Full wwPDB X-ray Structure Validation Report (i)

Nov 11, 2026 – 12:14 PM EST

PDB ID	:	11JH / pdb_000011jh
Title	:	Human MUTYH adenine glycosylase bound to DNA containing a transition state analog (1NBN) 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	:	2.00 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 (i) 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 (i)) were used in the production of this report:

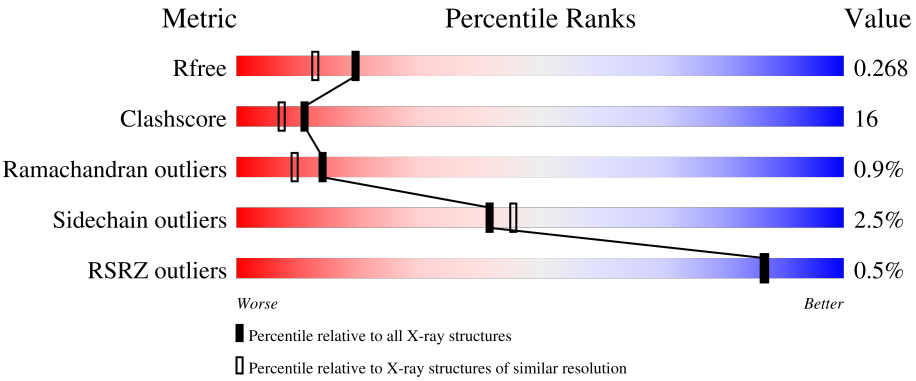
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	60% 28% • 11%
1	D	459	61% 26% • 11%
2	B	11	27% 55% 18%
2	E	11	9% 45% 45%
3	C	11	27% 36% 36%

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Mol	Chain	Length	Quality of chain
3	F	11	9% 55% 36%

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
4	SF4	A	601	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 14118 atoms, of which 6651 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	408	Total	C	H	N	O	S	0	1	0
			6206	1989	3055	570	575	17			
1	D	408	Total	C	H	N	O	S	0	1	0
			6225	1989	3074	570	577	15			

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

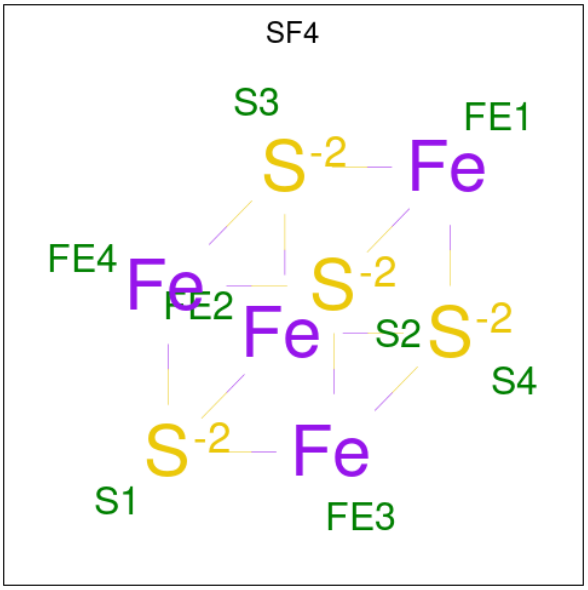
- Molecule 2 is a DNA chain called DNA('-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-').

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('-D(*TP*GP*TP*CP*CP*AP*(A1DE2)P*GP*TP*CP*TP)-').

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	11	Total C H N O P 349 109 132 33 65 10	0	0	0
3	F	11	Total C H N O P 334 104 126 31 63 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 8 4 4	0	0
4	D	1	Total Fe S 8 4 4	0	0

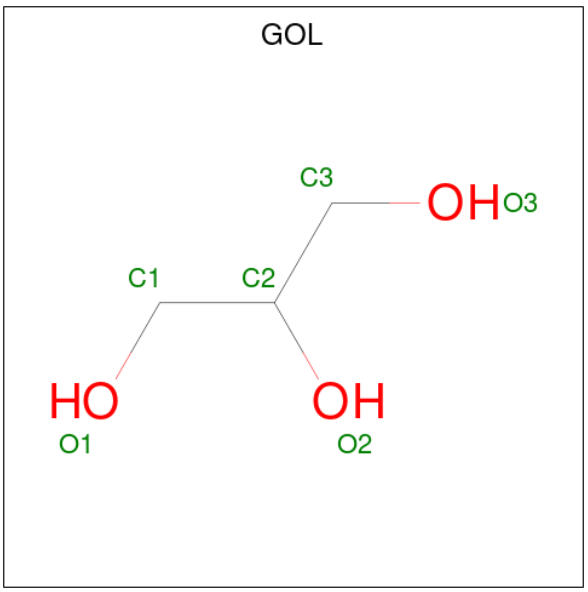
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

