Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 11:20 PM EDT

PDB ID	:	6EDW
Title	:	Crystal structure of Mycobacterium tuberculosis ICL2 in the apo form
Authors	:	Bashiri, G.; Bhusal, R.; Leung, I.
Deposited on	:	2018-08-12
Resolution	:	1.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

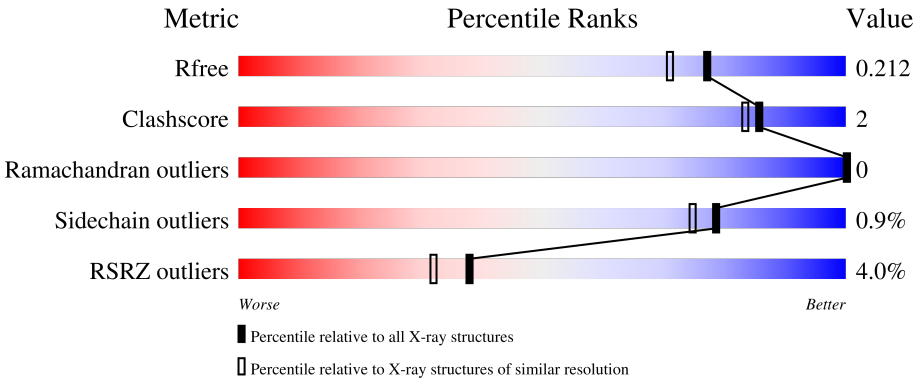
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	786	5% 89% 5% 6%
1	B	786	% 90% 5% 5%
1	C	786	7% 88% • 8%
1	D	786	2% 89% 6% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26840 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 Isocitrate lyase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	742	Total	C	N	O	S	0	6	0
			5877	3709	1052	1094	22			
1	B	746	Total	C	N	O	S	0	5	0
			5885	3714	1050	1099	22			
1	C	724	Total	C	N	O	S	0	5	0
			5710	3607	1020	1061	22			
1	D	741	Total	C	N	O	S	0	6	0
			5863	3700	1053	1088	22			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8VJU4
A	-18	GLY	-	expression tag	UNP Q8VJU4
A	-17	SER	-	expression tag	UNP Q8VJU4
A	-16	SER	-	expression tag	UNP Q8VJU4
A	-15	HIS	-	expression tag	UNP Q8VJU4
A	-14	HIS	-	expression tag	UNP Q8VJU4
A	-13	HIS	-	expression tag	UNP Q8VJU4
A	-12	HIS	-	expression tag	UNP Q8VJU4
A	-11	HIS	-	expression tag	UNP Q8VJU4
A	-10	HIS	-	expression tag	UNP Q8VJU4
A	-9	SER	-	expression tag	UNP Q8VJU4
A	-8	SER	-	expression tag	UNP Q8VJU4
A	-7	GLY	-	expression tag	UNP Q8VJU4
A	-6	LEU	-	expression tag	UNP Q8VJU4
A	-5	VAL	-	expression tag	UNP Q8VJU4
A	-4	PRO	-	expression tag	UNP Q8VJU4
A	-3	ARG	-	expression tag	UNP Q8VJU4
A	-2	GLY	-	expression tag	UNP Q8VJU4
A	-1	SER	-	expression tag	UNP Q8VJU4
A	0	HIS	-	expression tag	UNP Q8VJU4
B	-19	MET	-	initiating methionine	UNP Q8VJU4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q8VJU4
B	-17	SER	-	expression tag	UNP Q8VJU4
B	-16	SER	-	expression tag	UNP Q8VJU4
B	-15	HIS	-	expression tag	UNP Q8VJU4
B	-14	HIS	-	expression tag	UNP Q8VJU4
B	-13	HIS	-	expression tag	UNP Q8VJU4
B	-12	HIS	-	expression tag	UNP Q8VJU4
B	-11	HIS	-	expression tag	UNP Q8VJU4
B	-10	HIS	-	expression tag	UNP Q8VJU4
B	-9	SER	-	expression tag	UNP Q8VJU4
B	-8	SER	-	expression tag	UNP Q8VJU4
B	-7	GLY	-	expression tag	UNP Q8VJU4
B	-6	LEU	-	expression tag	UNP Q8VJU4
B	-5	VAL	-	expression tag	UNP Q8VJU4
B	-4	PRO	-	expression tag	UNP Q8VJU4
B	-3	ARG	-	expression tag	UNP Q8VJU4
B	-2	GLY	-	expression tag	UNP Q8VJU4
B	-1	SER	-	expression tag	UNP Q8VJU4
B	0	HIS	-	expression tag	UNP Q8VJU4
C	-19	MET	-	initiating methionine	UNP Q8VJU4
C	-18	GLY	-	expression tag	UNP Q8VJU4
C	-17	SER	-	expression tag	UNP Q8VJU4
C	-16	SER	-	expression tag	UNP Q8VJU4
C	-15	HIS	-	expression tag	UNP Q8VJU4
C	-14	HIS	-	expression tag	UNP Q8VJU4
C	-13	HIS	-	expression tag	UNP Q8VJU4
C	-12	HIS	-	expression tag	UNP Q8VJU4
C	-11	HIS	-	expression tag	UNP Q8VJU4
C	-10	HIS	-	expression tag	UNP Q8VJU4
C	-9	SER	-	expression tag	UNP Q8VJU4
C	-8	SER	-	expression tag	UNP Q8VJU4
C	-7	GLY	-	expression tag	UNP Q8VJU4
C	-6	LEU	-	expression tag	UNP Q8VJU4
C	-5	VAL	-	expression tag	UNP Q8VJU4
C	-4	PRO	-	expression tag	UNP Q8VJU4
C	-3	ARG	-	expression tag	UNP Q8VJU4
C	-2	GLY	-	expression tag	UNP Q8VJU4
C	-1	SER	-	expression tag	UNP Q8VJU4
C	0	HIS	-	expression tag	UNP Q8VJU4
D	-19	MET	-	initiating methionine	UNP Q8VJU4
D	-18	GLY	-	expression tag	UNP Q8VJU4
D	-17	SER	-	expression tag	UNP Q8VJU4

