Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 05:40 PM JST

PDB ID	:	5GOR
Title	:	Crystal structure of alkaline invertase InvA from Anabaena sp. PCC 7120
Authors	:	Xie, J.; Cai, K.; Hu, H.X.; Jiang, Y.L.; Yang, F.; Hu, P.F.; Chen, Y.; Zhou, C.Z.
Deposited on	:	2016-07-28
Resolution	:	2.67 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 (i)) were used in the production of this report:

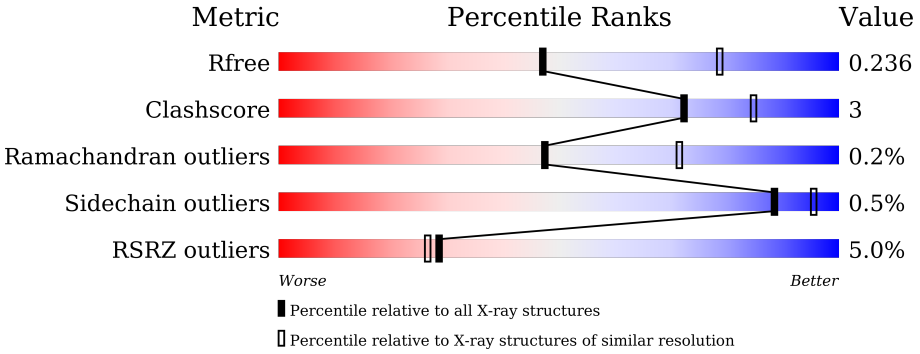
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	476	5% 88% 8% ·
1	B	476	6% 87% 9% ·
1	C	476	4% 87% 9% ·
1	D	476	5% 85% 11% ·
1	E	476	4% 88% 8% ·
1	F	476	6% 88% 8% ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22286 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 Alkaline Invertase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	457	3666	2380	610	657	19	0	0	0
1	B	457	3666	2380	610	657	19	0	0	0
1	C	457	3666	2380	610	657	19	0	0	0
1	D	455	3652	2371	608	654	19	0	0	0
1	E	457	3677	2390	611	657	19	0	1	0
1	F	457	3666	2380	610	657	19	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q8YWS9
A	-6	GLY	-	expression tag	UNP Q8YWS9
A	-5	HIS	-	expression tag	UNP Q8YWS9
A	-4	HIS	-	expression tag	UNP Q8YWS9
A	-3	HIS	-	expression tag	UNP Q8YWS9
A	-2	HIS	-	expression tag	UNP Q8YWS9
A	-1	HIS	-	expression tag	UNP Q8YWS9
A	0	HIS	-	expression tag	UNP Q8YWS9
B	-7	MET	-	expression tag	UNP Q8YWS9
B	-6	GLY	-	expression tag	UNP Q8YWS9
B	-5	HIS	-	expression tag	UNP Q8YWS9
B	-4	HIS	-	expression tag	UNP Q8YWS9
B	-3	HIS	-	expression tag	UNP Q8YWS9
B	-2	HIS	-	expression tag	UNP Q8YWS9
B	-1	HIS	-	expression tag	UNP Q8YWS9
B	0	HIS	-	expression tag	UNP Q8YWS9
C	-7	MET	-	expression tag	UNP Q8YWS9

