



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:13 pm BST

PDB ID : 3GA6  
Title : Mth0212 in complex with two DNA helices  
Authors : Lakomek, K.; Dickmanns, A.; Ficner, R.  
Deposited on : 2009-02-16  
Resolution : 1.90 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

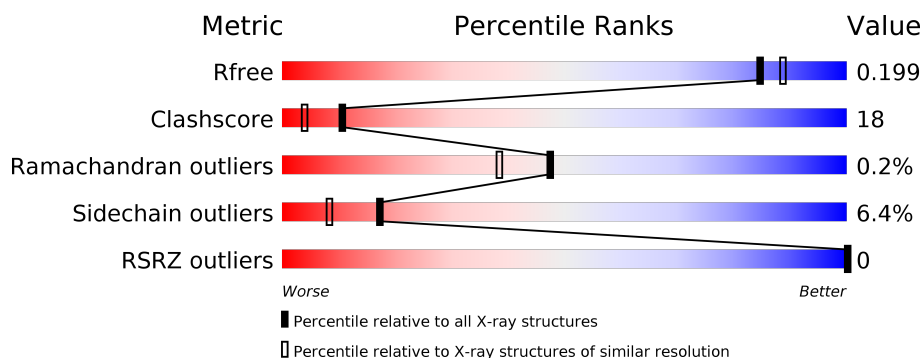
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	<div> <div>71%</div> <div>23%</div> <div>• •</div> </div>
1	B	265	<div> <div>63%</div> <div>30%</div> <div>• •</div> </div>
2	F	12	<div> <div>33%</div> <div>50%</div> <div>8% 8%</div> </div>
2	H	12	<div> <div>42%</div> <div>42%</div> <div>8% 8%</div> </div>
3	D	12	<div> <div>17%</div> <div>50%</div> <div>33%</div> </div>
3	G	12	<div> <div>50%</div> <div>42%</div> <div>8%</div> </div>

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	GOL	A	7002	-	-	X	-
4	GOL	A	7031	-	-	X	-
4	GOL	B	7022	-	-	X	-
4	GOL	B	7033	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5629 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	254	Total	C	N	O	S	0	0	0
			2122	1362	372	380	8			
1	B	255	Total	C	N	O	S	0	0	0
			2127	1365	373	381	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1002	ALA	THR	ENGINEERED MUTATION	UNP O26314
A	1151	ASN	ASP	ENGINEERED MUTATION	UNP O26314
A	1258	LEU	-	EXPRESSION TAG	UNP O26314
A	1259	GLU	-	EXPRESSION TAG	UNP O26314
A	1260	HIS	-	EXPRESSION TAG	UNP O26314
A	1261	HIS	-	EXPRESSION TAG	UNP O26314
A	1262	HIS	-	EXPRESSION TAG	UNP O26314
A	1263	HIS	-	EXPRESSION TAG	UNP O26314
A	1264	HIS	-	EXPRESSION TAG	UNP O26314
A	1265	HIS	-	EXPRESSION TAG	UNP O26314
B	2002	ALA	THR	ENGINEERED MUTATION	UNP O26314
B	2151	ASN	ASP	ENGINEERED MUTATION	UNP O26314
B	2258	LEU	-	EXPRESSION TAG	UNP O26314
B	2259	GLU	-	EXPRESSION TAG	UNP O26314
B	2260	HIS	-	EXPRESSION TAG	UNP O26314
B	2261	HIS	-	EXPRESSION TAG	UNP O26314
B	2262	HIS	-	EXPRESSION TAG	UNP O26314
B	2263	HIS	-	EXPRESSION TAG	UNP O26314
B	2264	HIS	-	EXPRESSION TAG	UNP O26314
B	2265	HIS	-	EXPRESSION TAG	UNP O26314

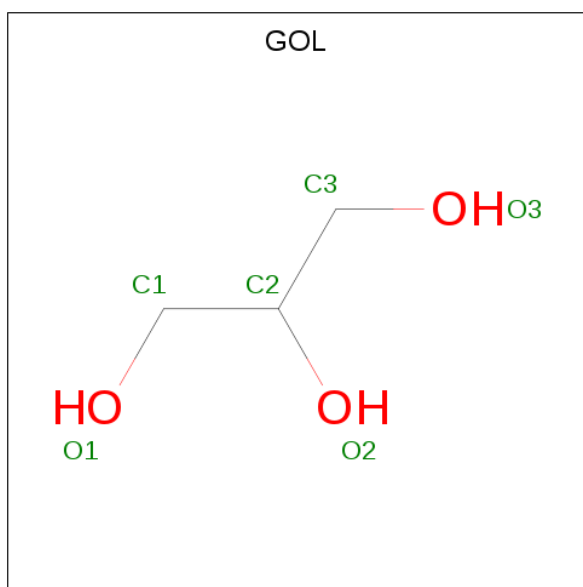
- Molecule 2 is a DNA chain called 5'-D(\*GP\*CP\*TP\*GP\*CP\*GP\*CP\*AP\*GP\*GP\*GP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	11	Total	C	N	O	P	0	0	0
			227	107	46	64	10			
2	H	11	Total	C	N	O	P	0	0	0
			227	106	44	66	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	12	Total	C	N	O	P	0	0	1
			207	95	36	65	11			
3	D	12	Total	C	N	O	P	0	0	0
			240	114	44	71	11			