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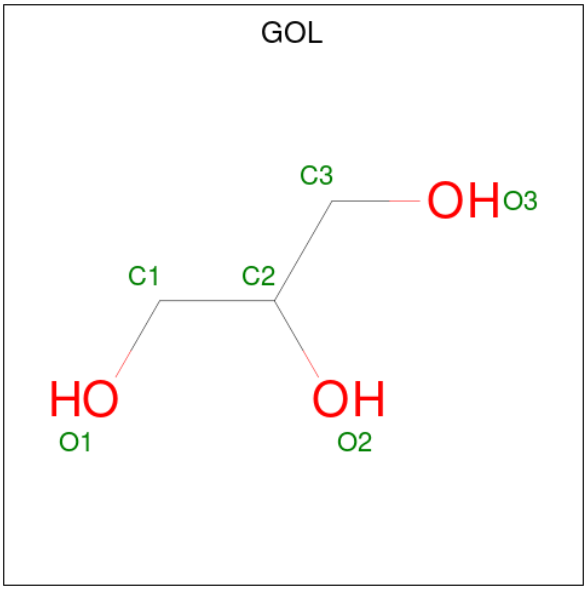
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q8VJU4
D	-15	HIS	-	expression tag	UNP Q8VJU4
D	-14	HIS	-	expression tag	UNP Q8VJU4
D	-13	HIS	-	expression tag	UNP Q8VJU4
D	-12	HIS	-	expression tag	UNP Q8VJU4
D	-11	HIS	-	expression tag	UNP Q8VJU4
D	-10	HIS	-	expression tag	UNP Q8VJU4
D	-9	SER	-	expression tag	UNP Q8VJU4
D	-8	SER	-	expression tag	UNP Q8VJU4
D	-7	GLY	-	expression tag	UNP Q8VJU4
D	-6	LEU	-	expression tag	UNP Q8VJU4
D	-5	VAL	-	expression tag	UNP Q8VJU4
D	-4	PRO	-	expression tag	UNP Q8VJU4
D	-3	ARG	-	expression tag	UNP Q8VJU4
D	-2	GLY	-	expression tag	UNP Q8VJU4
D	-1	SER	-	expression tag	UNP Q8VJU4
D	0	HIS	-	expression tag	UNP Q8VJU4

