



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:27 PM GMT

PDB ID : 1GW0
Title : CRYSTAL STRUCTURE OF LACCASE FROM MELANOCARPUS ALBOMYCES IN FOUR COPPER FORM
Authors : Hakulinen, N.; Kiiskinen, L.-L.; Kruus, K.; Saloheimo, M.; Koivula, A.; Rouvinen, J.
Deposited on : 2002-03-01
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

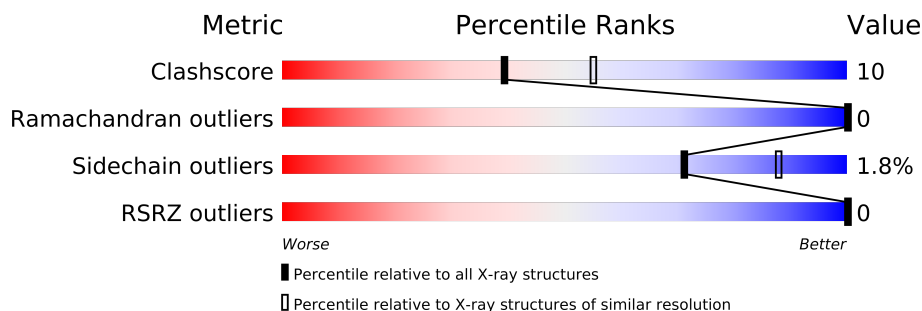
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	559	
1	B	559	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	SO4	A	1588	-	X
10	SO4	B	1584	-	X
2	OXY	A	620	-	X
5	NAG	A	1586	-	X
5	NAG	B	1566	-	X
5	NAG	B	1582	-	X
5	NAG	B	1583	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10060 atoms, of which 0 are hydrogen and 0 are deuterium.

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 LACCASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4369	2764	759	831	15			
1	B	559	Total	C	N	O	S	0	0	0
			4369	2764	759	831	15			

- Molecule 2 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



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

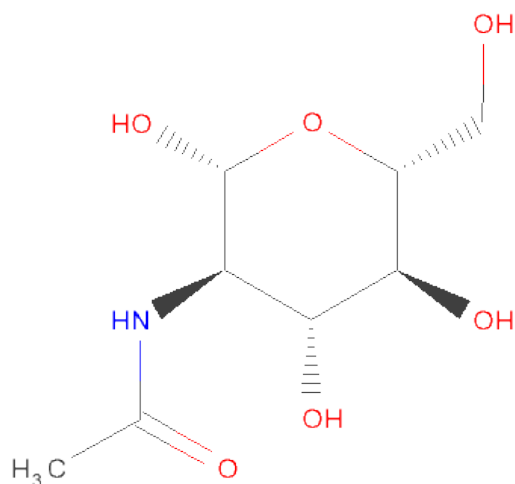
- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Cu	0	0
			4	4		
3	A	4	Total	Cu	0	0
			4	4		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	5	Total	C	N	O	0	0
			61	34	2	25		
8	B	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	2	Total	C	N	O	0	0
			28	16	2	10		
9	A	2	Total	C	N	O	0	0
			28	16	2	10		
9	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	406	Total	O	0	0
			406	406		
12	B	389	Total	O	0	0
			389	389		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

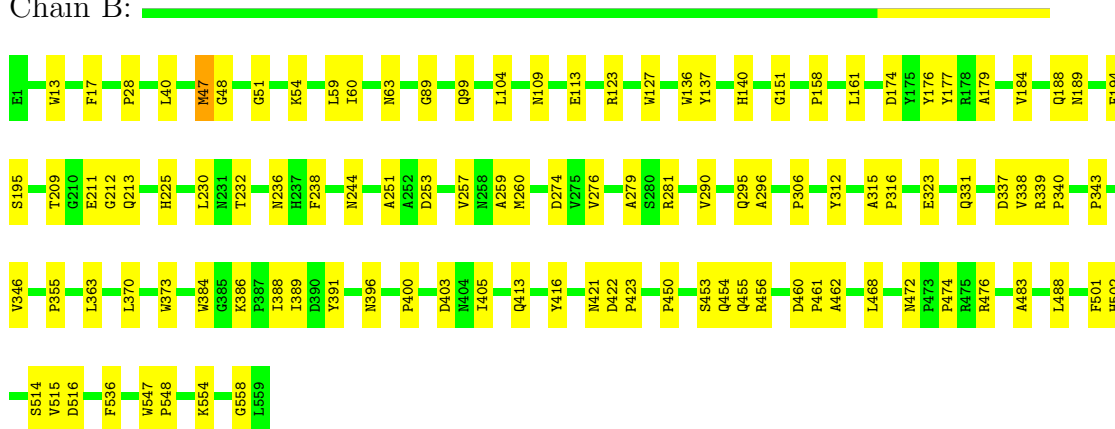
• Molecule 1: LACCASE-1

Chain A:



• Molecule 1: LACCASE-1

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.51Å 72.30Å 88.94Å 110.40° 95.23° 109.74°	Depositor
Resolution (Å)	100.00 – 2.40 80.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.0 (100.00-2.40) 89.2 (80.99-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.189 , 0.248 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 49561 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10060	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, NAG, CL, OXY, SO4, CU, MAN

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	0.34	0/4506	0.64	1/6191 (0.0%)
1	B	0.34	0/4506	0.63	1/6191 (0.0%)
All	All	0.34	0/9012	0.64	2/12382 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	GLY	N-CA-C	-5.81	98.57	113.10
1	B	89	GLY	N-CA-C	-5.02	100.56	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4369	0	4111	98	0
1	B	4369	0	4110	75	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	28	0	26	2	0
5	B	70	0	65	2	0
6	A	83	0	70	8	0
7	A	39	0	34	1	0
8	A	61	0	52	1	0
8	B	61	0	52	3	0
9	A	56	0	50	2	0
9	B	28	0	25	0	0
10	A	10	0	0	0	0
10	B	5	0	0	0	0
11	B	72	0	61	1	0
12	A	406	0	0	8	0
12	B	389	0	0	8	0
All	All	10060	0	8656	172	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (172) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:247:MET:HB3	1:A:275:VAL:HG11	1.39	0.99
1:A:1:GLU:HB2	1:A:2:PRO:HD2	1.47	0.93
1:A:185:HIS:CD2	6:A:1573:BMA:H2	2.04	0.92
1:A:400:PRO:HG2	1:A:403:ASP:OD2	1.82	0.79
1:B:453:SER:HB3	1:B:455:GLN:HG3	1.66	0.78
1:A:257:VAL:HG23	1:A:339:ARG:O	1.85	0.76
6:A:1571:MAN:H62	6:A:1573:BMA:O2	1.85	0.75
1:A:387:PRO:HG2	1:A:536:PHE:HZ	1.53	0.74
1:A:99:GLN:HE22	1:A:127:TRP:HB3	1.52	0.73
1:B:48:GLY:HA3	12:B:2049:HOH:O	1.87	0.72
1:A:13:TRP:HB2	1:A:158:PRO:HG3	1.71	0.71
1:B:13:TRP:HB2	1:B:158:PRO:HG3	1.73	0.70
1:A:339:ARG:HH21	1:A:474:PRO:HD3	1.56	0.69
1:B:281:ARG:NH2	5:B:1583:NAG:H82	2.08	0.69
1:A:323:GLU:OE1	8:A:1578:NAG:H61	1.93	0.69
1:A:251:ALA:HB3	1:A:274:ASP:HB2	1.76	0.68
1:B:338:VAL:HG23	1:B:474:PRO:HB3	1.75	0.68
1:A:190:ASN:HD21	6:A:1573:BMA:H5	1.58	0.68
1:B:212:GLY:O	1:B:213:GLN:HG2	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:354:ARG:HH11	1:A:354:ARG:HB3	1.60	0.66