- 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		

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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	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		
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		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

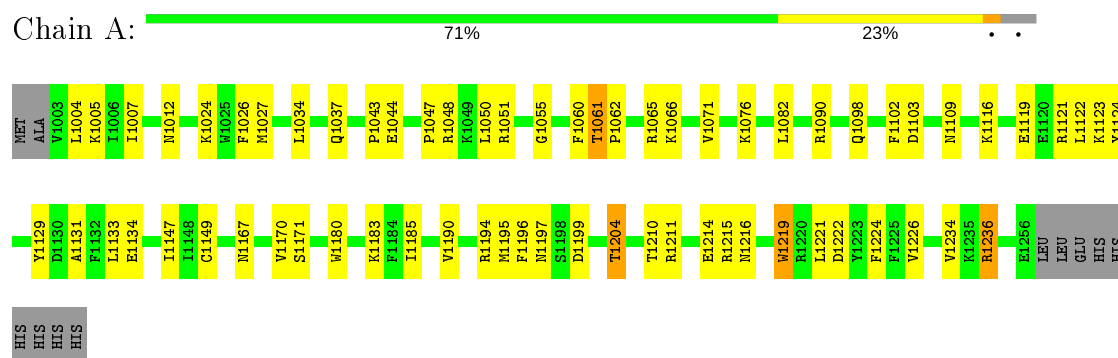
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	157	Total	O	0	0
			157	157		
7	B	155	Total	O	0	0
			155	155		
7	F	6	Total	O	0	0
			6	6		
7	G	13	Total	O	0	0
			13	13		
7	H	16	Total	O	0	0
			16	16		
7	D	7	Total	O	0	0
			7	7		

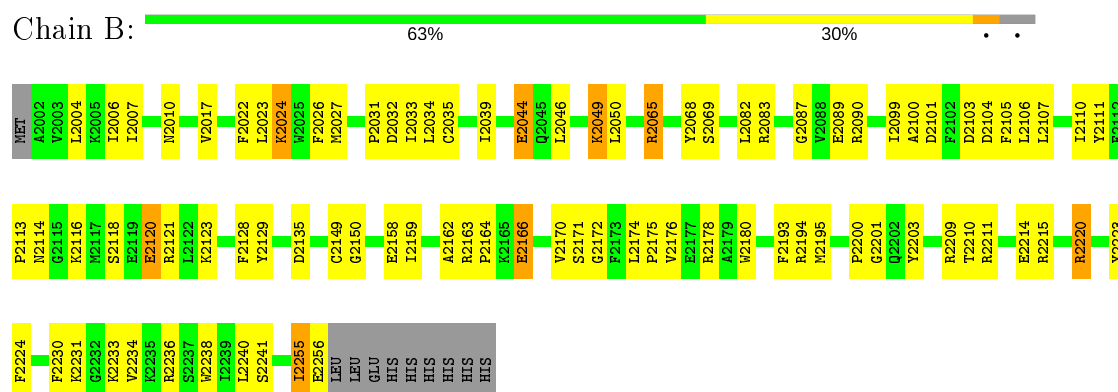
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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\*C)-3'



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



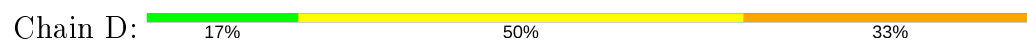




- Molecule 3: 5'-D(\*GP\*CP\*CP\*CP\*TP\*GP\*UP\*GP\*CP\*AP\*GP\*C)-3'



