



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:05 PM UTC

PDB ID : 5SWI / pdb_00005swi
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)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

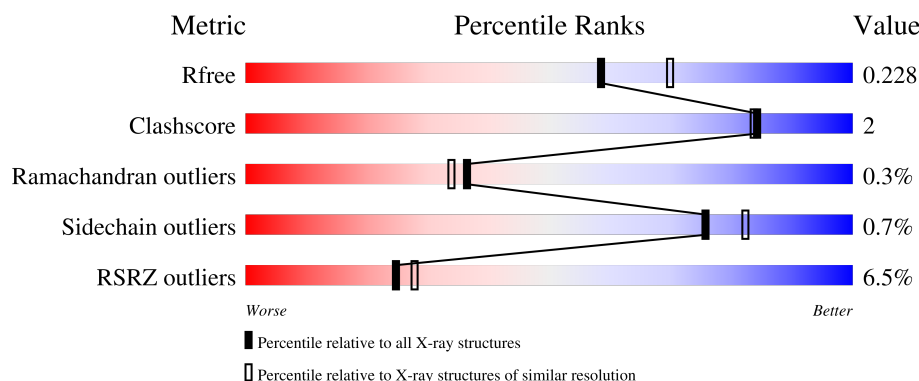
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 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 $\leq 5\%$. 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	717	 3% 91% 5% •
1	B	717	 4% 92% 5% •
1	C	717	 7% 89% 5% 5%
1	D	717	 11% 90% 5% 5%

2 Entry composition

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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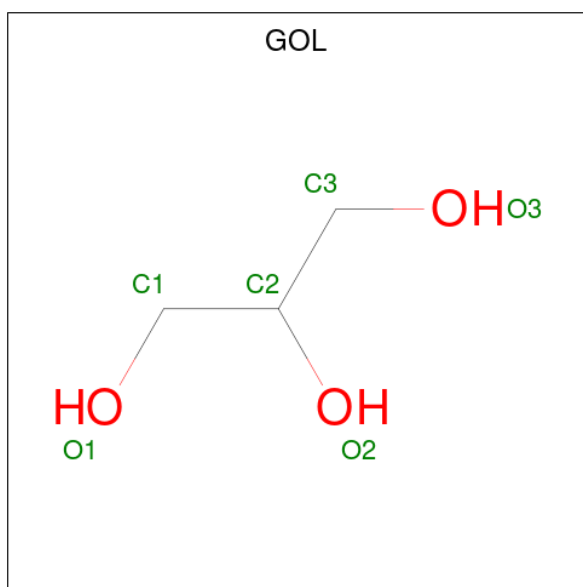
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP A0A0Y0HIE3
C	-4	SER	-	expression tag	UNP A0A0Y0HIE3
C	-3	HIS	-	expression tag	UNP A0A0Y0HIE3
C	-2	MET	-	expression tag	UNP A0A0Y0HIE3
C	-1	ALA	-	expression tag	UNP A0A0Y0HIE3
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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



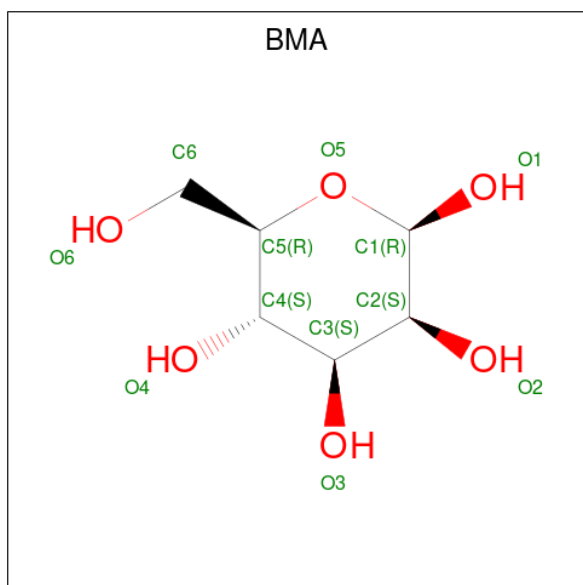
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total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

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

- Molecule 4 is beta-D-mannopyranose (CCD ID: BMA) (formula: C₆H₁₂O₆).



