Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2026 – 12:14 PM EST

PDB ID	:	11IP / pdb_000011ip
Title	:	Human MUTYH adenine glycosylase bound to DNA containing a product analog (THF) paired with d(8-oxo-G) with full Zinc coordination
Authors	:	Trasvina-Arenas, C.H.; David, S.S.; Hashemian, M.; Fisher, A.J.; Malek, M.
Deposited on	:	2026-02-25
Resolution	:	1.70 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:

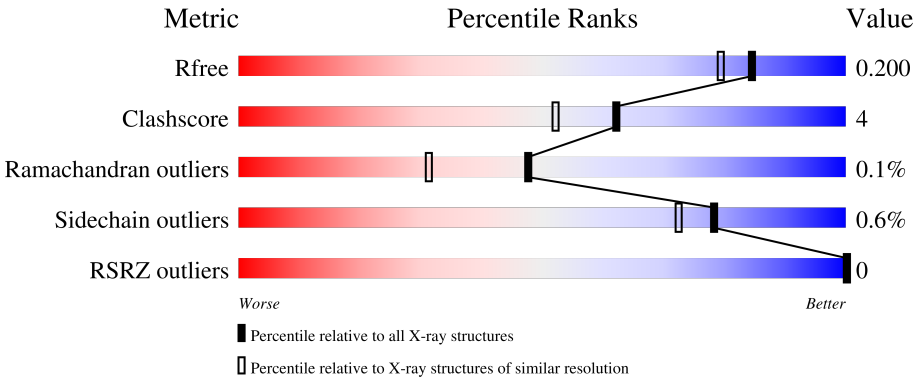
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	83% 6% 10%
1	D	459	82% 7% 11%
2	B	11	18% 82%
2	E	11	45% 55%
3	C	11	55% 45%

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Mol	Chain	Length	Quality of chain
3	F	11	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 15089 atoms, of which 6852 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	412	Total	C	H	N	O	S	0	9	0
			6457	2055	3194	592	599	17			
1	D	410	Total	C	H	N	O	S	0	8	0
			6345	2021	3138	580	589	17			

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

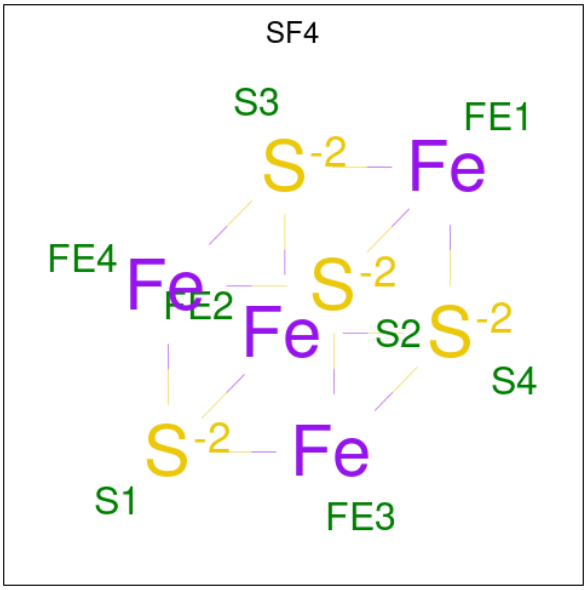
- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3').

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*(3DR)P*GP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	11	Total	C	H	N	O	P	0	0	0
			334	102	124	32	66	10			
3	F	11	Total	C	H	N	O	P	0	0	0
			334	102	124	32	66	10			

