Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:09 pm BST

PDB ID	:	3T0U
Title	:	Hansenula polymorpha copper amine oxidase-1 in complex with Cu(I)
Authors	:	Klema, V.J.; Wilmot, C.M.
Deposited on	:	2011-07-20
Resolution	:	1.90 Å(reported)

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

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

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

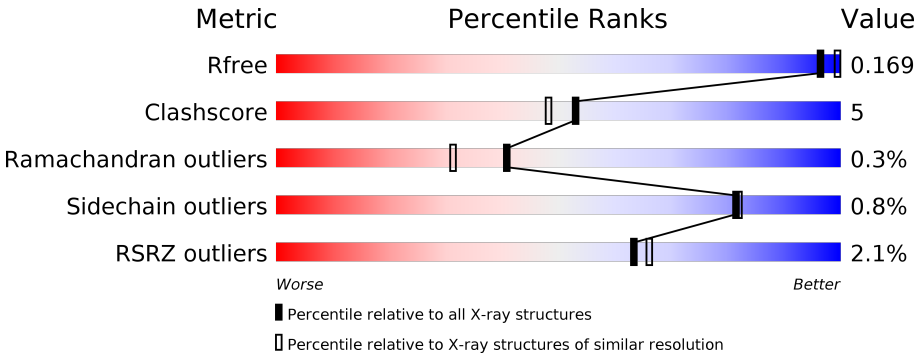
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

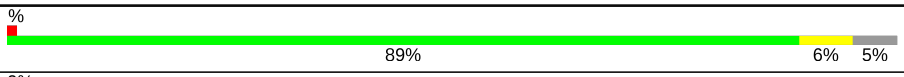
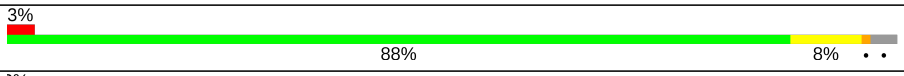
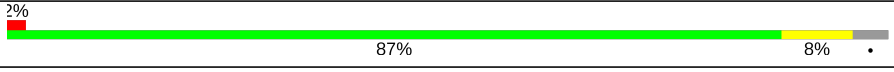
The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	692	
1	B	692	
1	C	692	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18801 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.

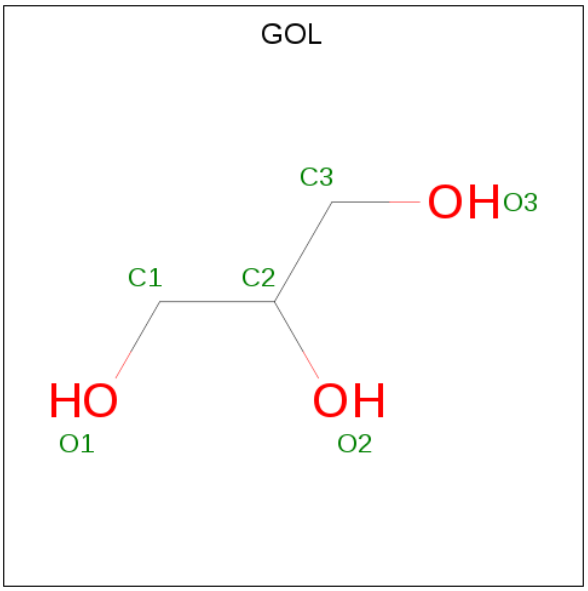
- Molecule 1 is a protein called Peroxisomal primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	657	Total	C	N	O	S	0	15	0
			5276	3366	902	981	27			
1	B	668	Total	C	N	O	S	0	16	0
			5350	3409	913	999	29			
1	C	665	Total	C	N	O	S	0	16	0
			5317	3391	907	991	28			

- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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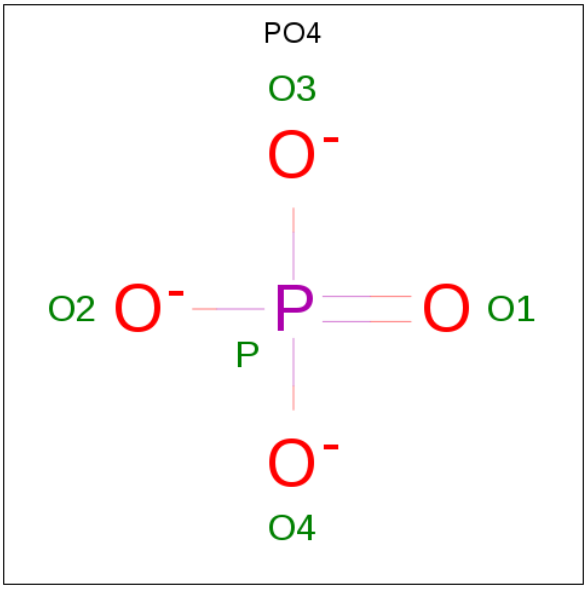
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