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

- Molecule 5 is water.

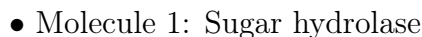
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	363	Total	O	0	0
			363	363		
5	A	393	Total	O	0	0
			393	393		
5	C	354	Total	O	0	0
			354	354		

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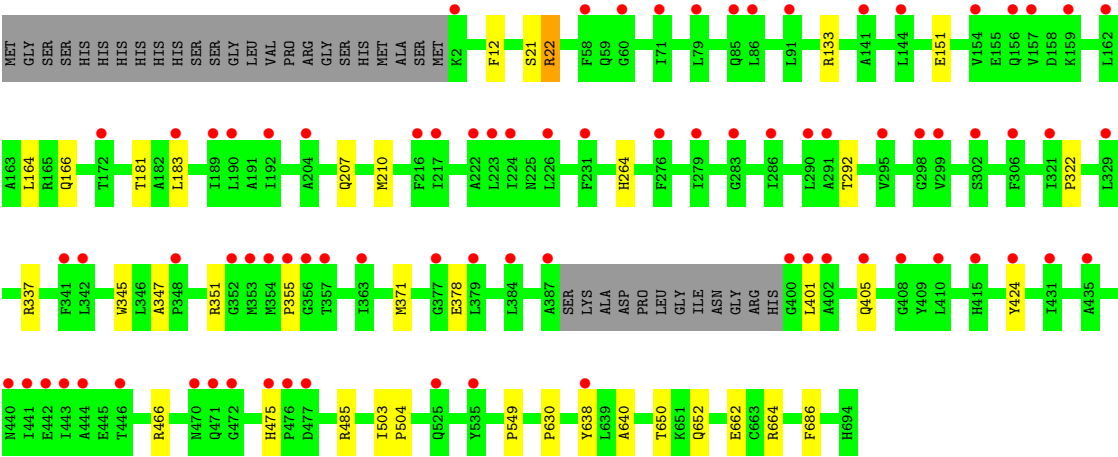
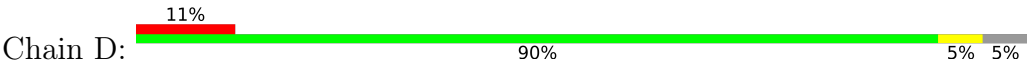
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	254	Total 254	O 254	0	0

- Molecule 1: Sugar hydrolase





● Molecule 1: Sugar hydrolase



4 Data and refinement statistics

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 – 2.15 127.76 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (127.76-2.15) 99.9 (127.76-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.99%)	wwPDB-VP
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 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.64	0/5753	0.74	0/7825
1	B	0.60	0/5688	0.73	0/7744
1	C	0.64	0/5597	0.74	0/7620
1	D	0.63	0/5592	0.73	0/7615
All	All	0.63	0/22630	0.73	0/30804

There are no bond length outliers.

There are no bond angle outliers.

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	33	0
1	B	5525	0	5218	18	0
1	C	5438	0	5139	26	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	30	3	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	97	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 (97) 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:C:510:MET:HE1	1:C:519:TYR:CD2	2.17	0.78
1:D:183:LEU:HD22	1:D:210:MET:HE2	1.69	0.74
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
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:HB3	1:A:355[B]:PRO:HD2	1.83	0.61
1:A:354[B]:MET:SD	1:A:355[B]:PRO:HD3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:THR:CG2	5:C:1140:HOH:O	2.49	0.59
1:D:183:LEU:HD13	1:D:210:MET:HE1	1.85	0.58
1:A:354[B]:MET:CB	1:A:355[B]:PRO:HD3	2.31	0.58
1:A:353[A]:MET:HA	1:A:353[A]:MET:HE3	1.85	0.57
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:D:322:PRO:HB3	1:D:371:MET:HE1	1.89	0.54
1:A:322:PRO:HB3	1:A:371:MET:HE1	1.90	0.54
1:B:322:PRO:HB3	1:B:371:MET:HE1	1.90	0.53
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:C:322:PRO:HB3	1:C:371:MET:HE1	1.91	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: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:H	1:A:401:LEU:HD12	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: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
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:C:638:TYR:CE2	1:C:640:ALA:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:151:GLU:O	1:B:166:GLN:HA	2.19	0.43
1:A:151:GLU:O	1:A:166:GLN:HA	2.18	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:22:ARG:HD2	1:A:22:ARG:HA	1.82	0.42
1:A:164:LEU:HB2	1:A:181:THR:HB	2.01	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:353[A]:MET:HA	1:A:353[A]:MET:CE	2.47	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
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: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
1:D:503:ILE:N	1:D:504:PRO:CD	2.85	0.40
1:A:21:SER:C	1:A:22:ARG:HD2	2.46	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%)	36	34
1	B	691/717 (96%)	674 (98%)	15 (2%)	2 (0%)	36	34
1	C	677/717 (94%)	661 (98%)	14 (2%)	2 (0%)	36	34
1	D	678/717 (95%)	662 (98%)	14 (2%)	2 (0%)	36	34
All	All	2744/2868 (96%)	2673 (97%)	63 (2%)	8 (0%)	36	34