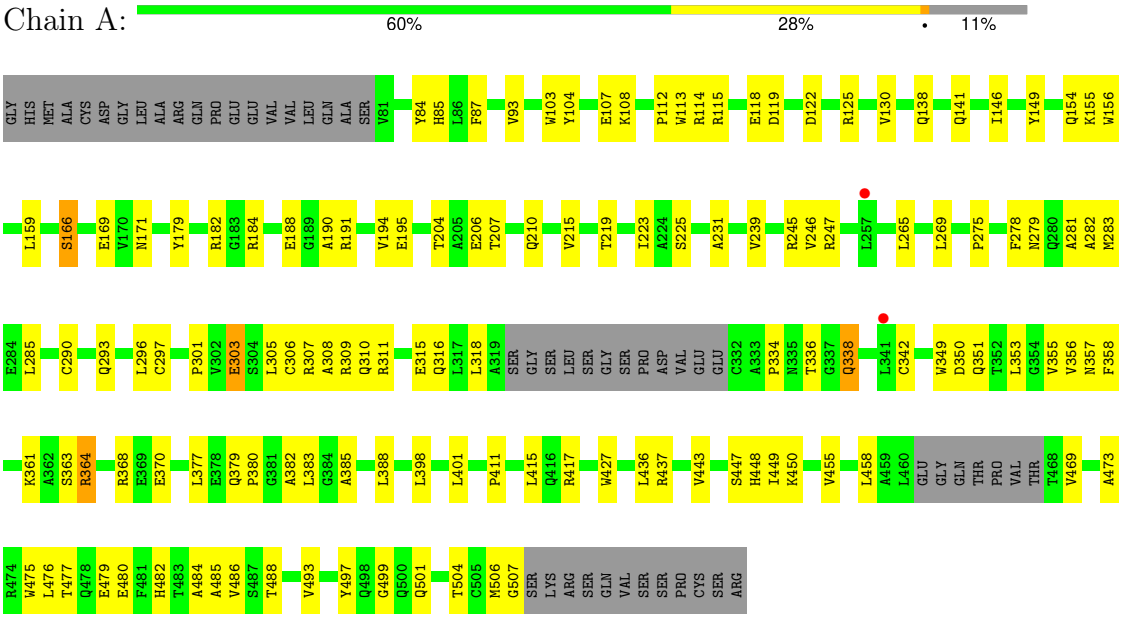
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	96	Total O 96 96	0	0
8	B	7	Total O 7 7	0	0
8	C	5	Total O 5 5	0	0
8	D	132	Total O 132 132	0	0
8	E	6	Total O 6 6	0	0
8	F	7	Total O 7 7	0	0

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.

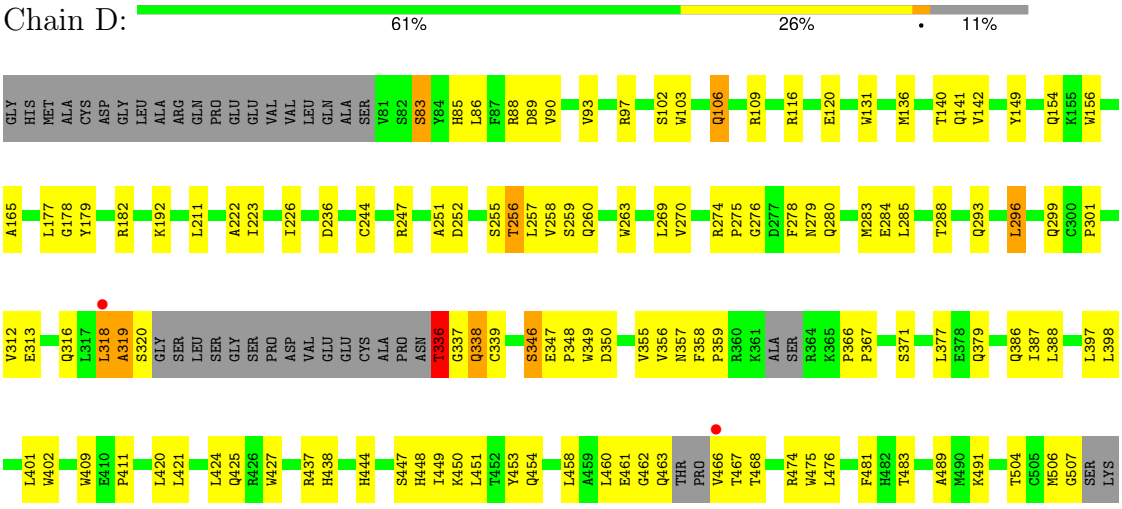
• Molecule 1: Isoform Alpha-1 of Adenine DNA glycosylase

Chain A:



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

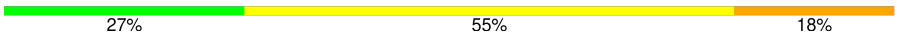
Chain D:

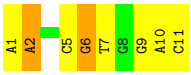




• Molecule 2: DNA('-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-')

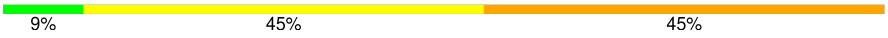
Chain B:





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

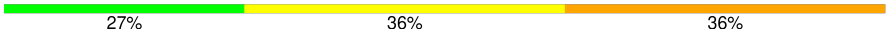
Chain E:

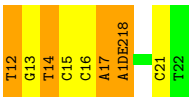




• Molecule 3: DNA('-D(*TP*GP*TP*CP*CP*AP*(A1DE2)P*GP*TP*CP*TP)-')

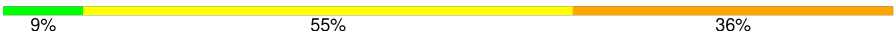
Chain C:

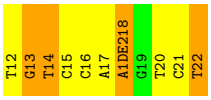




• Molecule 3: DNA('-D(*TP*GP*TP*CP*CP*AP*(A1DE2)P*GP*TP*CP*TP)-')

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	88.01Å 117.41Å 118.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.62 – 2.00 37.62 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (37.62-2.00) 94.4 (37.62-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.207 , 0.261 0.218 , 0.268	Depositor DCC
R_{free} test set	3936 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 30.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.368 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14118	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: 8OG, A1DE2, ZN, NA, SF4, GOL

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	0.63	0/3227	0.79	0/4400
1	D	0.65	0/3224	0.82	2/4394 (0.0%)
2	B	1.51	1/230 (0.4%)	1.34	3/351 (0.9%)
2	E	1.75	2/230 (0.9%)	1.43	4/351 (1.1%)
3	C	1.79	5/220 (2.3%)	1.47	3/335 (0.9%)
3	F	1.82	6/210 (2.9%)	1.65	7/319 (2.2%)
All	All	0.85	14/7341 (0.2%)	0.92	19/10150 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	13	DG	N9-C4	-7.62	1.31	1.38
2	E	8	DG	C3'-O3'	-7.48	1.34	1.44
3	C	17	DA	N9-C4	-6.48	1.33	1.37
3	F	13	DG	C5'-C4'	-6.34	1.47	1.51
2	E	3	DG	N9-C4	-6.23	1.32	1.38
3	F	21	DC	C3'-O3'	-6.09	1.36	1.44
3	F	13	DG	C2-N3	-5.81	1.28	1.32
3	C	17	DA	C3'-O3'	-5.47	1.36	1.44
3	F	22	DT	C1'-N1	-5.39	1.39	1.47
2	B	7	DT	C3'-C2'	5.38	1.56	1.52
3	F	14	DT	C3'-O3'	-5.37	1.36	1.44
3	C	14	DT	C1'-N1	5.24	1.54	1.47
3	C	14	DT	C3'-O3'	-5.22	1.37	1.44
3	C	21	DC	C3'-O3'	5.18	1.50	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	5	DC	O4'-C1'-N1	7.45	113.21	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	336	THR	OG1-CB-CG2	6.86	123.01	109.30
3	C	12	DT	O4'-C1'-N1	6.71	112.70	108.00
3	F	14	DT	O4'-C1'-N1	6.66	112.66	108.00
3	F	13	DG	O4'-C4'-C3'	-6.54	102.08	106.00
1	D	358	PHE	C-N-CD	-6.11	107.17	120.60
3	F	13	DG	C4'-C3'-C2'	-6.07	97.64	103.10
2	B	5	DC	O4'-C1'-N1	5.96	112.17	108.00
2	E	11	DC	O5'-C5'-C4'	5.83	114.06	109.40
3	F	12	DT	O4'-C4'-C3'	-5.56	102.66	106.00
3	F	16	DC	O5'-C5'-C4'	5.52	113.81	109.40
3	F	20	DT	N3-C4-O4	5.51	123.21	119.90
2	E	7	DT	O5'-C5'-C4'	5.51	113.81	109.40
3	C	12	DT	C3'-C2'-C1'	-5.46	95.94	102.50
2	B	5	DC	O5'-C5'-C4'	5.29	113.63	109.40
3	C	21	DC	O5'-C5'-C4'	5.22	113.58	109.40
2	B	2	DA	O4'-C1'-N9	5.19	111.64	108.00
2	E	5	DC	O4'-C1'-C2'	-5.08	101.84	105.90
3	F	13	DG	N9-C1'-C2'	-5.06	107.21	114.30

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	3151	3055	3061	96	1
1	D	3151	3074	3071	99	1
2	B	228	124	124	6	0
2	E	228	124	124	10	0
3	C	217	132	116	15	0
3	F	208	126	110	13	0
4	A	8	0	0	3	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	6	8	8	0	0
7	F	6	8	8	1	0
8	A	96	0	0	7	0
8	B	7	0	0	0	0
8	C	5	0	0	0	0
8	D	132	0	0	6	0
8	E	6	0	0	0	0
8	F	7	0	0	0	0
All	All	7467	6651	6622	221	1

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 16.

