



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 11:25 pm BST

PDB ID : 3G0R  
Title : Complex of Mth0212 and an 8bp dsDNA with distorted ends  
Authors : Lakomek, K.; Dickmanns, A.; Ficner, R.  
Deposited on : 2009-01-28  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

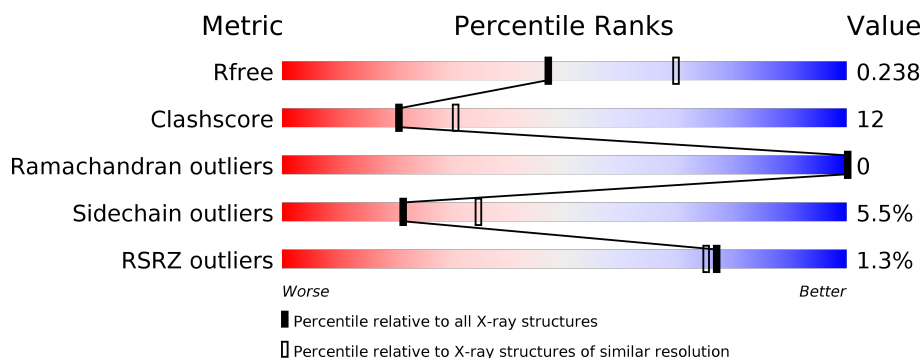
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	265	
1	B	265	
2	G	13	
3	K	11	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	267	-	-	X	-
4	GOL	A	268	-	-	X	-
4	GOL	A	269	-	-	X	-
4	GOL	A	270	-	-	X	-
4	GOL	A	271	-	-	X	-
4	GOL	B	266	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5093 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Exodeoxyribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	2	0
			2130	1368	373	381	8			
1	B	254	Total	C	N	O	S	0	0	0
			2122	1362	372	380	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	ENGINEERED MUTATION	UNP O26314
A	151	ASN	ASP	ENGINEERED MUTATION	UNP O26314
A	258	LEU	-	EXPRESSION TAG	UNP O26314
A	259	GLU	-	EXPRESSION TAG	UNP O26314
A	260	HIS	-	EXPRESSION TAG	UNP O26314
A	261	HIS	-	EXPRESSION TAG	UNP O26314
A	262	HIS	-	EXPRESSION TAG	UNP O26314
A	263	HIS	-	EXPRESSION TAG	UNP O26314
A	264	HIS	-	EXPRESSION TAG	UNP O26314
A	265	HIS	-	EXPRESSION TAG	UNP O26314
B	2	ALA	THR	ENGINEERED MUTATION	UNP O26314
B	151	ASN	ASP	ENGINEERED MUTATION	UNP O26314
B	258	LEU	-	EXPRESSION TAG	UNP O26314
B	259	GLU	-	EXPRESSION TAG	UNP O26314
B	260	HIS	-	EXPRESSION TAG	UNP O26314
B	261	HIS	-	EXPRESSION TAG	UNP O26314
B	262	HIS	-	EXPRESSION TAG	UNP O26314
B	263	HIS	-	EXPRESSION TAG	UNP O26314
B	264	HIS	-	EXPRESSION TAG	UNP O26314
B	265	HIS	-	EXPRESSION TAG	UNP O26314

