W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2017 – 05:27 AM EST

|		
PDB ID	:	5SWI
Title	:	Crystal structure of SpGH92 in complex with mannose
Authors	:	Shapiro-Ward, S.; Boraston, A.B.
Deposited on	:	2016-08-08
Resolution	:	2.15 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
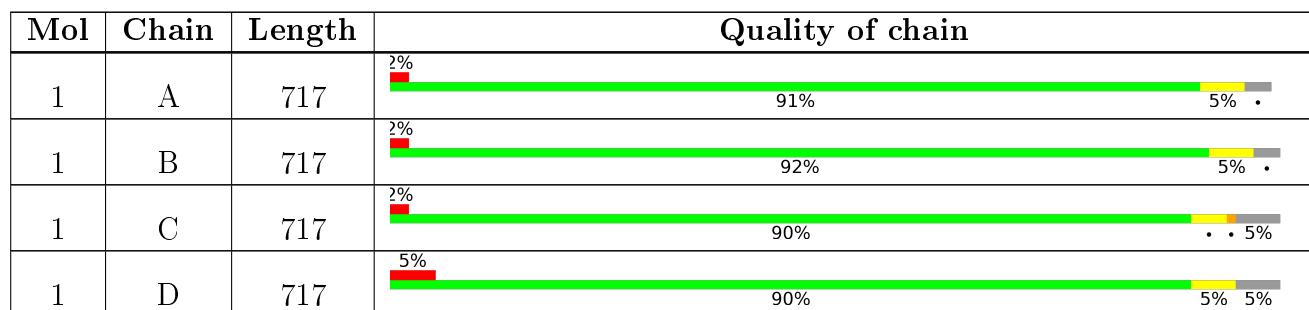
The reported resolution of this entry is 2.15 Å.

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	Percentile Ranks	Value
Rfree		0.228
Clashscore		2
Ramachandran outliers		0.3%
Sidechain outliers		0.8%
RSRZ outliers		2.5%

Worse   *Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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	717	2% · 91% · 5% ·
1	B	717	2% · 92% · 5% ·
1	C	717	2% · 90% · · 5%
1	D	717	5% · 90% · 5% 5%

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
3	GOL	A	702	-	-	-	X
3	GOL	A	703	-	-	-	X
3	GOL	A	704	-	-	-	X
3	GOL	A	706	-	-	-	X
3	GOL	B	702	-	-	-	X
3	GOL	B	704	-	-	-	X
3	GOL	B	705	-	-	-	X
3	GOL	D	702	-	-	-	X

2   Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23499 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 Sugar hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	693	Total	C	N	O	S	0	0	0
			5525	3544	911	1046	24			
1	A	692	Total	C	N	O	S	0	8	0
			5592	3578	924	1064	26			
1	C	680	Total	C	N	O	S	0	1	0
			5438	3489	897	1029	23			
1	D	681	Total	C	N	O	S	0	1	0
			5432	3485	895	1030	22			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	MET	-	initiating methionine	UNP A0A0Y0HIE3
B	-21	GLY	-	expression tag	UNP A0A0Y0HIE3
B	-20	SER	-	expression tag	UNP A0A0Y0HIE3
B	-19	SER	-	expression tag	UNP A0A0Y0HIE3
B	-18	HIS	-	expression tag	UNP A0A0Y0HIE3
B	-17	HIS	-	expression tag	UNP A0A0Y0HIE3
B	-16	HIS	-	expression tag	UNP A0A0Y0HIE3
B	-15	HIS	-	expression tag	UNP A0A0Y0HIE3
B	-14	HIS	-	expression tag	UNP A0A0Y0HIE3
B	-13	HIS	-	expression tag	UNP A0A0Y0HIE3
B	-12	SER	-	expression tag	UNP A0A0Y0HIE3
B	-11	SER	-	expression tag	UNP A0A0Y0HIE3
B	-10	GLY	-	expression tag	UNP A0A0Y0HIE3
B	-9	LEU	-	expression tag	UNP A0A0Y0HIE3
B	-8	VAL	-	expression tag	UNP A0A0Y0HIE3