All (221) 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:A:141:GLN:OE1	8:A:701:HOH:O	1.59	1.20
1:D:89:ASP:OD2	8:D:701:HOH:O	1.85	0.93
1:D:255:SER:O	1:D:257:LEU:N	2.11	0.83
1:D:468:THR:O	8:D:702:HOH:O	1.96	0.82
1:A:138:GLN:O	1:A:182:ARG:NH1	2.15	0.79
1:D:483:THR:HG22	1:D:483:THR:O	1.84	0.77
1:A:204:THR:HG22	1:A:207:THR:OG1	1.87	0.73
2:B:9:DG:H2"	2:B:10:DA:C8	2.23	0.73
3:C:14:DT:H2"	3:C:15:DC:C6	2.24	0.73
2:E:1:DA:H1'	2:E:2:DA:C5	2.27	0.70
1:D:86:LEU:O	1:D:247:ARG:NH1	2.24	0.69
1:A:310:GLN:O	8:A:703:HOH:O	2.13	0.67
3:F:13:DG:H3'	3:F:14:DT:H72	1.76	0.66
1:A:231:ALA:HA	1:A:275:PRO:HB3	1.78	0.65
1:D:274:ARG:O	1:D:278:PHE:HB2	1.98	0.63
3:C:13:DG:H2"	3:C:14:DT:H5'	1.81	0.63
3:C:14:DT:H2"	3:C:15:DC:C5	2.35	0.61
1:D:409:TRP:CZ3	1:D:411:PRO:HD3	2.36	0.61
1:A:484:ALA:HB3	1:A:486:VAL:HG13	1.83	0.60
1:D:483:THR:O	1:D:483:THR:CG2	2.48	0.59
1:D:285:LEU:HD11	1:D:301:PRO:HD2	1.85	0.59
1:D:438:HIS:NE2	1:D:454:GLN:OE1	2.35	0.59
1:D:103:TRP:HB2	1:D:301:PRO:HB3	1.85	0.58
1:A:107:GLU:OE2	1:A:107:GLU:HA	2.01	0.58
1:D:481:PHE:CD1	1:D:481:PHE:C	2.81	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HB2	1:A:357:ASN:ND2	2.19	0.57
2:B:1:DA:H1'	2:B:2:DA:C5	2.40	0.57
1:D:356:VAL:HG12	1:D:356:VAL:O	2.03	0.57
1:A:85:HIS:CE1	1:A:342:CYS:SG	2.98	0.56
3:F:13:DG:H4'	3:F:14:DT:OP1	2.06	0.56
1:A:368:ARG:NH1	1:A:370:GLU:OE1	2.39	0.56
1:A:103:TRP:NE1	8:A:710:HOH:O	2.33	0.55
1:A:246:VAL:HG12	1:A:247:ARG:HE	1.72	0.55
3:C:13:DG:C2'	3:C:14:DT:H5'	2.36	0.55
1:D:178:GLY:O	1:D:179:TYR:C	2.50	0.55
1:D:296:LEU:HD12	1:D:299:GLN:HB2	1.90	0.54
1:D:461:GLU:HG3	1:D:462:GLY:N	2.20	0.54
1:A:122:ASP:HB3	1:A:125:ARG:HB2	1.90	0.54
1:A:361:LYS:CB	3:C:16:DC:OP1	2.55	0.54
3:F:13:DG:H2"	3:F:14:DT:H5'	1.89	0.54
1:D:165:ALA:HB2	8:D:747:HOH:O	2.07	0.54
1:A:231:ALA:HA	1:A:275:PRO:CB	2.38	0.54
1:A:93:VAL:HG13	1:A:269:LEU:HD13	1.89	0.54
1:D:451:LEU:HD23	1:D:453:TYR:CZ	2.43	0.53
1:A:191:ARG:O	1:A:195:GLU:HG2	2.08	0.53
1:D:349:TRP:CZ3	1:D:357:ASN:HB2	2.43	0.53
1:A:278:PHE:CD1	1:A:278:PHE:C	2.87	0.52
1:A:316:GLN:HG2	1:D:438:HIS:O	2.09	0.52
1:D:259:SER:O	1:D:263:TRP:HD1	1.92	0.52
1:A:115:ARG:O	1:A:119:ASP:CG	2.53	0.52
3:C:12:DT:C2	3:C:13:DG:C8	2.98	0.52
1:A:190:ALA:O	1:A:194:VAL:HG23	2.10	0.52
1:A:382:ALA:C	1:A:383:LEU:HD12	2.35	0.51
1:D:83:SER:HB3	1:D:88:ARG:HG3	1.93	0.51
1:A:306:CYS:HB3	1:A:309:ARG:HB3	1.92	0.51
1:D:283:MET:HE2	3:F:18:A1DE2:C6	2.41	0.51
1:D:116:ARG:O	1:D:120:GLU:HB2	2.11	0.50
1:A:443:VAL:HG12	1:A:450:LYS:HZ2	1.76	0.50
1:A:479:GLU:HA	1:A:482[B]:HIS:ND1	2.26	0.50
1:D:192:LYS:HE2	1:D:211:LEU:O	2.12	0.50
1:A:103:TRP:NE1	1:A:107:GLU:HG3	2.27	0.49
2:E:2:DA:H2"	2:E:3:DG:C8	2.46	0.49
1:D:377:LEU:O	1:D:387:ILE:HA	2.12	0.49
1:D:504:THR:OG1	1:D:506:MET:HG3	2.13	0.49
1:A:206:GLU:O	1:A:210:GLN:HG3	2.13	0.49
1:D:278:PHE:CD1	1:D:278:PHE:C	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:TYR:CD1	1:A:281:ALA:HA	2.48	0.48
1:A:247:ARG:NH2	1:A:305:LEU:O	2.46	0.48
1:D:506:MET:O	1:D:507:GLY:C	2.56	0.48
1:A:155:LYS:HE2	1:A:156:TRP:CZ2	2.48	0.48
1:D:179:TYR:HB2	1:D:182:ARG:HE	1.78	0.48
1:A:112:PRO:HG2	1:A:146:ILE:HG23	1.96	0.48
1:A:308:ALA:HB2	1:A:358:PHE:CD2	2.49	0.48