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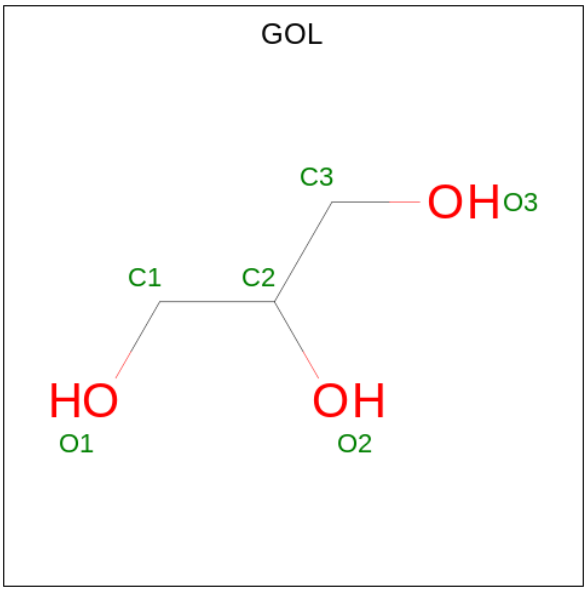
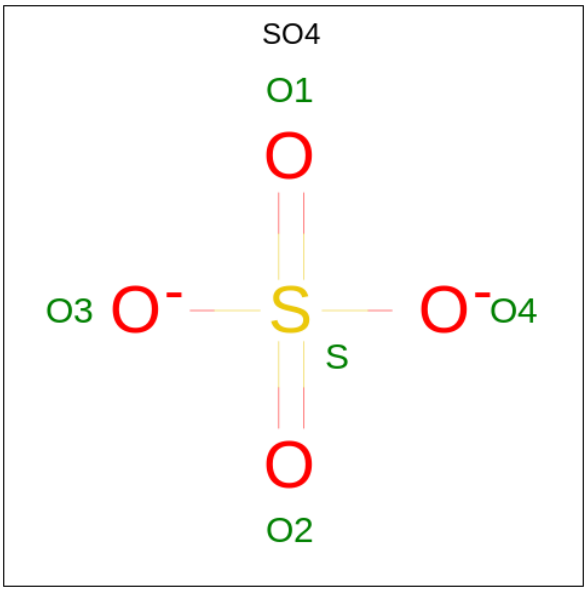
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	expression tag	UNP Q8YWS9
C	-5	HIS	-	expression tag	UNP Q8YWS9
C	-4	HIS	-	expression tag	UNP Q8YWS9
C	-3	HIS	-	expression tag	UNP Q8YWS9
C	-2	HIS	-	expression tag	UNP Q8YWS9
C	-1	HIS	-	expression tag	UNP Q8YWS9
C	0	HIS	-	expression tag	UNP Q8YWS9
D	-7	MET	-	expression tag	UNP Q8YWS9
D	-6	GLY	-	expression tag	UNP Q8YWS9
D	-5	HIS	-	expression tag	UNP Q8YWS9
D	-4	HIS	-	expression tag	UNP Q8YWS9
D	-3	HIS	-	expression tag	UNP Q8YWS9
D	-2	HIS	-	expression tag	UNP Q8YWS9
D	-1	HIS	-	expression tag	UNP Q8YWS9
D	0	HIS	-	expression tag	UNP Q8YWS9
E	-7	MET	-	expression tag	UNP Q8YWS9
E	-6	GLY	-	expression tag	UNP Q8YWS9
E	-5	HIS	-	expression tag	UNP Q8YWS9
E	-4	HIS	-	expression tag	UNP Q8YWS9
E	-3	HIS	-	expression tag	UNP Q8YWS9
E	-2	HIS	-	expression tag	UNP Q8YWS9
E	-1	HIS	-	expression tag	UNP Q8YWS9
E	0	HIS	-	expression tag	UNP Q8YWS9
F	-7	MET	-	expression tag	UNP Q8YWS9
F	-6	GLY	-	expression tag	UNP Q8YWS9
F	-5	HIS	-	expression tag	UNP Q8YWS9
F	-4	HIS	-	expression tag	UNP Q8YWS9
F	-3	HIS	-	expression tag	UNP Q8YWS9
F	-2	HIS	-	expression tag	UNP Q8YWS9
F	-1	HIS	-	expression tag	UNP Q8YWS9
F	0	HIS	-	expression tag	UNP Q8YWS9

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



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

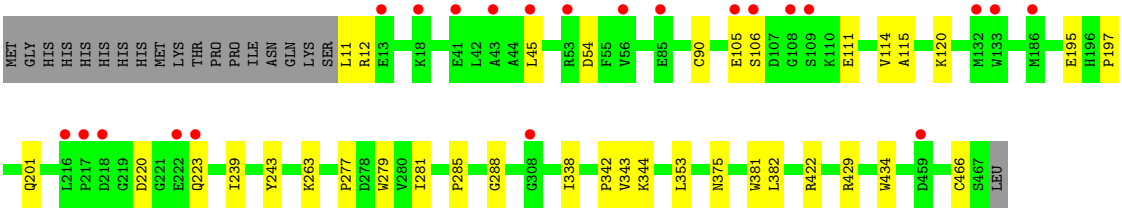
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	48	Total O 48 48	0	0
4	B	46	Total O 46 46	0	0
4	C	39	Total O 39 39	0	0
4	D	36	Total O 36 36	0	0
4	E	44	Total O 44 44	0	0
4	F	39	Total O 39 39	0	0

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.

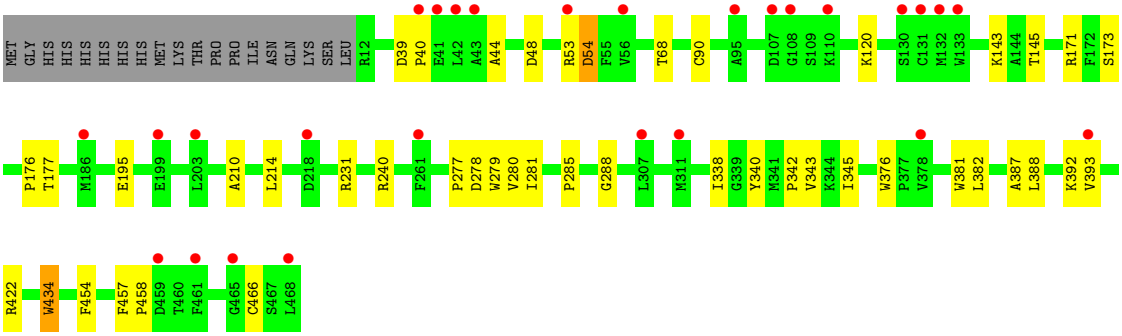
- Molecule 1: Alkaline Invertase

Chain A:



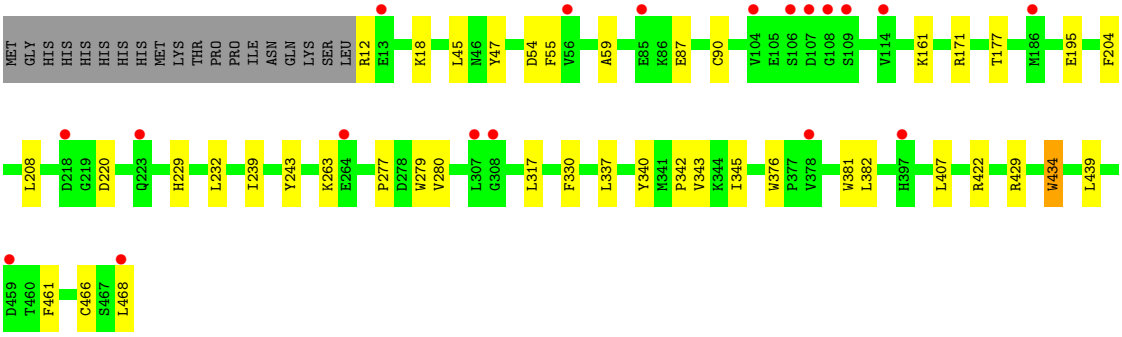
- Molecule 1: Alkaline Invertase

Chain B:



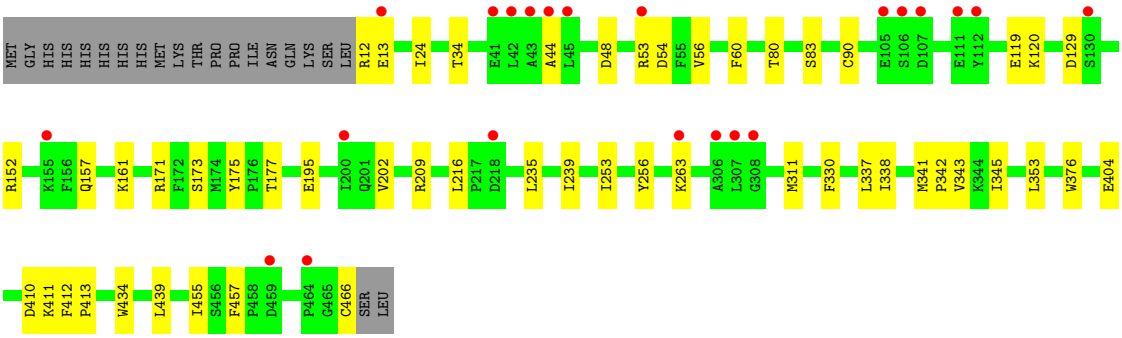
- Molecule 1: Alkaline Invertase

Chain C:



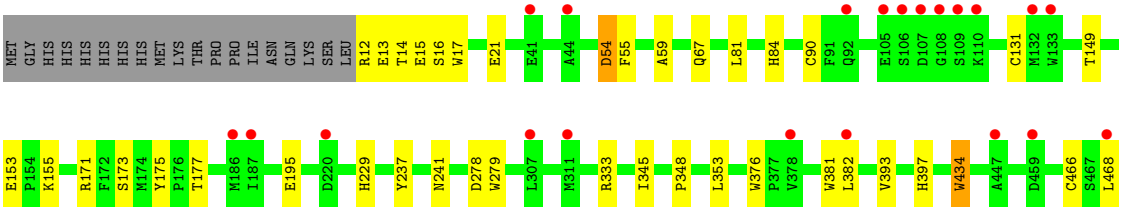
- Molecule 1: Alkaline Invertase

Chain D:



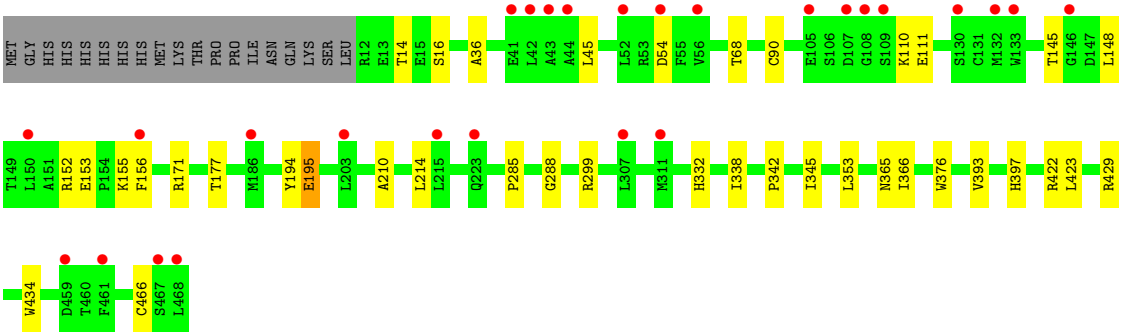
- Molecule 1: Alkaline Invertase

Chain E:



- Molecule 1: Alkaline Invertase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.17Å 179.28Å 96.36Å 90.00° 105.92° 90.00°	Depositor
Resolution (Å)	30.50 – 2.67 30.50 – 2.67	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.50-2.67) 95.2 (30.50-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.192 , 0.235 0.193 , 0.236	Depositor DCC
R_{free} test set	4215 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22286	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	0.33	0/3768	0.49	0/5112
1	B	0.34	0/3768	0.49	0/5112
1	C	0.34	0/3768	0.48	0/5112
1	D	0.33	0/3754	0.48	0/5093
1	E	0.34	0/3784	0.49	0/5135
1	F	0.33	0/3768	0.49	0/5112
All	All	0.34	0/22610	0.48	0/30676

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	3666	0	3602	23	0
1	B	3666	0	3602	28	0
1	C	3666	0	3602	26	0
1	D	3652	0	3586	32	0
1	E	3677	0	3612	30	0
1	F	3666	0	3602	24	0
2	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	8	2	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	0	0
2	F	6	0	8	0	0
3	C	5	0	0	0	0
4	A	48	0	0	0	0
4	B	46	0	0	1	0
4	C	39	0	0	0	0
4	D	36	0	0	0	0
4	E	44	0	0	3	0
4	F	39	0	0	2	0
All	All	22286	0	21654	148	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 3.