- Molecule 3: 5'-D(\*GP\*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, $\alpha$ , $\beta$ , $\gamma$	54.83Å 126.66Å 54.83Å 90.00° 93.14° 90.00°	Depositor
Resolution (Å)	33.71 – 1.90 33.71 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.4 (33.71-1.90) 95.5 (33.71-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 1.89Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.155 , 0.203 0.160 , 0.199	Depositor DCC
$R_{free}$ test set	3395 reflections (6.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.488 for l,-k,h	Xtriage
Reported twinning fraction	0.505 for l,-k,h	Depositor
Outliers	1 of 56227 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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, PO4, 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	0.40	0/2180	0.56	0/2939
1	B	0.39	0/2185	0.55	0/2946
2	F	0.63	0/255	1.28	1/393 (0.3%)
2	H	0.78	0/254	1.60	6/390 (1.5%)
3	D	0.59	0/268	1.57	6/411 (1.5%)
3	G	1.45	4/230 (1.7%)	1.78	5/354 (1.4%)
All	All	0.53	4/5372 (0.1%)	0.87	18/7433 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	DG	O3'-P	-10.34	1.48	1.61
3	G	11	DG	C3'-O3'	7.32	1.53	1.44
3	G	11	DG	N3-C4	5.93	1.39	1.35
3	G	11	DG	C6-N1	5.42	1.43	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	11	DG	P-O3'-C3'	15.09	137.81	119.70
3	D	10	DA	O4'-C4'-C3'	-9.99	100.01	106.00
3	D	4	DC	O4'-C1'-N1	9.32	114.53	108.00
2	H	11	DC	O4'-C1'-N1	7.70	113.39	108.00
3	D	10	DA	C4'-C3'-C2'	-6.93	96.86	103.10
2	H	2	DT	C1'-O4'-C4'	-6.88	103.22	110.10
2	H	9	DG	C1'-O4'-C4'	-6.75	103.35	110.10
3	D	6	DG	O4'-C1'-N9	6.72	112.70	108.00
2	H	2	DT	O4'-C1'-C2'	-6.14	100.99	105.90
2	H	9	DG	P-O3'-C3'	6.13	127.05	119.70
3	G	11	DG	O4'-C1'-N9	6.11	112.28	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	10	DA	O4'-C1'-N9	5.73	112.01	108.00
2	F	3	DT	N3-C4-O4	5.50	123.20	119.90
2	H	11	DC	C1'-O4'-C4'	-5.28	104.82	110.10
3	G	12	DC	O5'-P-OP1	-5.23	100.99	105.70
3	D	5	DT	N3-C4-O4	5.19	123.01	119.90
3	G	5	DT	O4'-C1'-N1	5.06	111.54	108.00
3	G	6	DG	O4'-C1'-N9	5.02	111.52	108.00

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	2122	0	2060	59	0
1	B	2127	0	2065	81	0
2	F	227	0	124	11	0
2	H	227	0	123	6	0
3	D	240	0	134	23	0
3	G	207	0	110	6	0
4	A	66	0	88	23	0
4	B	48	0	64	20	0
5	A	1	0	0	0	0
6	B	10	0	0	0	0
7	A	157	0	0	2	0
7	B	155	0	0	6	0
7	D	7	0	0	0	0
7	F	6	0	0	0	0
7	G	13	0	0	0	0
7	H	16	0	0	0	0
All	All	5629	0	4768	181	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 18.