1:A:354:ARG:NH1	1:A:354:ARG:HB3	2.11	0.65
1:B:386:LYS:HE3	1:B:391:TYR:CZ	2.31	0.65
1:B:453:SER:O	1:B:454:GLN:HB2	1.96	0.65
1:A:190:ASN:ND2	6:A:1573:BMA:H5	2.13	0.64
1:A:167:LEU:O	5:A:1586:NAG:H83	1.98	0.64
1:B:184:VAL:O	1:B:188:GLN:HG3	1.98	0.63
1:A:54:LYS:HD2	1:A:177:TYR:HA	1.81	0.63
1:B:405:ILE:HD13	1:B:516:ASP:HB3	1.81	0.62
1:A:295:GLN:HA	1:B:295:GLN:OE1	1.99	0.62
1:A:1:GLU:CB	1:A:2:PRO:HD2	2.27	0.61
1:B:54:LYS:HD2	1:B:177:TYR:HA	1.82	0.61
1:B:176:TYR:CE2	1:B:195:SER:HA	2.35	0.61
1:B:59:LEU:HD22	1:B:63:ASN:O	2.01	0.61
1:A:354:ARG:CB	1:A:354:ARG:HH11	2.14	0.61
1:A:247:MET:HB3	1:A:275:VAL:CG1	2.25	0.60
1:B:260:MET:HE1	1:B:337:ASP:C	2.22	0.60
1:A:185:HIS:NE2	6:A:1573:BMA:H2	2.17	0.59
1:B:257:VAL:HG12	1:B:340:PRO:HA	1.83	0.59
1:B:47:MET:HE1	1:B:51:GLY:O	2.03	0.58
1:A:399:TYR:HB2	12:A:2277:HOH:O	2.03	0.58
1:B:137:TYR:CZ	1:B:151:GLY:HA3	2.39	0.58
1:B:260:MET:HE1	1:B:338:VAL:N	2.18	0.58
1:A:1:GLU:HB2	1:A:2:PRO:CD	2.28	0.57
1:B:413:GLN:HG3	12:B:2284:HOH:O	2.04	0.57
1:A:48:GLY:HA3	12:A:2066:HOH:O	2.04	0.57
1:B:281:ARG:HH22	5:B:1583:NAG:H82	1.70	0.56
1:B:461:PRO:HD2	12:B:2312:HOH:O	2.05	0.56
1:A:91:SER:O	1:A:139:SER:HA	2.06	0.56
1:B:161:LEU:HD11	1:B:259:ALA:HB2	1.88	0.56
1:B:209:THR:OG1	1:B:211:GLU:HB2	2.06	0.56
1:B:355:PRO:HD2	12:B:2249:HOH:O	2.05	0.55
1:A:420:GLU:HG2	12:A:2298:HOH:O	2.06	0.55
1:A:67:PRO:HB3	12:A:2081:HOH:O	2.07	0.55
1:A:257:VAL:HG23	1:A:339:ARG:C	2.26	0.55
1:B:174:ASP:HB3	1:B:236:ASN:HB2	1.89	0.55
1:B:400:PRO:HG2	1:B:403:ASP:OD2	2.07	0.54
1:A:547:TRP:HB3	1:A:548:PRO:HD3	1.88	0.54
1:A:311:HIS:CD2	7:A:1574:NAG:H5	2.42	0.54
1:A:387:PRO:HG2	1:A:536:PHE:CZ	2.39	0.54
1:A:236:ASN:HB3	1:A:238:PHE:CE2	2.43	0.54
1:A:40:LEU:CD2	1:A:60:ILE:HG12	2.38	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:185:HIS:HD2	6:A:1573:BMA:H2	1.69	0.54
1:A:110:GLY:O	1:A:387:PRO:HA	2.08	0.54
1:A:263:ASP:OD1	8:B:1579:MAN:H4	2.08	0.54
1:B:290:VAL:HB	1:B:306:PRO:HG2	1.90	0.54
1:A:212:GLY:O	1:A:213:GLN:HG3	2.07	0.53
1:A:178:ARG:HH21	1:A:182:ASP:CG	2.11	0.53
1:A:184:VAL:O	1:A:188:GLN:HG3	2.07	0.53
1:B:450:PRO:HB2	1:B:453:SER:OG	2.08	0.53
1:A:190:ASN:HD21	6:A:1573:BMA:C5	2.20	0.53
1:A:348:VAL:HG12	1:A:443:LEU:HD13	1.91	0.53