B	-7	PRO	-	expression tag	UNP A0A0Y0HIE3
B	-6	ARG	-	expression tag	UNP A0A0Y0HIE3
B	-5	GLY	-	expression tag	UNP A0A0Y0HIE3
B	-4	SER	-	expression tag	UNP A0A0Y0HIE3
B	-3	HIS	-	expression tag	UNP A0A0Y0HIE3
B	-2	MET	-	expression tag	UNP A0A0Y0HIE3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ALA	-	expression tag	UNP A0A0Y0HIE3
B	0	SER	-	expression tag	UNP A0A0Y0HIE3
A	-22	MET	-	initiating methionine	UNP A0A0Y0HIE3
A	-21	GLY	-	expression tag	UNP A0A0Y0HIE3
A	-20	SER	-	expression tag	UNP A0A0Y0HIE3
A	-19	SER	-	expression tag	UNP A0A0Y0HIE3
A	-18	HIS	-	expression tag	UNP A0A0Y0HIE3
A	-17	HIS	-	expression tag	UNP A0A0Y0HIE3
A	-16	HIS	-	expression tag	UNP A0A0Y0HIE3
A	-15	HIS	-	expression tag	UNP A0A0Y0HIE3
A	-14	HIS	-	expression tag	UNP A0A0Y0HIE3
A	-13	HIS	-	expression tag	UNP A0A0Y0HIE3
A	-12	SER	-	expression tag	UNP A0A0Y0HIE3
A	-11	SER	-	expression tag	UNP A0A0Y0HIE3
A	-10	GLY	-	expression tag	UNP A0A0Y0HIE3
A	-9	LEU	-	expression tag	UNP A0A0Y0HIE3
A	-8	VAL	-	expression tag	UNP A0A0Y0HIE3
A	-7	PRO	-	expression tag	UNP A0A0Y0HIE3
A	-6	ARG	-	expression tag	UNP A0A0Y0HIE3
A	-5	GLY	-	expression tag	UNP A0A0Y0HIE3
A	-4	SER	-	expression tag	UNP A0A0Y0HIE3
A	-3	HIS	-	expression tag	UNP A0A0Y0HIE3
A	-2	MET	-	expression tag	UNP A0A0Y0HIE3
A	-1	ALA	-	expression tag	UNP A0A0Y0HIE3
A	0	SER	-	expression tag	UNP A0A0Y0HIE3
C	-22	MET	-	initiating methionine	UNP A0A0Y0HIE3
C	-21	GLY	-	expression tag	UNP A0A0Y0HIE3
C	-20	SER	-	expression tag	UNP A0A0Y0HIE3
C	-19	SER	-	expression tag	UNP A0A0Y0HIE3
C	-18	HIS	-	expression tag	UNP A0A0Y0HIE3
C	-17	HIS	-	expression tag	UNP A0A0Y0HIE3
C	-16	HIS	-	expression tag	UNP A0A0Y0HIE3
C	-15	HIS	-	expression tag	UNP A0A0Y0HIE3
C	-14	HIS	-	expression tag	UNP A0A0Y0HIE3
C	-13	HIS	-	expression tag	UNP A0A0Y0HIE3
C	-12	SER	-	expression tag	UNP A0A0Y0HIE3
C	-11	SER	-	expression tag	UNP A0A0Y0HIE3
C	-10	GLY	-	expression tag	UNP A0A0Y0HIE3
C	-9	LEU	-	expression tag	UNP A0A0Y0HIE3
C	-8	VAL	-	expression tag	UNP A0A0Y0HIE3
C	-7	PRO	-	expression tag	UNP A0A0Y0HIE3
C	-6	ARG	-	expression tag	UNP A0A0Y0HIE3