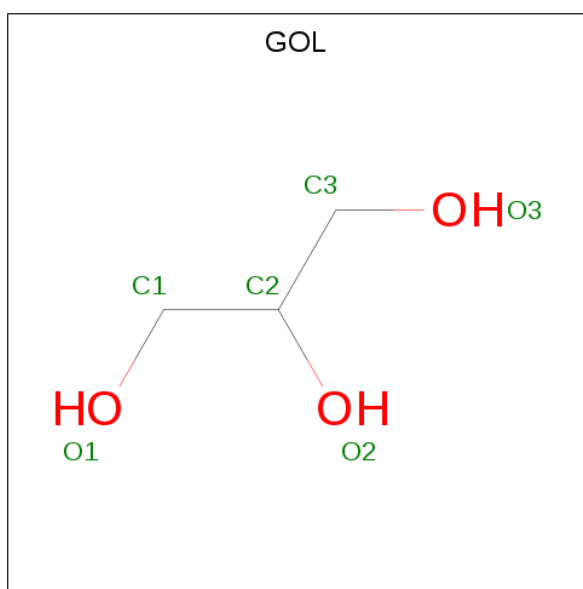
- Molecule 2 is a DNA chain called 5'-D(\*GP\*CP\*TP\*GP\*CP\*GP\*CP\*AP\*GP\*GP\*GP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	10	Total	C	N	O	P	0	0	0
			205	97	41	58	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	11	Total	C	N	O	P	0	0	0
			218	104	39	65	10			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



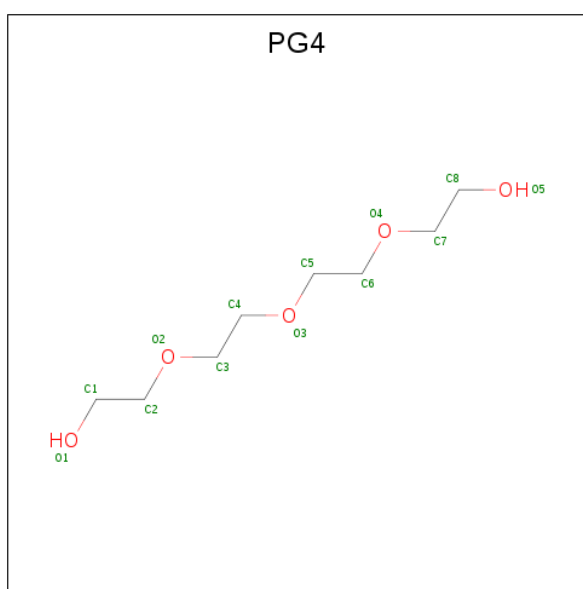
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	2	Total	Na	0	0
			2	2		

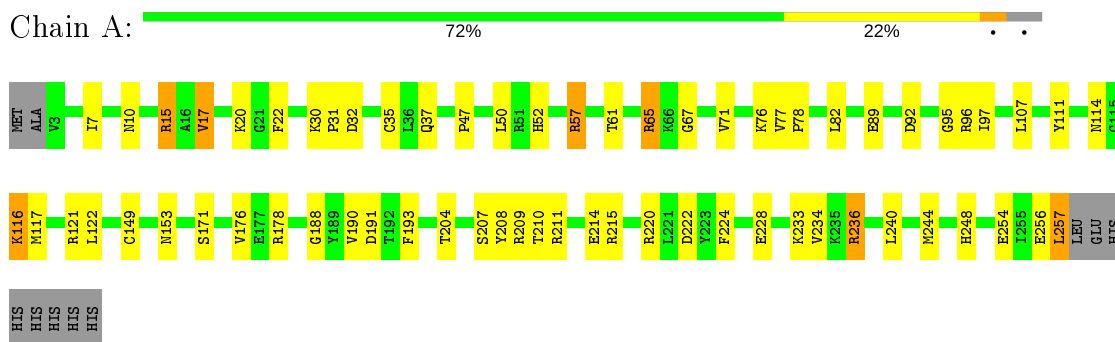
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	154	Total 154	O 154	0	0
7	B	115	Total 115	O 115	0	0
7	G	20	Total 20	O 20	0	0
7	K	16	Total 16	O 16	0	0