1:B:113:GLU:HA	1:B:536:PHE:CE1	2.44	0.53
1:A:137:TYR:CZ	1:A:151:GLY:HA3	2.44	0.53
1:A:422:ASP:N	1:A:423:PRO:HD3	2.24	0.52
1:B:47:MET:HE3	1:B:47:MET:HA	1.91	0.52
1:B:421:ASN:ND2	1:B:483:ALA:HA	2.24	0.52
1:B:40:LEU:HD22	1:B:60:ILE:HG12	1.92	0.52
1:B:113:GLU:HA	1:B:536:PHE:HE1	1.75	0.52
1:A:32:VAL:HB	1:A:75:ASP:OD1	2.10	0.52
1:A:2:PRO:HD3	1:A:13:TRP:CZ2	2.45	0.51
1:A:442:VAL:HB	1:A:474:PRO:HG2	1.92	0.51
1:A:510:SER:OG	1:A:556:ASP:OD1	2.26	0.51
1:A:336:LEU:O	1:A:339:ARG:NH2	2.42	0.51
1:B:236:ASN:HB3	1:B:238:PHE:CE2	2.46	0.50
1:A:315:ALA:HB1	1:A:316:PRO:HD2	1.93	0.50
1:A:260:MET:HE1	1:A:338:VAL:N	2.27	0.49
1:A:217:VAL:HG22	5:A:1586:NAG:O7	2.12	0.49
1:A:72:ASN:HB2	1:A:75:ASP:OD2	2.13	0.49
1:B:384:TRP:CZ3	1:B:554:LYS:HD2	2.47	0.49
1:A:311:HIS:HE1	1:A:315:ALA:O	1.96	0.48
1:B:40:LEU:CD2	1:B:60:ILE:HG12	2.43	0.48
1:A:388:ILE:HG12	1:A:405:ILE:HD11	1.95	0.48
1:A:174:ASP:HB3	1:A:236:ASN:HB2	1.96	0.48
1:B:456:ARG:HG3	1:B:456:ARG:HH11	1.77	0.48
1:B:253:ASP:OD2	1:B:476:ARG:HB2	2.14	0.48
1:A:340:PRO:HG2	1:A:472:ASN:OD1	2.13	0.48
1:A:396:ASN:ND2	9:A:1584:NAG:C7	2.76	0.48
1:A:257:VAL:HG22	1:A:258:ASN:N	2.28	0.48
1:A:346:VAL:HG22	1:A:416:TYR:OH	2.14	0.48
1:A:453:SER:OG	1:A:455:GLN:HG3	2.14	0.48
1:A:328:VAL:CG2	8:B:1579:MAN:H5	2.43	0.47
1:A:493:THR:HA	1:A:519:GLU:OE2	2.14	0.47
1:B:161:LEU:HD11	1:B:259:ALA:CB	2.43	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:502:HIS:CB	1:B:514:SER:HB2	2.45	0.47
1:B:502:HIS:HB3	1:B:514:SER:HB2	1.96	0.47
1:A:355:PRO:HD2	12:A:2248:HOH:O	2.14	0.47
1:A:179:ALA:CB	6:A:1568:NAG:H81	2.44	0.47
1:B:179:ALA:CB	11:B:1568:NAG:H81	2.44	0.47
1:B:547:TRP:HB3	1:B:548:PRO:HD3	1.97	0.47
1:B:340:PRO:HG2	1:B:472:ASN:OD1	2.16	0.46
1:A:338:VAL:CG2	1:A:474:PRO:HB3	2.45	0.46
1:A:386:LYS:HE2	9:A:1584:NAG:H61	1.96	0.46
1:A:282:ALA:HB1	12:A:2216:HOH:O	2.14	0.46
1:A:176:TYR:CE2	1:A:195:SER:HA	2.51	0.46
1:B:17:PHE:CE1	1:B:28:PRO:HB3	2.51	0.46
1:B:460:ASP:OD1	1:B:462:ALA:HB3	2.16	0.46
1:B:468:LEU:HD22	1:B:488:LEU:HD23	1.97	0.45
1:A:533:GLU:O	1:A:536:PHE:HB3	2.16	0.45
1:B:386:LYS:HE3	1:B:391:TYR:OH	2.16	0.44
1:A:2:PRO:HB3	1:A:13:TRP:CZ3	2.52	0.44
1:A:328:VAL:HG21	8:B:1579:MAN:H5	1.98	0.44
1:A:286:TYR:HA	12:A:2218:HOH:O	2.18	0.44