1:D:97:ARG:HA	1:D:278:PHE:HE2	1.78	0.48
1:D:141:GLN:HG2	3:F:17:DA:H1'	1.94	0.48
1:A:191:ARG:O	1:A:195:GLU:CG	2.62	0.48
1:D:279:ASN:O	1:D:283:MET:HG3	2.13	0.48
1:D:283:MET:HB3	3:F:18:A1DE2:C6	2.44	0.48
1:A:316:GLN:O	1:D:437:ARG:HA	2.14	0.48
1:A:388:LEU:HB2	1:A:475:TRP:CH2	2.49	0.48
1:A:499:GLY:HA2	1:D:296:LEU:HD13	1.96	0.48
1:A:455:VAL:HG13	1:A:493:VAL:HG13	1.94	0.47
1:D:252:ASP:HB3	1:D:255:SER:HB3	1.96	0.47
1:A:353:LEU:CB	1:A:357:ASN:ND2	2.77	0.47
1:A:398:LEU:HD12	1:A:401:LEU:HD12	1.97	0.47
1:D:397:LEU:O	1:D:398:LEU:C	2.56	0.47
1:A:484:ALA:CB	1:A:486:VAL:HG13	2.44	0.47
1:D:274:ARG:O	1:D:278:PHE:CB	2.61	0.47
1:D:451:LEU:HD23	1:D:453:TYR:OH	2.14	0.47
1:A:87:PHE:HB3	1:A:93:VAL:CG2	2.45	0.47
1:D:93:VAL:HG13	1:D:269:LEU:HD23	1.97	0.47
1:D:491:LYS:HD3	8:D:816:HOH:O	2.15	0.47
1:D:319:ALA:O	1:D:320:SER:CB	2.63	0.47
1:D:379:GLN:OE1	1:D:466:VAL:N	2.47	0.47
1:A:293:GLN:HA	1:A:293:GLN:OE1	2.13	0.47
1:D:402:TRP:CH2	1:D:474:ARG:HD2	2.50	0.46
1:D:409:TRP:CH2	1:D:411:PRO:HB3	2.50	0.46
1:A:171:ASN:HB3	1:A:485:ALA:HB1	1.96	0.46
1:A:225:SER:O	8:A:704:HOH:O	2.21	0.46
1:D:179:TYR:O	1:D:182:ARG:HG3	2.15	0.46
1:D:346:SER:OG	1:D:347:GLU:N	2.48	0.46
1:D:386:GLN:NE2	1:D:475:TRP:HB3	2.31	0.46
1:A:303:GLU:HA	4:A:601:SF4:S3	2.55	0.46
1:D:467:THR:OG1	1:D:468:THR:N	2.47	0.46
1:D:444:HIS:CD2	1:D:489:ALA:HB2	2.51	0.46
1:A:497:TYR:CZ	1:A:501:GLN:HG2	2.50	0.46
1:A:504:THR:OG1	1:A:506:MET:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:MET:O	1:D:182:ARG:NH1	2.46	0.45
1:A:385:ALA:HB3	1:A:506:MET:HE3	1.99	0.45
1:D:491:LYS:NZ	8:D:707:HOH:O	2.31	0.45
1:D:463:GLN:HE22	1:D:467:THR:HG22	1.81	0.45
3:C:12:DT:C2	3:C:13:DG:N7	2.85	0.45
3:C:13:DG:O4'	3:F:13:DG:H1'	2.16	0.45
1:D:255:SER:O	1:D:256:THR:HG22	2.15	0.45
1:D:338:GLN:O	1:D:339:CYS:C	2.59	0.45
1:A:279:ASN:O	1:A:283:MET:HG3	2.17	0.45
1:D:377:LEU:HD11	1:D:460:LEU:HD11	1.99	0.45
1:A:204:THR:HG23	1:A:207:THR:H	1.81	0.45
1:A:245:ARG:HD2	1:A:290:CYS:SG	2.56	0.45
1:A:448:HIS:C	1:A:449:ILE:HG13	2.42	0.45
1:A:103:TRP:CE3	1:A:104:TYR:N	2.85	0.45
1:A:155:LYS:CE	1:A:156:TRP:CZ2	2.99	0.45
1:A:507:GLY:C	8:A:762:HOH:O	2.60	0.45
1:D:251:ALA:HB3	1:D:258:VAL:HG21	1.98	0.45
1:A:363:SER:O	1:A:364:ARG:O	2.35	0.45
2:B:10:DA:C2	3:C:14:DT:O2	2.70	0.45
2:E:2:DA:C5	2:E:3:DG:C6	3.05	0.45
2:E:5:DC:H2"	2:E:6:8OG:O5'	2.17	0.45
3:C:17:DA:H2'	3:C:17:DA:N3	2.32	0.45
1:A:315:GLU:OE1	1:A:349:TRP:NE1	2.49	0.44
1:A:315:GLU:HA	1:A:318:LEU:HD13	1.99	0.44
1:D:388:LEU:HD21	1:D:427:TRP:HB2	1.98	0.44
1:A:411:PRO:HD2	1:A:415:LEU:HD13	1.99	0.44
3:C:12:DT:H3	3:F:13:DG:N2	2.15	0.44
1:D:256:THR:O	1:D:260:GLN:HB2	2.18	0.44
1:A:350:ASP:O	1:A:351:GLN:C	2.61	0.44
2:E:2:DA:N1	3:F:22:DT:C2	2.86	0.44
1:A:118:GLU:HB3	8:A:774:HOH:O	2.17	0.44
1:A:417:ARG:NH1	1:A:436:LEU:HD23	2.32	0.44
1:A:479:GLU:HA	1:A:482[B]:HIS:HD1	1.80	0.44
1:A:113:TRP:HB3	1:A:149:TYR:CE2	2.52	0.44
3:C:14:DT:OP2	3:C:14:DT:H6	2.00	0.44
1:A:84:TYR:O	1:A:307:ARG:NE	2.49	0.44
1:A:377:LEU:HD12	1:A:458:LEU:O	2.18	0.44
1:A:437:ARG:NH1	1:D:316:GLN:OE1	2.49	0.44
3:C:18:A1DE2:C6	3:C:18:A1DE2:C6'	2.96	0.44
1:A:87:PHE:HD1	1:A:265:LEU:CD2	2.31	0.43