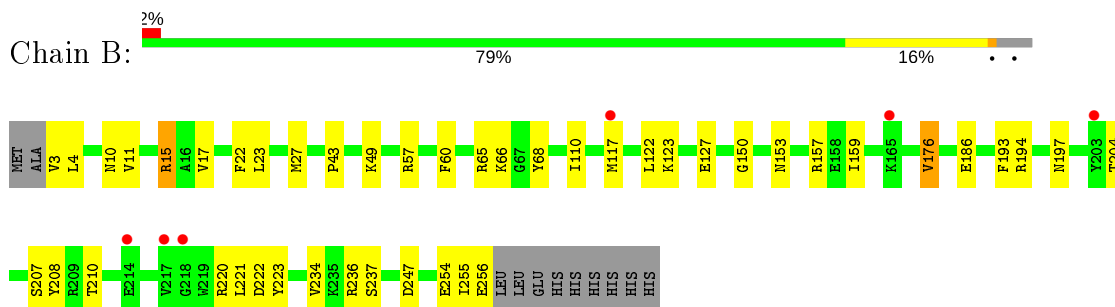
### 3 Residue-property plots [i](#)

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

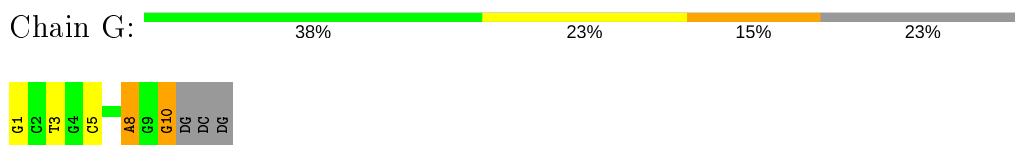
- Molecule 1: Exodeoxyribonuclease



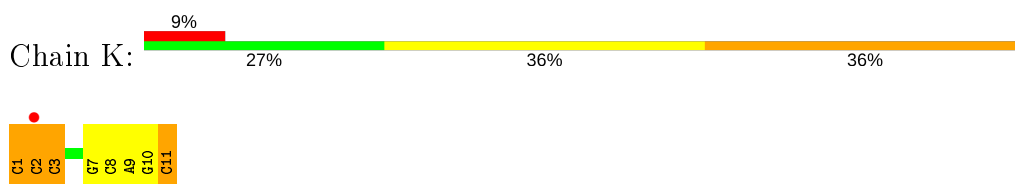
- Molecule 1: Exodeoxyribonuclease



- Molecule 2: 5'-D(\*GP\*CP\*TP\*GP\*CP\*GP\*CP\*AP\*GP\*GP\*GP\*CP\*G)-3'



- Molecule 3: 5'-D(\*CP\*CP\*CP\*TP\*GP\*UP\*GP\*CP\*AP\*GP\*C)-3'





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.75Å 80.76Å 105.21Å 90.00° 94.03° 90.00°	Depositor
Resolution (Å)	44.64 – 2.40 44.64 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.7 (44.64-2.40) 92.7 (44.64-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.39 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.178 , 0.243 0.176 , 0.238	Depositor DCC
$R_{free}$ test set	1391 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5093	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PG4, NA

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	0.71	0/2188	0.76	2/2950 (0.1%)
1	B	0.61	0/2180	0.71	3/2939 (0.1%)
2	G	1.21	0/230	2.15	14/354 (4.0%)
3	K	1.26	2/243 (0.8%)	1.80	6/372 (1.6%)
All	All	0.74	2/4841 (0.0%)	0.95	25/6615 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	11	DC	C3'-O3'	-6.60	1.35	1.44
3	K	3	DC	C3'-O3'	-5.22	1.37	1.44

