



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:14 AM UTC

PDB ID : 5ZN6 / pdb_00005zn6
Title : Crystal structure of GH31 alpha-xylosidase from a soil metagenome
Authors : Matsuzawa, T.; Nakamichi, Y.; Watanabe, M.; Yaoi, K.
Deposited on : 2018-04-07
Resolution : 1.80 Å(reported)

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

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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

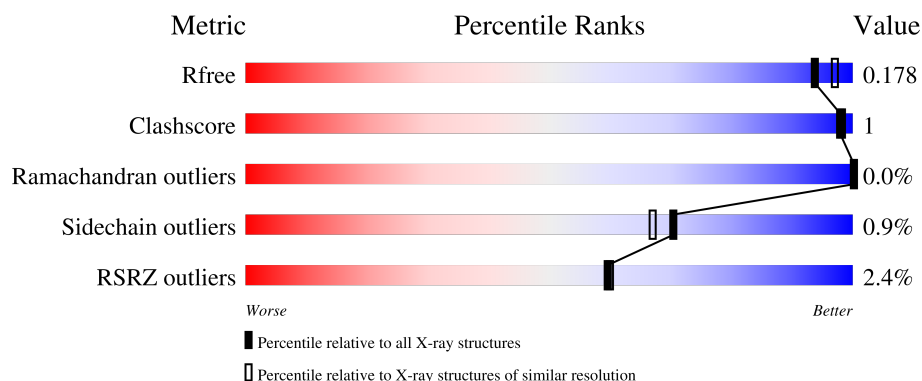
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	687	% 97% ..
1	B	687	2% 98% ..
1	C	687	% 96% ..
1	D	687	% 96% ..
1	E	687	6% 95% ..

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Mol	Chain	Length	Quality of chain
1	F	687	4% 95% ..
1	G	687	2% 95% ..
1	H	687	% 96% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47599 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 Alpha-xylosidase MeXyl31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	680	Total	C	N	O	S	0	1	0
			5461	3489	927	1013	32			
1	B	682	Total	C	N	O	S	0	3	0
			5496	3510	936	1018	32			
1	C	676	Total	C	N	O	S	0	2	0
			5438	3472	924	1010	32			
1	D	680	Total	C	N	O	S	0	0	0
			5454	3485	926	1011	32			
1	E	675	Total	C	N	O	S	0	1	0
			5429	3468	925	1004	32			
1	F	675	Total	C	N	O	S	0	0	0
			5418	3462	921	1003	32			
1	H	676	Total	C	N	O	S	0	1	0
			5430	3468	923	1007	32			
1	G	677	Total	C	N	O	S	0	0	0
			5432	3471	923	1006	32			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	567	Total O 567 567	0	0
3	B	474	Total O 474 474	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	528	Total 528	O 528	0	0
3	D	491	Total 491	O 491	0	0
3	E	338	Total 338	O 338	0	0
3	F	377	Total 377	O 377	0	0
3	H	519	Total 519	O 519	0	0
3	G	435	Total 435	O 435	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-xylosidase MeXyl31