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

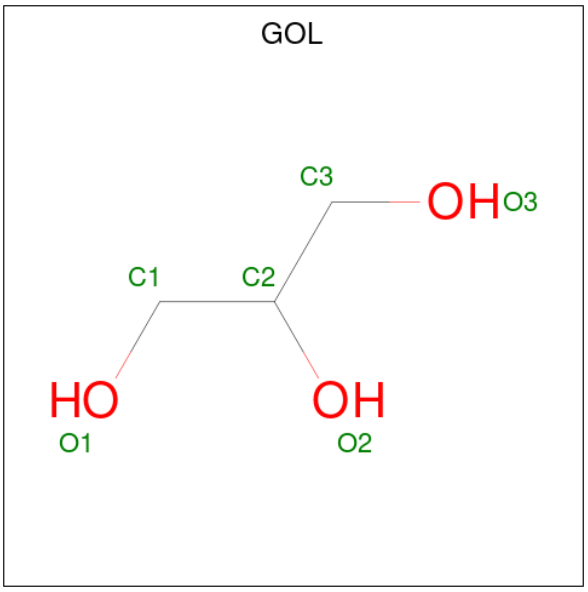


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		

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

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

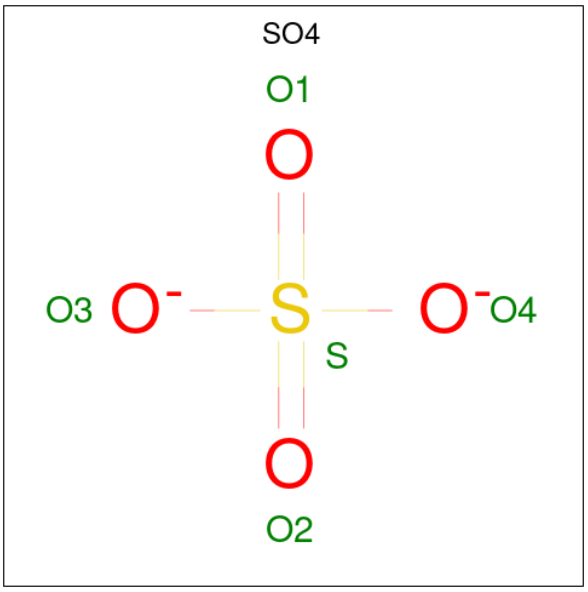


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 14 3 8 3	0	0
6	D	1	Total C H O 14 3 8 3	0	0
6	D	1	Total C H O 14 3 8 3	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O S 5 4 1	0	0
8	D	1	Total O S 5 4 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	363	Total O 363 363	0	0
9	B	25	Total O 25 25	0	0
9	C	32	Total O 32 32	0	0
9	D	369	Total O 369 369	0	0
9	E	29	Total O 29 29	0	0
9	F	26	Total O 26 26	0	0

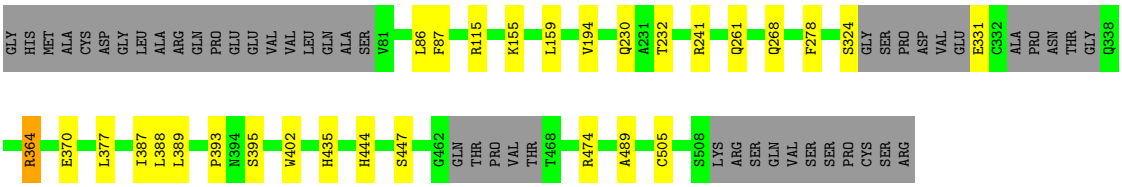
3 Residue-property plots (i)

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:

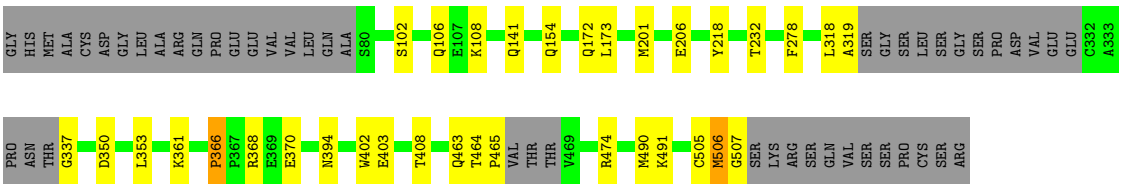




• Molecule 1: Isoform Alpha-1 of Adenine DNA glycosylase

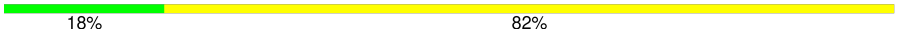
Chain D:





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

Chain B:

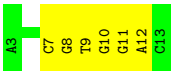




• Molecule 2: DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3')

Chain E:





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

Chain C:

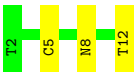




• Molecule 3: DNA (5'-D(*TP*GP*TP*CP*CP*AP*(3DR)P*GP*TP*CP*T)-3')