All (181) 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)
3:G:7:DU:H3	2:H:5:DG:H22	0.99	0.96
1:B:2175:PRO:HG2	4:B:7032:GOL:H12	1.46	0.94
1:B:2193:PHE:HB2	4:B:7033:GOL:H11	1.52	0.90
2:F:6:DG:H2''	2:F:7:DC:H5'	1.55	0.88
1:A:1131:ALA:HB1	4:A:7002:GOL:H31	1.56	0.87
1:A:1051:ARG:NH1	4:A:7015:GOL:H12	1.90	0.87
3:G:7:DU:H3	2:H:5:DG:N2	1.72	0.87
2:F:9:DG:H2''	2:F:10:DG:O4'	1.77	0.84
1:B:2193:PHE:HB2	4:B:7033:GOL:C1	2.10	0.81
1:A:1190:VAL:HG13	4:A:7031:GOL:H12	1.63	0.79
3:D:11:DG:H2''	3:D:12:DC:O5'	1.82	0.78
3:D:5:DT:C2'	3:D:6:DG:H5''	2.13	0.78
2:F:10:DG:H4'	2:F:10:DG:OP1	1.84	0.77
1:B:2163:ARG:HB3	1:B:2166:GLU:HG2	1.68	0.76
1:B:2210:THR:HG22	1:B:2215:ARG:HH21	1.52	0.75
3:D:4:DC:H2''	3:D:5:DT:H72	1.69	0.74
3:D:10:DA:H2''	3:D:11:DG:OP2	1.88	0.72
1:B:2163:ARG:HB3	1:B:2166:GLU:CG	2.21	0.71
1:A:1204:THR:HG21	1:A:1222:ASP:H	1.56	0.70
1:A:1180:TRP:HB2	4:A:7012:GOL:H31	1.73	0.70
1:B:2230:PHE:CE1	1:B:2233:LYS:HD2	2.27	0.70
1:B:2223:TYR:HA	4:B:7033:GOL:H2	1.75	0.69
2:F:11:DG:N2	3:D:2:DC:N3	2.34	0.68
1:A:1236:ARG:HG2	7:A:9104:HOH:O	1.92	0.68
4:A:7002:GOL:O2	1:B:2090:ARG:NH1	2.27	0.68
1:A:1185:ILE:HG23	4:A:7031:GOL:H32	1.76	0.68
3:D:9:DC:H2''	3:D:10:DA:C8	2.29	0.68
3:D:5:DT:H5''	3:D:5:DT:H6	1.60	0.67
2:F:11:DG:H1	3:D:2:DC:H42	1.43	0.66
1:A:1124:TYR:HA	4:A:7030:GOL:H32	1.79	0.65
3:D:5:DT:H2'	3:D:6:DG:H5''	1.77	0.65
1:B:2017:VAL:HG13	1:B:2022:PHE:HB2	1.80	0.64
1:A:1123:LYS:HE2	7:B:9076:HOH:O	1.97	0.64
1:A:1204:THR:HG22	1:A:1221:LEU:H	1.63	0.64
1:A:1124:TYR:HB2	4:A:7030:GOL:H2	1.80	0.64
1:A:1043:PRO:HD3	1:A:1062:PRO:HG3	1.79	0.64
3:D:6:DG:H2''	3:D:7:DU:O5'	1.97	0.63
1:A:1190:VAL:HA	4:A:7031:GOL:H31	1.80	0.63
2:F:5:DC:H2'	2:F:6:DG:C8	2.33	0.63
3:G:7:DU:C2	2:H:5:DG:H22	2.11	0.63
1:B:2116:LYS:HE3	1:B:2170:VAL:HG13	1.80	0.63
1:B:2210:THR:HG22	1:B:2210:THR:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:GLY:HA3	4:A:7004:GOL:H2	1.80	0.62
1:A:1051:ARG:HH12	4:A:7015:GOL:H12	1.66	0.61
1:B:2116:LYS:HD2	4:B:7022:GOL:H11	1.82	0.61
2:F:9:DG:C2'	2:F:10:DG:H5''	2.31	0.61
1:A:1090:ARG:NE	4:A:7030:GOL:O3	2.30	0.60
1:A:1183:LYS:HD3	4:A:7012:GOL:O2	2.00	0.60
1:B:2004:LEU:HB3	1:B:2255:ILE:CD1	2.32	0.60
4:B:7033:GOL:H12	7:B:9377:HOH:O	2.01	0.60
1:B:2083:ARG:NH2	1:B:2135:ASP:OD1	2.35	0.60
3:D:4:DC:H2''	3:D:5:DT:C7	2.32	0.60
1:B:2114:ASN:OD1	4:B:7022:GOL:H31	2.03	0.59
1:B:2159:ILE:HA	4:B:7021:GOL:H2	1.85	0.59
1:B:2083:ARG:HH22	1:B:2135:ASP:CG	2.06	0.59
1:A:1204:THR:HG23	1:A:1222:ASP:OD2	2.03	0.58
1:B:2101:ASP:HA	1:B:2106:LEU:HD23	1.85	0.58
3:G:6:DG:H2''	3:G:7:DU:H5'	1.84	0.58
3:D:10:DA:H5'	3:D:10:DA:C8	2.38	0.58
1:A:1131:ALA:CB	4:A:7002:GOL:H31	2.31	0.57
1:A:1219:TRP:CD1	1:A:1219:TRP:N	2.73	0.57
1:B:2158:GLU:HB3	4:B:7021:GOL:H31	1.87	0.56
1:A:1047:PRO:HD2	1:A:1050:LEU:HD23	1.86	0.56