- Molecule 1: Alpha-xylosidase MeXyl31



- Molecule 1: Alpha-xylosidase MeXyl31

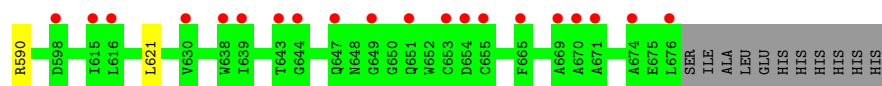


- Molecule 1: Alpha-xylosidase MeXyl31

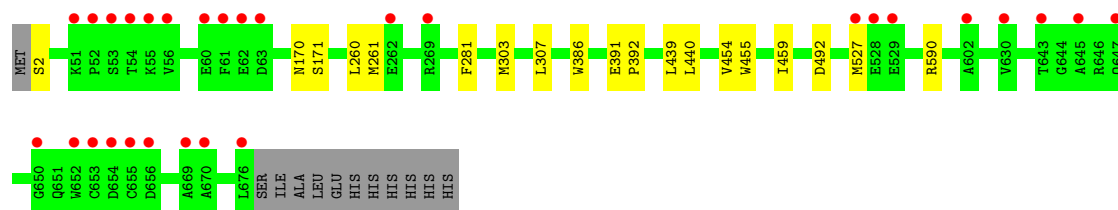


- Molecule 1: Alpha-xylosidase MeXyl31





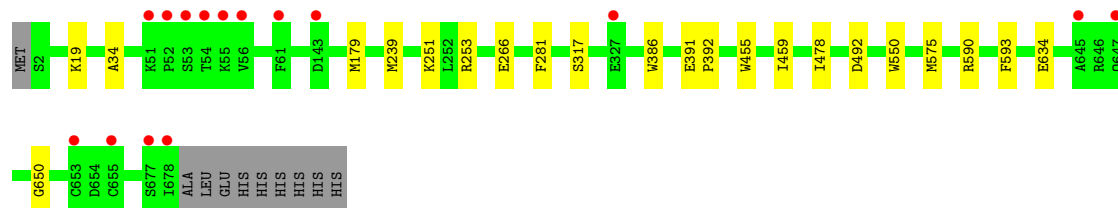
- Molecule 1: Alpha-xylosidase MeXyl31



- Molecule 1: Alpha-xylosidase MeXyl31



- Molecule 1: Alpha-xylosidase MeXyl31



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	173.15Å 124.17Å 177.45Å 90.00° 116.81° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-1.80) 91.1 (50.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.174 , 0.195 (Not available) , 0.178	Depositor DCC
R_{free} test set	27623 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	47599	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7799e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.56	0/5615	0.75	0/7633
1	B	0.56	0/5652	0.75	0/7682
1	C	0.57	0/5592	0.74	0/7601
1	D	0.55	0/5608	0.75	0/7623
1	E	0.57	0/5583	0.74	0/7588
1	F	0.55	0/5572	0.74	0/7574
1	G	0.54	0/5586	0.74	0/7593
1	H	0.56	0/5584	0.74	0/7590
All	All	0.56	0/44792	0.75	0/60884

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	5461	0	5230	7	0
1	B	5496	0	5260	5	0
1	C	5438	0	5198	6	0
1	D	5454	0	5224	8	0
1	E	5429	0	5198	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	5418	0	5186	11	0
1	G	5432	0	5202	9	0
1	H	5430	0	5195	9	0
2	A	54	0	72	0	0
2	B	48	0	64	0	0
2	C	48	0	64	0	0
2	D	36	0	48	1	0
2	E	30	0	40	0	0
2	F	12	0	16	0	0
2	G	36	0	48	0	0
2	H	48	0	64	0	0
3	A	567	0	0	0	0
3	B	474	0	0	0	0
3	C	528	0	0	0	0
3	D	491	0	0	0	0
3	E	338	0	0	0	0
3	F	377	0	0	0	0
3	G	435	0	0	0	0
3	H	519	0	0	0	0
All	All	47599	0	42109	57	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 1.