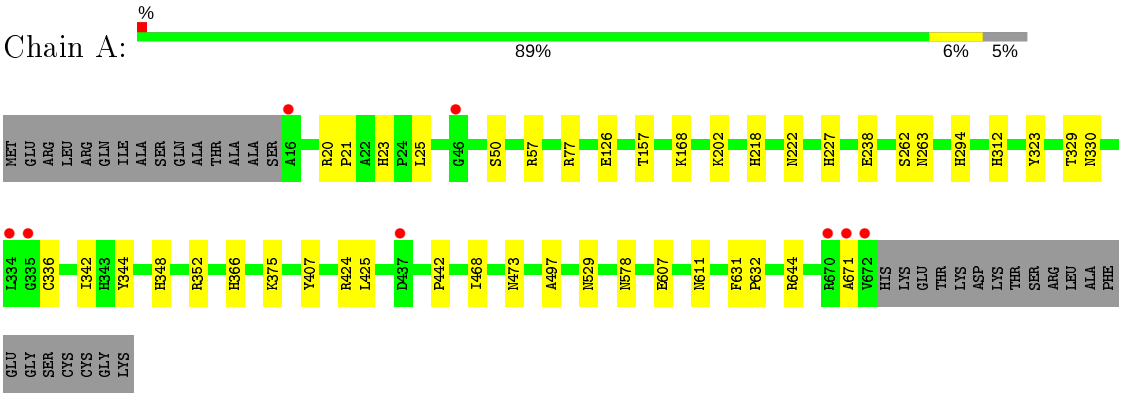
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	914	Total O 914 914	0	0
5	B	915	Total O 915 915	0	0
5	C	907	Total O 907 907	0	0

3 Residue-property plots (i)

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

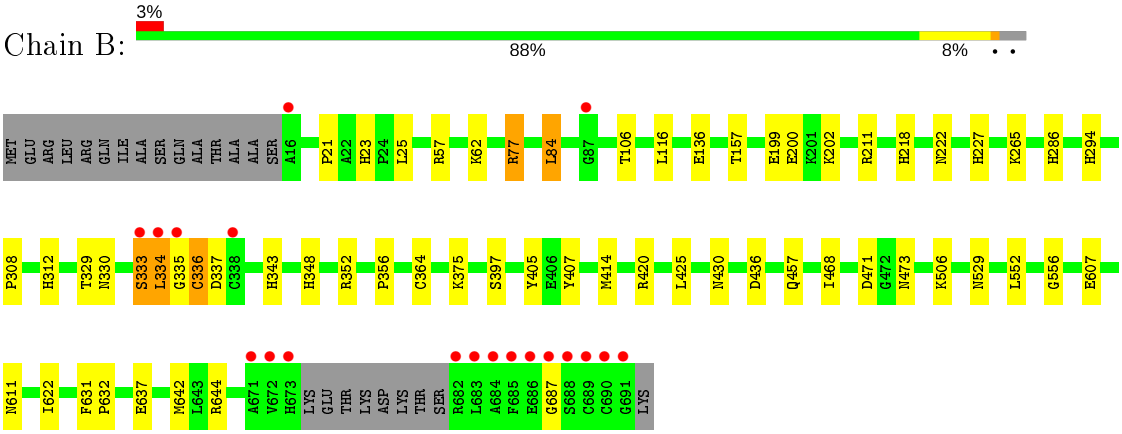
• Molecule 1: Peroxisomal primary amine oxidase

Chain A:



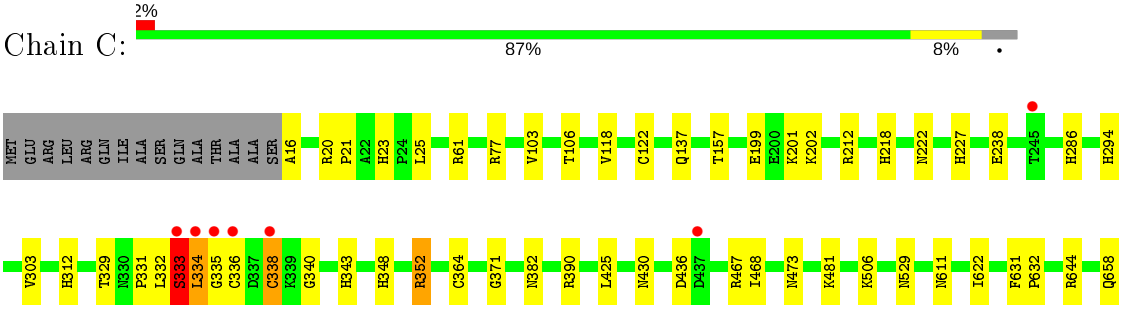
• Molecule 1: Peroxisomal primary amine oxidase