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	DG	O4'-C1'-C2'	-10.45	97.54	105.90
3	K	1	DC	O4'-C1'-N1	8.74	114.12	108.00
2	G	10	DG	N1-C6-O6	7.94	124.66	119.90
3	K	9	DA	P-O3'-C3'	7.89	129.17	119.70
2	G	10	DG	C4-C5-N7	7.04	113.62	110.80
2	G	3	DT	O4'-C4'-C3'	-7.03	101.69	104.50
2	G	10	DG	C5-N7-C8	-6.82	100.89	104.30
2	G	1	DG	C1'-O4'-C4'	-6.51	103.58	110.10
2	G	3	DT	C1'-O4'-C4'	-6.28	103.82	110.10
3	K	2	DC	C3'-C2'-C1'	-6.21	95.05	102.50
3	K	8	DC	P-O3'-C3'	5.80	126.67	119.70
3	K	2	DC	N1-C1'-C2'	5.75	123.52	112.60
2	G	5	DC	O4'-C1'-N1	5.64	111.95	108.00
1	B	15	ARG	NE-CZ-NH2	-5.53	117.53	120.30
2	G	1	DG	C2-N3-C4	5.51	114.66	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	LEU	CA-CB-CG	5.50	127.94	115.30
2	G	10	DG	C6-C5-N7	-5.48	127.11	130.40
2	G	10	DG	N3-C4-C5	5.45	131.32	128.60
2	G	1	DG	N3-C4-N9	5.41	129.25	126.00
2	G	1	DG	N3-C4-C5	-5.37	125.92	128.60
3	K	10	DG	O4'-C1'-C2'	-5.24	101.71	105.90
1	A	82	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	15	ARG	NE-CZ-NH2	-5.21	117.70	120.30
2	G	8	DA	P-O3'-C3'	5.20	125.94	119.70
1	B	15	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2130	0	2071	75	0
1	B	2122	0	2060	33	0
2	G	205	0	113	7	0
3	K	218	0	123	5	0
4	A	54	0	72	39	0
4	B	18	0	24	9	0
5	A	39	0	54	7	0
6	G	2	0	0	0	0
7	A	154	0	0	1	0
7	B	115	0	0	5	0
7	G	20	0	0	1	0
7	K	16	0	0	1	0
All	All	5093	0	4517	114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (114) 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:77:VAL:HB	4:A:267:GOL:H11	1.34	1.10
1:A:96:ARG:H	4:A:269:GOL:H31	1.10	1.08
1:A:193:PHE:CB	4:A:268:GOL:H11	1.85	1.06
1:A:193:PHE:HB2	4:A:268:GOL:H11	1.39	1.04
1:B:117:MET:HG2	7:K:252:HOH:O	1.58	1.01
1:B:17:VAL:HG12	1:B:22:PHE:HB2	1.43	1.00
1:A:193:PHE:HB2	4:A:268:GOL:H31	1.44	1.00
1:A:95:GLY:CA	4:A:269:GOL:H11	1.95	0.94
1:A:191:ASP:HB3	4:A:270:GOL:H2	1.51	0.92
1:A:208:TYR:CE2	4:A:271:GOL:H31	2.06	0.90
1:B:204:THR:HG21	1:B:222:ASP:H	1.38	0.89
1:A:95:GLY:HA2	4:A:269:GOL:H11	1.55	0.89
1:A:96:ARG:N	4:A:269:GOL:H31	1.88	0.89
1:A:153:ASN:OD1	2:G:10:DG:H3'	1.75	0.87
1:A:95:GLY:N	4:A:269:GOL:H11	1.91	0.86
1:B:204:THR:HG22	1:B:220:ARG:HA	1.57	0.85
1:A:193:PHE:HB3	4:A:268:GOL:H11	1.60	0.83
1:A:208:TYR:HE2	4:A:271:GOL:H31	1.43	0.81