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

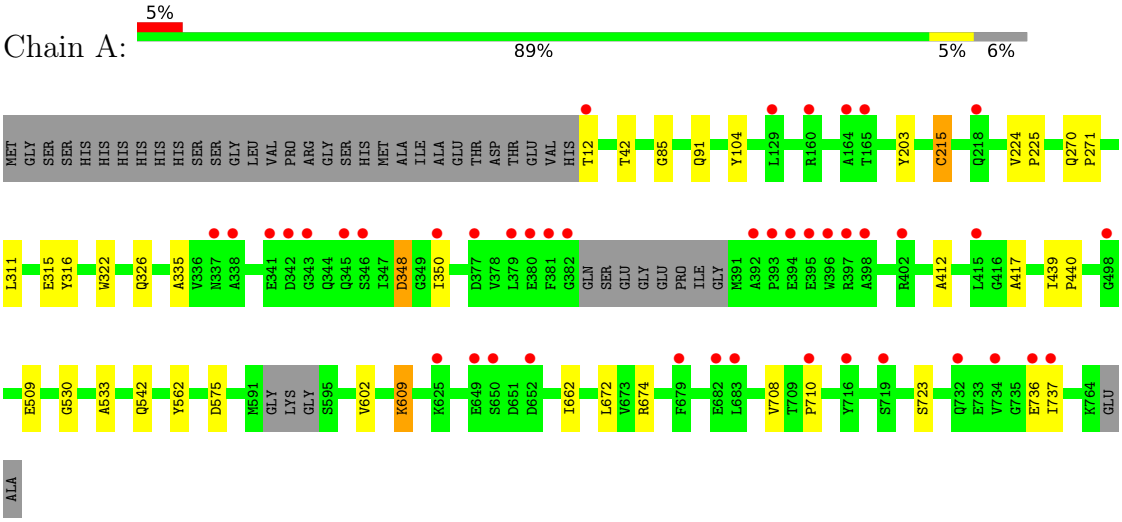
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	804	Total O 804 804	0	0
4	B	986	Total O 986 986	0	0
4	C	791	Total O 791 791	0	0
4	D	887	Total O 887 887	0	0

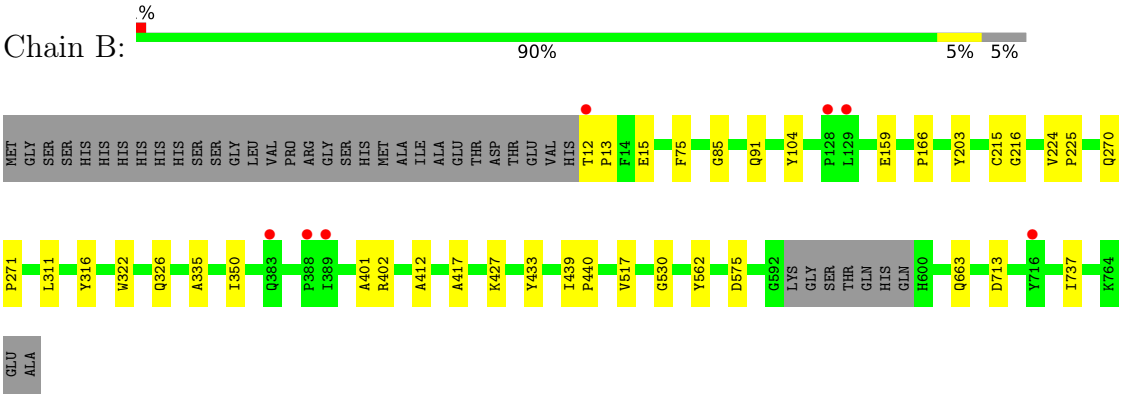
3 Residue-property plots (i)