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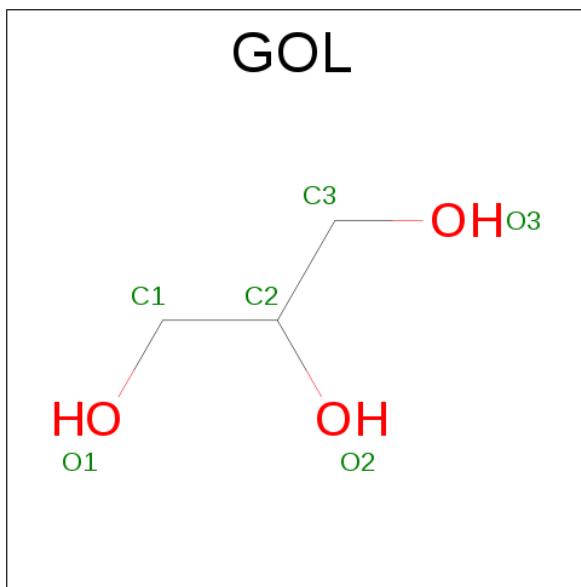
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP A0A0Y0HIE3
C	-4	SER	-	expression tag	UNP A0A0Y0HIE3
C	-3	HIS	-	expression tag	UNP A0A0Y0HIE3
C	-2	MET	-	expression tag	UNP A0A0Y0HIE3
C	-1	ALA	-	expression tag	UNP A0A0Y0HIE3
C	0	SER	-	expression tag	UNP A0A0Y0HIE3
D	-22	MET	-	initiating methionine	UNP A0A0Y0HIE3
D	-21	GLY	-	expression tag	UNP A0A0Y0HIE3
D	-20	SER	-	expression tag	UNP A0A0Y0HIE3
D	-19	SER	-	expression tag	UNP A0A0Y0HIE3
D	-18	HIS	-	expression tag	UNP A0A0Y0HIE3
D	-17	HIS	-	expression tag	UNP A0A0Y0HIE3
D	-16	HIS	-	expression tag	UNP A0A0Y0HIE3
D	-15	HIS	-	expression tag	UNP A0A0Y0HIE3
D	-14	HIS	-	expression tag	UNP A0A0Y0HIE3
D	-13	HIS	-	expression tag	UNP A0A0Y0HIE3
D	-12	SER	-	expression tag	UNP A0A0Y0HIE3
D	-11	SER	-	expression tag	UNP A0A0Y0HIE3
D	-10	GLY	-	expression tag	UNP A0A0Y0HIE3
D	-9	LEU	-	expression tag	UNP A0A0Y0HIE3
D	-8	VAL	-	expression tag	UNP A0A0Y0HIE3
D	-7	PRO	-	expression tag	UNP A0A0Y0HIE3
D	-6	ARG	-	expression tag	UNP A0A0Y0HIE3
D	-5	GLY	-	expression tag	UNP A0A0Y0HIE3
D	-4	SER	-	expression tag	UNP A0A0Y0HIE3
D	-3	HIS	-	expression tag	UNP A0A0Y0HIE3
D	-2	MET	-	expression tag	UNP A0A0Y0HIE3
D	-1	ALA	-	expression tag	UNP A0A0Y0HIE3
D	0	SER	-	expression tag	UNP A0A0Y0HIE3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Ca 1	0	0
2	A	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
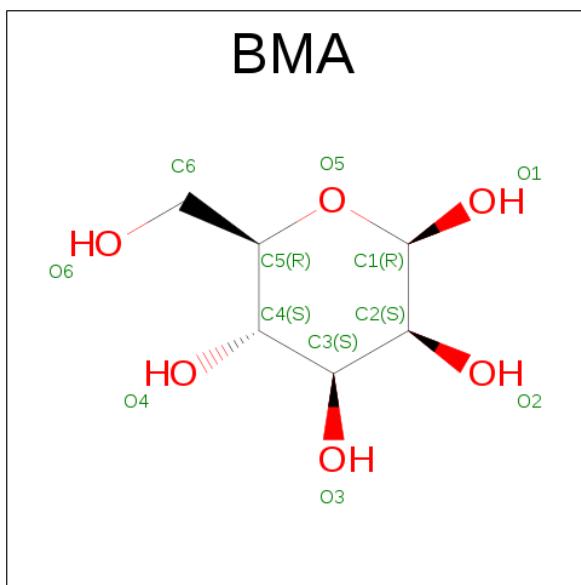
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0

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

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 12	C 6	O 6	0	0
4	A	1	Total 12	C 6	O 6	0	0
4	C	1	Total 12	C 6	O 6	0	0
4	D	1	Total 12	C 6	O 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	363	Total 363	O 363	0	0
5	A	393	Total 393	O 393	0	0
5	C	354	Total 354	O 354	0	0
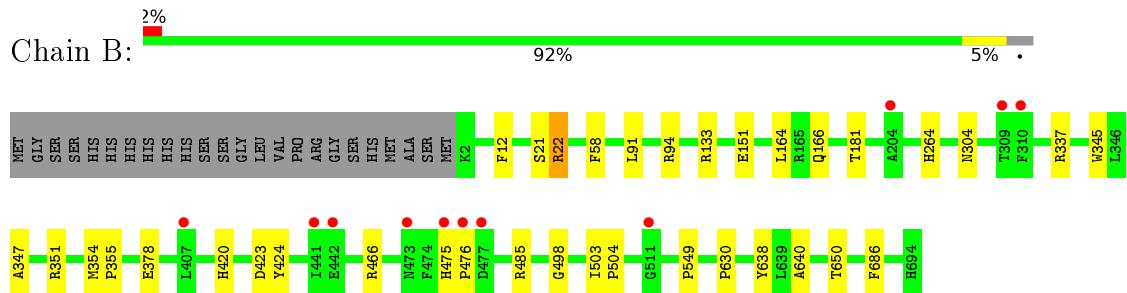
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	254	Total 254	O 254	0	0
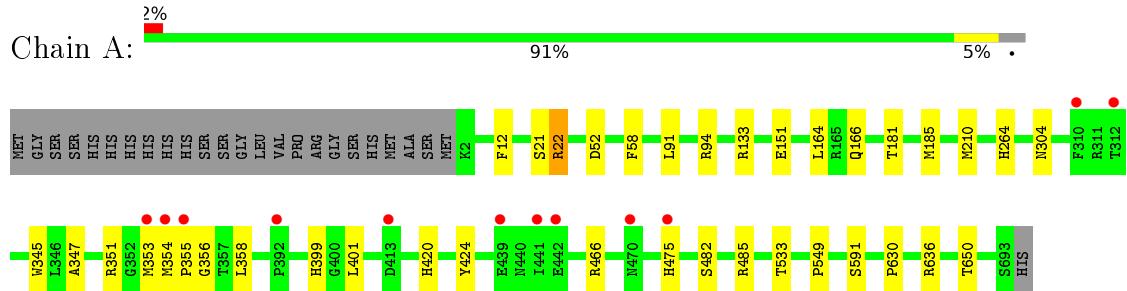
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
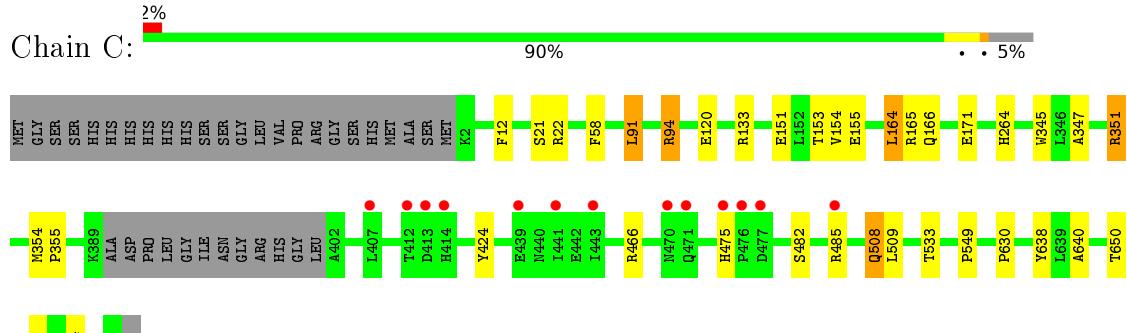