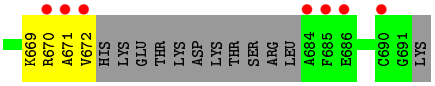
Chain B:



• Molecule 1: Peroxisomal primary amine oxidase

Chain C:




K669
R670
A671
V672
HIS
LYS
GLU
THR
LYS
ASP
LYS
THR
SER
ARG
LEU
A684
F685
E686
C690
G691
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	139.45Å 153.67Å 223.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.14 – 1.90 49.14 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.14-1.90) 99.9 (49.14-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.125 , 0.168 0.127 , 0.169	Depositor DCC
R_{free} test set	9388 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	12.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18801	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: GOL, PO4, CU1

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	0.68	0/5472	0.66	0/7446
1	B	0.69	0/5550	0.65	1/7549 (0.0%)
1	C	0.67	0/5516	0.66	1/7504 (0.0%)
All	All	0.68	0/16538	0.66	2/22499 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	77	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	C	352	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	333	SER	Peptide

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	5276	0	5160	49	0
1	B	5350	0	5210	71	0
1	C	5317	0	5201	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	30	0	40	1	0
3	B	36	0	48	4	0
3	C	48	0	64	3	0
4	B	5	0	0	0	0
5	A	914	0	0	20	5
5	B	915	0	0	29	2
5	C	907	0	0	30	4
All	All	18801	0	15723	169	7

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 5.