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

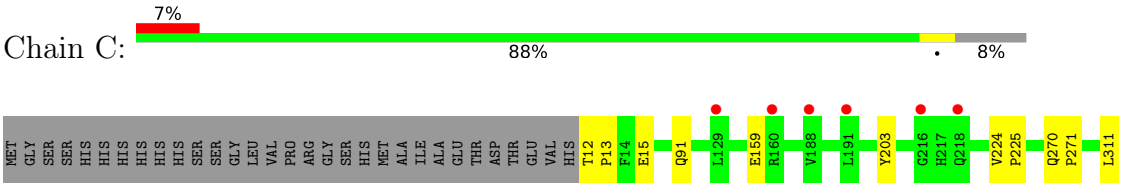
• Molecule 1: Isocitrate lyase 2

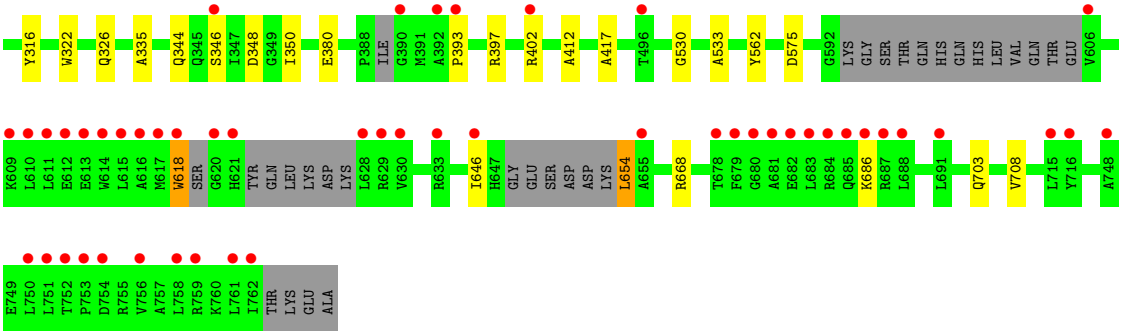


• Molecule 1: Isocitrate lyase 2

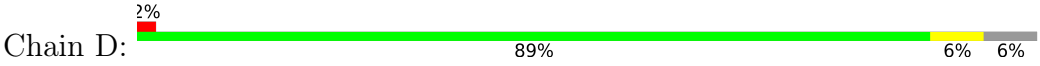


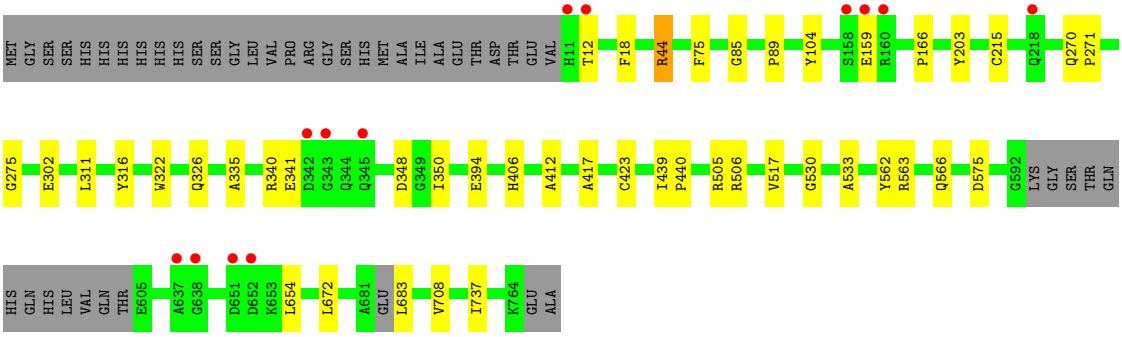
• Molecule 1: Isocitrate lyase 2





• Molecule 1: Isocitrate lyase 2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.82Å 136.08Å 138.92Å 90.00° 99.59° 90.00°	Depositor
Resolution (Å)	48.32 – 1.80 48.27 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.32-1.80) 99.9 (48.27-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.168 , 0.203 0.181 , 0.212	Depositor DCC
R_{free} test set	16234 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26840	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.36	0/6011	0.52	0/8136
1	B	0.37	0/6014	0.54	0/8142
1	C	0.37	0/5833	0.53	0/7893
1	D	0.39	0/5992	0.54	0/8108
All	All	0.37	0/23850	0.54	0/32279

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

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	5877	0	5797	30	0
1	B	5885	0	5796	28	0
1	C	5710	0	5618	31	0
1	D	5863	0	5778	43	0
2	A	12	0	16	0	0
2	C	12	0	16	1	0
2	D	6	0	8	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	804	0	0	4	0
4	B	986	0	0	4	0
4	C	791	0	0	4	0
4	D	887	0	0	6	0
All	All	26840	0	23029	104	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 2.