All (148) 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:E:14:THR:HB	1:E:17[A]:TRP:HD1	1.51	0.76
1:A:466:CYS:HB2	1:D:90:CYS:SG	2.26	0.75
1:E:90:CYS:SG	1:F:466:CYS:HB2	2.30	0.72
1:B:466:CYS:HB2	1:C:90:CYS:SG	2.30	0.71
1:F:148:LEU:O	1:F:152:ARG:HG2	1.90	0.70
1:A:11:LEU:HG	1:A:12:ARG:H	1.56	0.70
1:A:45:LEU:HD12	1:A:429:ARG:HH12	1.57	0.70
1:B:171:ARG:NH2	1:B:177:THR:O	2.25	0.69
1:D:12:ARG:HG3	1:D:13:GLU:H	1.57	0.69
1:A:281:ILE:HD13	1:F:423:LEU:HD11	1.76	0.67
1:C:171:ARG:NH2	1:C:177:THR:O	2.28	0.66
1:D:455:ILE:HG13	1:D:455:ILE:O	1.97	0.65
1:E:171:ARG:NH2	1:E:177:THR:O	2.30	0.65
1:C:161:LYS:NZ	1:C:220:ASP:OD1	2.28	0.64
1:C:232:LEU:HB3	1:C:461:PHE:HE2	1.63	0.62
1:E:173:SER:HG	1:E:175:TYR:HD1	1.46	0.62
1:E:153:GLU:OE1	1:E:155:LYS:HE2	2.01	0.61
1:F:153:GLU:OE1	1:F:155:LYS:HE2	2.01	0.61
1:D:157:GLN:O	1:D:161:LYS:HG3	2.00	0.60
1:E:466:CYS:HB2	1:F:90:CYS:SG	2.41	0.60
1:C:87:GLU:OE2	1:C:90:CYS:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:GLU:OE1	1:D:120:LYS:NZ	2.35	0.58
1:A:115:ALA:O	1:A:120:LYS:NZ	2.37	0.58
1:B:90:CYS:SG	1:C:466:CYS:HB2	2.44	0.57
1:A:12:ARG:HG3	1:A:12:ARG:O	2.04	0.57
1:E:171:ARG:HD2	4:E:643:HOH:O	2.04	0.56
1:B:240:ARG:NH2	4:B:601:HOH:O	2.39	0.56
1:E:278:ASP:OD1	1:E:279:TRP:N	2.39	0.56
1:D:410:ASP:O	1:D:411:LYS:HB2	2.05	0.55
1:F:36:ALA:O	4:F:601:HOH:O	2.18	0.55
1:E:12:ARG:HB3	1:E:17[A]:TRP:CD1	2.43	0.54
1:F:171:ARG:NH2	1:F:177:THR:O	2.40	0.54
1:B:53:ARG:HH11	2:B:501:GOL:H12	1.72	0.54
1:A:381:TRP:CE2	1:A:382:LEU:HD22	2.42	0.54
1:B:381:TRP:CE2	1:B:382:LEU:HD22	2.42	0.54
1:D:44:ALA:HB1	1:D:48:ASP:HB3	1.91	0.53
1:B:210:ALA:O	1:B:214:LEU:HD12	2.08	0.53
1:E:381:TRP:CE2	1:E:382:LEU:HD22	2.43	0.53
1:F:45:LEU:HD12	1:F:429:ARG:HH12	1.72	0.53
1:B:176:PRO:O	1:B:231:ARG:NH1	2.42	0.53
1:B:338:ILE:HG23	1:B:342:PRO:HB3	1.89	0.53
1:D:12:ARG:HG3	1:D:13:GLU:N	2.23	0.53
1:E:54:ASP:HA	1:E:434:TRP:CE3	2.44	0.53
1:C:381:TRP:CE2	1:C:382:LEU:HD22	2.44	0.52
1:B:44:ALA:HB1	1:B:48:ASP:HB3	1.93	0.51
1:D:171:ARG:NH2	1:D:177:THR:O	2.44	0.51
1:D:338:ILE:HG23	1:D:342:PRO:HB3	1.91	0.51
1:B:345:ILE:HB	1:B:376:TRP:CD1	2.46	0.50
1:C:47:TYR:CE1	1:C:429:ARG:NH2	2.79	0.50
1:D:24:ILE:HA	1:D:34:THR:HG22	1.94	0.50
1:D:345:ILE:HB	1:D:376:TRP:CD1	2.47	0.50
1:B:388:LEU:HD23	1:B:393:VAL:HG22	1.94	0.49
1:D:53:ARG:NH2	1:D:129:ASP:OD1	2.39	0.49