All (169) 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:157:THR:CG2	5:A:1786:HOH:O	1.78	1.28
1:A:607:GLU:HG2	5:A:1562:HOH:O	1.35	1.21
1:A:578[B]:ASN:ND2	5:A:1802:HOH:O	1.88	1.05
1:B:157:THR:HG22	5:B:1482:HOH:O	1.57	1.04
1:C:16:ALA:HB1	5:C:1291:HOH:O	1.64	0.96
1:A:644:ARG:NH2	1:B:637[B]:GLU:OE2	2.02	0.92
1:C:23:HIS:HD2	1:C:25:LEU:H	1.15	0.92
1:B:157:THR:CG2	5:B:1482:HOH:O	2.16	0.90
1:B:23:HIS:HD2	1:B:25:LEU:H	1.18	0.90
1:A:57:ARG:NH1	5:A:1803:HOH:O	1.84	0.90
1:C:468:ILE:H	1:C:473:ASN:HD21	1.17	0.89
1:A:23:HIS:HD2	1:A:25:LEU:H	1.16	0.87
1:C:16:ALA:HA	5:C:1427:HOH:O	1.75	0.86
1:C:506[A]:LYS:HE2	5:C:1517:HOH:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ILE:H	1:B:473:ASN:HD21	1.28	0.82
1:B:414[B]:MET:SD	1:B:420:ARG:NH1	2.52	0.82
1:A:157:THR:HG22	5:A:1786:HOH:O	1.55	0.82
1:C:670:ARG:C	1:C:672:VAL:H	1.86	0.79
1:C:382[B]:ASN:OD1	5:C:1711:HOH:O	2.01	0.78
1:A:348:HIS:HD2	5:A:1360:HOH:O	1.65	0.77
1:B:336:CYS:HB3	5:B:1792:HOH:O	1.85	0.76
1:B:529:ASN:HD21	1:B:611:ASN:HD21	1.31	0.76
1:A:238:GLU:HG3	5:A:1799:HOH:O	1.85	0.75
1:B:607[A]:GLU:OE1	5:B:1806:HOH:O	2.04	0.75
1:A:529:ASN:HD21	1:A:611:ASN:HD21	1.31	0.74
1:A:50:SER:HB2	1:A:352[A]:ARG:CG	2.19	0.73
1:A:468:ILE:H	1:A:473:ASN:HD21	1.34	0.73
1:C:529:ASN:HD21	1:C:611:ASN:HD21	1.37	0.72
1:A:50:SER:HB2	1:A:352[A]:ARG:HG3	1.73	0.71
1:B:343:HIS:HD2	5:B:1276:HOH:O	1.74	0.70
1:C:157:THR:HG22	5:C:1572:HOH:O	1.91	0.70
1:C:338:CYS:HG	1:C:364:CYS:CB	2.05	0.70
1:C:137:GLN:HE22	1:C:212:ARG:HH12	1.38	0.69
1:B:57:ARG:NH1	5:B:1372:HOH:O	2.07	0.68
1:A:126:GLU:HB2	1:B:687:GLY:HA3	1.76	0.67
1:C:333:SER:HB3	5:C:1389:HOH:O	1.93	0.67
1:B:506[A]:LYS:HE2	5:B:1249:HOH:O	1.95	0.67
1:C:286:HIS:HD2	5:C:1748:HOH:O	1.78	0.66
1:B:556:GLY:O	5:B:1392:HOH:O	2.13	0.66
1:C:332:LEU:HD13	5:C:1286:HOH:O	1.96	0.66
1:A:578[B]:ASN:ND2	5:A:1798:HOH:O	2.08	0.65
1:B:333:SER:O	1:B:334:LEU:HG	1.96	0.65
1:A:23:HIS:CD2	1:A:25:LEU:H	2.08	0.65
1:C:218:HIS:HE1	5:C:1526:HOH:O	1.79	0.64
1:C:436:ASP:O	5:C:1592:HOH:O	2.14	0.64
1:C:294:HIS:HD2	5:C:946:HOH:O	1.80	0.64
1:C:118[A]:VAL:HG22	5:C:1077:HOH:O	1.99	0.63
1:B:57:ARG:NH2	5:B:1279:HOH:O	2.30	0.62
1:B:335:GLY:HA3	1:B:337:ASP:N	2.14	0.62
1:A:336:CYS:SG	5:B:1779:HOH:O	2.47	0.62
1:B:348:HIS:HD2	5:B:1480:HOH:O	1.83	0.61
1:B:218:HIS:HE1	5:B:1255:HOH:O	1.84	0.60
1:C:20:ARG:NH2	5:C:1677:HOH:O	2.22	0.60
1:B:199:GLU:HG3	5:B:953:HOH:O	2.01	0.60
1:A:157:THR:HG22	1:A:323:TYR:OH	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:HIS:HE1	5:A:1523:HOH:O	1.85	0.59