All (104) 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:B:575[B]:ASP:OD1	1:D:215[B]:CSX:HB3	1.53	1.08
1:C:618:TRP:HZ3	1:C:686:LYS:O	1.37	1.06
1:C:618:TRP:CZ3	1:C:686:LYS:O	2.20	0.95
1:A:215[A]:CSX:HB3	1:C:575[A]:ASP:OD1	1.74	0.86
1:D:505[A]:ARG:HH22	1:D:506[A]:ARG:HH22	1.24	0.86
1:C:618:TRP:CH2	1:C:686:LYS:HB3	2.14	0.81
1:D:505[A]:ARG:HH22	1:D:506[A]:ARG:NH2	1.78	0.81
1:C:668:ARG:HD2	1:C:703:GLN:HG2	1.63	0.79
1:B:215[B]:CSX:HB3	1:D:575[B]:ASP:OD1	1.83	0.78
1:C:618:TRP:HH2	1:C:686:LYS:HB3	1.50	0.76
1:A:737:ILE:HD11	1:D:708:VAL:CG1	2.23	0.68
1:A:737:ILE:HD11	1:D:708:VAL:HG11	1.75	0.67
1:D:412:ALA:HB1	1:D:417:ALA:O	1.96	0.66
1:C:397:ARG:NH1	4:C:902:HOH:O	2.30	0.63
1:C:380:GLU:OE2	1:C:397:ARG:NH2	2.33	0.60
1:D:566:GLN:HG3	4:D:1089:HOH:O	2.03	0.59
1:B:216:GLY:N	1:D:566:GLN:HE22	2.01	0.58
1:C:159:GLU:CD	1:D:12:THR:HG21	2.23	0.58
1:C:646:ILE:O	1:C:654:LEU:HB3	2.04	0.58
1:A:708:VAL:HA	1:A:737:ILE:HD12	1.87	0.57
1:B:427:LYS:HD3	1:B:433:TYR:CZ	2.41	0.56
1:D:505[A]:ARG:NH2	1:D:506[A]:ARG:NH2	2.51	0.56
1:C:344:GLN:NE2	4:C:907:HOH:O	2.38	0.55
1:D:505[B]:ARG:NH1	4:D:909:HOH:O	2.38	0.55
1:B:166:PRO:HA	4:B:1008:HOH:O	2.06	0.55
1:B:737:ILE:HD11	1:C:708:VAL:HB	1.89	0.55
1:A:609:LYS:HD3	4:A:1391:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:VAL:HA	1:A:737:ILE:CD1	2.38	0.53
1:B:663:GLN:NE2	4:B:909:HOH:O	2.36	0.53
1:B:12:THR:OG1	1:B:13:PRO:HD2	2.09	0.53
1:C:618:TRP:CH2	1:C:686:LYS:CB	2.91	0.52
1:C:12:THR:OG1	1:C:13:PRO:HD2	2.10	0.51
1:C:393:PRO:O	1:C:397:ARG:HG3	2.11	0.51
1:B:575[B]:ASP:OD1	1:D:215[B]:CSX:CB	2.43	0.51
1:C:159:GLU:HG2	1:D:12:THR:HG21	1.94	0.50
1:A:710:PRO:HG3	1:A:736:GLU:HB3	1.93	0.49
1:C:335:ALA:HB1	1:C:350:ILE:CG2	2.43	0.49
1:A:42:THR:CG2	1:D:302:GLU:HB2	2.42	0.49
1:B:322:TRP:CE2	1:B:326:GLN:HG3	2.48	0.49
4:B:1021:HOH:O	1:D:89:PRO:HB2	2.13	0.48
1:D:505[A]:ARG:NH2	4:D:923:HOH:O	2.46	0.48
1:B:75:PHE:HB2	1:B:517:VAL:HG11	1.95	0.48
1:B:575[B]:ASP:CG	1:D:215[B]:CSX:HB3	2.29	0.48
1:A:602:VAL:HG23	4:A:1468:HOH:O	2.13	0.48
1:A:322:TRP:CE2	1:A:326:GLN:HG3	2.49	0.48
1:D:394:GLU:HG2	4:D:1417:HOH:O	2.14	0.47
1:B:562:TYR:CZ	1:D:530:GLY:HA3	2.49	0.47
1:D:322:TRP:CE2	1:D:326:GLN:HG3	2.49	0.47
1:A:530:GLY:HA3	1:C:562:TYR:CZ	2.50	0.47
1:A:737:ILE:HD11	1:D:708:VAL:HG13	1.96	0.47
1:B:12:THR:HG23	1:B:15:GLU:H	1.78	0.47
1:C:12:THR:HG23	1:C:15:GLU:H	1.78	0.47
1:D:166:PRO:HA	4:D:992:HOH:O	2.13	0.47
1:B:412:ALA:HB1	1:B:417:ALA:O	2.15	0.47
1:C:322:TRP:CE2	1:C:326:GLN:HG3	2.50	0.47