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
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%)	590 (99%)	5 (1%)	73	79
1	B	585/622 (94%)	580 (99%)	5 (1%)	70	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	579/622 (93%)	575 (99%)	4 (1%)	76	82
1	D	575/622 (92%)	572 (100%)	3 (0%)	81	87
All	All	2334/2488 (94%)	2317 (99%)	17 (1%)	76	82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	ARG
1	B	91	LEU
1	B	167	GLU
1	B	304	ASN
1	B	345	TRP
1	A	22	ARG
1	A	91	LEU
1	A	304	ASN
1	A	345	TRP
1	A	401	LEU
1	C	91	LEU
1	C	304	ASN
1	C	345	TRP
1	C	508	GLN
1	D	22	ARG
1	D	207	GLN
1	D	345	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	166	GLN
1	B	184	GLN
1	B	221	GLN
1	B	674	GLN
1	A	166	GLN
1	A	184	GLN
1	A	221	GLN
1	A	475	HIS
1	A	674	GLN
1	C	166	GLN
1	C	184	GLN
1	C	304	ASN

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Mol	Chain	Res	Type
1	C	324	HIS
1	C	674	GLN
1	D	166	GLN
1	D	184	GLN
1	D	207	GLN
1	D	221	GLN
1	D	304	ASN
1	D	324	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	BMA	D	704	-	12,12,12	0.58	0	17,17,17	1.09	1 (5%)
3	GOL	A	707	-	5,5,5	0.37	0	5,5,5	0.70	0
3	GOL	B	704	-	5,5,5	0.25	0	5,5,5	0.60	0
4	BMA	B	706	-	12,12,12	0.53	0	17,17,17	1.14	2 (11%)
3	GOL	A	702	-	5,5,5	0.39	0	5,5,5	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	702	-	5,5,5	0.55	0	5,5,5	0.81	0
3	GOL	A	706	-	5,5,5	0.34	0	5,5,5	0.35	0
3	GOL	B	703	-	5,5,5	0.43	0	5,5,5	0.78	0
4	BMA	A	708	-	12,12,12	0.69	0	17,17,17	1.83	3 (17%)
3	GOL	A	701	2	5,5,5	1.02	0	5,5,5	1.13	0
3	GOL	C	701	2	5,5,5	0.29	0	5,5,5	0.83	0
3	GOL	B	702	2	5,5,5	1.10	0	5,5,5	1.01	0
3	GOL	A	704	-	5,5,5	0.60	0	5,5,5	0.34	0
3	GOL	A	705	-	5,5,5	0.22	0	5,5,5	0.35	0
3	GOL	D	703	-	5,5,5	0.54	0	5,5,5	0.60	0
3	GOL	D	701	2	5,5,5	0.77	0	5,5,5	1.00	0
3	GOL	D	702	-	5,5,5	0.85	0	5,5,5	0.52	0
3	GOL	B	705	-	5,5,5	0.27	0	5,5,5	0.52	0
4	BMA	C	703	-	12,12,12	0.51	0	17,17,17	0.84	1 (5%)
3	GOL	A	703	-	5,5,5	0.43	0	5,5,5	0.73	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	BMA	D	704	-	-	0/2/22/22	0/1/1/1
3	GOL	A	707	-	-	3/4/4/4	-
3	GOL	B	704	-	-	3/4/4/4	-
4	BMA	B	706	-	-	2/2/22/22	0/1/1/1
3	GOL	A	702	-	-	0/4/4/4	-
3	GOL	C	702	-	-	2/4/4/4	-
3	GOL	A	706	-	-	3/4/4/4	-
3	GOL	B	703	-	-	2/4/4/4	-
4	BMA	A	708	-	-	0/2/22/22	0/1/1/1
3	GOL	A	701	2	-	2/4/4/4	-
3	GOL	C	701	2	-	4/4/4/4	-
3	GOL	B	702	2	-	2/4/4/4	-
3	GOL	A	704	-	-	3/4/4/4	-
3	GOL	A	705	-	-	1/4/4/4	-
3	GOL	D	703	-	-	2/4/4/4	-
3	GOL	D	701	2	-	2/4/4/4	-
3	GOL	D	702	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	705	-	-	2/4/4/4	-
4	BMA	C	703	-	-	0/2/22/22	0/1/1/1
3	GOL	A	703	-	-	2/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	708	BMA	O1-C1-C2	4.75	122.77	108.98
4	A	708	BMA	O5-C1-C2	3.39	116.27	110.30
4	B	706	BMA	O5-C1-C2	-2.81	105.35	110.30
4	D	704	BMA	C3-C4-C5	2.71	115.15	110.23
4	A	708	BMA	O1-C1-O5	2.61	118.17	110.41
4	C	703	BMA	O3-C3-C2	-2.40	104.71	110.38
4	B	706	BMA	C1-O5-C5	-2.39	109.02	113.65