1:B:2172:GLY:HA3	4:B:7022:GOL:H2	1.88	0.56
1:B:2193:PHE:HD2	1:B:2220:ARG:NH1	2.04	0.56
3:D:5:DT:C6	3:D:5:DT:H5''	2.41	0.56
1:A:1190:VAL:CG1	4:A:7031:GOL:H12	2.34	0.56
1:A:1076:LYS:HE2	4:A:7004:GOL:H12	1.88	0.56
3:D:5:DT:C3'	3:D:6:DG:H5''	2.36	0.55
1:B:2035:CYS:SG	1:B:2107:LEU:HD21	2.47	0.55
1:B:2121:ARG:HD3	4:B:7003:GOL:H12	1.88	0.55
1:B:2116:LYS:HG2	1:B:2171:SER:HB3	1.90	0.54
1:B:2236:ARG:HG2	1:B:2238:TRP:CE3	2.43	0.54
1:B:2193:PHE:CB	4:B:7033:GOL:H11	2.30	0.54
1:B:2223:TYR:HA	4:B:7033:GOL:C2	2.37	0.53
1:A:1051:ARG:HH11	4:A:7015:GOL:H12	1.73	0.53
1:B:2118:SER:OG	1:B:2120:GLU:HG3	2.08	0.53
3:D:10:DA:H1'	3:D:11:DG:H5'	1.91	0.53
1:B:2149:CYS:HB3	1:B:2224:PHE:CE2	2.44	0.53
1:B:2110:ILE:O	1:B:2150:GLY:HA3	2.09	0.53
1:B:2004:LEU:HB3	1:B:2255:ILE:HD13	1.90	0.53
1:B:2026:PHE:HE2	1:B:2031:PRO:HD2	1.74	0.53
1:A:1204:THR:HG21	1:A:1222:ASP:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2195:MET:HE1	1:B:2231:LYS:HG3	1.92	0.52
1:A:1210:THR:HG21	2:F:3:DT:H5'	1.92	0.51
1:A:1037:GLN:HA	1:A:1071:VAL:HG12	1.92	0.51
1:A:1210:THR:O	1:A:1210:THR:HG22	2.09	0.51
3:D:10:DA:H8	3:D:10:DA:H5'	1.74	0.51
1:A:1061:THR:HG23	1:A:1098:GLN:HE21	1.76	0.51
1:B:2017:VAL:HG13	1:B:2022:PHE:CB	2.40	0.51
1:A:1043:PRO:HG3	1:A:1060:PHE:HB2	1.92	0.50
1:B:2039:ILE:HG12	7:B:9165:HOH:O	2.10	0.50
1:B:2049:LYS:HD3	1:B:2049:LYS:H	1.77	0.50
1:A:1149:CYS:HB3	1:A:1224:PHE:CE2	2.46	0.50
1:B:2231:LYS:O	1:B:2234:VAL:HG12	2.12	0.50
1:B:2129:TYR:HB3	1:B:2180:TRP:CE2	2.47	0.49
1:B:2240:LEU:N	1:B:2240:LEU:HD12	2.27	0.49
1:A:1147:ILE:HG12	1:A:1226:VAL:HG12	1.94	0.49
1:B:2164:PRO:HD2	7:B:453:HOH:O	2.12	0.49
1:B:2120:GLU:OE1	4:B:7003:GOL:H11	2.13	0.49
1:A:1119:GLU:HG3	7:A:9063:HOH:O	2.11	0.49
1:B:2163:ARG:HB3	1:B:2166:GLU:HG3	1.95	0.48
2:F:6:DG:C2'	2:F:7:DC:H5'	2.37	0.48
1:A:1167:ASN:O	1:A:1170:VAL:HG12	2.13	0.48
1:A:1065:ARG:HG3	1:A:1066:LYS:N	2.28	0.48
1:B:2044:GLU:H	1:B:2044:GLU:CD	2.15	0.48
1:A:1131:ALA:HB2	4:A:7002:GOL:H12	1.96	0.48
2:F:9:DG:H2''	2:F:10:DG:H5''	1.95	0.47
1:A:1121:ARG:HA	1:A:1121:ARG:HD2	1.68	0.47
1:B:2082:LEU:HD23	1:B:2100:ALA:HB2	1.96	0.47
1:B:2004:LEU:HB3	1:B:2255:ILE:HD11	1.96	0.47
3:G:6:DG:H2''	3:G:7:DU:C5'	2.45	0.47
1:B:2129:TYR:HB3	1:B:2180:TRP:NE1	2.30	0.47
1:A:1185:ILE:CG2	4:A:7031:GOL:H32	2.45	0.46
1:B:2007:ILE:HD12	1:B:2031:PRO:HG3	1.96	0.46
1:B:2149:CYS:HB3	1:B:2224:PHE:CD2	2.50	0.46
1:A:1122:LEU:HD13	1:A:1171:SER:OG	2.16	0.46
2:H:10:DG:H2''	2:H:11:DC:H2'	1.97	0.46
1:A:1211:ARG:HB3	1:A:1214:GLU:OE1	2.15	0.46
1:B:2023:LEU:HA	1:B:2023:LEU:HD23	1.80	0.46
1:B:2210:THR:HG22	1:B:2215:ARG:NH2	2.26	0.46
3:D:9:DC:H2''	3:D:10:DA:N7	2.30	0.46
2:H:4:DC:H2''	2:H:5:DG:C8	2.51	0.46
1:B:2083:ARG:NH2	1:B:2099:ILE:HD13	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:11:DG:H2''	3:D:12:DC:O4'	2.16	0.46