1:A:412:ALA:HB1	1:A:417:ALA:O	2.16	0.46
1:D:75:PHE:HB2	1:D:517:VAL:HG11	1.98	0.46
1:A:335:ALA:HB1	1:A:350:ILE:CG2	2.46	0.46
1:B:216:GLY:N	1:D:566:GLN:NE2	2.65	0.45
1:A:42:THR:HG21	1:D:302:GLU:HB2	1.98	0.45
1:A:348:ASP:OD2	1:D:44:ARG:NH2	2.49	0.45
1:B:216:GLY:H	1:D:566:GLN:HE22	1.65	0.45
1:D:340:ARG:NH2	4:D:912:HOH:O	2.40	0.45
1:A:662:ILE:HD13	1:A:672:LEU:HD12	1.98	0.45
1:A:542:GLN:HG3	4:A:1409:HOH:O	2.16	0.45
1:B:401:ALA:O	4:B:901:HOH:O	2.21	0.44
1:B:530:GLY:HA3	1:D:562:TYR:CZ	2.53	0.44
1:A:270:GLN:N	1:A:271:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:LEU:HB3	1:B:316:TYR:CE2	2.53	0.43
1:C:270:GLN:N	1:C:271:PRO:CD	2.81	0.43
1:C:412:ALA:HB1	1:C:417:ALA:O	2.18	0.43
1:D:270:GLN:N	1:D:271:PRO:CD	2.81	0.43
2:C:802:GOL:H32	1:D:18:PHE:HA	1.99	0.43
1:A:562:TYR:CZ	1:C:530:GLY:HA3	2.54	0.43
1:C:350:ILE:HD13	4:C:1078:HOH:O	2.17	0.43
1:A:311:LEU:HB3	1:A:316:TYR:CE2	2.54	0.42
1:C:224:VAL:HB	1:C:225:PRO:HD2	2.01	0.42
1:B:270:GLN:N	1:B:271:PRO:CD	2.82	0.42
1:C:159:GLU:CG	1:D:12:THR:HG21	2.49	0.42
1:D:335:ALA:HB1	1:D:350:ILE:CG2	2.49	0.42
1:A:91:GLN:HG2	1:C:533:ALA:HB2	2.01	0.42
1:D:311:LEU:HB3	1:D:316:TYR:CE2	2.55	0.42
1:B:224:VAL:HB	1:B:225:PRO:HD2	2.00	0.42
1:A:224:VAL:HB	1:A:225:PRO:HD2	2.02	0.42
1:A:439:ILE:N	1:A:440:PRO:CD	2.83	0.42
1:A:85:GLY:HA2	1:A:104:TYR:O	2.21	0.41
1:A:533:ALA:HB2	1:C:91:GLN:HG2	2.01	0.41
1:D:439:ILE:N	1:D:440:PRO:CD	2.84	0.41
1:C:311:LEU:HB3	1:C:316:TYR:CE2	2.55	0.41
1:A:674:ARG:NH2	1:D:737:ILE:HD11	2.35	0.41
1:B:335:ALA:HB1	1:B:350:ILE:CG2	2.51	0.41
1:D:654:LEU:HB3	1:D:683:LEU:CD1	2.50	0.41
1:A:509:GLU:HB2	4:A:908:HOH:O	2.21	0.41
1:C:393:PRO:HB3	4:C:1473:HOH:O	2.21	0.41
1:D:85:GLY:HA2	1:D:104:TYR:O	2.21	0.41
1:B:439:ILE:N	1:B:440:PRO:CD	2.84	0.40
1:B:85:GLY:HA2	1:B:104:TYR:O	2.21	0.40
1:B:91:GLN:HG2	1:D:533:ALA:HB2	2.03	0.40
1:C:12:THR:HG21	1:D:159:GLU:OE1	2.20	0.40
1:A:12:THR:HG21	1:B:159:GLU:OE2	2.22	0.40
1:D:275:GLY:HA2	1:D:423:CYS:HA	2.04	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	741/786 (94%)	734 (99%)	7 (1%)	0	100	100
1	B	745/786 (95%)	736 (99%)	9 (1%)	0	100	100
1	C	715/786 (91%)	708 (99%)	7 (1%)	0	100	100
1	D	739/786 (94%)	732 (99%)	7 (1%)	0	100	100
All	All	2940/3144 (94%)	2910 (99%)	30 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	603/631 (96%)	598 (99%)	5 (1%)	81	78
1	B	602/631 (95%)	599 (100%)	3 (0%)	88	87
1	C	581/631 (92%)	575 (99%)	6 (1%)	76	71
1	D	598/631 (95%)	590 (99%)	8 (1%)	69	62
All	All	2384/2524 (94%)	2362 (99%)	22 (1%)	78	75