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	87.63Å 116.69Å 118.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.96 – 1.70 35.96 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.6 (35.96-1.70) 95.6 (35.96-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.168 , 0.200 0.168 , 0.200	Depositor DCC
R_{free} test set	6345 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.075 for -h,l,k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15089	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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, SO4, GOL, SF4, ZN, 3DR, 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	0.43	0/3359	0.57	0/4571
1	D	0.50	2/3317 (0.1%)	0.70	5/4515 (0.1%)
2	B	1.37	1/230 (0.4%)	1.31	3/351 (0.9%)
2	E	1.47	2/230 (0.9%)	1.22	1/351 (0.3%)
3	C	1.20	0/220	1.33	1/335 (0.3%)
3	F	1.27	0/220	1.21	0/335
All	All	0.64	5/7576 (0.1%)	0.75	10/10458 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	366	PRO	CG-CD	-8.04	1.23	1.50
2	E	10	DG	C3'-O3'	-5.25	1.37	1.44
2	E	9	DT	C3'-C2'	5.19	1.56	1.52
1	D	366	PRO	N-CA	5.12	1.57	1.46
2	B	9	DT	C3'-C2'	5.11	1.56	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	366	PRO	N-CD-CG	-14.44	81.54	103.20
1	D	366	PRO	CA-CB-CG	-11.68	82.31	104.50
2	B	7	DC	O4'-C1'-N1	8.78	114.14	108.00
2	E	7	DC	O4'-C1'-N1	8.56	113.99	108.00
3	C	6	DC	O4'-C1'-N1	8.03	113.62	108.00
1	D	366	PRO	CA-N-CD	-7.68	101.25	112.00
1	D	465	PRO	N-CA-CB	6.97	110.66	103.00
1	D	201	MET	CB-CG-SD	-6.00	94.69	112.70
2	B	9	DT	C1'-O4'-C4'	-5.96	104.14	110.10
2	B	13	DC	O4'-C1'-N1	5.11	111.58	108.00

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	3263	3194	3186	21	0
1	D	3207	3138	3107	27	0
2	B	228	124	124	4	0
2	E	228	124	124	2	0
3	C	210	124	124	2	0
3	F	210	124	124	2	0
4	A	8	0	0	0	0
4	D	8	0	0	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	6	8	8	0	0
6	D	12	16	16	1	0
7	A	1	0	0	0	0
8	C	5	0	0	0	0
8	D	5	0	0	0	0
9	A	363	0	0	8	2
9	B	25	0	0	2	0
9	C	32	0	0	0	0
9	D	369	0	0	15	2
9	E	29	0	0	2	0
9	F	26	0	0	2	0
All	All	8237	6852	6813	59	2

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 4.