- Molecule 1: Sugar hydrolase

- Molecule 1: Sugar hydrolase
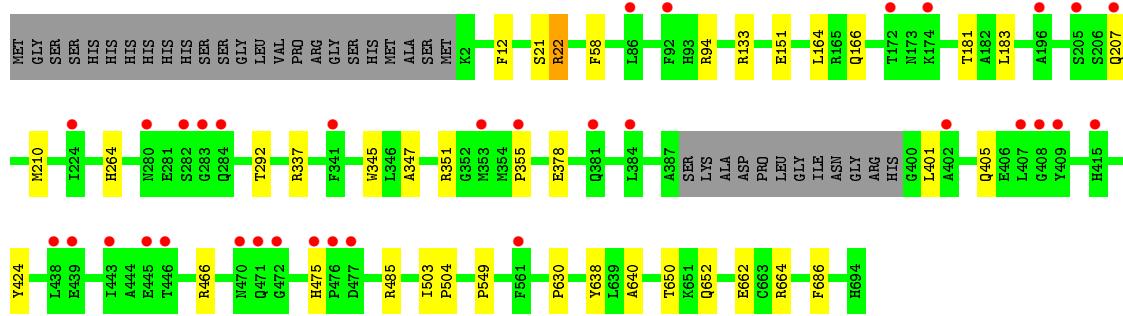
- Molecule 1: Sugar hydrolase

- Molecule 1: Sugar hydrolase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	130.00Å 161.71Å 208.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.76 – 2.15 38.84 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (127.76-2.15) 99.9 (38.84-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 2.16Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.221 0.203 , 0.228	Depositor DCC
R_{free} test set	11855 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.7	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23499	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.49	0/5753	0.65	4/7825 (0.1%)
1	B	0.46	0/5688	0.64	3/7744 (0.0%)
1	C	0.49	0/5597	0.65	5/7620 (0.1%)
1	D	0.47	0/5592	0.62	2/7615 (0.0%)
All	All	0.48	0/22630	0.64	14/30804 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	94	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	91	LEU	CA-CB-CG	5.94	128.96	115.30
1	D	94	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	91	LEU	CA-CB-CG	5.88	128.83	115.30
1	C	91	LEU	CA-CB-CG	5.81	128.67	115.30
1	B	94	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	94	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	164	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	94	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	B	94	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	D	94	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	94	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	52	ASP	CB-CG-OD1	5.15	122.94	118.30
1	C	351	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	5592	0	5290	30	0
1	B	5525	0	5218	17	0
1	C	5438	0	5139	24	1
1	D	5432	0	5109	20	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	42	0	54	1	0
3	B	24	0	30	4	0
3	C	12	0	16	0	0
3	D	18	0	23	0	0
4	A	12	0	12	0	0
4	B	12	0	12	0	0
4	C	12	0	12	0	0
4	D	12	0	12	0	0
5	A	393	0	0	3	0
5	B	363	0	0	1	0
5	C	354	0	0	10	0
5	D	254	0	0	2	0
All	All	23499	0	20927	92	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 2.