1:B:335:GLY:HA3	1:B:337:ASP:H	1.67	0.59
1:C:340:GLY:HA3	5:C:1641:HOH:O	2.02	0.59
1:C:436:ASP:H	3:C:808:GOL:H11	1.67	0.59
1:C:157:THR:CG2	5:C:1572:HOH:O	2.49	0.59
1:C:343:HIS:HD2	5:C:1463:HOH:O	1.86	0.59
1:C:201:LYS:HD3	5:C:1800:HOH:O	2.03	0.58
1:C:122[B]:CYS:SG	5:C:1418:HOH:O	2.47	0.58
1:C:23:HIS:CD2	1:C:25:LEU:H	2.07	0.58
1:C:670:ARG:C	1:C:672:VAL:N	2.56	0.58
1:B:116:LEU:HD12	1:B:157:THR:HB	1.85	0.57
1:B:200[B]:GLU:CD	1:B:202:LYS:NZ	2.58	0.57
1:C:468:ILE:N	1:C:473:ASN:HD21	1.96	0.57
1:A:342:ILE:HD11	1:A:344:TYR:CE2	2.40	0.57
1:A:644:ARG:CZ	1:B:637[B]:GLU:OE2	2.53	0.56
1:C:348:HIS:HD2	5:C:1243:HOH:O	1.87	0.56
1:A:424:ARG:NE	5:A:1458:HOH:O	2.38	0.56
1:B:506[A]:LYS:HD3	5:B:1304:HOH:O	2.06	0.56
1:A:407:TYR:CD2	1:A:425[B]:LEU:CD2	2.89	0.56
1:C:430:ASN:ND2	5:C:1799:HOH:O	2.10	0.56
1:B:333:SER:O	1:B:334:LEU:CB	2.54	0.55
1:B:294:HIS:HD2	5:B:913:HOH:O	1.89	0.55
1:B:23:HIS:CD2	1:B:25:LEU:H	2.11	0.55
1:C:371:GLY:HA2	1:C:390:ARG:NH2	2.22	0.55
1:B:106:THR:CG2	1:B:106:THR:O	2.55	0.55
1:A:157:THR:HG21	5:A:1786:HOH:O	1.68	0.54
1:B:106:THR:HG23	1:B:106:THR:O	2.07	0.54
1:B:352[B]:ARG:HG2	5:B:1629:HOH:O	2.07	0.54
1:A:126:GLU:HB2	1:B:687:GLY:CA	2.37	0.54
1:B:436:ASP:O	5:B:1391:HOH:O	2.19	0.53
1:B:506[A]:LYS:HE3	5:B:1443:HOH:O	2.09	0.53
1:A:424:ARG:CG	5:A:1458:HOH:O	2.56	0.53
1:A:20:ARG:HH11	1:A:20:ARG:HG3	1.73	0.52
1:B:436:ASP:H	3:B:806:GOL:H32	1.73	0.52
1:C:631:PHE:CG	1:C:632:PRO:HA	2.44	0.52
1:B:62:LYS:HE3	5:B:1352:HOH:O	2.09	0.52
1:A:21:PRO:HG3	1:A:77:ARG:CZ	2.40	0.52
1:A:375:LYS:NZ	1:B:330:ASN:HD22	2.08	0.52
1:C:669:LYS:O	1:C:672:VAL:HA	2.11	0.51
1:B:457:GLN:HE22	1:B:552:LEU:H	1.58	0.51
1:B:333:SER:O	1:B:334:LEU:CG	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:CYS:HB3	5:C:1389:HOH:O	2.10	0.51
1:A:342:ILE:HG22	1:A:366:HIS:HB3	1.92	0.51
1:B:506[B]:LYS:HE2	5:B:1329:HOH:O	2.11	0.50
1:A:442:PRO:HG3	3:B:807:GOL:H31	1.94	0.50
1:A:330:ASN:HD22	1:B:375:LYS:NZ	2.09	0.50
1:B:84:LEU:HD23	1:B:84:LEU:N	2.26	0.50
1:B:222:ASN:HB3	1:B:227:HIS:CG	2.48	0.49
1:C:137:GLN:HE21	1:C:212:ARG:HH22	1.59	0.49
1:C:468:ILE:H	1:C:473:ASN:ND2	1.96	0.49
1:C:312:HIS:HD2	5:C:1054:HOH:O	1.96	0.49
1:B:364[A]:CYS:SG	1:B:397:SER:OG	2.71	0.48
1:B:200[B]:GLU:CD	1:B:202:LYS:HZ2	2.14	0.48
1:C:16:ALA:CB	5:C:1291:HOH:O	2.40	0.48
1:C:338:CYS:HG	1:C:364:CYS:HB2	1.75	0.48
1:A:468:ILE:H	1:A:473:ASN:ND2	2.07	0.48
1:B:471:ASP:OD1	5:B:1501:HOH:O	2.20	0.48
