



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:20 AM UTC

PDB ID : 2XN1 / pdb_00002xn1
Title : Structure of alpha-galactosidase from Lactobacillus acidophilus NCFM with TRIS
Authors : Fredslund, F.; Abou Hachem, M.; Larsen, R.J.; Sorensen, P.G.; Lo Leggio, L.; Svensson, B.
Deposited on : 2010-07-30
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

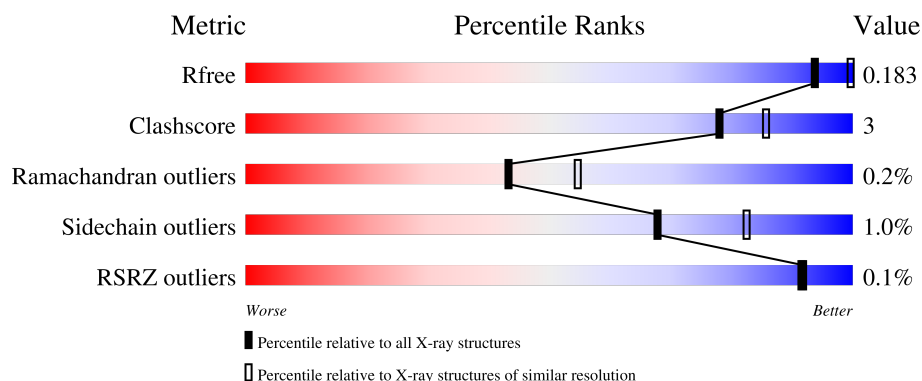
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

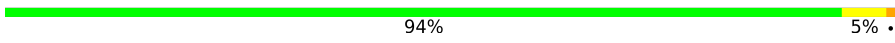
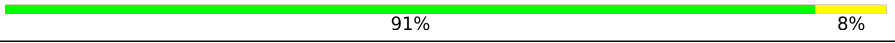
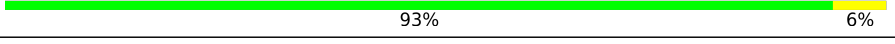
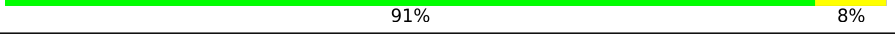
The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	732	
1	B	732	
1	C	732	
1	D	732	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	1736	-	-	X	-
3	GOL	C	1738	-	-	X	-

2 Entry composition [i](#)

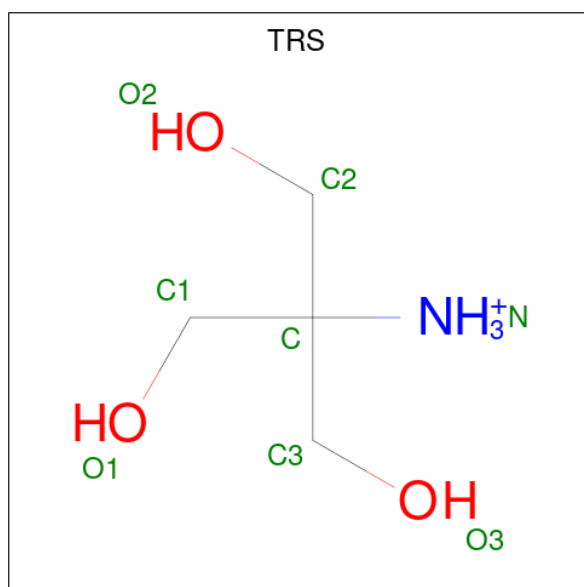
There are 4 unique types of molecules in this entry. The entry contains 48652 atoms, of which 22982 are hydrogens and 0 are deuteriums.

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 ALPHA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	729	Total	C	H	N	O	S	0	0	0
			11645	3770	5709	1008	1131	27			
1	B	729	Total	C	H	N	O	S	0	0	0
			11651	3770	5715	1008	1131	27			
1	C	729	Total	C	H	N	O	S	0	0	0
			11651	3770	5715	1008	1131	27			
1	D	729	Total	C	H	N	O	S	0	0	0
			11651	3770	5715	1008	1131	27			