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	GOL	C1-C2-C3-O3
3	B	704	GOL	C1-C2-C3-O3
3	B	704	GOL	O2-C2-C3-O3
3	A	703	GOL	O1-C1-C2-O2
3	A	703	GOL	O1-C1-C2-C3
3	A	704	GOL	C1-C2-C3-O3
3	A	707	GOL	C1-C2-C3-O3
3	C	701	GOL	O1-C1-C2-C3
3	C	701	GOL	C1-C2-C3-O3
3	D	701	GOL	O1-C1-C2-C3
3	D	703	GOL	C1-C2-C3-O3
3	C	701	GOL	O2-C2-C3-O3
4	B	706	BMA	C4-C5-C6-O6
3	B	703	GOL	C1-C2-C3-O3
3	B	705	GOL	C1-C2-C3-O3
3	A	704	GOL	O1-C1-C2-C3
3	A	706	GOL	O1-C1-C2-C3
3	C	702	GOL	O1-C1-C2-C3
3	B	705	GOL	O2-C2-C3-O3
3	A	704	GOL	O2-C2-C3-O3
3	C	701	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	701	GOL	O1-C1-C2-O2
3	B	702	GOL	O2-C2-C3-O3
3	A	707	GOL	O2-C2-C3-O3
3	D	703	GOL	O2-C2-C3-O3
4	B	706	BMA	O5-C5-C6-O6
3	A	706	GOL	O1-C1-C2-O2
3	B	703	GOL	O2-C2-C3-O3
3	B	704	GOL	O1-C1-C2-O2
3	A	701	GOL	O2-C2-C3-O3
3	A	705	GOL	O1-C1-C2-O2
3	A	701	GOL	C1-C2-C3-O3
3	C	702	GOL	O1-C1-C2-O2
3	A	706	GOL	O2-C2-C3-O3
3	A	707	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	707	GOL	1	0
3	B	704	GOL	2	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

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, 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%)	0.01	18 (2%) 57 61	13, 30, 49, 72	8 (1%)
1	B	693/717 (96%)	0.19	27 (3%) 43 48	22, 33, 55, 84	0
1	C	680/717 (94%)	0.48	53 (7%) 19 21	14, 33, 59, 81	1 (0%)
1	D	681/717 (94%)	0.90	80 (11%) 9 10	19, 40, 62, 86	1 (0%)
All	All	2746/2868 (95%)	0.39	178 (6%) 25 28	13, 34, 57, 86	10 (0%)