All (57) 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:H:471:MET:HA	1:H:471:MET:HE2	1.69	0.72
1:H:471:MET:HE1	1:H:606:GLU:O	1.96	0.66
1:F:261:MET:HE1	1:F:307:LEU:HD21	1.80	0.61
1:G:266:GLU:HG2	1:G:550:TRP:CZ2	2.39	0.57
1:D:418:ARG:NH1	2:D:705:GOL:O2	2.43	0.52
1:H:471:MET:HE2	1:H:471:MET:CA	2.39	0.52
1:F:261:MET:HA	1:F:261:MET:HE2	1.94	0.50
1:D:334:GLU:OE2	1:F:2:SER:N	2.46	0.48
1:A:323:ASP:O	1:A:326[A]:THR:HG22	2.13	0.47
1:E:327:GLU:O	1:E:331:ILE:HD12	2.15	0.47
1:A:2:SER:N	1:B:334:GLU:OE2	2.48	0.47
1:E:391:GLU:N	1:E:392:PRO:HA	2.30	0.47
1:F:391:GLU:N	1:F:392:PRO:HA	2.30	0.46
1:E:317:SER:HA	1:E:386:TRP:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:PRO:HB2	1:F:170:ASN:HB3	1.98	0.45
1:H:391:GLU:N	1:H:392:PRO:HA	2.32	0.45
1:C:317:SER:HA	1:C:386:TRP:HB3	1.99	0.45
1:F:261:MET:HE1	1:F:307:LEU:CG	2.48	0.44
1:E:440:LEU:O	1:E:454:VAL:HA	2.18	0.44
1:H:324:ASN:HA	1:H:329:TYR:CG	2.53	0.44
1:A:317:SER:HA	1:A:386:TRP:HB3	2.00	0.44
1:C:324:ASN:HA	1:C:329:TYR:CG	2.53	0.44
1:B:440:LEU:O	1:B:454:VAL:HA	2.18	0.44
1:D:391:GLU:N	1:D:392:PRO:HA	2.32	0.44
1:D:317:SER:HA	1:D:386:TRP:HB3	2.00	0.43
1:G:391:GLU:N	1:G:392:PRO:HA	2.34	0.43
1:B:391:GLU:N	1:B:392:PRO:HA	2.34	0.43
1:H:11:LEU:HD23	1:H:11:LEU:C	2.44	0.43
1:H:317:SER:HA	1:H:386:TRP:HB3	2.00	0.43
1:F:386:TRP:CD1	1:F:439:LEU:HD23	2.54	0.42
1:C:24:PRO:HG3	1:C:56:VAL:HG21	2.00	0.42
1:E:467[A]:ARG:HG2	1:E:621:LEU:HB3	2.01	0.42
1:G:251:LYS:O	1:G:253:ARG:HA	2.19	0.42
1:C:391:GLU:N	1:C:392:PRO:HA	2.35	0.42
1:F:260:LEU:HD23	1:F:261:MET:HE2	2.01	0.42
1:F:261:MET:HE1	1:F:307:LEU:CD2	2.46	0.42
1:G:179:MET:HE1	1:G:478:ILE:HD12	2.02	0.42
1:A:391:GLU:N	1:A:392:PRO:HA	2.35	0.42
1:B:400:GLU:H	1:B:400:GLU:CD	2.28	0.42
1:F:440:LEU:O	1:F:454:VAL:HA	2.19	0.42
1:G:19:LYS:O	1:G:34:ALA:HA	2.19	0.42
1:A:11:LEU:C	1:A:11:LEU:HD23	2.45	0.42
1:G:239:MET:HE3	1:G:575:MET:HE3	2.02	0.41
1:A:324:ASN:HA	1:A:329:TYR:CG	2.55	0.41
1:C:19:LYS:O	1:C:34:ALA:HA	2.20	0.41
1:D:170:ASN:HB3	1:H:116:PRO:HB2	2.02	0.41
1:B:317:SER:HA	1:B:386:TRP:HB3	2.02	0.41
1:G:179:MET:HE1	1:G:593:PHE:HE1	1.86	0.41
1:F:261:MET:HE3	1:F:303:MET:HG3	2.02	0.41
1:A:68:VAL:HG22	1:A:73:SER:HB3	2.03	0.41
1:G:634:GLU:HG2	1:G:650:GLY:CA	2.50	0.41
1:D:251:LYS:O	1:D:253:ARG:HA	2.21	0.41
1:D:439:LEU:HD11	1:D:455:TRP:HB3	2.03	0.41
1:D:19:LYS:O	1:D:34:ALA:HA	2.21	0.40
1:H:19:LYS:O	1:H:34:ALA:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:317:SER:HA	1:G:386:TRP:HB3	2.03	0.40
1:C:146:ILE:HD13	1:C:198:PHE:CD1	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	679/687 (99%)	663 (98%)	16 (2%)	0	100	100
1	B	683/687 (99%)	668 (98%)	15 (2%)	0	100	100
1	C	676/687 (98%)	658 (97%)	18 (3%)	0	100	100
1	D	678/687 (99%)	656 (97%)	22 (3%)	0	100	100
1	E	674/687 (98%)	654 (97%)	19 (3%)	1 (0%)	48	34
1	F	673/687 (98%)	653 (97%)	19 (3%)	1 (0%)	48	34
1	G	675/687 (98%)	660 (98%)	15 (2%)	0	100	100
1	H	675/687 (98%)	659 (98%)	16 (2%)	0	100	100
All	All	5413/5496 (98%)	5271 (97%)	140 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	171	SER
1	F	171	SER