1:A:76:LYS:HB2	4:A:267:GOL:H31	1.61	0.80
1:B:193:PHE:HB2	4:B:266:GOL:H31	1.65	0.78
1:B:204:THR:CG2	1:B:221:LEU:H	1.97	0.76
1:A:96:ARG:H	4:A:269:GOL:C3	1.95	0.76
1:A:190:VAL:HG13	4:A:270:GOL:H12	1.68	0.75
1:A:95:GLY:H	4:A:269:GOL:H11	1.51	0.74
1:A:211:ARG:HD3	1:A:214:GLU:OE2	1.90	0.71
1:A:193:PHE:CB	4:A:268:GOL:H31	2.21	0.70
1:A:32:ASP:HB3	4:A:267:GOL:H2	1.74	0.69
1:A:95:GLY:HA2	4:A:269:GOL:C1	2.23	0.68
1:B:15:ARG:HD3	7:G:19:HOH:O	1.92	0.68
1:A:77:VAL:HG23	4:A:267:GOL:H32	1.75	0.68
1:B:153:ASN:OD1	3:K:11:DC:H5''	1.95	0.67
1:A:220:ARG:NH2	4:A:268:GOL:H12	2.09	0.66
1:A:188:GLY:HA2	1:A:228:GLU:OE1	1.96	0.65
1:A:236:ARG:HB2	1:A:254:GLU:HB2	1.78	0.65
1:A:114:ASN:OD1	2:G:10:DG:H2'	1.98	0.64
1:B:66:LYS:CD	1:B:66:LYS:H	2.11	0.64
4:B:266:GOL:C3	7:B:300:HOH:O	2.49	0.61
1:A:209:ARG:HG3	1:A:210:THR:HG23	1.82	0.61
1:B:236:ARG:HB2	1:B:254:GLU:HB2	1.82	0.60
1:A:240:LEU:HG	4:A:273:GOL:H2	1.84	0.60
1:A:17:VAL:HG13	1:A:22:PHE:HB2	1.84	0.60
1:B:66:LYS:HD3	1:B:66:LYS:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:MET:HB2	7:A:351:HOH:O	2.01	0.59
4:B:266:GOL:H31	7:B:300:HOH:O	2.02	0.59
1:A:92:ASP:O	4:A:269:GOL:H2	2.03	0.59
1:A:193:PHE:HB2	4:A:268:GOL:C1	2.26	0.59
1:A:244:MET:HG2	5:A:277:PG4:H41	1.85	0.58
1:A:210:THR:O	1:A:215:ARG:NH2	2.28	0.57
1:A:61:THR:HG22	4:A:269:GOL:H12	1.86	0.57
1:B:23:LEU:CD1	1:B:49:LYS:HD3	2.34	0.57
1:A:97:ILE:HD12	4:A:269:GOL:H32	1.87	0.57
1:A:65:ARG:NH2	2:G:8:DA:OP1	2.38	0.56
1:A:193:PHE:HB2	4:A:268:GOL:C3	2.29	0.55
1:B:57:ARG:HG2	4:B:268:GOL:H2	1.89	0.55
1:A:209:ARG:HB2	3:K:2:DC:H5'	1.87	0.55
1:A:57[A]:ARG:HG3	1:A:78:PRO:HB3	1.88	0.55
1:B:3:VAL:HG22	1:B:3:VAL:O	2.07	0.55
1:B:223:TYR:HA	4:B:266:GOL:H32	1.88	0.54
1:A:188:GLY:HA2	1:A:228:GLU:CD	2.29	0.54
1:A:149:CYS:HB3	1:A:224:PHE:CE2	2.43	0.53
1:A:95:GLY:H	4:A:269:GOL:C1	2.19	0.53
1:B:193:PHE:CB	4:B:266:GOL:H31	2.36	0.52
1:B:176:VAL:HG22	7:B:309:HOH:O	2.09	0.52
1:A:20:LYS:NZ	4:A:271:GOL:H2	2.25	0.51
1:A:114:ASN:OD1	2:G:10:DG:H8	1.94	0.51
1:A:191:ASP:CB	4:A:270:GOL:H2	2.32	0.50
1:A:116:LYS:HG2	2:G:10:DG:C8	2.47	0.50
1:B:204:THR:HG23	1:B:221:LEU:H	1.72	0.50
1:A:193:PHE:CG	4:A:268:GOL:H31	2.46	0.49
1:A:67:GLY:HA3	3:K:7:DG:H5''	1.94	0.49