1:B:644:ARG:NH1	5:B:1533:HOH:O	2.47	0.48
1:A:424:ARG:HG2	5:A:1458:HOH:O	2.13	0.47
1:B:631:PHE:CG	1:B:632:PRO:HA	2.49	0.47
1:B:116:LEU:CD1	1:B:157:THR:HB	2.45	0.47
1:C:506[B]:LYS:HD2	5:C:1670:HOH:O	2.14	0.47
1:C:669:LYS:HE2	5:C:1755:HOH:O	2.14	0.47
1:B:468:ILE:H	1:B:473:ASN:ND2	2.04	0.47
1:B:405:TYR:CD1	1:B:425[A]:LEU:HD11	2.49	0.47
1:A:631:PHE:CG	1:A:632:PRO:HA	2.49	0.47
1:C:425[B]:LEU:HD12	1:C:622:ILE:HD11	1.97	0.47
1:A:294:HIS:HD2	5:A:1787:HOH:O	1.97	0.47
1:C:201:LYS:NZ	5:C:1521:HOH:O	2.47	0.47
3:B:805:GOL:H31	5:B:1315:HOH:O	2.15	0.47
1:B:211:ARG:NH2	5:B:1803:HOH:O	2.47	0.47
1:B:430:ASN:ND2	5:B:1802:HOH:O	2.23	0.46
1:A:50:SER:HB2	1:A:352[A]:ARG:HG2	1.94	0.46
1:B:312:HIS:HD2	5:B:1009:HOH:O	1.97	0.46
1:B:468:ILE:N	1:B:473:ASN:HD21	2.05	0.46
1:C:658:GLN:NE2	5:C:1790:HOH:O	2.12	0.46
1:C:23:HIS:HE1	3:C:806:GOL:O1	1.98	0.46
1:B:407:TYR:CD2	1:B:425[B]:LEU:CD2	2.98	0.46
1:A:312:HIS:HD2	5:A:973:HOH:O	1.98	0.46
1:C:303:VAL:HG23	5:C:1261:HOH:O	2.15	0.45
1:A:168:LYS:HE2	5:A:1570:HOH:O	2.15	0.45
1:A:342:ILE:CD1	1:A:344:TYR:CE2	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:CD2	1:B:84:LEU:N	2.79	0.45
5:A:1405:HOH:O	1:B:642:MET:CE	2.65	0.45
5:A:1419:HOH:O	1:B:286:HIS:HD2	2.00	0.44
1:B:407:TYR:CE2	1:B:425[B]:LEU:HD22	2.53	0.44
1:A:23:HIS:HE1	3:A:802:GOL:O1	2.00	0.44
1:B:265:LYS:NZ	5:B:1634:HOH:O	2.51	0.44
1:A:375:LYS:NZ	1:B:337:ASP:OD1	2.51	0.44
1:C:331:PRO:HD2	5:C:1315:HOH:O	2.17	0.44
1:C:61:ARG:NH2	1:C:467:ARG:HG3	2.33	0.43
1:C:670:ARG:O	1:C:672:VAL:N	2.49	0.43
1:B:506[B]:LYS:HD2	5:B:1330:HOH:O	2.19	0.43
1:B:21:PRO:HG3	1:B:77:ARG:CZ	2.48	0.43
1:A:330:ASN:HD22	1:B:375:LYS:HZ3	1.66	0.43
1:B:425[B]:LEU:HD12	1:B:622:ILE:HD11	2.01	0.43
1:A:497:ALA:HB2	1:B:308:PRO:HB3	2.00	0.42
1:B:200[B]:GLU:OE1	1:B:202:LYS:NZ	2.49	0.42
1:C:21:PRO:HG3	1:C:77:ARG:CZ	2.49	0.42
1:A:407:TYR:CD2	1:A:425[B]:LEU:HD22	2.55	0.41
1:B:136:GLU:HG3	5:B:1278:HOH:O	2.19	0.41
1:A:222:ASN:HB3	1:A:227:HIS:CG	2.55	0.41
1:B:631:PHE:CD1	1:B:632:PRO:HA	2.55	0.41
1:C:199:GLU:OE1	1:C:352:ARG:NH2	2.48	0.41
1:C:103:VAL:HG11	1:C:106[B]:THR:CG2	2.50	0.41
1:C:333:SER:HA	1:C:334:LEU:C	2.41	0.41
1:B:23:HIS:HE1	3:B:803:GOL:O3	2.03	0.41
1:A:238:GLU:CD	5:A:1799:HOH:O	2.58	0.40
1:C:222:ASN:HB3	1:C:227:HIS:CG	2.56	0.40
3:C:803:GOL:H12	5:C:1783:HOH:O	2.20	0.40
1:A:238:GLU:CG	5:A:1799:HOH:O	2.55	0.40
1:A:262:SER:O	1:A:263:ASN:HB2	2.21	0.40
1:C:506[B]:LYS:HD3	1:C:506[B]:LYS:HA	1.88	0.40
1:C:338:CYS:CB	1:C:364:CYS:SG	3.10	0.40