1:A:239:VAL:HG22	1:A:282:ALA:HB1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:O	1:A:118:GLU:HG3	2.18	0.43
1:D:116:ARG:HD2	1:D:149:TYR:HE2	1.84	0.43
2:B:11:DC:N3	3:C:13:DG:N2	2.60	0.43
1:D:468:THR:HA	8:D:727:HOH:O	2.18	0.43
2:E:2:DA:C2	3:F:22:DT:O2	2.71	0.43
1:A:296:LEU:O	1:A:297:CYS:C	2.60	0.43
1:A:356:VAL:HG12	1:A:356:VAL:O	2.18	0.43
1:D:312:VAL:HG21	1:D:355:VAL:HG13	2.00	0.43
1:A:215:VAL:HG13	1:A:219:THR:HG22	2.01	0.43
1:D:140:THR:HG21	1:D:177:LEU:CD2	2.49	0.42
1:D:312:VAL:O	1:D:313:GLU:C	2.60	0.42
1:A:265:LEU:O	1:A:269:LEU:HD23	2.19	0.42
1:D:276:GLY:O	1:D:280:GLN:HG3	2.19	0.42
1:A:166:SER:O	1:A:169:GLU:HB2	2.19	0.42
1:A:293:GLN:O	8:A:705:HOH:O	2.21	0.42
1:D:448:HIS:CD2	1:D:449:ILE:HG13	2.54	0.42
1:D:141:GLN:HE21	2:E:8:DG:H21	1.67	0.42
1:A:104:TYR:O	1:A:108:LYS:HB3	2.19	0.42
1:A:437:ARG:HD2	1:A:501:GLN:HE22	1.84	0.42
1:D:85:HIS:C	1:D:247:ARG:HD3	2.45	0.42
1:D:109:ARG:HE	1:D:284:GLU:CD	2.28	0.42
1:D:350:ASP:OD1	1:D:350:ASP:C	2.62	0.42
1:D:131:TRP:HA	1:D:223:ILE:HD11	2.01	0.42
1:D:420:LEU:O	1:D:424:LEU:HD12	2.20	0.42
1:A:349:TRP:CD1	1:A:349:TRP:C	2.98	0.42
1:D:141:GLN:HA	3:F:18:A1DE2:P	2.60	0.42
1:D:274:ARG:O	1:D:278:PHE:N	2.51	0.42
1:D:236:ASP:CG	1:D:283:MET:HE3	2.45	0.42
1:D:318:LEU:O	1:D:319:ALA:HB2	2.19	0.42
1:A:427:TRP:CE3	1:A:473:ALA:HB2	2.55	0.42
2:E:10:DA:C2	2:E:11:DC:C2	3.08	0.42
1:A:285:LEU:HD11	1:A:301:PRO:HD2	2.02	0.41
1:D:270:VAL:HG22	1:D:275:PRO:HA	2.02	0.41
1:D:397:LEU:HD12	2:E:5:DC:H3'	2.02	0.41
2:E:9:DG:H2"	2:E:10:DA:C8	2.55	0.41
3:C:14:DT:H2'	3:C:14:DT:O5'	2.19	0.41
1:D:102:SER:O	1:D:106:GLN:OE1	2.38	0.41
3:F:14:DT:H2"	3:F:15:DC:C6	2.55	0.41
1:A:379:GLN:HG2	1:A:380:PRO:O	2.20	0.41
2:B:6:8OG:O8	2:B:6:8OG:H2"	2.20	0.41
1:D:346:SER:O	1:D:348:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:VAL:HG13	1:A:469:VAL:O	2.21	0.41
1:D:398:LEU:HB3	1:D:401:LEU:HD12	2.02	0.41
1:D:222:ALA:O	1:D:226:ILE:HD12	2.19	0.41
1:D:466:VAL:HG12	1:D:467:THR:N	2.35	0.41
1:D:475:TRP:O	1:D:476:LEU:HD23	2.21	0.41
1:A:308:ALA:HB2	1:A:358:PHE:CE2	2.56	0.41
1:D:156:TRP:NE1	1:D:165:ALA:HB2	2.36	0.41
1:D:293:GLN:HE22	7:F:101:GOL:H12	1.86	0.41
1:A:184:ARG:O	1:A:188:GLU:HG3	2.20	0.41
1:A:245:ARG:HD3	4:A:601:SF4:S4	2.61	0.41
1:D:284:GLU:O	1:D:288:THR:OG1	2.35	0.41
1:D:366:PRO:HA	1:D:367:PRO:HD2	1.95	0.41
1:A:130:VAL:HG11	1:A:223:ILE:HA	2.02	0.41
1:A:336:THR:CB	1:A:338:GLN:HG3	2.51	0.41
1:A:383:LEU:HD12	1:A:383:LEU:N	2.36	0.41
2:B:1:DA:H4'	2:B:2:DA:OP1	2.21	0.41
1:D:90:VAL:HG22	1:D:90:VAL:O	2.22	0.41
1:D:421:LEU:O	1:D:425:GLN:OE1	2.39	0.41
1:D:257:LEU:HD12	1:D:257:LEU:O	2.21	0.40
1:D:336:THR:OG1	1:D:337:GLY:N	2.54	0.40
3:F:13:DG:H3'	3:F:14:DT:C7	2.47	0.40
1:D:109:ARG:HG3	1:D:284:GLU:OE2	2.22	0.40
1:A:355:VAL:HG21	4:A:601:SF4:S4	2.61	0.40
1:D:244:CYS:HB2	1:D:359:PRO:HD3	2.03	0.40
1:A:87:PHE:CD1	1:A:265:LEU:CD2	3.04	0.40
1:A:316:GLN:HB3	1:D:437:ARG:HB3	2.04	0.40
1:A:364:ARG:HB2	1:A:364:ARG:CZ	2.52	0.40
1:A:477:THR:OG1	1:A:480:GLU:HG3	2.22	0.40
1:D:103:TRP:CB	1:D:301:PRO:HB3	2.49	0.40
1:D:421:LEU:O	1:D:425:GLN:HG3	2.21	0.40
1:A:311:ARG:HD3	1:A:349:TRP:CZ3	2.56	0.40
1:A:476:LEU:HA	1:A:480:GLU:OE1	2.21	0.40