3:K:1:DC:H2'	3:K:3:DC:C4	2.48	0.49
1:A:244:MET:H	5:A:277:PG4:H51	1.77	0.48
1:B:204:THR:CG2	1:B:221:LEU:N	2.74	0.48
1:A:77:VAL:CG2	4:A:267:GOL:H32	2.43	0.48
1:A:244:MET:CG	5:A:277:PG4:H41	2.43	0.48
1:B:65:ARG:HG2	1:B:68:TYR:CB	2.44	0.48
1:B:3:VAL:HA	1:B:255:ILE:O	2.13	0.48
1:A:244:MET:H	5:A:277:PG4:C5	2.28	0.47
1:A:222:ASP:O	4:A:268:GOL:O2	2.24	0.47
1:B:123:LYS:O	1:B:127:GLU:HG3	2.15	0.47
1:A:57[A]:ARG:NH1	5:A:276:PG4:O3	2.47	0.47
1:A:220:ARG:HH22	4:A:268:GOL:H12	1.80	0.46
1:A:7:ILE:HG12	1:A:31:PRO:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:277:PG4:H22	5:A:277:PG4:H62	1.98	0.46
1:A:116:LYS:HE3	2:G:10:DG:C4	2.51	0.45
1:B:110:ILE:O	1:B:150:GLY:HA3	2.16	0.45
2:G:10:DG:N1	3:K:1:DC:C6	2.84	0.45
1:A:116:LYS:HB2	1:A:171:SER:HB3	1.98	0.44
1:A:35:CYS:SG	1:A:107:LEU:HD21	2.58	0.44
1:A:149:CYS:HB3	1:A:224:PHE:CD2	2.53	0.44
1:A:47:PRO:HD2	1:A:50:LEU:HD12	2.00	0.44
1:B:237:SER:OG	4:B:266:GOL:H11	2.18	0.44
1:A:204:THR:O	1:A:248:HIS:HA	2.18	0.43
1:A:116:LYS:CB	1:A:171:SER:HB3	2.48	0.43
1:A:37:GLN:HB3	1:A:111:TYR:HB2	1.99	0.43
1:B:66:LYS:N	1:B:66:LYS:HD3	2.33	0.43
1:B:194:ARG:HD3	1:B:197:ASN:O	2.18	0.43
1:B:208:TYR:CZ	1:B:247:ASP:HB3	2.54	0.43
1:B:157:ARG:HB2	1:B:159:ILE:HG22	2.00	0.43
1:B:23:LEU:HD11	1:B:49:LYS:HD3	1.99	0.43
1:A:61:THR:HB	1:A:71:VAL:HG23	2.00	0.42
4:B:266:GOL:H32	7:B:300:HOH:O	2.13	0.42
1:A:52:HIS:HD1	5:A:276:PG4:C2	2.32	0.42
1:A:20:LYS:HZ3	4:A:271:GOL:H2	1.84	0.42
1:B:43:PRO:HG3	1:B:60:PHE:HB2	2.02	0.42
1:A:178:ARG:NE	4:A:272:GOL:H31	2.35	0.42
1:A:121:ARG:HD2	1:A:121:ARG:HA	1.87	0.42
1:A:190:VAL:CG1	4:A:270:GOL:H12	2.45	0.42
1:A:257:LEU:HD12	1:A:257:LEU:HA	1.87	0.41
1:B:193:PHE:HB2	4:B:266:GOL:C3	2.44	0.41
1:A:204:THR:HG23	1:A:220:ARG:HG3	2.03	0.41
1:A:193:PHE:CD1	4:A:268:GOL:H31	2.57	0.40
1:B:65:ARG:HG2	1:B:68:TYR:HB2	2.02	0.40
1:B:186:GLU:CG	7:B:339:HOH:O	2.70	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	253/265 (96%)	242 (96%)	11 (4%)	0	100	100
1	B	252/265 (95%)	242 (96%)	10 (4%)	0	100	100
All	All	505/530 (95%)	484 (96%)	21 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	226/235 (96%)	210 (93%)	16 (7%)	14	23
1	B	225/235 (96%)	216 (96%)	9 (4%)	31	49
All	All	451/470 (96%)	426 (94%)	25 (6%)	21	35