All (92) 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:355[B]:PRO:HB3	1:A:420:HIS:CD2	2.25	0.72
1:A:355[B]:PRO:HB3	1:A:420:HIS:HD2	1.54	0.71
1:D:183:LEU:HD13	1:D:210:MET:CE	2.18	0.71
1:C:133:ARG:NH1	5:C:802:HOH:O	2.16	0.69
1:C:120:GLU:OE1	5:C:801:HOH:O	2.11	0.68
1:A:185:MET:HG3	1:A:210:MET:HG2	1.77	0.67
1:A:354[B]:MET:HB3	1:A:355[B]:PRO:CD	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:GLU:OE2	1:C:664:ARG:NH1	2.29	0.66
1:A:354[B]:MET:CB	1:A:355[B]:PRO:CD	2.73	0.64
1:B:420:HIS:NE2	3:B:705:GOL:O1	2.21	0.63
1:B:12:PHE:HB2	1:B:264:HIS:CE1	2.34	0.63
1:D:662:GLU:OE2	1:D:664:ARG:NH1	2.32	0.62
1:C:165:ARG:HD3	5:C:1098:HOH:O	1.99	0.62
1:D:12:PHE:HB2	1:D:264:HIS:CE1	2.35	0.61
1:A:133:ARG:NH1	5:A:801:HOH:O	2.09	0.61
1:A:354[B]:MET:SD	1:A:355[B]:PRO:HD3	2.41	0.61
1:A:354[B]:MET:HB3	1:A:355[B]:PRO:HD2	1.83	0.61
1:A:12:PHE:HB2	1:A:264:HIS:CE1	2.36	0.61
1:C:12:PHE:HB2	1:C:264:HIS:CE1	2.36	0.60
1:A:353[B]:MET:O	1:A:354[B]:MET:HB2	2.02	0.59
1:C:153:THR:CG2	5:C:1140:HOH:O	2.49	0.59
1:A:354[B]:MET:CB	1:A:355[B]:PRO:HD3	2.31	0.58
1:A:591:SER:HB2	3:A:707:GOL:H31	1.86	0.57
1:A:355[A]:PRO:HB3	1:A:399:HIS:CG	2.41	0.55
1:C:482:SER:OG	1:C:533:THR:OG1	2.23	0.53
1:C:153:THR:HG22	5:C:1140:HOH:O	2.10	0.52
1:A:355[A]:PRO:HB3	1:A:399:HIS:CD2	2.44	0.52
1:C:22[B]:ARG:HH11	1:C:22[B]:ARG:HA	1.74	0.52
1:C:355:PRO:HB2	1:C:424:TYR:OH	2.10	0.51
1:C:351:ARG:NH2	5:C:810:HOH:O	2.44	0.50
1:A:355[A]:PRO:HB2	1:A:424:TYR:OH	2.11	0.50
1:A:355[B]:PRO:CB	5:A:826:HOH:O	2.60	0.49
1:D:183:LEU:HD13	1:D:210:MET:HE1	1.93	0.49
1:D:355:PRO:HB2	1:D:424:TYR:OH	2.12	0.49
1:D:466:ARG:NH2	1:D:475:HIS:O	2.46	0.49
1:A:401:LEU:HD12	1:A:401:LEU:H	1.78	0.49
1:B:133:ARG:NH1	5:B:801:HOH:O	2.17	0.48
1:C:466:ARG:NH2	1:C:475:HIS:O	2.46	0.48
1:C:153:THR:HG21	5:C:1140:HOH:O	2.10	0.48
1:B:466:ARG:NH2	1:B:475:HIS:O	2.47	0.48
1:D:652:GLN:HG2	5:D:852:HOH:O	2.14	0.48
1:B:355:PRO:HB2	1:B:424:TYR:OH	2.15	0.47
1:C:153:THR:HG23	5:C:1057:HOH:O	2.14	0.47
1:D:183:LEU:HD22	1:D:210:MET:HE2	1.98	0.46
1:D:21:SER:O	1:D:22:ARG:HD2	2.16	0.46
1:A:356[B]:GLY:HA3	1:A:358:LEU:CD2	2.46	0.45
1:C:171:GLU:HG2	1:C:351:ARG:NH1	2.32	0.45
1:D:133:ARG:NH1	5:D:801:HOH:O	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:SER:O	1:A:22:ARG:HD2	2.17	0.45
1:A:482:SER:OG	1:A:533:THR:OG1	2.24	0.45
1:A:636:ARG:HD3	5:A:912:HOH:O	2.17	0.45
1:C:155:GLU:HG3	5:C:841:HOH:O	2.16	0.45
1:B:21:SER:O	1:B:22:ARG:HD2	2.16	0.45
1:B:630:PRO:HG2	1:B:650:THR:OG1	2.17	0.45
1:C:154:VAL:HG22	1:C:164:LEU:HD22	1.99	0.45
1:C:21:SER:O	1:C:22[B]:ARG:NH1	2.49	0.44
1:A:353[A]:MET:HA	1:A:353[A]:MET:CE	2.47	0.44
1:C:638:TYR:CE2	1:C:640:ALA:HA	2.53	0.44