1:A:344:LYS:NZ	1:A:375:ASN:OD1	2.44	0.49
1:F:14:THR:HG22	1:F:16:SER:H	1.76	0.49
1:C:239:ILE:O	1:C:243:TYR:HB2	2.14	0.48
1:D:152:ARG:HG2	1:D:216:LEU:HD21	1.95	0.48
1:D:235:LEU:O	1:D:239:ILE:HG12	2.12	0.48
1:A:338:ILE:HG23	1:A:342:PRO:HB3	1.96	0.48
1:B:277:PRO:O	1:B:280:VAL:HG12	2.13	0.48
1:C:330:PHE:HA	1:C:337:LEU:HD12	1.94	0.48
1:F:299:ARG:HD3	4:F:608:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:ARG:HB3	1:D:457:PHE:CE2	2.49	0.47
1:E:13:GLU:OE1	4:E:601:HOH:O	2.20	0.47
1:F:285:PRO:HB3	1:F:332:HIS:CG	2.49	0.47
1:B:277:PRO:HB2	1:B:279:TRP:CD1	2.48	0.47
1:B:278:ASP:OD1	1:B:278:ASP:N	2.47	0.47
1:C:204:PHE:O	1:C:208:LEU:HG	2.15	0.47
1:E:173:SER:OG	1:E:175:TYR:HD1	1.98	0.47
1:A:90:CYS:HB2	1:D:466:CYS:CB	2.45	0.47
1:E:17[B]:TRP:NE1	1:E:21:GLU:OE2	2.48	0.47
1:E:81:LEU:O	1:E:84:HIS:HB2	2.15	0.47
1:A:281:ILE:O	1:F:422:ARG:NH1	2.48	0.47
1:C:12:ARG:O	1:C:18:LYS:NZ	2.48	0.46
1:A:106:SER:HB3	1:A:111:GLU:HG2	1.98	0.46
1:D:80:THR:O	1:D:83:SER:OG	2.28	0.46
1:E:14:THR:HG22	1:E:15:GLU:N	2.30	0.46
1:A:120:LYS:HG2	1:D:263:LYS:HG3	1.98	0.46
1:B:342:PRO:HA	1:B:343:VAL:HA	1.77	0.46
1:E:229:HIS:NE2	1:E:468:LEU:HD22	2.29	0.46
1:F:110:LYS:HG2	1:F:111:GLU:N	2.31	0.46
1:E:237:TYR:O	1:E:241:ASN:ND2	2.37	0.46
1:D:404:GLU:HG2	1:D:439:LEU:HD21	1.98	0.46
1:E:55:PHE:CE2	1:E:59:ALA:HB2	2.51	0.46
1:A:342:PRO:HA	1:A:343:VAL:HA	1.76	0.46
1:C:277:PRO:HB2	1:C:279:TRP:CD1	2.51	0.45
1:E:131:CYS:HB3	4:E:611:HOH:O	2.16	0.45
1:E:353:LEU:HB3	1:F:353:LEU:HD23	1.98	0.45
1:F:155:LYS:HE3	1:F:156:PHE:CE1	2.51	0.45
1:F:393:VAL:HG12	1:F:397:HIS:CD2	2.51	0.45
1:C:54:ASP:HA	1:C:434:TRP:CE3	2.52	0.45
1:A:422:ARG:NH1	1:B:281:ILE:O	2.48	0.45
1:A:263:LYS:HE2	1:D:119:GLU:HG3	1.99	0.45
1:B:68:THR:HG21	1:B:145:THR:HG22	1.97	0.45
1:C:345:ILE:HB	1:C:376:TRP:CD1	2.52	0.45
1:A:220:ASP:O	1:A:223:GLN:HG2	2.17	0.45
1:B:340:TYR:CE2	1:B:422:ARG:HG3	2.53	0.44
1:C:47:TYR:CZ	1:C:429:ARG:NH2	2.85	0.44
1:C:340:TYR:CD2	1:C:422:ARG:HG3	2.52	0.44
1:C:342:PRO:HA	1:C:343:VAL:HA	1.78	0.44
1:C:239:ILE:HG21	1:C:317:LEU:HD21	2.00	0.44
1:C:407:LEU:HD12	1:C:439:LEU:HD22	2.00	0.44
1:D:202:VAL:HG11	1:D:311:MET:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:GLN:O	1:E:67:GLN:HG3	2.18	0.44
1:B:457:PHE:HA	1:B:458:PRO:HD3	1.86	0.44
1:F:210:ALA:O	1:F:214:LEU:HG	2.18	0.44
1:B:120:LYS:HE3	1:C:263:LYS:HE3	2.00	0.44