All (7) 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)
5:A:1570:HOH:O	5:A:1570:HOH:O[3_555]	1.65	0.55
5:B:1468:HOH:O	5:C:1725:HOH:O[3_555]	1.91	0.29
5:A:1777:HOH:O	5:B:1481:HOH:O[3_555]	1.91	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1359:HOH:O	5:C:1765:HOH:O[3_555]	2.01	0.19
5:A:1352:HOH:O	5:C:901:HOH:O[5_455]	2.06	0.14
5:A:1348:HOH:O	5:C:1585:HOH:O[5_555]	2.15	0.05
5:A:931:HOH:O	5:A:1433:HOH:O[4_565]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	670/692 (97%)	646 (96%)	23 (3%)	1 (0%)	51	43
1	B	680/692 (98%)	659 (97%)	19 (3%)	2 (0%)	41	31
1	C	677/692 (98%)	653 (96%)	21 (3%)	3 (0%)	34	24
All	All	2027/2076 (98%)	1958 (97%)	63 (3%)	6 (0%)	41	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	333	SER
1	B	334	LEU
1	C	333	SER
1	C	671	ALA
1	A	671	ALA
1	C	335	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	580/594 (98%)	578 (100%)	2 (0%)	92 93
1	B	588/594 (99%)	584 (99%)	4 (1%)	84 84
1	C	586/594 (99%)	579 (99%)	7 (1%)	71 70
All	All	1754/1782 (98%)	1741 (99%)	13 (1%)	81 84