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	564/570 (99%)	560 (99%)	4 (1%)	76	73
1	B	568/570 (100%)	564 (99%)	4 (1%)	76	73
1	C	562/570 (99%)	557 (99%)	5 (1%)	70	67
1	D	563/570 (99%)	557 (99%)	6 (1%)	65	60
1	E	560/570 (98%)	553 (99%)	7 (1%)	61	54
1	F	559/570 (98%)	553 (99%)	6 (1%)	65	60
1	G	561/570 (98%)	556 (99%)	5 (1%)	70	67
1	H	561/570 (98%)	556 (99%)	5 (1%)	70	67
All	All	4498/4560 (99%)	4456 (99%)	42 (1%)	70	67

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	PHE
1	A	455	TRP
1	A	492	ASP
1	A	590	ARG
1	B	281	PHE
1	B	455	TRP
1	B	459	ILE
1	B	590	ARG
1	C	281	PHE
1	C	308	LYS
1	C	455	TRP
1	C	459	ILE
1	C	590	ARG
1	D	2	SER
1	D	281	PHE
1	D	455	TRP
1	D	459	ILE
1	D	532	GLU
1	D	590	ARG
1	E	56	VAL
1	E	59	SER
1	E	281	PHE
1	E	455	TRP
1	E	459	ILE

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Mol	Chain	Res	Type
1	E	536	ASP
1	E	590	ARG
1	F	281	PHE
1	F	455	TRP
1	F	459	ILE
1	F	492	ASP
1	F	527	MET
1	F	590	ARG
1	H	2	SER
1	H	178	MET
1	H	281	PHE
1	H	471	MET
1	H	590	ARG
1	G	281	PHE
1	G	455	TRP
1	G	459	ILE
1	G	492	ASP
1	G	590	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	228	GLN
1	A	354	ASN
1	A	497	ASN
1	A	540	GLN
1	B	88	ASN
1	B	287	GLN
1	C	287	GLN
1	C	647	GLN
1	E	88	ASN
1	E	287	GLN
1	E	540	GLN
1	E	648	ASN
1	F	88	ASN
1	F	287	GLN
1	F	405	HIS
1	F	604	GLN
1	H	287	GLN
1	G	354	ASN
1	G	540	GLN

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Mol	Chain	Res	Type
1	G	642	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