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



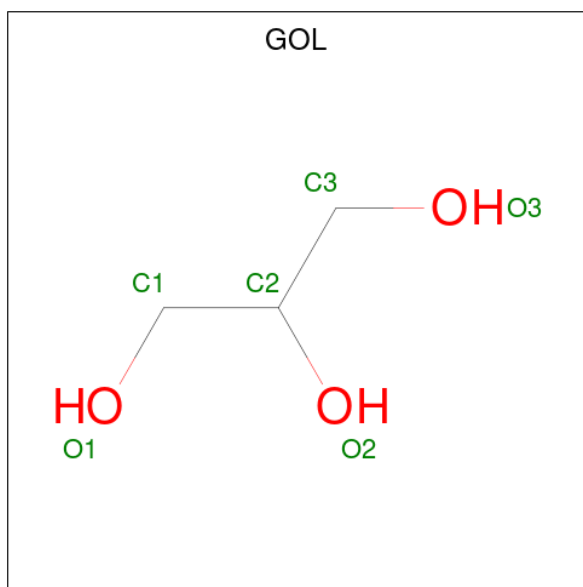
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	B	1	Total	C	N	O	0	0
			8	4	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			6	3	3			
3	A	1	Total	C	O		0	0
			6	3	3			
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	B	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0
3	C	1	Total C H O 14 3 8 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C H O 14 3 8 3	0	0
3	D	1	Total C H O 14 3 8 3	0	0
3	D	1	Total C H O 14 3 8 3	0	0

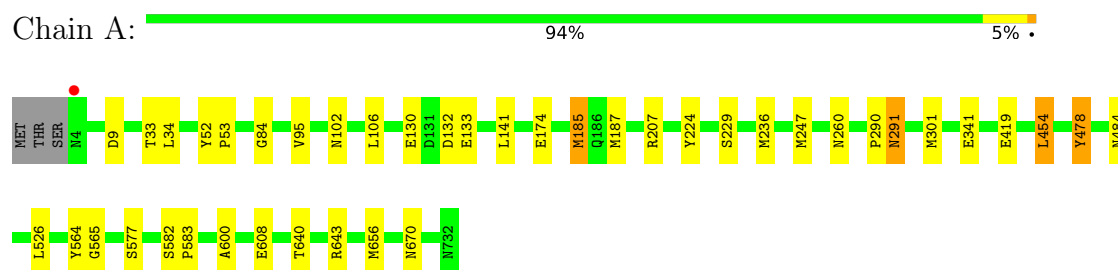
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	455	Total O 455 455	0	0
4	B	439	Total O 439 439	0	0
4	C	484	Total O 484 484	0	0
4	D	390	Total O 390 390	0	0

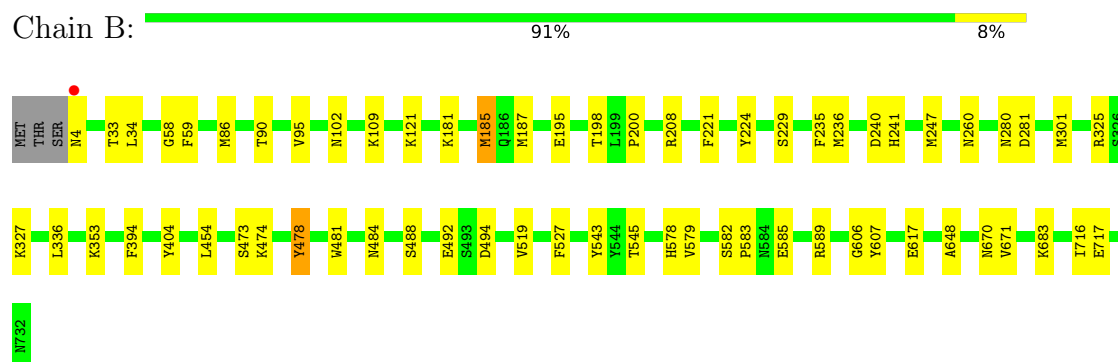
3 Residue-property plots [i](#)

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.

