



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:56 am BST

PDB ID : 5ZN6  
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.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

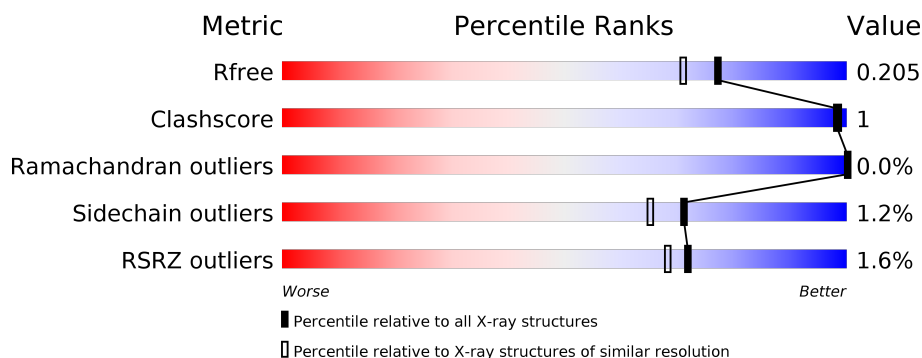
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 96%
1	B	687	 97%
1	C	687	 95%
1	D	687	 96%
1	E	687	 95%
1	F	687	 95%

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Mol	Chain	Length	Quality of chain
1	G	687	<div><div>%</div><div><div></div><div>96%</div><div></div></div><div><div></div><div></div><div></div></div></div>
1	H	687	<div><div>%</div><div><div></div><div>96%</div><div></div></div><div><div></div><div></div><div></div></div></div>

## 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 (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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 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.