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	15	ARG
1	A	17	VAL
1	A	30	LYS
1	A	57[A]	ARG
1	A	65	ARG
1	A	89	GLU
1	A	116	LYS
1	A	122	LEU
1	A	176	VAL
1	A	207	SER
1	A	233	LYS
1	A	234	VAL
1	A	236	ARG
1	A	256	GLU

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Mol	Chain	Res	Type
1	A	257	LEU
1	B	10	ASN
1	B	11	VAL
1	B	27	MET
1	B	122	LEU
1	B	176	VAL
1	B	207	SER
1	B	210	THR
1	B	234	VAL
1	B	256	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	167	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	GOL	A	266	-	5,5,5	0.39	0	5,5,5	0.22	0
4	GOL	A	269	-	5,5,5	0.72	0	5,5,5	1.37	0
4	GOL	A	270	-	5,5,5	0.48	0	5,5,5	0.48	0
4	GOL	B	267	-	5,5,5	0.35	0	5,5,5	0.64	0
5	PG4	A	275	-	12,12,12	0.76	0	11,11,11	0.55	0
5	PG4	A	277	-	12,12,12	1.05	0	11,11,11	0.86	0
4	GOL	A	267	-	5,5,5	0.56	0	5,5,5	0.64	0
4	GOL	A	273	-	5,5,5	0.43	0	5,5,5	0.34	0
4	GOL	A	274	-	5,5,5	0.35	0	5,5,5	0.30	0
4	GOL	B	266	-	5,5,5	0.53	0	5,5,5	0.38	0
4	GOL	A	268	-	5,5,5	0.48	0	5,5,5	0.57	0
4	GOL	B	268	-	5,5,5	0.47	0	5,5,5	0.19	0
5	PG4	A	276	-	12,12,12	0.84	0	11,11,11	0.69	0
4	GOL	A	272	-	5,5,5	0.49	0	5,5,5	0.45	0
4	GOL	A	271	-	5,5,5	0.43	0	5,5,5	0.54	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	GOL	A	266	-	-	2/4/4/4	-
4	GOL	A	269	-	-	2/4/4/4	-
4	GOL	A	270	-	-	0/4/4/4	-
4	GOL	B	267	-	-	1/4/4/4	-
5	PG4	A	275	-	-	8/10/10/10	-
5	PG4	A	277	-	-	6/10/10/10	-
4	GOL	A	267	-	-	2/4/4/4	-
4	GOL	A	273	-	-	4/4/4/4	-
4	GOL	A	274	-	-	3/4/4/4	-
4	GOL	B	266	-	-	0/4/4/4	-
4	GOL	A	268	-	-	4/4/4/4	-
4	GOL	B	268	-	-	4/4/4/4	-
5	PG4	A	276	-	-	7/10/10/10	-
4	GOL	A	272	-	-	1/4/4/4	-
4	GOL	A	271	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	266	GOL	O1-C1-C2-C3
4	A	269	GOL	O1-C1-C2-C3
4	B	267	GOL	O1-C1-C2-C3
4	A	274	GOL	O1-C1-C2-O2
4	A	274	GOL	O1-C1-C2-C3
4	A	268	GOL	O1-C1-C2-C3
4	A	268	GOL	C1-C2-C3-O3
4	A	268	GOL	O2-C2-C3-O3
4	B	268	GOL	O1-C1-C2-C3
4	A	271	GOL	O1-C1-C2-C3
4	A	271	GOL	O2-C2-C3-O3
5	A	275	PG4	O2-C3-C4-O3
5	A	277	PG4	O3-C5-C6-O4
5	A	276	PG4	O2-C3-C4-O3
5	A	275	PG4	O3-C5-C6-O4
4	A	269	GOL	O1-C1-C2-O2
4	B	268	GOL	O1-C1-C2-O2
4	B	268	GOL	O2-C2-C3-O3
4	A	271	GOL	O1-C1-C2-O2
5	A	276	PG4	C6-C5-O3-C4
5	A	276	PG4	O3-C5-C6-O4
5	A	277	PG4	O2-C3-C4-O3
5	A	277	PG4	O1-C1-C2-O2
4	A	267	GOL	C1-C2-C3-O3
4	A	273	GOL	O1-C1-C2-C3
4	A	273	GOL	C1-C2-C3-O3
4	B	268	GOL	C1-C2-C3-O3
4	A	272	GOL	C1-C2-C3-O3
4	A	271	GOL	C1-C2-C3-O3
4	A	266	GOL	O1-C1-C2-O2
4	A	273	GOL	O1-C1-C2-O2
4	A	273	GOL	O2-C2-C3-O3
4	A	268	GOL	O1-C1-C2-O2
5	A	275	PG4	O1-C1-C2-O2
5	A	275	PG4	O4-C7-C8-O5
4	A	274	GOL	C1-C2-C3-O3
5	A	277	PG4	C8-C7-O4-C6
5	A	275	PG4	C1-C2-O2-C3
5	A	276	PG4	C1-C2-O2-C3
5	A	275	PG4	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
5	A	275	PG4	C5-C6-O4-C7
5	A	276	PG4	C8-C7-O4-C6
5	A	277	PG4	C6-C5-O3-C4
4	A	267	GOL	O2-C2-C3-O3
5	A	275	PG4	C8-C7-O4-C6
5	A	276	PG4	C4-C3-O2-C2
5	A	277	PG4	C4-C3-O2-C2
5	A	276	PG4	C5-C6-O4-C7