1:C:508:GLN:HG3	1:C:509:LEU:N	2.33	0.44
1:D:630:PRO:HG2	1:D:650:THR:OG1	2.18	0.44
1:A:151:GLU:O	1:A:166:GLN:HA	2.18	0.43
1:B:151:GLU:O	1:B:166:GLN:HA	2.19	0.43
1:D:151:GLU:O	1:D:166:GLN:HA	2.17	0.43
1:B:347:ALA:HB3	1:B:351:ARG:HG3	2.00	0.43
1:B:423:ASP:OD1	3:B:704:GOL:O2	2.36	0.43
1:C:151:GLU:O	1:C:166:GLN:HA	2.18	0.43
1:C:630:PRO:HG2	1:C:650:THR:OG1	2.18	0.43
1:A:630:PRO:HG2	1:A:650:THR:OG1	2.17	0.43
1:A:466:ARG:NH2	1:A:475:HIS:O	2.52	0.43
1:D:638:TYR:CE2	1:D:640:ALA:HA	2.54	0.43
1:A:164:LEU:HB2	1:A:181:THR:HB	2.01	0.42
1:A:22:ARG:HA	1:A:22:ARG:HD2	1.82	0.42
1:A:347:ALA:HB3	1:A:351:ARG:HG3	2.00	0.42
1:B:475:HIS:CG	1:B:476:PRO:HD2	2.54	0.42
1:A:354[B]:MET:HA	1:A:355[B]:PRO:HD3	1.48	0.42
1:C:347:ALA:HB3	1:C:351:ARG:HG3	2.01	0.42
1:D:164:LEU:HB2	1:D:181:THR:HB	2.01	0.42
1:B:164:LEU:HB2	1:B:181:THR:HB	2.02	0.42
3:B:704:GOL:HO2	3:B:704:GOL:HO1	1.58	0.42
1:B:337:ARG:NH1	1:B:378:GLU:OE2	2.53	0.41
1:B:503:ILE:N	1:B:504:PRO:CD	2.84	0.41
1:D:183:LEU:HB3	1:D:210:MET:HE2	2.01	0.41
1:C:94:ARG:HD2	5:C:1054:HOH:O	2.19	0.41
1:B:638:TYR:CE2	1:B:640:ALA:HA	2.55	0.41
1:B:630:PRO:HG3	1:B:686:PHE:CD1	2.56	0.41
1:D:401:LEU:O	1:D:405:GLN:CG	2.69	0.41
1:B:498:GLY:O	3:B:704:GOL:H32	2.21	0.41
1:D:347:ALA:HB3	1:D:351:ARG:HG3	2.02	0.41
1:D:630:PRO:HG3	1:D:686:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:ILE:N	1:D:504:PRO:CD	2.85	0.40
1:A:354[B]:MET:SD	1:A:355[B]:PRO:CD	3.08	0.40
1:D:337:ARG:NH1	1:D:378:GLU:OE2	2.54	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:C:664:ARG:NH2	1:D:292:THR:O[4_545]	2.09	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	698/717 (97%)	676 (97%)	20 (3%)	2 (0%)	46	42
1	B	691/717 (96%)	674 (98%)	15 (2%)	2 (0%)	46	42
1	C	677/717 (94%)	661 (98%)	14 (2%)	2 (0%)	46	42
1	D	678/717 (95%)	662 (98%)	14 (2%)	2 (0%)	46	42
All	All	2744/2868 (96%)	2673 (97%)	63 (2%)	8 (0%)	46	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	485	ARG
1	A	485	ARG
1	C	485	ARG
1	D	485	ARG
1	B	549	PRO
1	A	549	PRO
1	C	549	PRO

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Mol	Chain	Res	Type
1	D	549	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	595/622 (96%)	591 (99%)	4 (1%)	88	93
1	B	585/622 (94%)	580 (99%)	5 (1%)	84	89
1	C	579/622 (93%)	574 (99%)	5 (1%)	84	89
1	D	575/622 (92%)	571 (99%)	4 (1%)	88	93
All	All	2334/2488 (94%)	2316 (99%)	18 (1%)	86	91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	ARG
1	B	58	PHE
1	B	304	ASN
1	B	345	TRP
1	B	354	MET
1	A	22	ARG
1	A	58	PHE
1	A	304	ASN
1	A	345	TRP
1	C	58	PHE
1	C	91	LEU
1	C	345	TRP
1	C	354	MET
1	C	508	GLN
1	D	22	ARG
1	D	58	PHE
1	D	207	GLN
1	D	345	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	304	ASN