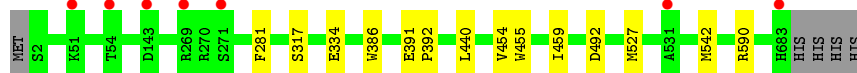
- Molecule 1: Alpha-xylosidase MeXyl31

Chain A:  96%



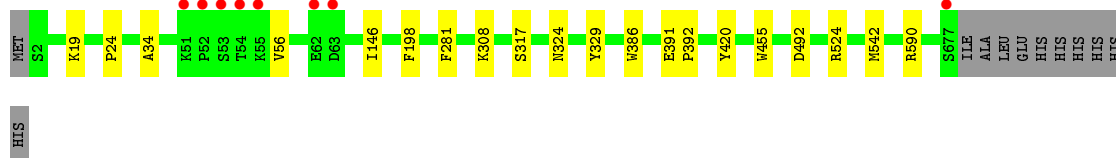
- Molecule 1: Alpha-xylosidase MeXyl31

Chain B:  97%



- Molecule 1: Alpha-xylosidase MeXyl31

Chain C:  95%



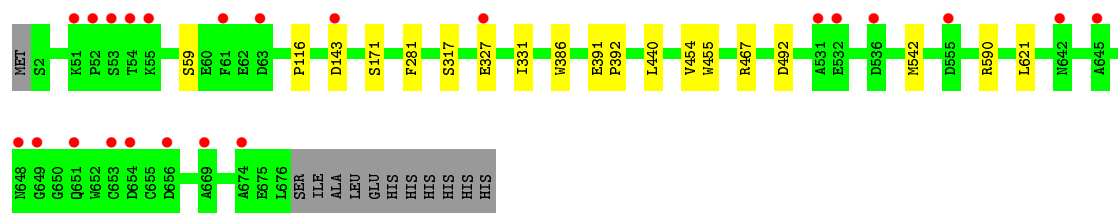
- Molecule 1: Alpha-xylosidase MeXyl31

Chain D:  96%

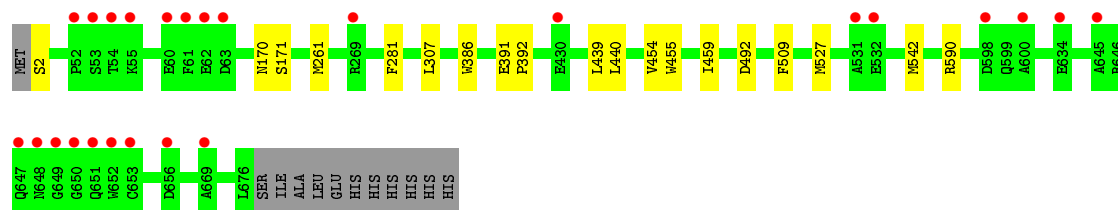


- Molecule 1: Alpha-xylosidase MeXyl31

Chain E:  95%



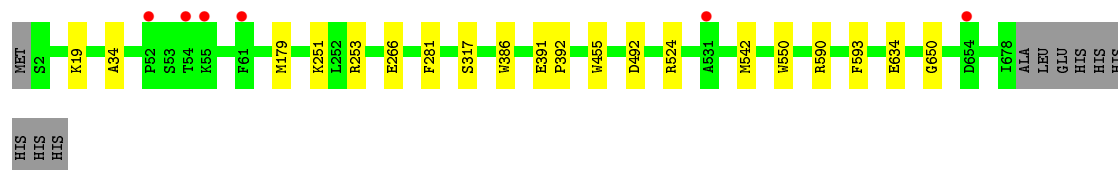
- Molecule 1: Alpha-xylosidase MeXyl31



- 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, $\alpha$ , $\beta$ , $\gamma$	173.15Å 124.17Å 177.45Å 90.00° 116.81° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 39.98 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-1.80) 91.1 (39.98-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.174 , 0.195 0.186 , 0.205	Depositor DCC
$R_{free}$ test set	27623 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.4	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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

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	0.44	0/5615	0.71	2/7633 (0.0%)
1	B	0.43	0/5652	0.68	0/7682
1	C	0.44	0/5592	0.69	3/7601 (0.0%)
1	D	0.42	0/5608	0.67	0/7623
1	E	0.44	0/5583	0.65	0/7588
1	F	0.42	0/5572	0.65	0/7574
1	G	0.42	0/5586	0.67	1/7593 (0.0%)
1	H	0.43	0/5584	0.68	0/7590
All	All	0.43	0/44792	0.67	6/60884 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	C	524	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	449	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	420	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	C	524	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	G	524	ARG	NE-CZ-NH1	5.01	122.80	120.30

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	5461	0	5230	6	0
1	B	5496	0	5260	4	0
1	C	5438	0	5198	6	0
1	D	5454	0	5224	8	0
1	E	5429	0	5198	6	0
1	F	5418	0	5186	7	0
1	G	5432	0	5202	7	0
1	H	5430	0	5195	8	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	48	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 (48) 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:N	1:H:471:MET:HE2	2.17	0.59
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:HE3	1:H:606:GLU:O	2.13	0.49
1:G:179:MET:HE1	1:G:593:PHE:HE1	1.77	0.49
1:F:261:MET:HE2	1:F:307:LEU:HD21	1.95	0.48
1:D:334:GLU:OE2	1:F:2:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:A:391:GLU:N	1:A:392:PRO:HA	2.35	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: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:F:261:MET:HE1	1:F:307:LEU:HD11	2.02	0.41
1:H:471:MET:HE2	1:H:471:MET:CA	2.51	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: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
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%)	51	36
1	F	673/687 (98%)	653 (97%)	19 (3%)	1 (0%)	51	36
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%)	558 (99%)	6 (1%)	73	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	568/570 (100%)	561 (99%)	7 (1%)	71	65
1	C	562/570 (99%)	556 (99%)	6 (1%)	73	68
1	D	563/570 (99%)	554 (98%)	9 (2%)	62	54
1	E	560/570 (98%)	553 (99%)	7 (1%)	69	62
1	F	559/570 (98%)	551 (99%)	8 (1%)	67	59
1	G	561/570 (98%)	556 (99%)	5 (1%)	78	75
1	H	561/570 (98%)	554 (99%)	7 (1%)	71	65
All	All	4498/4560 (99%)	4443 (99%)	55 (1%)	71	65

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	MET
1	A	281	PHE
1	A	455	TRP
1	A	492	ASP
1	A	542	MET
1	A	590	ARG
1	B	281	PHE
1	B	455	TRP
1	B	459	ILE
1	B	492	ASP
1	B	527	MET
1	B	542	MET
1	B	590	ARG
1	C	281	PHE
1	C	308	LYS
1	C	455	TRP
1	C	492	ASP
1	C	542	MET
1	C	590	ARG
1	D	2	SER
1	D	178	MET
1	D	281	PHE
1	D	455	TRP
1	D	459	ILE
1	D	492	ASP
1	D	532	GLU
1	D	542	MET
1	D	590	ARG