1:A:113:GLU:HA	1:A:536:PHE:CE1	2.52	0.44
1:B:388:ILE:HD11	1:B:403:ASP:CG	2.38	0.44
1:A:328:VAL:HG23	12:B:2381:HOH:O	2.17	0.44
1:B:296:ALA:N	12:B:2220:HOH:O	2.42	0.43
1:B:99:GLN:HE22	1:B:127:TRP:HB3	1.84	0.43
1:A:239:GLN:HB2	1:A:291:THR:O	2.17	0.43
1:B:422:ASP:N	1:B:423:PRO:HD3	2.33	0.43
1:A:275:VAL:HG12	1:A:276:VAL:N	2.34	0.43
1:B:502:HIS:HB3	1:B:514:SER:CB	2.48	0.43
1:B:225:HIS:O	1:B:276:VAL:HA	2.19	0.43
1:B:391:TYR:HB3	1:B:396:ASN:O	2.18	0.43
1:B:343:PRO:HA	1:B:472:ASN:OD1	2.19	0.43
1:A:453:SER:O	1:A:454:GLN:HB2	2.19	0.43
1:A:91:SER:OG	1:A:109:ASN:HB3	2.19	0.42
1:B:251:ALA:HB3	1:B:274:ASP:HB2	2.01	0.42
1:B:47:MET:HB3	12:B:2045:HOH:O	2.19	0.42
1:B:331:GLN:OE1	1:B:450:PRO:HA	2.19	0.42
1:B:501:PHE:HB3	1:B:515:VAL:HG22	2.00	0.42
1:B:501:PHE:HB3	1:B:515:VAL:CG2	2.49	0.42
1:A:380:ILE:HG22	1:A:512:GLY:HA2	2.02	0.42
1:A:122:GLN:O	1:A:538:ARG:NH2	2.43	0.42
1:A:17:PHE:CE1	1:A:28:PRO:HB3	2.54	0.42
1:A:257:VAL:HG21	1:A:338:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:136:TRP:CE3	1:B:232:THR:HG22	2.55	0.41
1:A:1:GLU:N	12:A:2002:HOH:O	2.52	0.41
1:B:363:LEU:HD13	1:B:373:TRP:CE2	2.54	0.41
1:B:189:ASN:ND2	1:B:370:LEU:H	2.18	0.41
1:A:172:ILE:HG22	1:A:238:PHE:CE1	2.55	0.41
1:A:380:ILE:HG21	1:A:514:SER:HB3	2.02	0.41
1:A:467:ARG:HG2	1:A:467:ARG:HH11	1.85	0.41
1:B:279:ALA:HA	1:B:312:TYR:OH	2.21	0.41
1:A:453:SER:HA	1:B:194:PHE:CD1	2.55	0.41
1:B:389:ILE:HA	1:B:389:ILE:HD13	1.81	0.41
1:A:339:ARG:NH2	1:A:474:PRO:HD3	2.31	0.41
1:B:338:VAL:CG2	1:B:474:PRO:HB3	2.44	0.41
1:A:509:VAL:HG13	1:A:510:SER:N	2.36	0.41
1:B:315:ALA:HB1	1:B:316:PRO:HD2	2.03	0.41
1:B:257:VAL:HA	1:B:340:PRO:HA	2.02	0.41
1:B:346:VAL:HG22	1:B:416:TYR:OH	2.21	0.41
1:A:389:ILE:HA	1:A:389:ILE:HD13	1.87	0.41
1:A:251:ALA:HA	1:A:257:VAL:HG12	2.03	0.41
1:B:554:LYS:HE2	1:B:558:GLY:CA	2.52	0.41
1:A:225:HIS:O	1:A:276:VAL:HA	2.20	0.40
1:A:180:ALA:O	1:A:184:VAL:HG23	2.21	0.40
1:A:248:THR:HA	1:A:261:THR:HA	2.03	0.40
1:B:295:GLN:O	1:B:296:ALA:HB3	2.22	0.40
1:A:174:ASP:CG	1:A:233:SER:HB3	2.41	0.40
1:A:13:TRP:HB3	1:A:17:PHE:O	2.22	0.40
1:B:323:GLU:HG3	12:B:2210:HOH:O	2.20	0.40
1:A:421:ASN:HB2	1:A:481:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