1:B:285:PRO:HG2	1:B:288:GLY:HA3	2.00	0.44
1:E:149:THR:O	1:E:153:GLU:HG3	2.18	0.43
1:D:253:ILE:HA	1:D:256:TYR:CD2	2.53	0.43
1:D:341:MET:SD	1:D:342:PRO:HD2	2.58	0.43
1:B:53:ARG:HD2	2:B:501:GOL:O1	2.17	0.43
1:E:345:ILE:HB	1:E:376:TRP:CD1	2.53	0.43
1:F:155:LYS:HE3	1:F:156:PHE:HE1	1.82	0.43
1:E:279:TRP:CZ2	1:E:348:PRO:HD3	2.53	0.43
1:F:338:ILE:HG23	1:F:342:PRO:HB3	2.01	0.43
1:A:197:PRO:O	1:A:201:GLN:HG2	2.19	0.43
1:A:239:ILE:O	1:A:243:TYR:HB2	2.18	0.43
1:B:120:LYS:HG2	1:C:263:LYS:HG3	2.01	0.43
1:A:353:LEU:HD23	1:D:353:LEU:HB3	2.01	0.42
1:C:229:HIS:CE1	1:C:468:LEU:HD23	2.54	0.42
1:E:12:ARG:HG3	1:E:13:GLU:H	1.84	0.42
1:B:143:LYS:HD3	1:B:454:PHE:HA	2.02	0.42
1:C:55:PHE:CE2	1:C:59:ALA:HB2	2.55	0.42
1:F:194:TYR:CD1	1:F:195:GLU:HB2	2.54	0.42
1:A:105:GLU:HG3	1:A:114:VAL:HG21	2.01	0.42
1:D:173:SER:HB3	1:D:175:TYR:HD1	1.84	0.42
1:F:285:PRO:HG2	1:F:288:GLY:HA3	2.01	0.42
1:C:45:LEU:HD12	1:C:429:ARG:HH11	1.85	0.42
1:C:277:PRO:O	1:C:280:VAL:HG12	2.20	0.41
1:D:412:PHE:N	1:D:413:PRO:HD3	2.35	0.41
1:D:56:VAL:HG12	1:D:60:PHE:CE2	2.56	0.41
1:B:54:ASP:HA	1:B:434:TRP:CE3	2.55	0.41
1:D:152:ARG:HD3	1:D:216:LEU:HD21	2.03	0.41
1:B:387:ALA:HB1	1:B:392:LYS:O	2.21	0.41
1:D:342:PRO:HA	1:D:343:VAL:HA	1.73	0.41
1:D:152:ARG:CD	1:D:216:LEU:HD21	2.50	0.41
1:E:333:ARG:HD3	1:E:333:ARG:HA	1.85	0.41
1:F:345:ILE:HB	1:F:376:TRP:CD1	2.55	0.41
1:E:393:VAL:HG12	1:E:397:HIS:CD2	2.56	0.41
1:A:277:PRO:HB2	1:A:279:TRP:CD1	2.56	0.41
1:D:330:PHE:HA	1:D:337:LEU:HD12	2.03	0.41
1:E:14:THR:HB	1:E:17[A]:TRP:CD1	2.43	0.41
1:E:14:THR:HG22	1:E:16:SER:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:365:ASN:O	1:F:366:ILE:O	2.39	0.41
1:B:39:ASP:HA	1:B:40:PRO:HD3	1.95	0.40
1:F:68:THR:HG21	1:F:145:THR:HG22	2.02	0.40
1:A:285:PRO:HG2	1:A:288:GLY:HA3	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	455/476 (96%)	443 (97%)	11 (2%)	1 (0%)	47	71
1	B	455/476 (96%)	445 (98%)	9 (2%)	1 (0%)	47	71
1	C	455/476 (96%)	444 (98%)	10 (2%)	1 (0%)	47	71
1	D	453/476 (95%)	445 (98%)	7 (2%)	1 (0%)	47	71
1	E	456/476 (96%)	445 (98%)	10 (2%)	1 (0%)	47	71
1	F	455/476 (96%)	446 (98%)	8 (2%)	1 (0%)	47	71
All	All	2729/2856 (96%)	2668 (98%)	55 (2%)	6 (0%)	47	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	195	GLU
1	E	195	GLU
1	F	195	GLU
1	A	195	GLU
1	B	195	GLU
1	D	195	GLU