All (1) 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)
1:A:154:GLN:HE22	1:D:154:GLN:O[4_545]	1.49	0.11

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	403/459 (88%)	383 (95%)	17 (4%)	3 (1%)	18 14
1	D	401/459 (87%)	375 (94%)	22 (6%)	4 (1%)	12 8
All	All	804/918 (88%)	758 (94%)	39 (5%)	7 (1%)	14 9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ARG
1	D	256	THR
1	D	319	ALA
1	D	318	LEU
1	D	338	GLN
1	A	179	TYR
1	A	334	PRO

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	324/380 (85%)	318 (98%)	6 (2%)	50 56
1	D	326/380 (86%)	316 (97%)	10 (3%)	35 37
All	All	650/760 (86%)	634 (98%)	16 (2%)	42 45

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LEU
1	A	166	SER
1	A	303	GLU
1	A	338	GLN
1	A	447	SER
1	A	488	THR
1	D	83	SER
1	D	106	GLN
1	D	142	VAL
1	D	296	LEU
1	D	336	THR
1	D	346	SER
1	D	371	SER
1	D	447	SER
1	D	450	LYS
1	D	458	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	435	HIS
1	A	500	GLN
1	D	141	GLN
1	D	200	HIS
1	D	260	GLN
1	D	261	GLN
1	D	338	GLN
1	D	416	GLN
1	D	500	GLN