There are no ring outliers.

11 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	269	GOL	12	0
4	A	270	GOL	4	0
5	A	277	PG4	5	0
4	A	267	GOL	5	0
4	A	273	GOL	1	0
4	B	266	GOL	8	0
4	A	268	GOL	12	0
4	B	268	GOL	1	0
5	A	276	PG4	2	0
4	A	272	GOL	1	0
4	A	271	GOL	4	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<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	255/265 (96%)	-0.47	0 100 100	9, 21, 33, 43	2 (0%)
1	B	254/265 (95%)	-0.31	6 (2%) 59 57	20, 32, 46, 53	0
2	G	10/13 (76%)	-0.48	0 100 100	21, 27, 39, 57	0
3	K	10/11 (90%)	-0.13	1 (10%) 7 6	19, 27, 39, 49	0
All	All	529/554 (95%)	-0.39	7 (1%) 77 75	9, 26, 43, 57	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	2	DC	3.3
1	B	117	MET	2.7
1	B	214	GLU	2.2
1	B	203	TYR	2.1
1	B	217	VAL	2.1
1	B	218	GLY	2.0
1	B	165	LYS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	273	6/6	0.70	0.22	49,53,54,54	0
4	GOL	B	267	6/6	0.74	0.27	43,44,46,47	0
4	GOL	B	268	6/6	0.78	0.31	64,64,66,66	0
5	PG4	A	277	13/13	0.79	0.24	43,50,56,57	0
5	PG4	A	276	13/13	0.80	0.20	51,58,63,63	0
4	GOL	A	274	6/6	0.81	0.29	47,51,52,53	0
4	GOL	A	267	6/6	0.83	0.32	33,36,37,38	0
4	GOL	A	270	6/6	0.88	0.25	29,33,33,34	0
5	PG4	A	275	13/13	0.89	0.15	54,58,59,60	0
4	GOL	B	266	6/6	0.90	0.43	32,35,36,37	0
4	GOL	A	271	6/6	0.90	0.22	45,47,49,50	0
4	GOL	A	268	6/6	0.93	0.21	20,25,26,28	0
4	GOL	A	272	6/6	0.94	0.33	23,29,33,33	0
4	GOL	A	269	6/6	0.95	0.33	24,26,28,28	0
4	GOL	A	266	6/6	0.97	0.17	35,36,37,38	0
6	NA	G	15	1/1	0.98	0.10	12,12,12,12	0
6	NA	G	14	1/1	1.00	0.20	14,14,14,14	0

## 6.5 Other polymers

There are no such residues in this entry.