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	557/559 (100%)	531 (95%)	26 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	557/559 (100%)	531 (95%)	26 (5%)	0	100	100
All	All	1114/1118 (100%)	1062 (95%)	52 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	478/478 (100%)	469 (98%)	9 (2%)	69	87
1	B	478/478 (100%)	470 (98%)	8 (2%)	73	89
All	All	956/956 (100%)	939 (98%)	17 (2%)	71	88

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

Mol	Chain	Res	Type
1	A	109	ASN
1	A	119	LYS
1	A	123	ARG
1	A	140	HIS
1	A	145	TYR
1	A	224	ARG
1	A	230	LEU
1	A	388	ILE
1	A	538	ARG
1	B	47	MET
1	B	104	LEU
1	B	109	ASN
1	B	123	ARG
1	B	140	HIS
1	B	230	LEU
1	B	244	ASN
1	B	339	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	99	GLN
1	A	144	GLN
1	A	189	ASN
1	A	190	ASN
1	A	208	ASN
1	A	236	ASN
1	A	244	ASN
1	A	413	GLN
1	A	530	GLN
1	B	20	ASN
1	B	99	GLN
1	B	144	GLN
1	B	189	ASN
1	B	208	ASN
1	B	236	ASN
1	B	455	GLN
1	B	530	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

32 carbohydrates 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	$\# Z > 2$
6	NAG	A	1567	1,6	12,14,15	0.48	0	15,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1568	6	12,14,15	0.44	0	15,19,21	0.75	1 (6%)
6	BMA	A	1569	6	10,11,12	0.48	0	11,15,17	0.28	0
6	MAN	A	1570	6	10,11,12	0.39	0	11,15,17	0.30	0
6	MAN	A	1571	6	10,11,12	0.56	0	11,15,17	0.50	0
6	MAN	A	1572	6	10,11,12	0.38	0	11,15,17	0.22	0
6	BMA	A	1573	6	10,11,12	0.38	0	11,15,17	0.37	0
7	NAG	A	1574	1,7	12,14,15	0.50	0	15,19,21	0.69	0
7	NAG	A	1575	7	12,14,15	0.47	0	15,19,21	0.67	0
7	BMA	A	1576	7	10,11,12	0.40	0	11,15,17	0.24	0
8	NAG	A	1577	1,8	12,14,15	0.45	0	15,19,21	0.83	1 (6%)
8	NAG	A	1578	8	12,14,15	0.47	0	15,19,21	0.68	0
8	BMA	A	1579	8	10,11,12	0.45	0	11,15,17	0.31	0
8	MAN	A	1580	8	10,11,12	0.40	0	11,15,17	0.29	0
8	MAN	A	1581	8	10,11,12	0.39	0	11,15,17	0.30	0
9	NAG	A	1582	1,9	12,14,15	0.55	0	15,19,21	0.87	0
9	NAG	A	1583	9	12,14,15	0.41	0	15,19,21	0.77	1 (6%)
9	NAG	A	1584	1,9	12,14,15	0.46	0	15,19,21	0.64	0
9	NAG	A	1585	9	12,14,15	0.43	0	15,19,21	0.75	1 (6%)
11	NAG	B	1567	1,11	12,14,15	0.47	0	15,19,21	0.67	0
11	NAG	B	1568	11	12,14,15	0.47	0	15,19,21	0.67	0
11	BMA	B	1569	11	10,11,12	0.45	0	11,15,17	0.38	0
11	MAN	B	1570	11	10,11,12	0.44	0	11,15,17	0.27	0
11	MAN	B	1571	11	10,11,12	0.44	0	11,15,17	0.36	0
11	MAN	B	1572	11	10,11,12	0.39	0	11,15,17	0.23	0
9	NAG	B	1573	1,9	12,14,15	0.56	0	15,19,21	0.66	0
9	NAG	B	1574	9	12,14,15	0.44	0	15,19,21	0.72	0
8	NAG	B	1575	1,8	12,14,15	0.50	0	15,19,21	0.85	1 (6%)
8	NAG	B	1576	8	12,14,15	0.51	0	15,19,21	0.78	0
8	BMA	B	1577	8	10,11,12	0.45	0	11,15,17	0.19	0
8	MAN	B	1578	8	10,11,12	0.43	0	11,15,17	0.35	0
8	MAN	B	1579	8	10,11,12	0.38	0	11,15,17	0.22	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
6	NAG	A	1567	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1568	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1569	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	1570	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1571	6	-	0/2/19/22	0/1/1/1
6	MAN	A	1572	6	-	0/2/19/22	0/1/1/1
6	BMA	A	1573	6	-	0/2/19/22	0/1/1/1
7	NAG	A	1574	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	1575	7	-	0/6/23/26	0/1/1/1
7	BMA	A	1576	7	-	0/2/19/22	0/1/1/1
8	NAG	A	1577	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	1578	8	-	0/6/23/26	0/1/1/1
8	BMA	A	1579	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1580	8	-	0/2/19/22	0/1/1/1
8	MAN	A	1581	8	-	0/2/19/22	0/1/1/1
9	NAG	A	1582	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	1583	9	-	0/6/23/26	0/1/1/1
9	NAG	A	1584	1,9	-	2/6/23/26	0/1/1/1
9	NAG	A	1585	9	-	0/6/23/26	0/1/1/1
11	NAG	B	1567	1,11	-	0/6/23/26	0/1/1/1
11	NAG	B	1568	11	-	0/6/23/26	0/1/1/1
11	BMA	B	1569	11	-	0/2/19/22	0/1/1/1
11	MAN	B	1570	11	-	0/2/19/22	0/1/1/1
11	MAN	B	1571	11	-	0/2/19/22	0/1/1/1
11	MAN	B	1572	11	-	0/2/19/22	0/1/1/1
9	NAG	B	1573	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	1574	9	-	0/6/23/26	0/1/1/1
8	NAG	B	1575	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1576	8	-	0/6/23/26	0/1/1/1
8	BMA	B	1577	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1578	8	-	0/2/19/22	0/1/1/1
8	MAN	B	1579	8	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1575	NAG	C3-C2-N2	-2.28	108.29	111.76
9	A	1583	NAG	C2-N2-C7	-2.07	119.62	123.09
9	A	1585	NAG	C2-N2-C7	-2.06	119.64	123.09
6	A	1568	NAG	C3-C2-N2	-2.04	108.66	111.76
8	A	1577	NAG	C3-C2-N2	-2.01	108.71	111.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1584	NAG	C1-C2-N2-C7
9	A	1584	NAG	O7-C7-N2-C2