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	A1DE2	F	18	3	16,19,20	0.67	0	15,25,28	1.30	3 (20%)
2	8OG	B	6	3,2	22,25,26	0.74	1 (4%)	26,37,40	1.19	2 (7%)
2	8OG	E	6	3,2	22,25,26	0.85	2 (9%)	26,37,40	1.28	3 (11%)
3	A1DE2	C	18	3	16,19,20	0.91	1 (6%)	15,25,28	0.98	1 (6%)

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	A1DE2	F	18	3	-	2/7/21/22	0/2/2/2
2	8OG	B	6	3,2	-	1/7/21/22	0/3/3/3
2	8OG	E	6	3,2	-	1/7/21/22	0/3/3/3
3	A1DE2	C	18	3	-	3/7/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	6	8OG	C5-C4	2.78	1.41	1.37
2	E	6	8OG	C8-N9	-2.53	1.36	1.40
2	B	6	8OG	C5-C4	2.39	1.40	1.37
3	C	18	A1DE2	C6'-C4'	-2.37	1.49	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	6	8OG	N7-C8-N9	4.29	111.39	106.61
2	E	6	8OG	N7-C8-N9	3.66	110.69	106.61
2	E	6	8OG	C5-N7-C8	-3.18	105.09	109.47
2	E	6	8OG	C4-C5-N7	2.55	110.74	106.06
3	C	18	A1DE2	C6'-N1'-C2'	2.50	107.76	104.12
3	F	18	A1DE2	C5-N1'-C2'	-2.42	108.72	113.39
3	F	18	A1DE2	C5-N1'-C6'	-2.40	108.77	113.39
2	B	6	8OG	C5-N7-C8	-2.40	106.16	109.47
3	F	18	A1DE2	C6'-N1'-C2'	2.27	107.42	104.12

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	18	A1DE2	C6'-C4'-C5'-O5'
3	F	18	A1DE2	C6'-C4'-C5'-O5'
2	E	6	8OG	C4'-C5'-O5'-P
2	B	6	8OG	C4'-C5'-O5'-P
3	C	18	A1DE2	C3'-C4'-C5'-O5'
3	F	18	A1DE2	C3'-C4'-C5'-O5'
3	C	18	A1DE2	C4-C5-N1'-C6'

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	18	A1DE2	3	0
2	B	6	8OG	1	0
2	E	6	8OG	1	0
3	C	18	A1DE2	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
7	GOL	D	603	-	5,5,5	1.01	0	5,5,5	1.12	0
7	GOL	F	101	-	5,5,5	1.22	1 (20%)	5,5,5	0.73	0
4	SF4	D	601	1	0,12,12	-	-	-		
4	SF4	A	601	1	0,12,12	-	-	-		

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
7	GOL	D	603	-	-	3/4/4/4	-
7	GOL	F	101	-	-	0/4/4/4	-
4	SF4	D	601	1	-	-	0/6/5/5
4	SF4	A	601	1	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	101	GOL	C1-C2	2.22	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	101	GOL	1	0
4	A	601	SF4	3	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	408/459 (88%)	-0.14	2 (0%)	87	87	26, 44, 80, 156	1 (0%)
1	D	408/459 (88%)	-0.19	2 (0%)	87	87	22, 41, 70, 128	1 (0%)
2	B	10/11 (90%)	-0.28	0	100	100	46, 60, 76, 82	0
2	E	10/11 (90%)	-0.43	0	100	100	38, 53, 74, 94	0
3	C	10/11 (90%)	-0.18	0	100	100	38, 59, 93, 115	0
3	F	10/11 (90%)	-0.47	0	100	100	39, 52, 78, 87	0
All	All	856/962 (88%)	-0.17	4 (0%)	87	87	22, 43, 78, 156	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	LEU	2.2
1	A	341	LEU	2.1
1	D	318	LEU	2.1
1	D	466	VAL	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. 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	A1DE2	C	18	18/19	0.97	0.08	32,38,46,46	0
2	8OG	E	6	23/24	0.98	0.06	32,36,44,44	0
2	8OG	B	6	23/24	0.98	0.06	40,44,53,54	0
3	A1DE2	F	18	18/19	0.98	0.06	33,39,45,46	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	GOL	F	101	6/6	0.92	0.11	63,76,79,79	0
7	GOL	D	603	6/6	0.97	0.06	46,55,62,62	0
6	NA	A	603	1/1	0.98	0.05	44,44,44,44	0
4	SF4	A	601	8/8	0.99	0.03	27,35,38,38	0
4	SF4	D	601	8/8	0.99	0.04	26,33,34,40	0
5	ZN	D	602	1/1	0.99	0.02	41,41,41,41	0
5	ZN	A	602	1/1	1.00	0.03	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.