1:A:1061:THR:CG2	1:A:1098:GLN:HE21	2.27	0.46
1:B:2089:GLU:HA	4:B:7011:GOL:H12	1.97	0.46
1:B:2046:LEU:HD22	1:B:2050:LEU:HD23	1.97	0.46
1:A:1219:TRP:HD1	1:A:1219:TRP:N	2.14	0.46
1:B:2174:LEU:O	1:B:2178:ARG:HG3	2.15	0.46
1:B:2024:LYS:O	1:B:2027:MET:HB3	2.16	0.45
1:B:2193:PHE:CB	4:B:7033:GOL:H32	2.46	0.45
1:B:2087:GLY:C	4:B:7011:GOL:H31	2.37	0.45
1:A:1102:PHE:O	1:A:1103:ASP:HB3	2.16	0.45
1:A:1194:ARG:HD3	1:A:1197:ASN:O	2.17	0.45
1:B:2159:ILE:HG13	1:B:2200:PRO:HB3	1.98	0.45
1:B:2026:PHE:CE2	1:B:2031:PRO:HD2	2.50	0.45
4:A:7002:GOL:C2	1:B:2090:ARG:HH22	2.30	0.45
1:B:2158:GLU:HG2	1:B:2164:PRO:HB3	1.99	0.45
1:B:2201:GLY:HA2	1:B:2203:TYR:CZ	2.52	0.45
1:B:2175:PRO:CD	4:B:7032:GOL:H31	2.46	0.45
1:A:1204:THR:CG2	1:A:1221:LEU:H	2.29	0.44
1:A:1004:LEU:HD11	4:A:7006:GOL:H32	1.98	0.44
1:A:1211:ARG:O	1:A:1214:GLU:HG2	2.17	0.44
1:A:1210:THR:HG22	1:A:1215:ARG:NH2	2.32	0.44
4:A:7002:GOL:H2	1:B:2090:ARG:HH22	1.83	0.44
1:B:2006:ILE:CD1	1:B:2033:ILE:HD12	2.48	0.44
1:A:1024:LYS:HE3	1:A:1024:LYS:HB2	1.70	0.43
1:A:1204:THR:CG2	1:A:1222:ASP:OD2	2.67	0.43
2:F:6:DG:H1'	2:F:7:DC:H5''	1.99	0.43
1:B:2113:PRO:HD3	1:B:2128:PHE:CD2	2.53	0.43
1:B:2210:THR:CG2	1:B:2215:ARG:HH21	2.27	0.43
1:A:1061:THR:HG23	1:A:1098:GLN:NE2	2.34	0.43
1:A:1066:LYS:HB3	1:A:1066:LYS:HE2	1.93	0.43
1:B:2123:LYS:HD2	1:B:2123:LYS:HA	1.76	0.43
3:D:11:DG:H2'	3:D:12:DC:C6	2.53	0.43
1:B:2162:ALA:C	1:B:2164:PRO:HD3	2.39	0.42
1:A:1061:THR:O	1:A:1061:THR:OG1	2.34	0.42
1:A:1005:LYS:HD3	1:A:1007:ILE:HD11	2.01	0.42
1:A:1214:GLU:H	1:A:1214:GLU:HG2	1.63	0.42
3:D:10:DA:C2'	3:D:11:DG:OP2	2.65	0.42
3:D:11:DG:H2'	3:D:12:DC:H6	1.85	0.42
1:B:2172:GLY:CA	4:B:7022:GOL:H2	2.48	0.42
1:B:2255:ILE:HG12	1:B:2256:GLU:N	2.35	0.41
3:D:8:DG:H2''	3:D:9:DC:O5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2069:SER:HG	1:B:2111:TYR:HD2	1.64	0.41
4:B:7033:GOL:C1	7:B:9377:HOH:O	2.62	0.41
1:A:1116:LYS:HE3	1:A:1116:LYS:HB3	1.88	0.41
1:B:2065:ARG:HG2	1:B:2068:TYR:CB	2.50	0.41
3:G:7:DU:H3	2:H:5:DG:H1	1.69	0.41
3:D:10:DA:C4	3:D:11:DG:C8	3.09	0.41
1:A:1098:GLN:HB2	1:A:1109:ASN:HB3	2.02	0.40
1:B:2083:ARG:NH2	1:B:2135:ASP:CG	2.71	0.40
1:B:2194:ARG:HD3	1:B:2194:ARG:HA	1.77	0.40
1:A:1134:GLU:OE2	4:A:7002:GOL:H11	2.21	0.40
1:B:2039:ILE:HD12	1:B:2039:ILE:C	2.42	0.40
1:A:1195:MET:HE2	1:A:1196:PHE:CZ	2.57	0.40
1:B:2004:LEU:HD23	1:B:2032:ASP:HB2	2.03	0.40
1:B:2103:ASP:HB2	7:B:9101:HOH:O	2.22	0.40
1:B:2104:ASP:O	1:B:2105:PHE:HB3	2.21	0.40
1:B:2211:ARG:O	1:B:2215:ARG:HG3	2.22	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	252/265 (95%)	243 (96%)	8 (3%)	1 (0%)	34	24
1	B	253/265 (96%)	243 (96%)	10 (4%)	0	100	100
All	All	505/530 (95%)	486 (96%)	18 (4%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1216	ASN