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	380/398 (96%)	378 (100%)	2 (0%)	88	95
1	B	380/398 (96%)	377 (99%)	3 (1%)	81	92
1	C	380/398 (96%)	379 (100%)	1 (0%)	92	97
1	D	378/398 (95%)	376 (100%)	2 (0%)	88	95
1	E	381/398 (96%)	379 (100%)	2 (0%)	88	95
1	F	380/398 (96%)	378 (100%)	2 (0%)	88	95
All	All	2279/2388 (95%)	2267 (100%)	12 (0%)	88	95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	434	TRP
1	B	54	ASP
1	B	173	SER
1	B	434	TRP
1	C	434	TRP
1	D	54	ASP
1	D	434	TRP
1	E	54	ASP
1	E	434	TRP
1	F	54	ASP
1	F	434	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands 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	$\#\|Z\| > 2$
2	GOL	A	501	-	5,5,5	0.18	0	5,5,5	0.33	0
2	GOL	E	501	-	5,5,5	0.21	0	5,5,5	0.32	0
2	GOL	D	501	-	5,5,5	0.18	0	5,5,5	0.33	0
2	GOL	F	501	-	5,5,5	0.20	0	5,5,5	0.37	0
2	GOL	C	501	-	5,5,5	0.20	0	5,5,5	0.30	0
3	SO4	C	502	-	4,4,4	0.27	0	6,6,6	0.29	0
2	GOL	B	501	-	5,5,5	0.23	0	5,5,5	0.30	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	501	-	-	0/4/4/4	-
2	GOL	E	501	-	-	0/4/4/4	-
2	GOL	D	501	-	-	0/4/4/4	-
2	GOL	F	501	-	-	0/4/4/4	-
2	GOL	C	501	-	-	0/4/4/4	-
2	GOL	B	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	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, 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	457/476 (96%)	0.07	22 (4%)	30	28	42, 60, 88, 119	1 (0%)
1	B	457/476 (96%)	0.16	27 (5%)	22	20	41, 63, 87, 115	1 (0%)
1	C	457/476 (96%)	0.06	19 (4%)	36	34	42, 60, 88, 122	1 (0%)
1	D	455/476 (95%)	0.15	22 (4%)	30	28	42, 65, 93, 121	1 (0%)
1	E	457/476 (96%)	0.08	21 (4%)	32	30	43, 63, 87, 109	0
1	F	457/476 (96%)	0.13	27 (5%)	22	20	42, 65, 95, 116	1 (0%)
All	All	2740/2856 (95%)	0.11	138 (5%)	28	26	41, 63, 90, 122	5 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	107	ASP	6.1
1	C	109	SER	5.3
1	F	43	ALA	5.3
1	D	41	GLU	5.1
1	F	109	SER	4.6
1	F	56	VAL	4.1
1	E	109	SER	4.0
1	A	459	ASP	3.9
1	C	218	ASP	3.9
1	E	468	LEU	3.9
1	E	108	GLY	3.8
1	A	43	ALA	3.8
1	F	108	GLY	3.8
1	B	133	TRP	3.8
1	B	186	MET	3.8
1	B	132	MET	3.7
1	B	261	PHE	3.7
1	C	13	GLU	3.7
1	D	464	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	106	SER	3.7
1	E	107	ASP	3.6
1	B	107	ASP	3.6
1	D	43	ALA	3.5
1	B	41	GLU	3.4
1	A	108	GLY	3.4
1	B	56	VAL	3.3
1	F	44	ALA	3.3
1	F	468	LEU	3.3
1	A	41	GLU	3.3
1	D	45	LEU	3.2
1	C	106	SER	3.2
1	A	218	ASP	3.2
1	E	459	ASP	3.2
1	B	40	PRO	3.2
1	F	307	LEU	3.2
1	C	108	GLY	3.1
1	D	44	ALA	3.1
1	F	459	ASP	3.1
1	D	307	LEU	3.1
1	D	107	ASP	3.1
1	F	133	TRP	3.1
1	A	85	GLU	3.1
1	F	41	GLU	3.0
1	B	307	LEU	3.0
1	A	109	SER	3.0
1	B	465	GLY	2.9
1	A	45	LEU	2.9
1	A	132	MET	2.9
1	D	13	GLU	2.9
1	F	107	ASP	2.9
1	F	223	GLN	2.8
1	C	307	LEU	2.8
1	F	186	MET	2.8
1	A	106	SER	2.8
1	A	133	TRP	2.8
1	A	18	LYS	2.8
1	D	112	TYR	2.7
1	D	459	ASP	2.7
1	E	307	LEU	2.7
1	E	106	SER	2.7
1	B	311	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	56	VAL	2.7
1	B	461	PHE	2.7
1	B	130	SER	2.7
1	C	378	VAL	2.7
1	C	468	LEU	2.6
1	E	447	ALA	2.6
1	B	378	VAL	2.6
1	D	42	LEU	2.5
1	F	105	GLU	2.5
1	D	105	GLU	2.5
1	B	110	LYS	2.5
1	D	111	GLU	2.5
1	E	105	GLU	2.5
1	C	85	GLU	2.4
1	E	41	GLU	2.4
1	F	54	ASP	2.4
1	C	186	MET	2.4
1	B	95	ALA	2.4
1	F	203	LEU	2.4
1	B	468	LEU	2.4
1	E	133	TRP	2.4
1	F	311	MET	2.4
1	B	203	LEU	2.4
1	B	53	ARG	2.4
1	F	52	LEU	2.3
1	F	461	PHE	2.3
1	E	186	MET	2.3
1	B	218	ASP	2.3
1	D	218	ASP	2.3
1	B	199	GLU	2.3
1	D	306	ALA	2.3
1	A	308	GLY	2.3
1	C	223	GLN	2.3
1	C	56	VAL	2.3
1	A	186	MET	2.3
1	B	42	LEU	2.3
1	F	42	LEU	2.3
1	A	13	GLU	2.2
1	D	155	LYS	2.2
1	F	156	PHE	2.2
1	D	263	LYS	2.2
1	B	108	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	104	VAL	2.2
1	C	264	GLU	2.2
1	B	459	ASP	2.2
1	E	110	LYS	2.2
1	F	215	LEU	2.2
1	B	43	ALA	2.2
1	C	459	ASP	2.2
1	F	130	SER	2.2
1	F	467	SER	2.2
1	F	146	GLY	2.2
1	E	378	VAL	2.2
1	D	308	GLY	2.2
1	F	132	MET	2.2
1	D	130	SER	2.1
1	A	223	GLN	2.1
1	C	397	HIS	2.1
1	A	216	LEU	2.1
1	C	308	GLY	2.1
1	D	53	ARG	2.1
1	A	105	GLU	2.1
1	E	311	MET	2.1
1	B	393	VAL	2.1
1	E	382	LEU	2.1
1	A	217	PRO	2.1
1	A	222	GLU	2.1
1	C	114	VAL	2.1
1	F	150	LEU	2.1
1	B	131	CYS	2.1
1	E	92	GLN	2.0
1	E	187	ILE	2.0
1	A	53	ARG	2.0
1	D	200	ILE	2.0
1	E	44	ALA	2.0
1	E	220	ASP	2.0
1	E	132	MET	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 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, 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	SO4	C	502	5/5	0.88	0.29	67,68,75,92	0
2	GOL	E	501	6/6	0.92	0.36	54,59,59,61	0
2	GOL	A	501	6/6	0.93	0.39	56,58,60,60	0
2	GOL	C	501	6/6	0.93	0.32	59,59,64,66	0
2	GOL	B	501	6/6	0.94	0.35	54,60,63,64	0
2	GOL	F	501	6/6	0.94	0.42	59,61,64,68	0
2	GOL	D	501	6/6	0.94	0.44	59,60,62,63	0

6.5 Other polymers (i)

There are no such residues in this entry.