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	LYS
1	A	329	THR
1	B	84	LEU
1	B	329	THR
1	B	336	CYS
1	B	356	PRO
1	C	202	LYS
1	C	238	GLU
1	C	329	THR
1	C	334	LEU
1	C	338	CYS
1	C	481	LYS
1	C	644	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	218	HIS
1	A	286	HIS
1	A	294	HIS
1	A	312	HIS
1	A	330	ASN
1	A	343	HIS
1	A	348	HIS
1	A	361	ASN
1	A	450	ASN
1	A	473	ASN
1	A	529	ASN
1	B	23	HIS
1	B	66	GLN
1	B	70	GLN
1	B	218	HIS

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Mol	Chain	Res	Type
1	B	286	HIS
1	B	294	HIS
1	B	312	HIS
1	B	330	ASN
1	B	343	HIS
1	B	348	HIS
1	B	450	ASN
1	B	457	GLN
1	B	473	ASN
1	B	529	ASN
1	B	547	GLN
1	C	23	HIS
1	C	70	GLN
1	C	137	GLN
1	C	218	HIS
1	C	286	HIS
1	C	288	ASN
1	C	294	HIS
1	C	312	HIS
1	C	330	ASN
1	C	343	HIS
1	C	348	HIS
1	C	361	ASN
1	C	450	ASN
1	C	473	ASN
1	C	529	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 3 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	C	806	-	5,5,5	0.35	0	5,5,5	0.61	0
3	GOL	A	802	-	5,5,5	0.30	0	5,5,5	0.60	0
3	GOL	B	806	-	5,5,5	0.46	0	5,5,5	0.23	0
3	GOL	C	802	-	5,5,5	0.44	0	5,5,5	0.66	0
3	GOL	C	809	-	5,5,5	0.34	0	5,5,5	0.30	0
3	GOL	B	805	-	5,5,5	0.47	0	5,5,5	0.33	0
3	GOL	B	802	-	5,5,5	0.29	0	5,5,5	0.53	0
3	GOL	C	807	-	5,5,5	0.35	0	5,5,5	0.62	0
3	GOL	A	806	-	5,5,5	0.47	0	5,5,5	0.32	0
3	GOL	A	803	-	5,5,5	0.34	0	5,5,5	0.45	0
4	PO4	B	804	-	4,4,4	0.97	0	6,6,6	0.23	0
3	GOL	B	808	-	5,5,5	0.46	0	5,5,5	0.46	0
3	GOL	A	804	-	5,5,5	0.47	0	5,5,5	0.38	0
3	GOL	C	804	-	5,5,5	0.29	0	5,5,5	0.78	0
3	GOL	B	807	-	5,5,5	0.37	0	5,5,5	0.70	0
3	GOL	C	805	-	5,5,5	0.49	0	5,5,5	0.38	0
3	GOL	C	808	-	5,5,5	0.45	0	5,5,5	0.44	0
3	GOL	C	803	-	5,5,5	0.43	0	5,5,5	0.48	0
3	GOL	B	803	-	5,5,5	0.39	0	5,5,5	0.66	0
3	GOL	A	805	-	5,5,5	0.30	0	5,5,5	0.83	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
3	GOL	C	806	-	-	2/4/4/4	-
3	GOL	A	802	-	-	0/4/4/4	-
3	GOL	B	806	-	-	2/4/4/4	-
3	GOL	C	802	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	809	-	-	2/4/4/4	-
3	GOL	B	805	-	-	0/4/4/4	-
3	GOL	B	802	-	-	0/4/4/4	-
3	GOL	C	807	-	-	0/4/4/4	-
3	GOL	A	803	-	-	4/4/4/4	-
3	GOL	C	804	-	-	1/4/4/4	-
3	GOL	B	808	-	-	0/4/4/4	-
3	GOL	A	804	-	-	2/4/4/4	-
3	GOL	A	806	-	-	0/4/4/4	-
3	GOL	B	807	-	-	4/4/4/4	-
3	GOL	C	805	-	-	0/4/4/4	-
3	GOL	C	808	-	-	1/4/4/4	-
3	GOL	C	803	-	-	2/4/4/4	-
3	GOL	B	803	-	-	0/4/4/4	-
3	GOL	A	805	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	806	GOL	O1-C1-C2-C3
3	A	803	GOL	O1-C1-C2-O2
3	A	803	GOL	O1-C1-C2-C3
3	A	803	GOL	C1-C2-C3-O3
3	B	807	GOL	O1-C1-C2-C3
3	B	807	GOL	C1-C2-C3-O3
3	B	807	GOL	O2-C2-C3-O3
3	C	802	GOL	O1-C1-C2-C3
3	C	809	GOL	O1-C1-C2-C3
3	C	806	GOL	O1-C1-C2-C3
3	C	803	GOL	O1-C1-C2-C3
3	A	803	GOL	O2-C2-C3-O3
3	B	807	GOL	O1-C1-C2-O2
3	C	802	GOL	O1-C1-C2-O2
3	C	809	GOL	O1-C1-C2-O2
3	A	805	GOL	O1-C1-C2-O2
3	B	806	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	805	GOL	O2-C2-C3-O3
3	C	803	GOL	O1-C1-C2-O2
3	A	805	GOL	O1-C1-C2-C3
3	C	806	GOL	O1-C1-C2-O2
3	A	804	GOL	O1-C1-C2-O2
3	C	804	GOL	O2-C2-C3-O3
3	A	804	GOL	O1-C1-C2-C3
3	C	808	GOL	C1-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	806	GOL	1	0
3	A	802	GOL	1	0
3	B	806	GOL	1	0
3	B	805	GOL	1	0
3	B	807	GOL	1	0
3	C	808	GOL	1	0
3	C	803	GOL	1	0
3	B	803	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	657/692 (94%)	-0.46	8 (1%) 79 81	4, 11, 25, 55	0
1	B	668/692 (96%)	-0.39	19 (2%) 53 56	5, 11, 28, 68	0
1	C	665/692 (96%)	-0.49	14 (2%) 63 66	4, 10, 27, 63	0
All	All	1990/2076 (95%)	-0.45	41 (2%) 63 66	4, 10, 27, 68	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	683	LEU	7.4
1	B	673	HIS	7.1
1	C	672	VAL	6.8
1	B	333	SER	6.7
1	B	682	ARG	6.5
1	B	334	LEU	5.9
1	A	672	VAL	5.7
1	B	685	PHE	5.3
1	B	684	ALA	4.5
1	B	689	CYS	4.3
1	C	334	LEU	4.3
1	C	684	ALA	4.2
1	B	672	VAL	4.0
1	C	335	GLY	3.7
1	B	16	ALA	3.7
1	A	335	GLY	3.6
1	B	690	CYS	3.4
1	B	686	GLU	3.3
1	B	338[A]	CYS	3.1
1	B	687	GLY	2.7
1	A	437	ASP	2.6
1	C	336	CYS	2.6
1	B	688	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	16	ALA	2.5
1	A	671	ALA	2.5
1	A	670	ARG	2.5
1	A	334	LEU	2.5
1	C	671	ALA	2.4
1	C	245	THR	2.4
1	A	46	GLY	2.4
1	C	686	GLU	2.3
1	B	691	GLY	2.3
1	B	87	GLY	2.2
1	C	333	SER	2.2
1	C	338	CYS	2.2
1	C	670	ARG	2.2
1	C	437	ASP	2.2
1	C	690	CYS	2.2
1	B	335	GLY	2.1
1	B	671	ALA	2.1
1	C	685	PHE	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. 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	GOL	C	808	6/6	0.74	0.19	37,39,41,43	0
3	GOL	A	804	6/6	0.78	0.28	61,64,65,65	0
3	GOL	C	807	6/6	0.80	0.17	28,36,42,45	0
3	GOL	B	805	6/6	0.82	0.22	54,58,59,61	0
3	GOL	A	803	6/6	0.86	0.20	36,41,45,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	806	6/6	0.87	0.15	28,37,38,39	0
3	GOL	B	807	6/6	0.88	0.15	36,43,46,46	0
3	GOL	A	805	6/6	0.89	0.21	29,34,36,37	0
4	PO4	B	804	5/5	0.89	0.22	33,49,52,52	0
3	GOL	C	803	6/6	0.89	0.18	47,53,56,57	0
3	GOL	C	804	6/6	0.90	0.15	31,36,39,44	0
3	GOL	C	809	6/6	0.92	0.15	35,37,40,44	0
3	GOL	C	802	6/6	0.92	0.15	32,39,40,41	0
3	GOL	C	806	6/6	0.95	0.11	17,25,31,37	0
3	GOL	A	802	6/6	0.95	0.18	20,25,28,29	0
3	GOL	A	806	6/6	0.95	0.13	15,21,22,23	0
3	GOL	B	808	6/6	0.96	0.10	12,16,21,22	0
3	GOL	B	802	6/6	0.97	0.08	13,22,25,30	0
3	GOL	B	803	6/6	0.97	0.12	21,25,27,30	0
3	GOL	C	805	6/6	0.98	0.09	14,16,20,22	0
2	CU1	B	801	1/1	1.00	0.05	9,9,9,9	0
2	CU1	A	801	1/1	1.00	0.07	9,9,9,9	0
2	CU1	C	801	1/1	1.00	0.06	9,9,9,9	0

6.5 Other polymers (i)

There are no such residues in this entry.