1	D	36	ASN
1	D	207	GLN
1	D	304	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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
3	GOL	A	701	2	5,5,5	0.94	0	5,5,5	1.01	0
3	GOL	A	702	-	5,5,5	0.36	0	5,5,5	0.68	0
3	GOL	A	703	-	5,5,5	0.39	0	5,5,5	0.62	0
3	GOL	A	704	-	5,5,5	0.53	0	5,5,5	0.40	0
3	GOL	A	705	-	5,5,5	0.18	0	5,5,5	0.28	0
3	GOL	A	706	-	5,5,5	0.29	0	5,5,5	0.31	0
3	GOL	A	707	-	5,5,5	0.32	0	5,5,5	0.64	0
4	BMA	A	708	-	12,12,12	0.63	0	17,17,17	1.93	3 (17%)
3	GOL	B	702	2	5,5,5	1.03	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	B	703	-	5,5,5	0.36	0	5,5,5	0.73	0
3	GOL	B	704	-	5,5,5	0.23	0	5,5,5	0.48	0
3	GOL	B	705	-	5,5,5	0.22	0	5,5,5	0.45	0
4	BMA	B	706	-	12,12,12	0.50	0	17,17,17	1.14	2 (11%)
3	GOL	C	701	2	5,5,5	0.25	0	5,5,5	0.73	0
3	GOL	C	702	-	5,5,5	0.49	0	5,5,5	0.75	0
4	BMA	C	703	-	12,12,12	0.54	0	17,17,17	0.89	1 (5%)
3	GOL	D	701	2	5,5,5	0.70	0	5,5,5	0.92	0
3	GOL	D	702	-	5,5,5	0.79	0	5,5,5	0.55	0
3	GOL	D	703	-	5,5,5	0.49	0	5,5,5	0.58	0
4	BMA	D	704	-	12,12,12	0.57	0	17,17,17	1.12	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	701	2	-	0/4/4/4	0/0/0/0
3	GOL	A	702	-	-	0/4/4/4	0/0/0/0
3	GOL	A	703	-	-	0/4/4/4	0/0/0/0
3	GOL	A	704	-	-	0/4/4/4	0/0/0/0
3	GOL	A	705	-	-	0/4/4/4	0/0/0/0
3	GOL	A	706	-	-	0/4/4/4	0/0/0/0
3	GOL	A	707	-	-	0/4/4/4	0/0/0/0
4	BMA	A	708	-	-	0/2/22/22	0/1/1/1
3	GOL	B	702	2	-	0/4/4/4	0/0/0/0
3	GOL	B	703	-	-	0/4/4/4	0/0/0/0
3	GOL	B	704	-	-	0/4/4/4	0/0/0/0
3	GOL	B	705	-	-	0/4/4/4	0/0/0/0
4	BMA	B	706	-	-	0/2/22/22	0/1/1/1
3	GOL	C	701	2	-	0/4/4/4	0/0/0/0
3	GOL	C	702	-	-	0/4/4/4	0/0/0/0
4	BMA	C	703	-	-	0/2/22/22	0/1/1/1
3	GOL	D	701	2	-	0/4/4/4	0/0/0/0
3	GOL	D	702	-	-	0/4/4/4	0/0/0/0
3	GOL	D	703	-	-	0/4/4/4	0/0/0/0
4	BMA	D	704	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	706	BMA	O5-C1-C2	-2.66	105.35	110.00
4	C	703	BMA	O3-C3-C2	-2.51	104.71	110.36
4	B	706	BMA	C1-O5-C5	-2.36	109.02	113.54
4	D	704	BMA	O3-C3-C2	-2.04	105.75	110.36
4	D	704	BMA	C3-C4-C5	2.76	115.15	110.23
4	A	708	BMA	O1-C1-O5	2.82	118.17	110.33
4	A	708	BMA	O5-C1-C2	3.58	116.27	110.00
4	A	708	BMA	O1-C1-C2	4.96	122.77	109.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	707	GOL	1	0
3	B	704	GOL	3	0
3	B	705	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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, 95th 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	692/717 (96%)	-0.16	12 (1%)	73	80	18, 30, 49, 72	0
1	B	693/717 (96%)	-0.15	11 (1%)	74	81	22, 33, 55, 84	0
1	C	680/717 (94%)	-0.02	13 (1%)	70	78	19, 33, 59, 81	0
1	D	681/717 (94%)	0.26	34 (4%)	32	43	21, 40, 62, 86	0