All (59) 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:106:GLN:NE2	9:D:702:HOH:O	1.88	1.07
2:E:12:DA:OP1	9:E:101:HOH:O	1.82	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:ASN:OD1	9:D:701:HOH:O	1.84	0.95
3:F:5:DC:OP1	9:F:101:HOH:O	1.89	0.89
1:D:206:GLU:OE1	9:D:703:HOH:O	1.94	0.85
3:F:12:DT:OP2	9:F:102:HOH:O	2.01	0.77
1:D:108:LYS:NZ	9:D:705:HOH:O	2.17	0.77
1:D:337:GLY:N	9:D:706:HOH:O	2.22	0.71
2:B:12:DA:OP1	9:B:101:HOH:O	2.10	0.68
2:B:5:DG:OP2	9:B:102:HOH:O	2.12	0.68
1:A:505:CYS:SG	9:A:1029:HOH:O	2.53	0.67
1:A:159[B]:LEU:HD11	1:A:194:VAL:HG23	1.77	0.67
1:A:232[A]:THR:OG1	9:A:702:HOH:O	2.14	0.66
1:A:230:GLN:HG2	1:A:232[B]:THR:HG23	1.77	0.65
1:A:364:ARG:NH2	1:A:447:SER:O	2.29	0.65
1:D:368:ARG:NH1	1:D:370:GLU:OE2	2.32	0.63
2:E:11:DG:OP1	9:E:102:HOH:O	2.15	0.63
1:D:232[B]:THR:HG23	9:D:998:HOH:O	1.97	0.63
1:A:86:LEU:HD11	1:A:261:GLN:OE1	2.01	0.61
1:A:159[B]:LEU:CD1	1:A:194:VAL:HG23	2.30	0.60
1:A:370:GLU:OE1	9:A:703:HOH:O	2.16	0.58
1:D:350:ASP:HB3	1:D:353:LEU:HD12	1.88	0.55
1:D:463:GLN:O	1:D:464:THR:HG23	2.06	0.55
1:A:364:ARG:NE	9:A:710:HOH:O	2.40	0.55
1:D:172:GLN:NE2	9:D:712:HOH:O	2.40	0.53
1:D:318:LEU:O	1:D:319:ALA:HB3	2.08	0.53
1:A:324:SER:OG	9:A:704:HOH:O	2.18	0.51
1:D:154[B]:GLN:NE2	9:D:713:HOH:O	2.41	0.50
1:A:388:LEU:C	1:A:389:LEU:HD22	2.38	0.48
2:B:11:DG:H2"	2:B:12:DA:H5"	1.97	0.47
2:B:3:DA:H1'	2:B:4:DA:C5	2.49	0.47
1:D:318:LEU:O	1:D:319:ALA:CB	2.64	0.46
1:A:444:HIS:CD2	1:A:489:ALA:HB2	2.52	0.45
1:A:402:TRP:CH2	1:A:474:ARG:HD2	2.51	0.45
1:D:102[B]:SER:O	1:D:106:GLN:HG2	2.16	0.45
1:D:402:TRP:CH2	1:D:474:ARG:HD2	2.51	0.45
1:D:408:THR:HG23	9:D:892:HOH:O	2.16	0.45
1:A:324:SER:HB2	9:A:941:HOH:O	2.16	0.45
1:D:141:GLN:NE2	9:D:718:HOH:O	2.46	0.44
3:C:3:DG:H2'	3:C:4:DT:C6	2.53	0.43
1:D:366:PRO:O	1:D:366:PRO:HG2	2.19	0.43
1:D:102[A]:SER:O	1:D:106:GLN:HG2	2.18	0.43
1:A:87:PHE:O	1:A:268:GLN:NE2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:NZ	9:A:712:HOH:O	2.42	0.42
1:A:278:PHE:CD1	1:A:278:PHE:C	2.98	0.42
1:D:278:PHE:CD1	1:D:278:PHE:C	2.97	0.42
1:D:505:CYS:C	9:D:747:HOH:O	2.62	0.42
1:A:241:ARG:NH1	3:C:7:DA:OP1	2.40	0.42
1:A:393:PRO:C	1:A:395:SER:H	2.28	0.42
1:D:361:LYS:HE3	9:D:851:HOH:O	2.19	0.42
1:D:491:LYS:HE2	9:D:829:HOH:O	2.18	0.42
1:A:377:LEU:O	1:A:387:ILE:HA	2.21	0.41
1:D:506:MET:O	1:D:507:GLY:C	2.64	0.41
6:D:604:GOL:H11	9:D:771:HOH:O	2.21	0.41
1:A:435:HIS:ND1	9:A:701:HOH:O	2.03	0.41
1:D:402:TRP:CH2	1:D:474:ARG:CD	3.04	0.41
1:D:218:TYR:CD2	1:D:218:TYR:C	2.99	0.40
1:D:403:GLU:HA	1:D:490:MET:HG3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:853:HOH:O	9:D:960:HOH:O[4_545]	1.93	0.27
9:A:986:HOH:O	9:D:988:HOH:O[4_545]	1.97	0.23

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	413/459 (90%)	407 (98%)	6 (2%)	0	100	100
1	D	410/459 (89%)	401 (98%)	8 (2%)	1 (0%)	43	28
All	All	823/918 (90%)	808 (98%)	14 (2%)	1 (0%)	48	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	506	MET

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	345/380 (91%)	342 (99%)	3 (1%)	70	62
1	D	338/380 (89%)	337 (100%)	1 (0%)	86	83
All	All	683/760 (90%)	679 (99%)	4 (1%)	78	72