### 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	225/235 (96%)	210 (93%)	15 (7%)	16	7
1	B	225/235 (96%)	211 (94%)	14 (6%)	18	9
All	All	450/470 (96%)	421 (94%)	29 (6%)	17	8

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1012	ASN
1	A	1026	PHE
1	A	1027	MET
1	A	1034	LEU
1	A	1044	GLU
1	A	1048	ARG
1	A	1061	THR
1	A	1082	LEU
1	A	1129	TYR
1	A	1133	LEU
1	A	1199	ASP
1	A	1204	THR
1	A	1219	TRP
1	A	1234	VAL
1	A	1236	ARG
1	B	2010	ASN
1	B	2024	LYS
1	B	2034	LEU
1	B	2044	GLU
1	B	2049	LYS
1	B	2065	ARG
1	B	2120	GLU
1	B	2166	GLU
1	B	2176	VAL
1	B	2209	ARG
1	B	2214	GLU
1	B	2220	ARG

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Mol	Chain	Res	Type
1	B	2241	SER
1	B	2255	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1012	ASN
1	A	1018	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](#)

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 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	7012	-	5,5,5	0.46	0	5,5,5	0.22	0
4	GOL	A	7024	-	5,5,5	0.36	0	5,5,5	0.15	0
4	GOL	B	7022	-	5,5,5	0.48	0	5,5,5	0.58	0
4	GOL	A	7004	-	5,5,5	0.43	0	5,5,5	0.42	0
4	GOL	A	7020	-	5,5,5	0.42	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	B	7003	-	5,5,5	0.32	0	5,5,5	0.21	0
4	GOL	B	7027	-	5,5,5	0.33	0	5,5,5	0.30	0
4	GOL	A	7013	-	5,5,5	0.32	0	5,5,5	0.43	0
4	GOL	A	7030	-	5,5,5	0.43	0	5,5,5	0.38	0
4	GOL	B	7009	-	5,5,5	0.35	0	5,5,5	0.25	0
4	GOL	A	7010	-	5,5,5	0.40	0	5,5,5	0.56	0
4	GOL	A	7002	-	5,5,5	0.53	0	5,5,5	0.42	0
4	GOL	B	7033	-	5,5,5	0.42	0	5,5,5	0.33	0
4	GOL	A	7031	-	5,5,5	0.63	0	5,5,5	0.40	0
6	PO4	B	7204	-	4,4,4	0.85	0	6,6,6	0.57	0
4	GOL	B	7011	-	5,5,5	0.36	0	5,5,5	0.25	0
6	PO4	B	7205	-	4,4,4	0.90	0	6,6,6	0.45	0
4	GOL	B	7032	-	5,5,5	0.39	0	5,5,5	0.23	0
4	GOL	A	7006	5	5,5,5	0.34	0	5,5,5	0.44	0
4	GOL	A	7015	-	5,5,5	0.46	0	5,5,5	0.71	0
4	GOL	B	7021	-	5,5,5	0.44	0	5,5,5	0.27	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	7012	-	-	2/4/4/4	-
4	GOL	A	7024	-	-	3/4/4/4	-
4	GOL	B	7022	-	-	2/4/4/4	-
4	GOL	A	7004	-	-	4/4/4/4	-
4	GOL	A	7020	-	-	2/4/4/4	-
4	GOL	B	7003	-	-	0/4/4/4	-
4	GOL	B	7027	-	-	0/4/4/4	-
4	GOL	A	7013	-	-	2/4/4/4	-
4	GOL	A	7030	-	-	0/4/4/4	-
4	GOL	B	7009	-	-	2/4/4/4	-
4	GOL	A	7010	-	-	3/4/4/4	-
4	GOL	A	7002	-	-	4/4/4/4	-
4	GOL	B	7033	-	-	0/4/4/4	-
4	GOL	A	7031	-	-	2/4/4/4	-
4	GOL	B	7011	-	-	2/4/4/4	-
4	GOL	A	7006	5	-	4/4/4/4	-
4	GOL	B	7032	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	7015	-	-	2/4/4/4	-
4	GOL	B	7021	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	7022	GOL	O1-C1-C2-C3
4	A	7020	GOL	O1-C1-C2-C3
4	A	7006	GOL	O1-C1-C2-C3
4	A	7002	GOL	O1-C1-C2-C3
4	B	7032	GOL	O1-C1-C2-C3
4	A	7004	GOL	O1-C1-C2-C3
4	B	7009	GOL	O1-C1-C2-C3
4	B	7021	GOL	O1-C1-C2-C3
4	A	7024	GOL	O1-C1-C2-C3
4	B	7022	GOL	O1-C1-C2-O2
4	A	7006	GOL	O1-C1-C2-O2
4	B	7011	GOL	O2-C2-C3-O3
4	A	7012	GOL	C1-C2-C3-O3
4	A	7006	GOL	C1-C2-C3-O3
4	A	7002	GOL	C1-C2-C3-O3
4	A	7004	GOL	C1-C2-C3-O3
4	B	7011	GOL	C1-C2-C3-O3
4	A	7013	GOL	O1-C1-C2-C3
4	A	7010	GOL	O1-C1-C2-C3
4	A	7020	GOL	O1-C1-C2-O2
4	A	7002	GOL	O1-C1-C2-O2
4	B	7032	GOL	O1-C1-C2-O2
4	A	7004	GOL	O2-C2-C3-O3
4	B	7009	GOL	O1-C1-C2-O2
4	A	7015	GOL	O1-C1-C2-O2
4	B	7021	GOL	O1-C1-C2-O2
4	A	7024	GOL	O1-C1-C2-O2
4	A	7013	GOL	O1-C1-C2-O2
4	A	7010	GOL	O1-C1-C2-O2
4	A	7002	GOL	O2-C2-C3-O3
4	A	7031	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	7010	GOL	O2-C2-C3-O3
4	A	7004	GOL	O1-C1-C2-O2
4	A	7024	GOL	C1-C2-C3-O3
4	A	7015	GOL	O1-C1-C2-C3
4	A	7012	GOL	O2-C2-C3-O3
4	A	7006	GOL	O2-C2-C3-O3
4	A	7031	GOL	O1-C1-C2-C3