There are no ring outliers.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 10 are monoatomic - leaving 12 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	$\# Z > 2$
5	NAG	A	1566	1	12,14,15	0.42	0	15,19,21	0.70	0
5	NAG	A	1586	1	12,14,15	0.44	0	15,19,21	0.80	1 (6%)
10	SO4	A	1587	-	4,4,4	0.25	0	6,6,6	0.12	0
10	SO4	A	1588	-	4,4,4	0.24	0	6,6,6	0.08	0
2	OXY	A	620	3	1,1,1	0.54	0	0,0,0	0.00	-
5	NAG	B	1566	1	12,14,15	0.49	0	15,19,21	0.78	0
5	NAG	B	1580	1	12,14,15	0.44	0	15,19,21	0.69	0
5	NAG	B	1581	1	12,14,15	0.41	0	15,19,21	0.63	0
5	NAG	B	1582	1	12,14,15	0.43	0	15,19,21	0.85	0
5	NAG	B	1583	1	12,14,15	0.41	0	15,19,21	0.70	0
10	SO4	B	1584	-	4,4,4	0.27	0	6,6,6	0.08	0
2	OXY	B	620	3	1,1,1	0.52	0	0,0,0	0.00	-

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
5	NAG	A	1566	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1586	1	-	0/6/23/26	0/1/1/1
10	SO4	A	1587	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	SO4	A	1588	-	-	0/0/0/0	0/0/0/0
2	OXY	A	620	3	-	0/0/0/0	0/0/0/0
5	NAG	B	1566	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1580	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1581	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1582	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1583	1	-	0/6/23/26	0/1/1/1
10	SO4	B	1584	-	-	0/0/0/0	0/0/0/0
2	OXY	B	620	3	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1586	NAG	C2-N2-C7	-2.17	119.44	123.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1581	NAG	O7-C7-N2-C2

There are no ring outliers.