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353[A]	MET	8.0
1	A	355[A]	PRO	7.1
1	A	354[A]	MET	4.7
1	D	159	LYS	4.6
1	D	355	PRO	4.5
1	D	401	LEU	4.4
1	C	444	ALA	4.0
1	A	476	PRO	3.9
1	B	357	THR	3.9
1	D	192	ILE	3.9
1	B	356	GLY	3.9
1	C	402	ALA	3.8
1	D	295	VAL	3.7
1	D	217	ILE	3.7
1	D	357	THR	3.7
1	C	669	LEU	3.6
1	B	401	LEU	3.6
1	C	471	GLN	3.6
1	D	471	GLN	3.6
1	D	353	MET	3.6
1	D	400	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	384	LEU	3.5
1	A	475	HIS	3.4
1	B	402	ALA	3.3
1	B	414	HIS	3.3
1	D	387	ALA	3.3
1	C	354	MET	3.3
1	D	189	ILE	3.3
1	C	624	SER	3.2
1	A	693	SER	3.2
1	C	389	LYS	3.2
1	D	475	HIS	3.1
1	D	354	MET	3.1
1	C	22[A]	ARG	3.1
1	D	444	ALA	3.0
1	D	352	GLY	3.0
1	D	440	ASN	3.0
1	B	354	MET	3.0
1	C	353	MET	3.0
1	C	450	ALA	3.0
1	C	693	SER	3.0
1	A	477	ASP	3.0
1	D	402	ALA	2.9
1	C	438	LEU	2.9
1	D	441	ILE	2.9
1	C	415	HIS	2.9
1	A	470	ASN	2.9
1	D	341	PHE	2.9
1	C	449	ALA	2.9
1	D	470	ASN	2.8
1	D	91	LEU	2.8
1	D	85	GLN	2.8
1	C	477	ASP	2.8
1	D	283	GLY	2.8
1	C	373	PRO	2.8
1	C	408	GLY	2.8
1	B	405	GLN	2.7
1	B	525	GLN	2.7
1	D	216	PHE	2.7
1	C	460	ALA	2.7
1	C	407	LEU	2.7
1	D	231	PHE	2.7
1	C	442	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	395	ILE	2.7
1	D	356	GLY	2.7
1	B	399	HIS	2.6
1	C	475	HIS	2.6
1	B	440	ASN	2.6
1	B	473	ASN	2.6
1	B	397	GLY	2.6
1	D	222	ALA	2.6
1	D	363	ILE	2.6
1	B	463	GLY	2.6
1	B	282	SER	2.5
1	D	190	LEU	2.5
1	C	458	PHE	2.5
1	D	154	VAL	2.5
1	C	424	TYR	2.5
1	D	446	THR	2.5
1	B	470	ASN	2.5
1	C	445	GLU	2.5
1	D	442	GLU	2.5
1	A	392	PRO	2.5
1	C	367	ALA	2.5
1	B	393	LEU	2.5
1	B	407	LEU	2.5
1	D	183	LEU	2.5
1	D	290	LEU	2.5
1	A	352[A]	GLY	2.5
1	A	441	ILE	2.5
1	D	424	TYR	2.4
1	D	348	PRO	2.4
1	C	510	MET	2.4
1	D	204	ALA	2.4
1	A	393	LEU	2.4
1	D	2	LYS	2.4
1	D	162	LEU	2.4
1	D	60	GLY	2.4
1	D	298	GLY	2.4
1	C	381	GLN	2.4
1	D	431	ILE	2.4
1	D	443	ILE	2.4
1	B	355	PRO	2.4
1	C	384	LEU	2.4
1	D	79	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	408	GLY	2.4
1	D	286	ILE	2.4
1	D	535	TYR	2.4
1	D	223	LEU	2.4
1	A	440	ASN	2.4
1	B	458	PHE	2.4
1	A	399	HIS	2.4
1	B	406	GLU	2.3
1	C	440	ASN	2.3
1	C	448	LYS	2.3
1	C	443	ILE	2.3
1	D	321	ILE	2.3
1	D	415	HIS	2.3