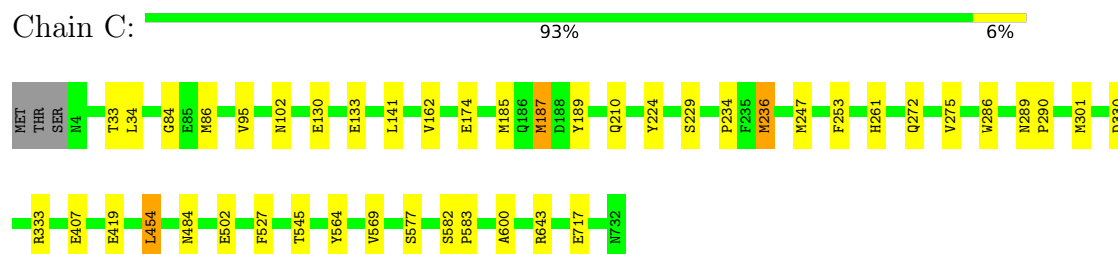
• Molecule 1: ALPHA-GALACTOSIDASE



• Molecule 1: ALPHA-GALACTOSIDASE

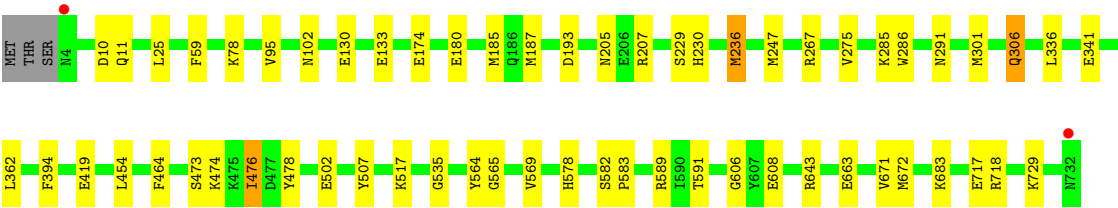


• Molecule 1: ALPHA-GALACTOSIDASE



• Molecule 1: ALPHA-GALACTOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.92Å 150.68Å 126.68Å 90.00° 94.29° 90.00°	Depositor
Resolution (Å)	21.98 – 2.30 21.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (21.98-2.30) 99.5 (21.98-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.78 (at 2.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.147 , 0.187 (Not available) , 0.183	Depositor DCC
R_{free} test set	2010 reflections (1.11%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	48652	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.92	0/6084	0.92	1/8220 (0.0%)
1	B	0.91	1/6084 (0.0%)	0.89	6/8220 (0.1%)
1	C	0.93	0/6084	0.89	3/8220 (0.0%)
1	D	0.87	2/6084 (0.0%)	0.90	3/8220 (0.0%)
All	All	0.91	3/24336 (0.0%)	0.90	13/32880 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	519	VAL	CA-CB	5.32	1.61	1.54
1	D	671	VAL	CA-C	5.21	1.59	1.52
1	D	25	LEU	CA-C	5.00	1.58	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	569	VAL	CB-CA-C	-7.40	103.65	110.91
1	C	333	ARG	CA-C-N	6.43	126.39	119.76
1	C	333	ARG	C-N-CA	6.43	126.39	119.76
1	B	484	ASN	N-CA-C	5.60	119.42	112.59
1	D	394	PHE	CA-C-N	5.52	124.98	119.24
1	D	394	PHE	C-N-CA	5.52	124.98	119.24
1	B	90	THR	CA-C-N	5.51	125.27	119.76
1	B	90	THR	C-N-CA	5.51	125.27	119.76
1	B	394	PHE	CA-C-N	5.41	125.23	119.28
1	B	394	PHE	C-N-CA	5.41	125.23	119.28
1	A	484	ASN	N-CA-C	5.13	118.85	112.59
1	C	484	ASN	N-CA-C	5.10	118.99	112.26
1	B	648	ALA	N-CA-C	-5.02	106.42	112.54