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Mol	Chain	Res	Type
1	E	59	SER
1	E	143	ASP
1	E	281	PHE
1	E	455	TRP
1	E	492	ASP
1	E	542	MET
1	E	590	ARG
1	F	281	PHE
1	F	455	TRP
1	F	459	ILE
1	F	492	ASP
1	F	509	PHE
1	F	527	MET
1	F	542	MET
1	F	590	ARG
1	H	2	SER
1	H	178	MET
1	H	281	PHE
1	H	455	TRP
1	H	492	ASP
1	H	542	MET
1	H	590	ARG
1	G	281	PHE
1	G	455	TRP
1	G	492	ASP
1	G	542	MET
1	G	590	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	604	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	C	703	-	5,5,5	0.18	0	5,5,5	0.33	0
2	GOL	B	707	-	5,5,5	0.30	0	5,5,5	0.33	0
2	GOL	G	703	-	5,5,5	0.37	0	5,5,5	0.48	0
2	GOL	E	703	-	5,5,5	0.43	0	5,5,5	0.43	0
2	GOL	A	709	-	5,5,5	0.26	0	5,5,5	0.37	0
2	GOL	D	706	-	5,5,5	0.36	0	5,5,5	0.38	0
2	GOL	D	705	-	5,5,5	0.25	0	5,5,5	0.27	0
2	GOL	D	702	-	5,5,5	0.26	0	5,5,5	0.26	0
2	GOL	C	701	-	5,5,5	0.36	0	5,5,5	0.63	0
2	GOL	G	706	-	5,5,5	0.32	0	5,5,5	0.29	0
2	GOL	C	705	-	5,5,5	0.37	0	5,5,5	0.55	0
2	GOL	A	702	-	5,5,5	0.29	0	5,5,5	0.39	0
2	GOL	G	702	-	5,5,5	0.35	0	5,5,5	0.49	0
2	GOL	C	707	-	5,5,5	0.40	0	5,5,5	0.49	0
2	GOL	A	707	-	5,5,5	0.30	0	5,5,5	0.46	0
2	GOL	G	704	-	5,5,5	0.56	0	5,5,5	0.75	0
2	GOL	F	702	-	5,5,5	0.34	0	5,5,5	0.37	0
2	GOL	E	705	-	5,5,5	0.32	0	5,5,5	0.27	0
2	GOL	D	701	-	5,5,5	0.29	0	5,5,5	0.37	0
2	GOL	H	702	-	5,5,5	0.43	0	5,5,5	0.23	0
2	GOL	A	708	-	5,5,5	0.25	0	5,5,5	0.26	0
2	GOL	C	702	-	5,5,5	0.35	0	5,5,5	0.20	0
2	GOL	B	702	-	5,5,5	0.60	0	5,5,5	0.93	0
2	GOL	C	706	-	5,5,5	0.58	0	5,5,5	0.47	0
2	GOL	E	702	-	5,5,5	0.35	0	5,5,5	0.28	0
2	GOL	H	704	-	5,5,5	0.62	0	5,5,5	0.51	0
2	GOL	A	704	-	5,5,5	0.17	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	H	706	-	5,5,5	0.31	0	5,5,5	0.27	0
2	GOL	C	704	-	5,5,5	0.24	0	5,5,5	0.51	0
2	GOL	B	706	-	5,5,5	0.22	0	5,5,5	0.36	0
2	GOL	A	701	-	5,5,5	0.41	0	5,5,5	0.48	0
2	GOL	B	708	-	5,5,5	0.37	0	5,5,5	0.62	0
2	GOL	F	701	-	5,5,5	0.28	0	5,5,5	0.24	0
2	GOL	E	701	-	5,5,5	0.27	0	5,5,5	0.35	0
2	GOL	H	701	-	5,5,5	0.43	0	5,5,5	0.55	0
2	GOL	H	708	-	5,5,5	0.41	0	5,5,5	0.53	0
2	GOL	H	705	-	5,5,5	0.26	0	5,5,5	0.25	0
2	GOL	A	706	-	5,5,5	0.36	0	5,5,5	0.23	0
2	GOL	B	703	-	5,5,5	0.25	0	5,5,5	0.49	0
2	GOL	B	704	-	5,5,5	0.32	0	5,5,5	0.44	0
2	GOL	C	708	-	5,5,5	0.26	0	5,5,5	0.36	0
2	GOL	A	703	-	5,5,5	0.32	0	5,5,5	0.20	0
2	GOL	D	703	-	5,5,5	0.33	0	5,5,5	0.16	0
2	GOL	E	704	-	5,5,5	0.28	0	5,5,5	0.24	0
2	GOL	H	703	-	5,5,5	0.37	0	5,5,5	0.27	0
2	GOL	H	707	-	5,5,5	0.24	0	5,5,5	0.58	0
2	GOL	B	701	-	5,5,5	0.37	0	5,5,5	0.17	0
2	GOL	G	705	-	5,5,5	0.28	0	5,5,5	0.22	0