52 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	E	705	-	5,5,5	0.33	0	5,5,5	0.28	0
2	GOL	A	705	-	5,5,5	0.18	0	5,5,5	0.39	0
2	GOL	H	708	-	5,5,5	0.42	0	5,5,5	0.54	0
2	GOL	B	706	-	5,5,5	0.21	0	5,5,5	0.39	0
2	GOL	C	707	-	5,5,5	0.41	0	5,5,5	0.51	0
2	GOL	B	704	-	5,5,5	0.32	0	5,5,5	0.47	0
2	GOL	H	706	-	5,5,5	0.32	0	5,5,5	0.29	0
2	GOL	A	704	-	5,5,5	0.17	0	5,5,5	0.42	0
2	GOL	A	706	-	5,5,5	0.37	0	5,5,5	0.22	0
2	GOL	D	703	-	5,5,5	0.34	0	5,5,5	0.17	0
2	GOL	A	702	-	5,5,5	0.30	0	5,5,5	0.42	0
2	GOL	B	703	-	5,5,5	0.25	0	5,5,5	0.54	0
2	GOL	D	705	-	5,5,5	0.26	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	E	703	-	5,5,5	0.44	0	5,5,5	0.45	0
2	GOL	H	703	-	5,5,5	0.38	0	5,5,5	0.29	0
2	GOL	H	701	-	5,5,5	0.44	0	5,5,5	0.56	0
2	GOL	E	702	-	5,5,5	0.36	0	5,5,5	0.31	0
2	GOL	D	704	-	5,5,5	0.26	0	5,5,5	0.68	0
2	GOL	H	702	-	5,5,5	0.44	0	5,5,5	0.24	0
2	GOL	D	706	-	5,5,5	0.36	0	5,5,5	0.40	0
2	GOL	G	703	-	5,5,5	0.38	0	5,5,5	0.50	0
2	GOL	G	701	-	5,5,5	0.36	0	5,5,5	0.17	0
2	GOL	B	708	-	5,5,5	0.38	0	5,5,5	0.66	0
2	GOL	A	707	-	5,5,5	0.31	0	5,5,5	0.50	0
2	GOL	B	702	-	5,5,5	0.61	0	5,5,5	0.97	0
2	GOL	G	702	-	5,5,5	0.36	0	5,5,5	0.53	0
2	GOL	D	702	-	5,5,5	0.27	0	5,5,5	0.29	0
2	GOL	H	707	-	5,5,5	0.25	0	5,5,5	0.62	0
2	GOL	C	703	-	5,5,5	0.18	0	5,5,5	0.36	0
2	GOL	E	701	-	5,5,5	0.27	0	5,5,5	0.39	0
2	GOL	A	701	-	5,5,5	0.42	0	5,5,5	0.51	0
2	GOL	A	708	-	5,5,5	0.26	0	5,5,5	0.30	0
2	GOL	C	705	-	5,5,5	0.38	0	5,5,5	0.56	0
2	GOL	H	705	-	5,5,5	0.26	0	5,5,5	0.27	0
2	GOL	C	701	-	5,5,5	0.37	0	5,5,5	0.66	0
2	GOL	B	701	-	5,5,5	0.38	0	5,5,5	0.18	0
2	GOL	C	706	-	5,5,5	0.59	0	5,5,5	0.48	0
2	GOL	E	704	-	5,5,5	0.29	0	5,5,5	0.26	0
2	GOL	A	703	-	5,5,5	0.33	0	5,5,5	0.23	0
2	GOL	C	702	-	5,5,5	0.36	0	5,5,5	0.20	0
2	GOL	B	705	-	5,5,5	0.25	0	5,5,5	0.33	0
2	GOL	A	709	-	5,5,5	0.26	0	5,5,5	0.40	0
2	GOL	C	708	-	5,5,5	0.27	0	5,5,5	0.40	0
2	GOL	D	701	-	5,5,5	0.30	0	5,5,5	0.40	0
2	GOL	G	705	-	5,5,5	0.28	0	5,5,5	0.22	0
2	GOL	B	707	-	5,5,5	0.30	0	5,5,5	0.35	0
2	GOL	G	704	-	5,5,5	0.57	0	5,5,5	0.78	0
2	GOL	C	704	-	5,5,5	0.25	0	5,5,5	0.56	0
2	GOL	G	706	-	5,5,5	0.32	0	5,5,5	0.32	0
2	GOL	F	701	-	5,5,5	0.28	0	5,5,5	0.28	0
2	GOL	H	704	-	5,5,5	0.63	0	5,5,5	0.53	0
2	GOL	F	702	-	5,5,5	0.35	0	5,5,5	0.40	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	E	705	-	-	1/4/4/4	-
2	GOL	A	705	-	-	0/4/4/4	-
2	GOL	H	708	-	-	2/4/4/4	-
2	GOL	B	706	-	-	2/4/4/4	-
2	GOL	C	707	-	-	1/4/4/4	-
2	GOL	B	704	-	-	0/4/4/4	-
2	GOL	H	706	-	-	0/4/4/4	-
