1	0,12,12	-	-	-		
7	SO4	A	605	-	4,4,4	0.27	0	6,6,6	0.20	0
8	GOL	D	603	-	5,5,5	1.64	2 (40%)	5,5,5	0.59	0
4	SF4	A	601[A]	1	0,12,12	-	-	-		
7	SO4	D	605	-	4,4,4	0.27	0	6,6,6	0.28	0
4	SF4	A	601[B]	1	0,12,12	-	-	-		
7	SO4	A	606	-	4,4,4	0.25	0	6,6,6	0.16	0
7	SO4	A	607	-	4,4,4	0.35	0	6,6,6	0.24	0
8	GOL	D	604	-	5,5,5	0.93	0	5,5,5	0.85	0
7	SO4	A	604	-	4,4,4	0.22	0	6,6,6	0.38	0
8	GOL	A	608	-	5,5,5	1.08	0	5,5,5	0.86	0

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	D	601	1	-	-	0/6/5/5
8	GOL	D	603	-	-	4/4/4/4	-
4	SF4	A	601[A]	1	-	-	0/6/5/5
4	SF4	A	601[B]	1	-	-	0/6/5/5
8	GOL	D	604	-	-	4/4/4/4	-
8	GOL	A	608	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	603	GOL	C3-C2	2.47	1.61	1.51
8	D	603	GOL	C1-C2	2.01	1.59	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	603	GOL	O1-C1-C2-C3
8	D	603	GOL	C1-C2-C3-O3
8	D	604	GOL	O1-C1-C2-O2
8	A	608	GOL	O1-C1-C2-C3
8	D	604	GOL	O1-C1-C2-C3
8	D	604	GOL	C1-C2-C3-O3
8	A	608	GOL	O1-C1-C2-O2
8	A	608	GOL	O2-C2-C3-O3
8	D	603	GOL	O1-C1-C2-O2
8	D	603	GOL	O2-C2-C3-O3
8	A	608	GOL	C1-C2-C3-O3
8	D	604	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	603	GOL	1	0
4	A	601[A]	SF4	1	0
4	A	601[B]	SF4	1	0

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^{th} 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	406/459 (88%)	0.03	16 (3%) 43 47	13, 38, 71, 98	7 (1%)
1	D	407/459 (88%)	0.01	19 (4%) 36 39	19, 36, 71, 108	4 (0%)
2	B	10/11 (90%)	0.27	0 100 100	29, 46, 74, 80	0
2	E	10/11 (90%)	0.15	0 100 100	30, 50, 71, 80	0
3	C	10/11 (90%)	0.34	1 (10%) 12 12	30, 50, 75, 86	0
3	F	10/11 (90%)	0.22	0 100 100	29, 47, 74, 77	0
All	All	853/962 (88%)	0.03	36 (4%) 40 44	13, 37, 73, 108	11 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86[A]	LEU	4.5
1	A	508	SER	4.5
1	D	507	GLY	4.1
1	A	462	GLY	4.0
1	D	466	VAL	3.9
1	A	84	TYR	3.9
1	D	319	ALA	3.9
1	D	362	ALA	3.8
1	A	362	ALA	3.6
1	D	465	PRO	3.5
1	D	340	HIS	3.3
1	D	361	LYS	3.3
1	D	467	THR	3.3
1	A	364	ARG	3.2
1	D	464	THR	3.1
1	A	83	SER	3.1
1	A	323	LEU	2.9
1	D	345	PRO	2.9
1	D	84	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	341	LEU	2.7
1	A	257	LEU	2.7
1	D	83	SER	2.6
1	D	505	CYS	2.6
3	C	12	DT	2.5
1	D	82	SER	2.5
1	A	394	ASN	2.4
1	D	339	CYS	2.3
1	D	341	LEU	2.3
1	A	256	THR	2.3
1	A	347	GLU	2.3
1	A	340	HIS	2.3
1	D	348	PRO	2.2
1	A	260	GLN	2.1
1	A	345	PRO	2.1
1	D	461	GLU	2.0
1	D	468	THR	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^{th} 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^2)	Q<0.9
2	8OG	B	6	23/24	0.98	0.04	22,27,33,38	0
2	8OG	E	6	23/24	0.98	0.06	22,28,34,34	0
3	NRI	C	18	11/12	0.98	0.06	21,26,32,33	0
3	NRI	F	18	11/12	0.98	0.04	22,27,31,32	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (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^{th} 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^2)	Q<0.9
7	SO4	A	606	5/5	0.71	0.12	65,69,87,91	5
8	GOL	D	603	6/6	0.75	0.20	43,71,87,87	0
7	SO4	A	607	5/5	0.78	0.16	43,51,58,72	5
8	GOL	D	604	6/6	0.80	0.12	70,84,96,96	0
8	GOL	A	608	6/6	0.81	0.17	51,77,93,93	0
7	SO4	D	605	5/5	0.82	0.12	54,70,87,92	0
7	SO4	A	604	5/5	0.84	0.13	50,56,68,70	5
7	SO4	A	605	5/5	0.84	0.14	45,48,54,57	5
4	SF4	A	601[A]	8/8	0.98	0.04	21,24,26,26	8
4	SF4	A	601[B]	8/8	0.98	0.04	21,23,25,25	8
4	SF4	D	601	8/8	0.98	0.04	24,25,25,26	0
5	ZN	A	602	1/1	0.98	0.04	50,50,50,50	1
5	ZN	D	602	1/1	0.99	0.04	36,36,36,36	1
6	NA	A	603	1/1	0.99	0.12	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.