1	C	405	GLN	2.3
1	C	505	GLY	2.3
1	C	621	GLY	2.3
1	D	525	GLN	2.3
1	B	475	HIS	2.3
1	D	58	PHE	2.3
1	B	476	PRO	2.3
1	D	477	ASP	2.3
1	C	377	GLY	2.3
1	D	144	LEU	2.3
1	D	342	LEU	2.3
1	C	447	TYR	2.3
1	C	406	GLU	2.2
1	D	156	GLN	2.2
1	C	435	ALA	2.2
1	D	329	LEU	2.2
1	C	427	SER	2.2
1	D	276	PHE	2.2
1	C	439	GLU	2.2
1	D	226	LEU	2.2
1	D	410	LEU	2.2
1	D	306	PHE	2.2
1	D	472	GLY	2.2
1	C	86	LEU	2.2
1	D	172	THR	2.2
1	D	476	PRO	2.1
1	C	380	PHE	2.1
1	A	397	GLY	2.1
1	A	669	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	383	MET	2.1
1	C	409	TYR	2.1
1	D	638	TYR	2.1
1	B	477	ASP	2.1
1	C	374	ASP	2.1
1	C	462	THR	2.1
1	A	194	GLN	2.1
1	C	478	PHE	2.1
1	D	279	ILE	2.1
1	D	405	GLN	2.1
1	D	157	VAL	2.1
1	D	377	GLY	2.1
1	D	141	ALA	2.1
1	D	435	ALA	2.1
1	C	375	LEU	2.1
1	D	302	SER	2.1
1	D	379	LEU	2.1
1	B	508	GLN	2.1
1	C	484	GLY	2.1
1	C	525	GLN	2.1
1	C	446	THR	2.1
1	B	511	GLY	2.1
1	A	394	GLY	2.1
1	D	71	ILE	2.1
1	D	224	ILE	2.1
1	D	299	VAL	2.1
1	D	291	ALA	2.1
1	D	86	LEU	2.0
1	C	414	HIS	2.0
1	B	2	LYS	2.0
1	C	485	ARG	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
3	GOL	D	702	6/6	0.76	0.20	47,51,52,56	0
3	GOL	A	707	6/6	0.78	0.16	54,57,58,62	0
3	GOL	B	702	6/6	0.80	0.19	35,40,43,44	0
3	GOL	B	704	6/6	0.81	0.17	46,50,52,54	0
3	GOL	D	703	6/6	0.81	0.20	55,60,60,62	0
3	GOL	A	704	6/6	0.85	0.15	51,52,53,54	0
3	GOL	D	701	6/6	0.86	0.15	36,40,43,45	0
3	GOL	A	705	6/6	0.87	0.19	60,62,63,65	0
3	GOL	A	701	6/6	0.88	0.14	28,34,35,38	0
3	GOL	A	702	6/6	0.89	0.13	40,40,41,42	0
3	GOL	B	705	6/6	0.91	0.14	51,59,62,62	0
3	GOL	A	706	6/6	0.91	0.13	54,58,59,60	0
3	GOL	B	703	6/6	0.92	0.14	45,47,50,54	0
3	GOL	A	703	6/6	0.92	0.17	37,42,44,46	0
3	GOL	C	701	6/6	0.92	0.14	35,45,50,53	0
4	BMA	B	706	12/12	0.92	0.09	36,43,46,48	0
4	BMA	A	708	12/12	0.92	0.09	27,33,35,39	0
4	BMA	D	704	12/12	0.93	0.09	38,42,44,46	0
3	GOL	C	702	6/6	0.94	0.09	42,45,47,48	0
4	BMA	C	703	12/12	0.95	0.07	31,37,38,43	0
2	CA	D	705	1/1	0.98	0.03	27,27,27,27	0
2	CA	C	704	1/1	0.99	0.02	24,24,24,24	0
2	CA	A	709	1/1	0.99	0.03	17,17,17,17	0
2	CA	B	701	1/1	1.00	0.02	23,23,23,23	0

6.5 Other polymers

There are no such residues in this entry.