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	5936	5709	5712	29	0
1	B	5936	5715	5712	42	0
1	C	5936	5715	5712	28	0
1	D	5936	5715	5712	34	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
2	C	8	0	12	0	0
2	D	8	0	12	0	0
3	A	30	24	40	9	0
3	B	42	48	56	5	0
3	C	30	32	40	6	0
3	D	24	24	32	3	0
4	A	455	0	0	2	0
4	B	439	0	0	7	0
4	C	484	0	0	3	0
4	D	390	0	0	4	0
All	All	25670	22982	23064	131	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 (131) 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:327:LYS:O	4:B:2217:HOH:O	1.93	0.85
1:C:162:VAL:O	4:C:2107:HOH:O	1.95	0.85
1:B:187:MET:HE1	1:B:301:MET:HE1	1.63	0.80
1:D:187:MET:HE1	1:D:301:MET:HE1	1.71	0.73
1:C:141:LEU:HD13	3:C:1738:GOL:H32	1.72	0.71
1:A:247:MET:HE3	1:D:247:MET:HE3	1.73	0.70
1:B:33:THR:HA	3:B:1740:GOL:H11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:683:LYS:NZ	4:D:2364:HOH:O	2.26	0.69
1:A:34:LEU:H	3:A:1736:GOL:H31	1.58	0.69
1:B:240:ASP:OD2	4:B:2165:HOH:O	2.11	0.68
1:C:187:MET:CE	1:C:301:MET:HE1	2.23	0.67
1:D:187:MET:CE	1:D:301:MET:HE1	2.25	0.67
1:D:362:LEU:O	4:D:2209:HOH:O	2.12	0.67
4:A:2299:HOH:O	3:B:1739:GOL:H2	1.96	0.66
1:A:670:ASN:HB3	4:A:2411:HOH:O	1.96	0.65
1:B:187:MET:HE1	1:B:301:MET:CE	2.27	0.65
1:A:187:MET:HE1	1:A:301:MET:HE1	1.79	0.64
1:C:187:MET:HE1	1:C:301:MET:HE1	1.80	0.63
1:A:187:MET:CE	1:A:301:MET:HE1	2.29	0.62
1:D:78:LYS:HD2	3:D:1737:GOL:H12	1.83	0.61
1:B:247:MET:HE3	1:C:247:MET:HE3	1.85	0.59
1:C:236:MET:HE1	1:C:275:VAL:HG13	1.85	0.59
1:B:86:MET:O	1:B:86:MET:HG3	2.03	0.58
1:D:95:VAL:O	1:D:102:ASN:HA	2.05	0.57
1:B:34:LEU:H	3:B:1740:GOL:H11	1.70	0.57
1:D:130:GLU:O	1:D:133:GLU:HG2	2.05	0.57
1:A:419:GLU:HG2	1:A:454:LEU:HD11	1.87	0.57
1:C:34:LEU:H	3:C:1738:GOL:H31	1.69	0.56
1:A:185:MET:HE3	1:A:185:MET:C	2.31	0.56
1:C:289:ASN:HB3	1:C:290:PRO:HD2	1.88	0.55
1:B:109:LYS:HE3	4:B:2079:HOH:O	2.05	0.55
1:D:473:SER:O	1:D:474:LYS:HB2	2.05	0.55
1:B:582:SER:HA	1:B:583:PRO:C	2.32	0.55
1:D:286:TRP:CE3	1:D:502:GLU:HG2	2.41	0.54
1:D:419:GLU:HG2	1:D:454:LEU:HD11	1.89	0.54
3:A:1734:GOL:H31	1:B:58:GLY:HA2	1.89	0.54
1:B:473:SER:O	1:B:474:LYS:HB2	2.07	0.54
3:D:1735:GOL:H32	4:D:2049:HOH:O	2.08	0.54
1:D:10:ASP:OD1	1:D:11:GLN:NE2	2.41	0.54
1:C:95:VAL:O	1:C:102:ASN:HA	2.08	0.54
1:B:200:PRO:HD2	1:B:208:ARG:O	2.09	0.53
1:C:236:MET:HE1	1:C:275:VAL:CG1	2.39	0.53
1:C:253:PHE:HE2	1:C:301:MET:HE3	1.74	0.53
1:B:95:VAL:O	1:B:102:ASN:HA	2.10	0.52
1:C:272:GLN:HB3	4:C:2192:HOH:O	2.08	0.52
1:C:286:TRP:CE3	1:C:502:GLU:HG2	2.45	0.51
1:B:578:HIS:HA	1:B:606:GLY:O	2.10	0.51
1:A:207:ARG:O	1:A:565:GLY:HA3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD13	3:A:1736:GOL:H32	1.91	0.50
1:C:582:SER:HA	1:C:583:PRO:C	2.36	0.50
1:A:564:TYR:CZ	1:A:643:ARG:HD2	2.47	0.50
1:D:582:SER:HA	1:D:583:PRO:C	2.36	0.50
1:D:236:MET:HE1	1:D:275:VAL:CG1	2.42	0.49
1:D:683:LYS:CE	4:D:2364:HOH:O	2.61	0.49
1:C:84:GLY:HA2	3:C:1737:GOL:O3	2.13	0.49
1:B:195:GLU:OE2	1:B:241:HIS:ND1	2.43	0.48
1:B:198:THR:HG21	1:B:221:PHE:CD1	2.48	0.48
1:B:478:TYR:C	1:B:478:TYR:CD1	2.91	0.48
1:B:492:GLU:HG2	1:B:494:ASP:OD1	2.13	0.48
1:B:716:ILE:C	1:B:717:GLU:HG2	2.37	0.48
1:B:187:MET:HE3	1:B:187:MET:HB2	1.64	0.48
1:C:33:THR:HG23	3:C:1738:GOL:H2	1.94	0.47
1:C:234:PRO:HB3	1:C:261:HIS:CD2	2.49	0.47
1:D:578:HIS:HA	1:D:606:GLY:O	2.14	0.47