2	GOL	B	705	-	5,5,5	0.24	0	5,5,5	0.30	0
2	GOL	A	705	-	5,5,5	0.18	0	5,5,5	0.35	0
2	GOL	G	701	-	5,5,5	0.36	0	5,5,5	0.15	0
2	GOL	D	704	-	5,5,5	0.25	0	5,5,5	0.63	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	C	703	-	-	0/4/4/4	-
2	GOL	B	707	-	-	0/4/4/4	-
2	GOL	G	703	-	-	2/4/4/4	-
2	GOL	E	703	-	-	0/4/4/4	-
2	GOL	A	709	-	-	1/4/4/4	-
2	GOL	D	706	-	-	0/4/4/4	-
2	GOL	D	705	-	-	0/4/4/4	-
2	GOL	D	702	-	-	0/4/4/4	-
2	GOL	C	701	-	-	2/4/4/4	-
2	GOL	G	706	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	705	-	-	4/4/4/4	-
2	GOL	A	702	-	-	1/4/4/4	-
2	GOL	G	702	-	-	0/4/4/4	-
2	GOL	C	707	-	-	2/4/4/4	-
2	GOL	A	707	-	-	0/4/4/4	-
2	GOL	G	704	-	-	3/4/4/4	-
2	GOL	F	702	-	-	0/4/4/4	-
2	GOL	E	705	-	-	1/4/4/4	-
2	GOL	D	701	-	-	0/4/4/4	-
2	GOL	H	702	-	-	0/4/4/4	-
2	GOL	A	708	-	-	0/4/4/4	-
2	GOL	C	702	-	-	0/4/4/4	-
2	GOL	B	702	-	-	3/4/4/4	-
2	GOL	C	706	-	-	0/4/4/4	-
2	GOL	E	702	-	-	0/4/4/4	-
2	GOL	H	704	-	-	0/4/4/4	-
2	GOL	A	704	-	-	0/4/4/4	-
2	GOL	H	706	-	-	0/4/4/4	-
2	GOL	C	704	-	-	0/4/4/4	-
2	GOL	B	706	-	-	3/4/4/4	-
2	GOL	A	701	-	-	2/4/4/4	-
2	GOL	B	708	-	-	0/4/4/4	-
2	GOL	F	701	-	-	0/4/4/4	-
2	GOL	E	701	-	-	0/4/4/4	-
2	GOL	H	701	-	-	0/4/4/4	-
2	GOL	H	708	-	-	2/4/4/4	-
2	GOL	H	705	-	-	2/4/4/4	-
2	GOL	A	706	-	-	0/4/4/4	-
2	GOL	B	703	-	-	0/4/4/4	-
2	GOL	B	704	-	-	0/4/4/4	-
2	GOL	C	708	-	-	0/4/4/4	-
2	GOL	A	703	-	-	0/4/4/4	-
2	GOL	D	703	-	-	0/4/4/4	-
2	GOL	E	704	-	-	0/4/4/4	-
2	GOL	H	703	-	-	0/4/4/4	-
2	GOL	H	707	-	-	0/4/4/4	-
2	GOL	B	701	-	-	0/4/4/4	-
2	GOL	G	705	-	-	2/4/4/4	-
2	GOL	B	705	-	-	2/4/4/4	-
2	GOL	A	705	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	G	701	-	-	0/4/4/4	-
2	GOL	D	704	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	705	GOL	O1-C1-C2-C3
2	G	704	GOL	C1-C2-C3-O3
2	B	702	GOL	O1-C1-C2-C3
2	H	708	GOL	O1-C1-C2-C3
2	B	705	GOL	O1-C1-C2-C3
2	A	709	GOL	C1-C2-C3-O3
2	C	705	GOL	C1-C2-C3-O3
2	G	704	GOL	O1-C1-C2-C3
2	E	705	GOL	C1-C2-C3-O3
2	B	702	GOL	C1-C2-C3-O3
2	A	701	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	G	704	GOL	O2-C2-C3-O3
2	B	702	GOL	O1-C1-C2-O2
2	H	705	GOL	O2-C2-C3-O3
2	B	705	GOL	O1-C1-C2-O2
2	G	703	GOL	O2-C2-C3-O3
2	C	701	GOL	O2-C2-C3-O3
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	G	703	GOL	C1-C2-C3-O3
2	A	702	GOL	O1-C1-C2-C3
2	D	704	GOL	O1-C1-C2-C3
2	C	705	GOL	O2-C2-C3-O3
2	A	701	GOL	O2-C2-C3-O3
2	B	706	GOL	O1-C1-C2-O2
2	C	701	GOL	C1-C2-C3-O3
2	C	707	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	B	706	GOL	O1-C1-C2-C3