2	GOL	A	704	-	-	0/4/4/4	-
2	GOL	A	706	-	-	0/4/4/4	-
2	GOL	D	703	-	-	0/4/4/4	-
2	GOL	A	702	-	-	1/4/4/4	-
2	GOL	B	703	-	-	0/4/4/4	-
2	GOL	D	705	-	-	0/4/4/4	-
2	GOL	E	703	-	-	0/4/4/4	-
2	GOL	H	703	-	-	0/4/4/4	-
2	GOL	H	701	-	-	0/4/4/4	-
2	GOL	E	702	-	-	0/4/4/4	-
2	GOL	D	704	-	-	0/4/4/4	-
2	GOL	H	702	-	-	0/4/4/4	-
2	GOL	D	706	-	-	0/4/4/4	-
2	GOL	G	703	-	-	1/4/4/4	-
2	GOL	G	701	-	-	0/4/4/4	-
2	GOL	B	708	-	-	0/4/4/4	-
2	GOL	A	707	-	-	0/4/4/4	-
2	GOL	B	702	-	-	4/4/4/4	-
2	GOL	G	702	-	-	0/4/4/4	-
2	GOL	D	702	-	-	0/4/4/4	-
2	GOL	H	707	-	-	0/4/4/4	-
2	GOL	C	703	-	-	0/4/4/4	-
2	GOL	E	701	-	-	0/4/4/4	-
2	GOL	A	701	-	-	2/4/4/4	-
2	GOL	A	708	-	-	0/4/4/4	-
2	GOL	C	705	-	-	4/4/4/4	-
2	GOL	H	705	-	-	2/4/4/4	-
2	GOL	C	701	-	-	1/4/4/4	-
2	GOL	B	701	-	-	0/4/4/4	-
2	GOL	C	706	-	-	0/4/4/4	-
2	GOL	E	704	-	-	0/4/4/4	-
2	GOL	A	703	-	-	0/4/4/4	-
2	GOL	C	702	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	705	-	-	2/4/4/4	-
2	GOL	A	709	-	-	1/4/4/4	-
2	GOL	C	708	-	-	0/4/4/4	-
2	GOL	D	701	-	-	0/4/4/4	-
2	GOL	G	705	-	-	2/4/4/4	-
2	GOL	B	707	-	-	0/4/4/4	-
2	GOL	G	704	-	-	3/4/4/4	-
2	GOL	C	704	-	-	0/4/4/4	-
2	GOL	G	706	-	-	0/4/4/4	-
2	GOL	F	701	-	-	0/4/4/4	-
2	GOL	H	704	-	-	0/4/4/4	-
2	GOL	F	702	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	702	GOL	O1-C1-C2-C3
2	B	705	GOL	O1-C1-C2-C3
2	C	705	GOL	O1-C1-C2-C3
2	H	708	GOL	O1-C1-C2-C3
2	G	704	GOL	C1-C2-C3-O3
2	A	701	GOL	C1-C2-C3-O3
2	A	709	GOL	C1-C2-C3-O3
2	B	702	GOL	C1-C2-C3-O3
2	C	705	GOL	C1-C2-C3-O3
2	E	705	GOL	C1-C2-C3-O3
2	H	705	GOL	C1-C2-C3-O3
2	G	705	GOL	C1-C2-C3-O3
2	C	705	GOL	O1-C1-C2-O2
2	H	708	GOL	O1-C1-C2-O2
2	B	702	GOL	O1-C1-C2-O2
2	B	705	GOL	O1-C1-C2-O2
2	H	705	GOL	O2-C2-C3-O3
2	G	704	GOL	O2-C2-C3-O3
2	G	704	GOL	O1-C1-C2-C3
2	C	701	GOL	O2-C2-C3-O3
2	G	703	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	706	GOL	C1-C2-C3-O3
2	C	707	GOL	O1-C1-C2-O2
2	G	705	GOL	O2-C2-C3-O3
2	A	702	GOL	O1-C1-C2-C3
2	A	701	GOL	O2-C2-C3-O3
2	C	705	GOL	O2-C2-C3-O3
2	B	706	GOL	O1-C1-C2-O2
2	B	702	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	705	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	680/687 (98%)	-0.49	9 (1%) 75 75	6, 11, 23, 45	1 (0%)
1	B	682/687 (99%)	-0.19	11 (1%) 70 71	6, 15, 27, 46	3 (0%)
1	C	676/687 (98%)	-0.53	9 (1%) 75 75	4, 10, 21, 50	2 (0%)
1	D	680/687 (98%)	-0.26	10 (1%) 72 72	8, 15, 29, 46	0
1	E	675/687 (98%)	0.51	39 (5%) 29 27	11, 23, 38, 63	1 (0%)
1	F	675/687 (98%)	0.29	29 (4%) 40 39	11, 22, 39, 64	0