There are no ring outliers.

13 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	7012	GOL	2	0
4	B	7022	GOL	4	0
4	A	7004	GOL	2	0
4	B	7003	GOL	2	0
4	A	7030	GOL	3	0
4	A	7002	GOL	7	0
4	B	7033	GOL	8	0
4	A	7031	GOL	5	0
4	B	7011	GOL	2	0
4	B	7032	GOL	2	0
4	A	7006	GOL	1	0
4	A	7015	GOL	3	0
4	B	7021	GOL	2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	254/265 (95%)	-0.69	0 100 100	17, 30, 48, 75	2 (0%)
1	B	255/265 (96%)	-0.70	0 100 100	18, 30, 49, 72	3 (1%)
2	F	11/12 (91%)	-0.35	0 100 100	46, 79, 88, 113	0
2	H	11/12 (91%)	-0.70	0 100 100	30, 38, 43, 99	0
3	D	11/12 (91%)	-0.61	0 100 100	40, 61, 87, 99	0
3	G	11/12 (91%)	-0.61	0 100 100	37, 41, 60, 133	0
All	All	553/578 (95%)	-0.68	0 100 100	17, 31, 56, 133	5 (0%)

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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<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	B	7009	6/6	0.58	0.20	76,79,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	7003	6/6	0.72	0.24	65,72,74,79	0
4	GOL	A	7004	6/6	0.76	0.13	48,52,54,54	0
4	GOL	A	7024	6/6	0.82	0.15	57,58,59,59	0
4	GOL	A	7015	6/6	0.85	0.17	32,42,45,45	0
4	GOL	B	7032	6/6	0.86	0.19	67,68,71,71	0
6	PO4	B	7205	5/5	0.87	0.18	101,103,103,103	0
4	GOL	A	7002	6/6	0.89	0.15	38,46,50,50	0
4	GOL	A	7010	6/6	0.90	0.14	36,40,45,48	0
6	PO4	B	7204	5/5	0.91	0.16	86,88,90,90	0
4	GOL	B	7022	6/6	0.92	0.11	35,41,44,48	0
4	GOL	B	7027	6/6	0.92	0.16	56,60,61,63	0
4	GOL	A	7031	6/6	0.93	0.17	21,34,35,39	0
4	GOL	A	7030	6/6	0.93	0.15	37,39,41,42	0
4	GOL	A	7012	6/6	0.93	0.14	37,38,41,41	0
4	GOL	A	7006	6/6	0.93	0.13	32,45,46,51	0
4	GOL	A	7013	6/6	0.94	0.09	41,43,46,46	0
4	GOL	B	7021	6/6	0.95	0.15	39,44,44,45	0
4	GOL	A	7020	6/6	0.95	0.10	27,31,37,38	0
4	GOL	B	7011	6/6	0.96	0.12	28,34,38,41	0
4	GOL	B	7033	6/6	0.98	0.12	32,36,37,37	0
5	NA	A	7401	1/1	0.99	0.06	30,30,30,30	0

## 6.5 Other polymers

There are no such residues in this entry.