1:D:663:GLU:CD	1:D:729:LYS:HE2	2.40	0.47
1:B:481:TRP:CD1	1:B:481:TRP:C	2.92	0.47
1:C:224:TYR:HE1	3:D:1735:GOL:O2	1.97	0.47
1:B:336:LEU:C	1:B:336:LEU:HD12	2.40	0.47
1:C:330:ASP:HB2	4:C:2229:HOH:O	2.14	0.47
1:D:236:MET:HE1	1:D:275:VAL:HG13	1.97	0.47
1:C:130:GLU:O	1:C:133:GLU:HG2	2.15	0.46
1:A:174:GLU:HB2	3:A:1735:GOL:H31	1.97	0.46
1:B:181:LYS:HG3	1:B:281:ASP:HB3	1.98	0.46
1:C:253:PHE:CE2	1:C:301:MET:HE3	2.51	0.45
1:D:341:GLU:HB2	1:D:608:GLU:HG2	1.98	0.45
1:C:86:MET:HG3	1:C:86:MET:O	2.16	0.45
1:C:564:TYR:CZ	1:C:643:ARG:HD2	2.51	0.45
1:D:187:MET:HE3	1:D:187:MET:HB2	1.85	0.45
1:A:640:THR:O	1:A:656:MET:HA	2.17	0.45
1:B:185:MET:O	1:B:185:MET:HE3	2.17	0.45
1:A:187:MET:HB2	1:A:187:MET:HE3	1.78	0.45
3:A:1734:GOL:H11	1:B:59:PHE:CE1	2.52	0.45
1:B:109:LYS:HE2	4:B:2100:HOH:O	2.17	0.44
1:A:95:VAL:O	1:A:102:ASN:HA	2.17	0.44
1:B:4:ASN:N	4:B:2001:HOH:O	2.49	0.44
1:A:290:PRO:O	1:A:291:ASN:HB2	2.17	0.44
3:A:1738:GOL:H31	1:B:488:SER:HA	1.99	0.44
1:A:130:GLU:HB3	1:A:132:ASP:OD2	2.17	0.44
1:B:527:PHE:HB3	1:B:545:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:TYR:HA	1:A:260:ASN:CG	2.43	0.43
1:A:106:LEU:O	3:A:1736:GOL:O3	2.37	0.43
1:A:577:SER:HB2	1:A:600:ALA:HA	2.00	0.43
1:A:84:GLY:H	3:A:1738:GOL:H11	1.83	0.43
1:B:187:MET:CE	1:B:301:MET:HE1	2.42	0.43
1:A:130:GLU:O	1:A:133:GLU:HG2	2.19	0.43
1:A:582:SER:HA	1:A:583:PRO:C	2.44	0.43
1:B:589:ARG:NH2	1:D:672:MET:HE3	2.34	0.43
1:B:683:LYS:NZ	4:B:2407:HOH:O	2.52	0.43
1:D:193:ASP:HA	1:D:267:ARG:HH22	1.84	0.43
1:C:527:PHE:HB3	1:C:545:THR:HG22	2.01	0.43
1:D:230:HIS:CE1	1:D:535:GLY:HA3	2.54	0.43
1:D:564:TYR:CZ	1:D:643:ARG:HD2	2.54	0.43
1:B:585:GLU:O	1:D:718:ARG:NH1	2.52	0.42
1:B:670:ASN:HB3	4:B:2403:HOH:O	2.20	0.42
1:A:52:TYR:HA	1:A:53:PRO:HD3	1.97	0.42
1:B:224:TYR:HA	1:B:260:ASN:OD1	2.19	0.42
1:B:325:ARG:CZ	1:B:543:TYR:CE2	3.03	0.42
1:D:464:PHE:CZ	1:D:517:LYS:HE2	2.55	0.42
1:D:507:TYR:CD1	1:D:507:TYR:C	2.98	0.42
1:A:33:THR:HG23	3:A:1736:GOL:H2	2.02	0.42
1:D:306:GLN:O	1:D:306:GLN:CG	2.66	0.42
1:D:476:ILE:N	1:D:476:ILE:HD12	2.35	0.42
1:A:478:TYR:HA	1:A:526:LEU:O	2.20	0.42
3:C:1734:GOL:H11	1:D:59:PHE:CE1	2.55	0.42
1:A:9:ASP:OD1	1:A:9:ASP:C	2.62	0.41
1:A:224:TYR:HE1	3:B:1739:GOL:O2	2.02	0.41
1:C:419:GLU:HG2	1:C:454:LEU:HD11	2.01	0.41
1:B:33:THR:HA	3:B:1740:GOL:C1	2.48	0.41
1:A:341:GLU:HB2	1:A:608:GLU:HG2	2.02	0.41
1:D:180:GLU:OE2	1:D:285:LYS:HE3	2.21	0.41
1:C:577:SER:HB2	1:C:600:ALA:HA	2.03	0.41
1:D:336:LEU:C	1:D:336:LEU:HD12	2.46	0.41
1:B:353:LYS:HG2	1:B:404:TYR:CD2	2.56	0.41
1:C:141:LEU:CD1	3:C:1738:GOL:H32	2.48	0.41
1:B:235:PHE:CG	1:B:236:MET:N	2.89	0.40
1:C:187:MET:HG2	1:C:189:TYR:CE1	2.56	0.40
1:A:564:TYR:CE1	1:A:643:ARG:HD2	2.57	0.40
1:D:589:ARG:HG2	1:D:591:THR:HG23	2.02	0.40
1:D:207:ARG:O	1:D:565:GLY:HA3	2.22	0.40
1:B:260:ASN:HB3	1:B:280:ASN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:VAL:HB	1:B:607:TYR:CD2	2.57	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	727/732 (99%)	699 (96%)	27 (4%)	1 (0%)	48	60
1	B	727/732 (99%)	696 (96%)	29 (4%)	2 (0%)	36	46
1	C	727/732 (99%)	702 (97%)	24 (3%)	1 (0%)	48	60
1	D	727/732 (99%)	698 (96%)	27 (4%)	2 (0%)	36	46
All	All	2908/2928 (99%)	2795 (96%)	107 (4%)	6 (0%)	43	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	SER
1	B	229	SER
1	C	229	SER
1	D	205	ASN
1	D	229	SER
1	B	671	VAL