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	TYR
1	A	315	GLU

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Mol	Chain	Res	Type
1	A	348	ASP
1	A	609	LYS
1	A	723	SER
1	B	203	TYR
1	B	402	ARG
1	B	713	ASP
1	C	203	TYR
1	C	346	SER
1	C	348	ASP
1	C	402	ARG
1	C	618	TRP
1	C	654	LEU
1	D	44	ARG
1	D	203	TYR
1	D	341	GLU
1	D	348	ASP
1	D	406[A]	HIS
1	D	406[B]	HIS
1	D	563	ARG
1	D	672	LEU

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

Mol	Chain	Res	Type
1	D	566	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CSX	B	215[A]	-	3,6,7	0.80	0	1,6,8	1.93	0
1	CSX	D	215[A]	-	3,6,7	0.59	0	1,6,8	1.95	0
1	CSX	C	215[B]	-	3,6,7	0.74	0	1,6,8	0.00	0
1	CSX	B	215[B]	-	3,6,7	0.79	0	1,6,8	0.59	0
1	CSX	D	215[B]	-	3,6,7	0.73	0	1,6,8	1.16	0
1	CSX	A	215[A]	-	3,6,7	0.71	0	1,6,8	2.04	1 (100%)
1	CSX	C	215[A]	-	3,6,7	0.74	0	1,6,8	1.49	0
1	CSX	A	215[B]	-	3,6,7	0.72	0	1,6,8	0.02	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
1	CSX	B	215[A]	-	-	0/1/5/7	-
1	CSX	D	215[A]	-	-	0/1/5/7	-
1	CSX	C	215[B]	-	-	0/1/5/7	-
1	CSX	B	215[B]	-	-	0/1/5/7	-
1	CSX	D	215[B]	-	-	0/1/5/7	-
1	CSX	A	215[A]	-	-	0/1/5/7	-
1	CSX	C	215[A]	-	-	0/1/5/7	-
1	CSX	A	215[B]	-	-	0/1/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	215[A]	CSX	CA-CB-SG	-2.04	108.89	113.36