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	680/687 (98%)	-0.54	3 (0%) 92 90	6, 11, 23, 45	0
1	B	682/687 (99%)	-0.35	7 (1%) 82 80	8, 15, 27, 46	0
1	C	676/687 (98%)	-0.48	8 (1%) 79 76	5, 10, 21, 50	0
1	D	680/687 (98%)	-0.45	8 (1%) 79 76	8, 15, 29, 46	0
1	E	675/687 (98%)	-0.04	23 (3%) 45 39	12, 23, 38, 63	0
1	F	675/687 (98%)	-0.04	25 (3%) 41 36	11, 22, 39, 64	0
1	G	677/687 (98%)	-0.38	6 (0%) 84 82	9, 16, 32, 57	0
1	H	676/687 (98%)	-0.42	9 (1%) 77 74	8, 13, 25, 55	0
All	All	5421/5496 (98%)	-0.34	89 (1%) 72 68	5, 15, 32, 64	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	54	THR	5.9
1	F	52	PRO	5.7
1	H	52	PRO	5.2
1	H	54	THR	5.2
1	F	55	LYS	5.0
1	F	61	PHE	4.9
1	C	55	LYS	4.7
1	C	52	PRO	4.5
1	C	54	THR	4.5
1	E	55	LYS	4.3
1	F	652	TRP	4.1
1	H	55	LYS	4.0
1	D	531	ALA	4.0
1	E	52	PRO	3.9
1	F	54	THR	3.9
1	G	55	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	54	THR	3.8
1	B	531	ALA	3.8
1	H	531	ALA	3.8
1	A	54	THR	3.7
1	D	52	PRO	3.7
1	G	54	THR	3.7
1	F	656	ASP	3.7
1	F	531	ALA	3.6
1	H	51	LYS	3.6
1	F	648	ASN	3.5
1	E	51	LYS	3.5
1	H	62	GLU	3.5
1	G	531	ALA	3.5
1	F	62	GLU	3.4
1	B	143	ASP	3.4
1	E	531	ALA	3.4
1	A	52	PRO	3.4
1	E	143	ASP	3.3
1	E	654	ASP	3.2
1	D	54	THR	2.9
1	C	51	LYS	2.9
1	H	53	SER	2.9
1	F	649	GLY	2.7
1	C	53	SER	2.7
1	E	669	ALA	2.7
1	F	600	ALA	2.7
1	E	327	GLU	2.6
1	D	143	ASP	2.6
1	E	674	ALA	2.6
1	F	650	GLY	2.6
1	E	61	PHE	2.5
1	B	269	ARG	2.5
1	E	645	ALA	2.5
1	E	63	ASP	2.5
1	F	53	SER	2.5
1	E	532	GLU	2.5
1	F	269	ARG	2.5
1	F	63	ASP	2.4
1	F	651	GLN	2.4
1	E	53	SER	2.4
1	A	55	LYS	2.4
1	D	51	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	677	SER	2.4
1	B	683	HIS	2.3
1	E	653	CYS	2.3
1	C	62	GLU	2.3
1	D	536	ASP	2.3
1	F	598	ASP	2.3
1	E	649	GLY	2.3
1	F	647	GLN	2.3
1	G	61	PHE	2.2
1	E	648	ASN	2.2
1	F	634	GLU	2.2
1	G	52	PRO	2.2
1	E	642	ASN	2.2
1	B	271	SER	2.2
1	D	309	GLU	2.2
1	F	430	GLU	2.1
1	H	532	GLU	2.1
1	E	536	ASP	2.1
1	F	669	ALA	2.1
1	E	555	ASP	2.1
1	G	654	ASP	2.1
1	F	532	GLU	2.1
1	D	55	LYS	2.1
1	C	677	SER	2.1
1	F	645	ALA	2.1
1	B	51	LYS	2.1
1	F	60	GLU	2.0
1	E	651	GLN	2.0
1	E	656	ASP	2.0
1	F	653	CYS	2.0
1	C	63	ASP	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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GOL	B	706	6/6	0.85	0.15	30,34,35,37	0