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, 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	559/559 (100%)	-0.76	0 100 100	10, 21, 38, 57	0
1	B	559/559 (100%)	-0.74	0 100 100	7, 22, 37, 58	0
All	All	1118/1118 (100%)	-0.75	0 100 100	7, 21, 37, 58	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	BMA	A	1573	11/12	0.34	14.53	84,85,88,89	0
6	MAN	A	1571	11/12	0.27	9.26	72,74,79,82	0
8	MAN	B	1579	11/12	0.23	8.78	71,72,74,74	0
9	NAG	A	1582	14/15	0.16	8.39	28,36,43,52	0
11	MAN	B	1571	11/12	0.32	8.23	86,89,92,92	0
8	MAN	A	1581	11/12	0.28	6.55	78,79,80,82	0
9	NAG	A	1583	14/15	0.34	5.61	57,60,64,65	0
11	MAN	B	1572	11/12	0.33	5.51	94,95,96,96	0
8	MAN	A	1580	11/12	0.25	5.00	71,72,74,76	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	BMA	A	1569	11/12	0.18	4.00	53,59,66,68	0
7	NAG	A	1575	14/15	0.16	2.44	50,53,57,60	0
6	MAN	A	1572	11/12	0.17	2.24	66,70,71,72	0
8	MAN	B	1578	11/12	0.18	2.04	65,67,68,70	0
9	NAG	A	1585	14/15	0.16	1.22	48,49,52,54	0
8	NAG	B	1576	14/15	0.13	1.06	36,38,44,51	0
9	NAG	B	1574	14/15	0.13	0.90	38,40,41,41	0
9	NAG	A	1584	14/15	0.12	0.67	39,43,45,48	0
7	NAG	A	1574	14/15	0.12	0.39	41,44,47,50	0
11	BMA	B	1569	11/12	0.15	0.30	59,67,74,81	0
6	NAG	A	1567	14/15	0.10	0.28	14,23,26,29	0
9	NAG	B	1573	14/15	0.12	0.27	35,37,37,39	0
6	NAG	A	1568	14/15	0.12	0.00	26,35,38,46	0
8	NAG	A	1578	14/15	0.11	-0.40	36,40,44,50	0
11	NAG	B	1568	14/15	0.10	-0.62	24,35,41,50	0
8	NAG	B	1575	14/15	0.09	-0.68	22,27,32,34	0
11	NAG	B	1567	14/15	0.08	-1.52	17,26,29,31	0
8	NAG	A	1577	14/15	0.08	-1.78	21,25,30,35	0
8	BMA	B	1577	11/12	0.20	-	53,59,61,63	0
8	BMA	A	1579	11/12	0.18	-	57,62,66,68	0
11	MAN	B	1570	11/12	0.27	-	76,79,80,80	0
7	BMA	A	1576	11/12	0.18	-	63,65,65,66	0
6	MAN	A	1570	11/12	0.24	-	70,73,74,74	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	OXY	A	620	2/2	0.15	5.52	22,22,22,25	0
10	SO4	A	1588	5/5	0.17	4.74	77,77,78,79	0
5	NAG	B	1566	14/15	0.15	4.73	34,36,39,40	0
5	NAG	A	1586	14/15	0.16	4.05	46,49,53,55	0
5	NAG	B	1583	14/15	0.20	2.90	55,57,60,60	0
5	NAG	B	1582	14/15	0.14	2.83	38,44,48,49	0
10	SO4	B	1584	5/5	0.13	2.36	73,74,74,74	0
5	NAG	B	1581	14/15	0.16	1.67	49,52,54,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	B	1580	14/15	0.13	1.47	26,30,34,35	0
5	NAG	A	1566	14/15	0.13	0.40	31,34,37,39	0
2	OXY	B	620	2/2	0.10	0.01	19,19,19,23	0
10	SO4	A	1587	5/5	0.11	-0.44	61,62,62,63	0
4	CL	A	1564	1/1	0.08	-1.42	31,31,31,31	0
4	CL	B	1564	1/1	0.08	-2.41	25,25,25,25	0
3	CU	A	1561	1/1	0.04	-2.97	23,23,23,23	0
3	CU	B	1560	1/1	0.06	-3.25	25,25,25,25	0
3	CU	A	1562	1/1	0.04	-3.26	25,25,25,25	0
3	CU	A	1560	1/1	0.03	-4.04	26,26,26,26	0
3	CU	A	1563	1/1	0.04	-4.16	26,26,26,26	0
3	CU	B	1561	1/1	0.05	-4.26	28,28,28,28	0
3	CU	B	1563	1/1	0.06	-4.78	27,27,27,27	0
3	CU	B	1562	1/1	0.04	-9.33	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.