1	G	677/687 (98%)	-0.10	15 (2%) 62 62	9, 16, 32, 57	0
1	H	676/687 (98%)	-0.36	10 (1%) 72 72	6, 13, 25, 55	1 (0%)
All	All	5421/5496 (98%)	-0.14	132 (2%) 59 60	4, 15, 32, 64	8 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	52	PRO	5.9
1	F	61	PHE	5.9
1	B	54	THR	4.8
1	H	54	THR	4.8
1	G	52	PRO	4.7
1	F	55	LYS	4.7
1	E	54	THR	4.7
1	F	52	PRO	4.6
1	F	54	THR	4.3
1	C	52	PRO	4.2
1	G	55	LYS	4.2
1	E	61	PHE	4.1
1	C	55	LYS	4.1
1	C	54	THR	4.1
1	G	54	THR	4.0
1	E	55	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	55	LYS	3.9
1	H	61	PHE	3.9
1	G	678	ILE	3.8
1	C	61	PHE	3.8
1	E	669	ALA	3.8
1	E	653	CYS	3.8
1	B	53	SER	3.7
1	H	62	GLU	3.7
1	D	54	THR	3.6
1	E	527	MET	3.6
1	E	676	LEU	3.6
1	B	143	ASP	3.6
1	C	677	SER	3.6
1	C	51	LYS	3.6
1	E	531	ALA	3.5
1	H	51	LYS	3.5
1	E	655	CYS	3.5
1	H	52	PRO	3.5
1	F	669	ALA	3.5
1	E	51	LYS	3.4
1	F	51	LYS	3.4
1	A	54	THR	3.4
1	E	143	ASP	3.3
1	E	674	ALA	3.3
1	H	55	LYS	3.3
1	F	53	SER	3.3
1	F	656	ASP	3.2
1	C	53	SER	3.2
1	F	645	ALA	3.1
1	E	56	VAL	3.1
1	A	326[A]	THR	3.1
1	E	644	GLY	3.1
1	F	676	LEU	3.0
1	E	62	GLU	3.0
1	B	531	ALA	3.0
1	H	53	SER	3.0
1	F	647	GLN	3.0
1	F	62	GLU	3.0
1	C	63	ASP	3.0
1	E	63	ASP	2.9
1	H	63	ASP	2.9
1	E	638	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	56	VAL	2.8
1	F	63	ASP	2.8
1	B	52	PRO	2.8
1	E	643	THR	2.8
1	D	52	PRO	2.8
1	E	654	ASP	2.8
1	E	651	GLN	2.7
1	A	52	PRO	2.7
1	B	527	MET	2.6
1	E	557	TYR	2.6
1	F	653	CYS	2.6
1	E	670	ALA	2.6
1	F	655	CYS	2.6
1	G	653	CYS	2.6
1	D	143	ASP	2.6
1	A	61	PHE	2.5
1	F	643	THR	2.5
1	E	467[A]	ARG	2.5
1	C	62	GLU	2.5
1	G	53	SER	2.5
1	G	56	VAL	2.5
1	B	655	CYS	2.4
1	D	680	LEU	2.4
1	E	53	SER	2.4
1	B	654	ASP	2.4
1	F	269	ARG	2.4
1	F	60	GLU	2.4
1	F	652	TRP	2.4
1	D	527	MET	2.4
1	B	51	LYS	2.4
1	G	655	CYS	2.4
1	G	143	ASP	2.3
1	A	327	GLU	2.3
1	G	647	GLN	2.3
1	E	647	GLN	2.3
1	F	602	ALA	2.3
1	G	645	ALA	2.3
1	G	677	SER	2.3
1	F	630	VAL	2.3
1	D	61	PHE	2.2
1	D	531	ALA	2.2
1	E	649	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	327	GLU	2.2
1	E	615	ILE	2.2
1	A	294	THR	2.2
1	A	143	ASP	2.2
1	H	677	SER	2.2
1	G	61	PHE	2.2
1	E	616	LEU	2.2
1	E	242	ASP	2.2
1	F	670	ALA	2.2
1	D	51	LYS	2.2
1	F	654	ASP	2.2
1	B	55	LYS	2.2
1	G	51	LYS	2.2
1	F	262	GLU	2.1
1	D	327	GLU	2.1
1	E	542	MET	2.1
1	F	528	GLU	2.1
1	E	434	THR	2.1
1	H	56	VAL	2.1
1	A	681	GLU	2.1
1	E	665	PHE	2.1
1	E	639	ILE	2.1
1	F	529	GLU	2.1
1	E	499	PRO	2.1
1	D	63	ASP	2.1
1	B	653	CYS	2.0
1	E	671	ALA	2.0
1	E	598	ASP	2.0
1	E	327	GLU	2.0
1	F	527	MET	2.0
1	F	650	GLY	2.0
1	E	630	VAL	2.0