2	GOL	B	705	6/6	0.86	0.18	25,29,30,34	0
2	GOL	G	706	6/6	0.88	0.14	36,41,42,43	0
2	GOL	G	705	6/6	0.88	0.18	34,37,38,39	0
2	GOL	G	704	6/6	0.88	0.13	19,22,23,24	0
2	GOL	C	707	6/6	0.89	0.12	24,27,27,28	0
2	GOL	H	705	6/6	0.89	0.14	24,28,29,30	0
2	GOL	A	709	6/6	0.89	0.15	29,33,35,35	0
2	GOL	B	702	6/6	0.89	0.15	20,24,25,27	0
2	GOL	C	705	6/6	0.90	0.14	19,23,24,24	0
2	GOL	D	705	6/6	0.90	0.11	23,25,25,27	0
2	GOL	E	703	6/6	0.91	0.11	25,27,28,29	0
2	GOL	H	708	6/6	0.91	0.14	27,30,31,31	0
2	GOL	A	708	6/6	0.91	0.11	20,21,21,21	0
2	GOL	D	706	6/6	0.91	0.16	31,32,32,33	0
2	GOL	H	704	6/6	0.91	0.11	18,20,21,22	0
2	GOL	A	705	6/6	0.91	0.14	26,29,30,31	0
2	GOL	B	708	6/6	0.92	0.10	25,26,26,27	0
2	GOL	A	702	6/6	0.92	0.11	20,21,22,23	0
2	GOL	C	706	6/6	0.92	0.12	14,16,17,18	0
2	GOL	B	703	6/6	0.92	0.11	21,21,22,23	0
2	GOL	E	705	6/6	0.92	0.11	32,33,33,34	0
2	GOL	H	706	6/6	0.92	0.11	24,26,27,30	0
2	GOL	B	707	6/6	0.92	0.10	26,27,28,30	0
2	GOL	E	702	6/6	0.93	0.10	25,26,26,27	0
2	GOL	B	701	6/6	0.93	0.10	18,19,19,20	0
2	GOL	A	707	6/6	0.93	0.11	19,19,19,20	0
2	GOL	G	702	6/6	0.93	0.08	19,20,21,21	0
2	GOL	C	704	6/6	0.93	0.09	18,19,21,21	0
2	GOL	E	704	6/6	0.94	0.08	29,29,29,30	0
2	GOL	F	702	6/6	0.94	0.09	21,22,23,24	0
2	GOL	C	701	6/6	0.94	0.11	12,13,13,13	0
2	GOL	D	701	6/6	0.94	0.10	16,17,17,18	0
2	GOL	C	708	6/6	0.94	0.10	23,24,24,25	0
2	GOL	C	702	6/6	0.95	0.09	13,14,14,15	0
2	GOL	D	703	6/6	0.95	0.09	25,25,26,26	0
2	GOL	F	701	6/6	0.95	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	H	707	6/6	0.95	0.09	24,26,26,26	0
2	GOL	E	701	6/6	0.95	0.10	23,24,25,27	0
2	GOL	C	703	6/6	0.95	0.10	20,21,21,22	0
2	GOL	H	702	6/6	0.95	0.09	14,14,15,16	0
2	GOL	G	703	6/6	0.95	0.09	17,18,19,19	0
2	GOL	D	704	6/6	0.95	0.08	17,18,20,21	0
2	GOL	B	704	6/6	0.96	0.09	18,19,19,21	0
2	GOL	H	703	6/6	0.96	0.08	16,18,18,18	0
2	GOL	A	704	6/6	0.96	0.08	13,14,15,17	0
2	GOL	D	702	6/6	0.96	0.09	18,19,20,20	0
2	GOL	A	703	6/6	0.97	0.09	16,16,17,19	0
2	GOL	G	701	6/6	0.97	0.10	17,17,18,18	0
2	GOL	H	701	6/6	0.97	0.06	21,21,21,21	0
2	GOL	A	701	6/6	0.98	0.09	12,13,13,13	0
2	GOL	A	706	6/6	0.98	0.08	14,14,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.