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	645/648 (100%)	640 (99%)	5 (1%)	73	86
1	B	645/648 (100%)	640 (99%)	5 (1%)	73	86
1	C	645/648 (100%)	636 (99%)	9 (1%)	59	76
1	D	645/648 (100%)	637 (99%)	8 (1%)	63	79
All	All	2580/2592 (100%)	2553 (99%)	27 (1%)	68	82

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	MET
1	A	236	MET
1	A	291	ASN
1	A	454	LEU
1	A	478	TYR
1	B	121	LYS
1	B	185	MET
1	B	454	LEU
1	B	478	TYR
1	B	617	GLU
1	C	174	GLU
1	C	185	MET
1	C	187	MET
1	C	210	GLN
1	C	236	MET
1	C	407	GLU
1	C	454	LEU
1	C	569	VAL
1	C	717	GLU
1	D	174	GLU
1	D	185	MET
1	D	236	MET
1	D	291	ASN
1	D	306	GLN
1	D	476	ILE
1	D	478	TYR
1	D	717	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	205	ASN
1	A	233	ASN
1	A	306	GLN
1	A	660	ASN
1	B	48	ASN
1	B	135	GLN
1	B	205	ASN
1	B	233	ASN
1	B	331	GLN
1	B	376	HIS
1	B	674	HIS
1	B	709	HIS
1	C	172	HIS
1	C	205	ASN
1	C	233	ASN
1	C	660	ASN
1	C	709	HIS
1	D	48	ASN
1	D	170	HIS
1	D	233	ASN
1	D	621	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 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	TRS	B	1733	-	7,7,7	0.35	0	9,9,9	1.05	0
3	GOL	A	1737	-	5,5,5	0.54	0	5,5,5	1.19	0
3	GOL	C	1737	-	5,5,5	0.80	0	5,5,5	0.96	0
2	TRS	C	1733	-	7,7,7	0.51	0	9,9,9	1.03	0
3	GOL	B	1739	-	5,5,5	0.75	0	5,5,5	1.23	0
3	GOL	B	1734	-	5,5,5	0.32	0	5,5,5	1.15	1 (20%)
2	TRS	D	1733	-	7,7,7	0.25	0	9,9,9	0.65	0
2	TRS	A	1733	-	7,7,7	0.44	0	9,9,9	1.00	0
3	GOL	C	1734	-	5,5,5	0.33	0	5,5,5	1.91	1 (20%)
3	GOL	D	1736	-	5,5,5	0.36	0	5,5,5	0.65	0
3	GOL	C	1736	-	5,5,5	0.39	0	5,5,5	0.69	0
3	GOL	A	1736	-	5,5,5	0.47	0	5,5,5	0.46	0
3	GOL	C	1738	-	5,5,5	0.36	0	5,5,5	0.56	0
3	GOL	A	1738	-	5,5,5	0.80	0	5,5,5	1.24	0
3	GOL	A	1734	-	5,5,5	0.27	0	5,5,5	1.61	0
3	GOL	D	1737	-	5,5,5	0.67	0	5,5,5	0.89	0
3	GOL	D	1734	-	5,5,5	0.36	0	5,5,5	1.13	0
3	GOL	C	1735	-	5,5,5	0.59	0	5,5,5	0.89	0
3	GOL	B	1735	-	5,5,5	0.35	0	5,5,5	1.25	1 (20%)
3	GOL	D	1735	-	5,5,5	0.81	0	5,5,5	0.76	0
3	GOL	B	1738	-	5,5,5	0.42	0	5,5,5	0.59	0
3	GOL	B	1740	-	5,5,5	0.50	0	5,5,5	0.81	0
3	GOL	B	1737	-	5,5,5	0.40	0	5,5,5	0.59	0
3	GOL	A	1735	-	5,5,5	0.58	0	5,5,5	0.78	0
3	GOL	B	1736	-	5,5,5	0.25	0	5,5,5	0.51	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	TRS	B	1733	-	-	1/9/9/9	-
3	GOL	A	1737	-	-	0/4/4/4	-
3	GOL	C	1737	-	-	4/4/4/4	-
2	TRS	C	1733	-	-	6/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1739	-	-	4/4/4/4	-
3	GOL	B	1734	-	-	2/4/4/4	-
2	TRS	D	1733	-	-	5/9/9/9	-
2	TRS	A	1733	-	-	4/9/9/9	-
3	GOL	C	1734	-	-	0/4/4/4	-
3	GOL	D	1736	-	-	2/4/4/4	-
3	GOL	C	1736	-	-	0/4/4/4	-
3	GOL	A	1736	-	-	0/4/4/4	-
3	GOL	C	1738	-	-	0/4/4/4	-
3	GOL	A	1738	-	-	4/4/4/4	-
3	GOL	A	1734	-	-	2/4/4/4	-
3	GOL	D	1737	-	-	0/4/4/4	-
3	GOL	D	1734	-	-	2/4/4/4	-
3	GOL	C	1735	-	-	2/4/4/4	-
3	GOL	B	1735	-	-	2/4/4/4	-
3	GOL	D	1735	-	-	2/4/4/4	-
3	GOL	B	1738	-	-	4/4/4/4	-
3	GOL	B	1740	-	-	4/4/4/4	-
3	GOL	B	1737	-	-	0/4/4/4	-
3	GOL	A	1735	-	-	2/4/4/4	-
3	GOL	B	1736	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1734	GOL	C3-C2-C1	-3.16	100.20	111.80
3	B	1735	GOL	C3-C2-C1	-2.37	103.10	111.80
3	B	1734	GOL	O1-C1-C2	-2.25	100.27	110.38