All	All	2746/2868 (95%)	-0.02	70 (2%)	61	69	18, 34, 57, 86	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355[A]	PRO	6.5
1	A	354[A]	MET	5.3
1	A	353[A]	MET	4.5
1	D	471	GLN	4.3
1	C	477	ASP	4.0
1	C	476	PRO	3.9
1	C	475	HIS	3.8
1	C	443	ILE	3.8
1	D	355	PRO	3.8
1	D	402	ALA	3.8
1	D	384	LEU	3.7
1	D	282	SER	3.6
1	D	477	ASP	3.6
1	B	473	ASN	3.6
1	D	472	GLY	3.5
1	B	476	PRO	3.4
1	D	476	PRO	3.3
1	A	441	ILE	3.3
1	C	485	ARG	3.2
1	A	475	HIS	3.1
1	D	172	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	353	MET	3.1
1	D	174	LYS	3.1
1	D	407	LEU	3.0
1	D	283	GLY	3.0
1	D	196	ALA	3.0
1	C	471	GLN	2.9
1	C	441	ILE	2.9
1	D	446	THR	2.8
1	D	443	ILE	2.8
1	C	414	HIS	2.8
1	D	470	ASN	2.8
1	D	439	GLU	2.8
1	D	475	HIS	2.8
1	B	477	ASP	2.7
1	A	442	GLU	2.6
1	C	413	ASP	2.6
1	D	381	GLN	2.6
1	D	561	PHE	2.6
1	C	470	ASN	2.6
1	D	415	HIS	2.5
1	A	470	ASN	2.5
1	C	412	THR	2.5
1	B	309	THR	2.5
1	B	475	HIS	2.5
1	D	86	LEU	2.4
1	C	407	LEU	2.4
1	A	392	PRO	2.4
1	A	310	PHE	2.4
1	D	341	PHE	2.3
1	D	408	GLY	2.3
1	D	92	PHE	2.3
1	D	409	TYR	2.3
1	D	445	GLU	2.3
1	C	439	GLU	2.3
1	A	439	GLU	2.2
1	B	442	GLU	2.2
1	B	441	ILE	2.2
1	B	511	GLY	2.2
1	B	310	PHE	2.2
1	D	284	GLN	2.1
1	D	438	LEU	2.1
1	D	205	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	280	ASN	2.1
1	D	224	ILE	2.1
1	A	413	ASP	2.1
1	B	407	LEU	2.0
1	B	204	ALA	2.0
1	A	312	THR	2.0
1	D	207	GLN	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors($Å^2$)	Q<0.9
3	GOL	B	705	6/6	0.86	0.33	9.90	51,59,62,62	0
3	GOL	A	706	6/6	0.91	0.23	7.84	54,58,59,60	0
3	GOL	A	703	6/6	0.92	0.16	3.27	37,42,44,46	0
3	GOL	A	702	6/6	0.88	0.30	3.22	40,40,41,42	0
3	GOL	B	704	6/6	0.88	0.31	3.17	46,50,52,54	0
3	GOL	B	702	6/6	0.80	0.29	3.09	35,40,43,44	0
3	GOL	D	702	6/6	0.74	0.20	2.65	47,51,52,56	0
3	GOL	A	704	6/6	0.86	0.17	2.33	51,52,53,54	0
3	GOL	A	705	6/6	0.86	0.14	1.61	60,62,63,65	0
3	GOL	B	703	6/6	0.94	0.14	1.55	45,47,50,54	0
3	GOL	C	701	6/6	0.91	0.19	1.27	35,45,50,53	0
3	GOL	D	701	6/6	0.89	0.18	0.62	36,40,43,45	0
4	BMA	C	703	12/12	0.92	0.12	0.51	31,37,38,43	0
3	GOL	A	701	6/6	0.90	0.23	0.30	28,34,35,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
3	GOL	D	703	6/6	0.86	0.16	0.26	55,60,60,62	0
2	CA	A	709	1/1	0.99	0.14	-0.19	17,17,17,17	0
4	BMA	A	708	12/12	0.92	0.12	-0.38	27,33,35,39	0
3	GOL	C	702	6/6	0.94	0.10	-0.87	42,45,47,48	0
2	CA	D	705	1/1	0.97	0.12	-0.92	27,27,27,27	0
4	BMA	B	706	12/12	0.93	0.09	-1.17	36,43,46,48	0
4	BMA	D	704	12/12	0.93	0.09	-1.18	38,42,44,46	0
2	CA	B	701	1/1	0.99	0.14	-1.28	23,23,23,23	0
2	CA	C	704	1/1	0.99	0.10	-2.13	24,24,24,24	0
3	GOL	A	707	6/6	0.82	0.21	-	54,57,58,62	0

6.5 Other polymers (i)

There are no such residues in this entry.