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	331	GLU
1	A	364	ARG
1	D	173	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	260	GLN
1	A	310	GLN
1	A	394	ASN
1	A	478	GLN
1	A	500	GLN
1	D	238	ASN
1	D	338	GLN
1	D	351	GLN
1	D	422	GLN
1	D	435	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	3DR	F	8	3	8,11,12	1.88	1 (12%)	7,14,17	1.53	2 (28%)
3	3DR	C	8	3	8,11,12	1.77	2 (25%)	7,14,17	1.17	1 (14%)
2	8OG	B	8	2	22,25,26	0.61	0	26,37,40	1.42	4 (15%)
2	8OG	E	8	2	22,25,26	0.66	0	26,37,40	1.38	3 (11%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	8	3DR	O5'-C5'	-4.41	1.31	1.44
3	C	8	3DR	O5'-C5'	-4.16	1.32	1.44
3	C	8	3DR	O4'-C1'	-2.12	1.36	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	8	8OG	N7-C8-N9	4.45	111.56	106.61
2	E	8	8OG	N7-C8-N9	4.44	111.55	106.61
2	B	8	8OG	C5-N7-C8	-3.44	104.73	109.47
2	E	8	8OG	C5-N7-C8	-3.32	104.90	109.47
3	F	8	3DR	C1'-O4'-C4'	-3.04	103.58	108.37
2	B	8	8OG	C4-C5-N7	2.57	110.76	106.06
2	E	8	8OG	C4-C5-N7	2.55	110.73	106.06
3	C	8	3DR	O4'-C4'-C3'	2.27	107.07	103.73
3	F	8	3DR	O4'-C4'-C3'	2.14	106.88	103.73
2	B	8	8OG	C1'-N9-C4	-2.08	123.22	126.88

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	8	8OG	C4'-C5'-O5'-P
2	B	8	8OG	C4'-C5'-O5'-P
3	C	8	3DR	C4'-C5'-O5'-P
3	F	8	3DR	C3'-C4'-C5'-O5'

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 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
8	SO4	C	101	-	4,4,4	0.30	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	D	603	-	5,5,5	1.30	0	5,5,5	1.40	1 (20%)
6	GOL	A	603	-	5,5,5	1.00	0	5,5,5	1.32	1 (20%)
8	SO4	D	605	-	4,4,4	0.28	0	6,6,6	0.14	0
4	SF4	A	601	1	0,12,12	-	-	-		
4	SF4	D	601	1	0,12,12	-	-	-		
6	GOL	D	604	-	5,5,5	1.27	1 (20%)	5,5,5	1.15	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
6	GOL	D	603	-	-	2/4/4/4	-
6	GOL	A	603	-	-	0/4/4/4	-
4	SF4	A	601	1	-	-	0/6/5/5
4	SF4	D	601	1	-	-	0/6/5/5
6	GOL	D	604	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	604	GOL	C3-C2	2.14	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	603	GOL	C3-C2-C1	-2.56	102.42	111.80
6	D	603	GOL	C3-C2-C1	-2.42	102.93	111.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	604	GOL	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	412/459 (89%)	-1.14	0	100	100	15, 31, 63, 90	7 (1%)
1	D	410/459 (89%)	-1.16	0	100	100	15, 30, 60, 97	4 (0%)
2	B	10/11 (90%)	-1.29	0	100	100	26, 40, 65, 71	0
2	E	10/11 (90%)	-1.23	0	100	100	24, 44, 66, 76	0
3	C	10/11 (90%)	-1.23	0	100	100	27, 39, 58, 79	0
3	F	10/11 (90%)	-1.24	0	100	100	27, 41, 58, 73	0
All	All	862/962 (89%)	-1.15	0	100	100	15, 31, 63, 97	11 (1%)

There are no RSRZ outliers to report.

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. 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
3	3DR	F	8	11/12	0.99	0.03	22,27,34,34	0
2	8OG	E	8	23/24	1.00	0.02	19,23,29,30	0
3	3DR	C	8	11/12	1.00	0.03	22,29,33,34	0
2	8OG	B	8	23/24	1.00	0.02	19,23,26,27	0

6.3 Carbohydrates

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
6	GOL	A	603	6/6	0.96	0.06	46,64,79,79	0
6	GOL	D	603	6/6	0.96	0.07	41,51,62,68	0
8	SO4	C	101	5/5	0.97	0.07	61,62,77,101	0
8	SO4	D	605	5/5	0.98	0.06	53,67,100,102	0
6	GOL	D	604	6/6	0.99	0.05	41,54,63,76	0
4	SF4	D	601	8/8	1.00	0.02	20,21,22,22	0
5	ZN	A	602	1/1	1.00	0.02	37,37,37,37	0
7	NA	A	604	1/1	1.00	0.04	25,25,25,25	0
5	ZN	D	602	1/1	1.00	0.02	31,31,31,31	0
4	SF4	A	601	8/8	1.00	0.02	21,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.