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 ⓘ

There are no oligosaccharides in this entry.

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. 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
2	GOL	G	706	6/6	0.83	0.17	36,41,42,43	0
2	GOL	B	702	6/6	0.84	0.14	20,24,25,27	0
2	GOL	H	704	6/6	0.85	0.12	18,20,21,22	0
2	GOL	A	705	6/6	0.86	0.13	26,29,30,31	0
2	GOL	H	705	6/6	0.86	0.12	24,28,29,30	0
2	GOL	D	706	6/6	0.86	0.13	31,32,32,33	0
2	GOL	H	708	6/6	0.87	0.12	27,30,31,31	0
2	GOL	B	706	6/6	0.88	0.13	30,34,35,37	0
2	GOL	C	704	6/6	0.88	0.09	18,19,21,21	0
2	GOL	A	709	6/6	0.88	0.14	29,33,35,35	0
2	GOL	G	704	6/6	0.88	0.12	19,22,23,24	0
2	GOL	E	703	6/6	0.88	0.12	25,27,28,29	0
2	GOL	D	705	6/6	0.89	0.10	23,25,25,27	0
2	GOL	G	705	6/6	0.89	0.13	34,37,38,39	0
2	GOL	B	705	6/6	0.89	0.14	25,29,30,34	0
2	GOL	H	706	6/6	0.90	0.11	24,26,27,30	0
2	GOL	E	702	6/6	0.90	0.10	25,26,26,27	0
2	GOL	C	706	6/6	0.90	0.10	14,16,17,18	0
2	GOL	B	703	6/6	0.90	0.09	21,21,22,23	0
2	GOL	A	708	6/6	0.90	0.11	20,21,21,21	0
2	GOL	G	702	6/6	0.91	0.08	19,20,21,21	0
2	GOL	C	707	6/6	0.91	0.10	24,27,27,28	0
2	GOL	A	707	6/6	0.91	0.10	19,19,19,20	0
2	GOL	B	708	6/6	0.91	0.10	25,26,26,27	0
2	GOL	F	702	6/6	0.92	0.09	21,22,23,24	0
2	GOL	A	702	6/6	0.92	0.09	20,21,22,23	0
2	GOL	E	705	6/6	0.92	0.10	32,33,33,34	0
2	GOL	B	704	6/6	0.93	0.09	18,19,19,21	0
2	GOL	B	707	6/6	0.93	0.10	26,27,28,30	0
2	GOL	B	701	6/6	0.93	0.09	18,19,19,20	0
2	GOL	H	707	6/6	0.93	0.09	24,26,26,26	0
2	GOL	C	708	6/6	0.93	0.09	23,24,24,25	0
2	GOL	E	704	6/6	0.93	0.09	29,29,29,30	0
2	GOL	D	701	6/6	0.93	0.08	16,17,17,18	0
2	GOL	D	704	6/6	0.93	0.08	17,18,20,21	0
2	GOL	H	702	6/6	0.93	0.08	14,14,15,16	0
2	GOL	F	701	6/6	0.94	0.08	21,22,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	G	703	6/6	0.94	0.07	17,18,19,19	0
2	GOL	C	705	6/6	0.94	0.09	19,23,24,24	0
2	GOL	D	703	6/6	0.94	0.09	25,25,26,26	0
2	GOL	C	701	6/6	0.94	0.07	12,13,13,13	0
2	GOL	E	701	6/6	0.95	0.08	23,24,25,27	0
2	GOL	D	702	6/6	0.95	0.07	18,19,20,20	0
2	GOL	C	702	6/6	0.96	0.06	13,14,14,15	0
2	GOL	C	703	6/6	0.96	0.07	20,21,21,22	0
2	GOL	G	701	6/6	0.96	0.06	17,17,18,18	0
2	GOL	A	703	6/6	0.96	0.06	16,16,17,19	0
2	GOL	H	703	6/6	0.96	0.06	16,18,18,18	0
2	GOL	A	704	6/6	0.96	0.06	13,14,15,17	0
2	GOL	A	701	6/6	0.96	0.06	12,13,13,13	0
2	GOL	A	706	6/6	0.96	0.06	14,14,15,15	0
2	GOL	H	701	6/6	0.97	0.05	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.