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1733	TRS	C1-C-C3-O3
3	A	1734	GOL	C1-C2-C3-O3
3	A	1735	GOL	O1-C1-C2-C3
3	A	1738	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	1738	GOL	C1-C2-C3-O3
3	B	1735	GOL	O1-C1-C2-O2
3	B	1735	GOL	O1-C1-C2-C3
3	B	1738	GOL	O1-C1-C2-C3
3	B	1739	GOL	C1-C2-C3-O3
3	B	1740	GOL	O1-C1-C2-C3
3	B	1740	GOL	C1-C2-C3-O3
3	C	1735	GOL	C1-C2-C3-O3
3	C	1737	GOL	C1-C2-C3-O3
3	D	1736	GOL	O1-C1-C2-C3
3	B	1739	GOL	O2-C2-C3-O3
3	B	1734	GOL	C1-C2-C3-O3
3	B	1738	GOL	C1-C2-C3-O3
3	B	1739	GOL	O1-C1-C2-C3
3	C	1737	GOL	O1-C1-C2-C3
3	D	1734	GOL	C1-C2-C3-O3
3	D	1735	GOL	O1-C1-C2-C3
3	A	1738	GOL	O1-C1-C2-O2
3	A	1738	GOL	O2-C2-C3-O3
3	B	1734	GOL	O2-C2-C3-O3
3	B	1738	GOL	O1-C1-C2-O2
3	B	1740	GOL	O1-C1-C2-O2
3	C	1735	GOL	O2-C2-C3-O3
3	C	1737	GOL	O2-C2-C3-O3
3	D	1736	GOL	O1-C1-C2-O2
2	D	1733	TRS	C2-C-C3-O3
3	A	1734	GOL	O2-C2-C3-O3
3	B	1739	GOL	O1-C1-C2-O2
3	D	1734	GOL	O2-C2-C3-O3
3	B	1740	GOL	O2-C2-C3-O3
3	C	1737	GOL	O1-C1-C2-O2
2	A	1733	TRS	N-C-C3-O3
2	C	1733	TRS	N-C-C3-O3
3	D	1735	GOL	O1-C1-C2-O2
3	A	1735	GOL	O1-C1-C2-O2
2	A	1733	TRS	C1-C-C3-O3
2	A	1733	TRS	C2-C-C3-O3
2	C	1733	TRS	C1-C-C3-O3
2	C	1733	TRS	C2-C-C3-O3
2	D	1733	TRS	C2-C-C1-O1
2	D	1733	TRS	N-C-C1-O1
2	D	1733	TRS	N-C-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	1738	GOL	O2-C2-C3-O3
2	A	1733	TRS	C1-C-C2-O2
2	B	1733	TRS	C1-C-C3-O3
2	C	1733	TRS	C2-C-C1-O1
2	C	1733	TRS	C1-C-C2-O2
2	C	1733	TRS	N-C-C1-O1