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
1	B	215[B]	CSX	1	0
1	D	215[B]	CSX	3	0
1	A	215[A]	CSX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
2	GOL	A	802	-	5,5,5	0.36	0	5,5,5	0.56	0
2	GOL	C	802	-	5,5,5	0.29	0	5,5,5	0.40	0
2	GOL	C	801	-	5,5,5	0.43	0	5,5,5	0.27	0
2	GOL	A	801	-	5,5,5	0.27	0	5,5,5	0.39	0
2	GOL	D	801	-	5,5,5	0.32	0	5,5,5	0.25	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
2	GOL	A	802	-	-	0/4/4/4	-
2	GOL	C	802	-	-	2/4/4/4	-
2	GOL	C	801	-	-	0/4/4/4	-
2	GOL	A	801	-	-	0/4/4/4	-
2	GOL	D	801	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	802	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	C	802	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	802	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	741/786 (94%)	0.06	43 (5%) 23 18	13, 28, 64, 95	0
1	B	745/786 (94%)	-0.24	7 (0%) 84 82	13, 23, 52, 86	0
1	C	723/786 (91%)	0.16	56 (7%) 13 10	12, 25, 70, 108	0
1	D	740/786 (94%)	-0.18	13 (1%) 68 64	13, 24, 54, 86	0
All	All	2949/3144 (93%)	-0.05	119 (4%) 38 32	12, 24, 60, 108	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	618	TRP	6.4
1	A	381	PHE	6.3
1	C	616	ALA	5.9
1	A	734	VAL	5.9
1	C	685	GLN	5.7
1	C	615	LEU	5.4
1	B	389	ILE	5.0
1	C	620	GLY	4.6
1	D	160	ARG	4.4
1	C	683	LEU	4.3
1	C	609	LYS	4.1
1	C	682	GLU	4.0
1	C	628	LEU	4.0
1	C	684	ARG	3.8
1	C	762	ILE	3.8
1	A	393	PRO	3.8
1	A	341	GLU	3.8
1	C	610	LEU	3.7
1	A	392	ALA	3.7
1	A	382	GLY	3.7
1	B	12	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	680	GLY	3.6
1	A	343	GLY	3.6
1	C	761	LEU	3.6
1	A	716	TYR	3.5
1	A	379	LEU	3.5
1	C	681	ALA	3.5
1	A	160	ARG	3.5
1	A	346[A]	SER	3.5
1	C	688	LEU	3.4
1	A	719	SER	3.3
1	C	218	GLN	3.3
1	C	393	PRO	3.3
1	C	679	PHE	3.2
1	C	686	LYS	3.2
1	C	629	ARG	3.2
1	A	402	ARG	3.1
1	A	415	LEU	3.1
1	C	606	VAL	3.1
1	C	691	LEU	3.0
1	A	164	ALA	3.0
1	A	380	GLU	3.0
1	C	646	ILE	3.0
1	B	716	TYR	3.0
1	C	687	ARG	3.0
1	C	614	TRP	3.0
1	A	345	GLN	2.9
1	A	394	GLU	2.9
1	C	756	VAL	2.9
1	A	338	ALA	2.8
1	C	758	LEU	2.8
1	C	716	TYR	2.8
1	C	346	SER	2.8
1	D	345	GLN	2.8
1	C	655	ALA	2.7
1	C	750	LEU	2.7
1	A	342	ASP	2.7
1	C	390	GLY	2.7
1	C	392	ALA	2.6
1	A	710	PRO	2.6
1	C	759	ARG	2.6
1	A	679	PHE	2.6
1	C	633	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	682	GLU	2.5
1	C	129	LEU	2.5
1	D	218	GLN	2.5
1	B	388	PRO	2.5
1	D	343	GLY	2.5
1	D	158	SER	2.5
1	C	612	GLU	2.5
1	C	751	LEU	2.5
1	B	129	LEU	2.5
1	A	625	LYS	2.4
1	A	683	LEU	2.4
1	D	651	ASP	2.4
1	D	638	GLY	2.4
1	A	395	GLU	2.4
1	C	754	ASP	2.4
1	A	736	GLU	2.4
1	C	630	VAL	2.3
1	A	737	ILE	2.3
1	C	617	MET	2.3
1	D	342	ASP	2.3
1	D	637	ALA	2.3
1	C	752	THR	2.3
1	A	129	LEU	2.3
1	C	611	LEU	2.3
1	A	649	GLU	2.3
1	A	396	TRP	2.3
1	A	165	THR	2.3
1	C	191	LEU	2.3
1	A	377	ASP	2.3
1	C	188	VAL	2.2
1	A	350	ILE	2.2
1	C	613	GLU	2.2
1	C	715	LEU	2.2
1	A	397	ARG	2.2
1	A	12	THR	2.2
1	C	621	HIS	2.2
1	D	11	HIS	2.2
1	C	216	GLY	2.2
1	A	732	GLN	2.2
1	B	383	GLN	2.1
1	C	402	ARG	2.1
1	D	12	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	398	ALA	2.1
1	C	748	ALA	2.1
1	A	337	ASN	2.1
1	A	218	GLN	2.1
1	C	496	THR	2.1
1	C	753	PRO	2.1
1	C	160	ARG	2.0
1	C	678	THR	2.0
1	D	159	GLU	2.0
1	D	652	ASP	2.0
1	B	128	PRO	2.0
1	A	498	GLY	2.0
1	A	652	ASP	2.0
1	A	650	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSX	D	215[A]	7/8	0.88	0.16	28,34,39,39	4
1	CSX	D	215[B]	7/8	0.88	0.16	28,34,39,39	4
1	CSX	A	215[A]	7/8	0.90	0.13	26,38,44,52	4
1	CSX	A	215[B]	7/8	0.90	0.13	29,31,38,38	4
1	CSX	C	215[A]	7/8	0.91	0.11	40,41,47,50	4
1	CSX	C	215[B]	7/8	0.91	0.11	33,37,40,50	4
1	CSX	B	215[A]	7/8	0.94	0.09	25,32,39,42	4
1	CSX	B	215[B]	7/8	0.94	0.09	24,29,33,34	4

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	804	1/1	0.86	0.26	30,30,30,30	0
2	GOL	C	801	6/6	0.90	0.30	34,51,60,61	0
3	MG	A	804	1/1	0.92	0.28	30,30,30,30	0
2	GOL	A	802	6/6	0.95	0.15	25,37,38,43	0
2	GOL	A	801	6/6	0.95	0.15	25,40,41,45	0
3	MG	D	803	1/1	0.95	0.16	30,30,30,30	0
2	GOL	D	801	6/6	0.96	0.14	25,36,39,49	0
2	GOL	C	802	6/6	0.96	0.13	24,31,37,40	0
3	MG	A	803	1/1	0.98	0.10	21,21,21,21	0
3	MG	B	801	1/1	0.99	0.03	20,20,20,20	0
3	MG	D	802	1/1	0.99	0.04	23,23,23,23	0
3	MG	C	803	1/1	0.99	0.10	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.