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1737	GOL	1	0
3	B	1739	GOL	2	0
3	C	1734	GOL	1	0
3	A	1736	GOL	4	0
3	C	1738	GOL	4	0
3	A	1738	GOL	2	0
3	A	1734	GOL	2	0
3	D	1737	GOL	1	0
3	D	1735	GOL	2	0
3	B	1740	GOL	3	0
3	A	1735	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 [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	729/732 (99%)	-0.92	1 (0%) 92 91	10, 23, 49, 79	0
1	B	729/732 (99%)	-0.91	1 (0%) 92 91	11, 25, 50, 94	0
1	C	729/732 (99%)	-0.94	0 100 100	10, 23, 50, 87	0
1	D	729/732 (99%)	-0.83	2 (0%) 90 90	12, 29, 58, 117	0
All	All	2916/2928 (99%)	-0.90	4 (0%) 92 91	10, 25, 53, 117	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	732	ASN	3.8
1	B	4	ASN	2.6
1	A	4	ASN	2.6
1	D	4	ASN	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
3	GOL	A	1734	6/6	0.85	0.16	25,47,60,63	0
3	GOL	B	1735	6/6	0.86	0.15	40,55,64,69	0
3	GOL	A	1735	6/6	0.87	0.19	48,58,63,63	0
3	GOL	B	1737	6/6	0.87	0.15	63,76,88,90	0
3	GOL	D	1734	6/6	0.89	0.19	38,65,77,85	0
3	GOL	C	1734	6/6	0.90	0.13	21,45,56,57	0
3	GOL	A	1738	6/6	0.91	0.19	30,49,64,64	0
3	GOL	B	1734	6/6	0.91	0.19	29,50,69,69	0
3	GOL	A	1737	6/6	0.91	0.12	29,46,55,58	0
3	GOL	D	1735	6/6	0.91	0.20	27,49,59,59	0
3	GOL	C	1735	6/6	0.92	0.10	33,44,59,71	0
3	GOL	C	1737	6/6	0.92	0.18	30,50,60,62	0
3	GOL	B	1738	6/6	0.92	0.12	45,59,77,86	0
3	GOL	B	1736	6/6	0.92	0.09	40,50,60,60	0
3	GOL	D	1737	6/6	0.92	0.20	31,51,62,62	0
3	GOL	D	1736	6/6	0.93	0.10	37,52,65,65	0
3	GOL	C	1736	6/6	0.94	0.11	31,61,74,80	0
3	GOL	A	1736	6/6	0.94	0.20	52,65,76,91	0
3	GOL	B	1740	6/6	0.94	0.19	31,42,63,70	0
3	GOL	B	1739	6/6	0.95	0.15	23,48,65,65	0
2	TRS	B	1733	8/8	0.95	0.07	20,30,31,33	0
2	TRS	D	1733	8/8	0.96	0.09	25,38,39,41	0
3	GOL	C	1738	6/6	0.96	0.18	37,45,60,72	0
2	TRS	A	1733	8/8	0.97	0.07	19,26,31,35	0
2	TRS	C	1733	8/8	0.97	0.07	16,23,27,36	0

6.5 Other polymers

There are no such residues in this entry.