



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:41 PM GMT

PDB ID : 1E6X
Title : MYROSINASE FROM SINAPIS ALBA WITH A BOUND TRANSITION
STATE ANALOGUE,D-GLUCONO-1,5-LACTONE
Authors : Burmeister, W.P.
Deposited on : 2000-08-23
Resolution : 1.60 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>

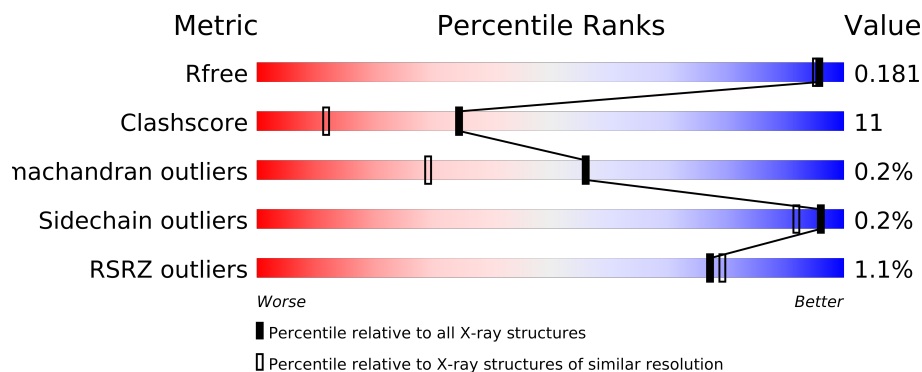
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.60 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}	66092	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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	M	501	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	M	901	-	X
2	NAG	M	911	-	X
2	NAG	M	931	-	X
2	NAG	M	961	-	X
2	NAG	M	971	-	X
2	NAG	M	991	-	X
6	LGC	M	999	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
8	SO4	M	1503	-	X
8	SO4	M	1504	-	X
8	SO4	M	1505	-	X
8	SO4	M	1507	-	X
8	SO4	M	1508	-	X
8	SO4	M	1510	-	X
9	GOL	M	1511	-	X
9	GOL	M	1512[A]	-	X
9	GOL	M	1512[B]	-	X
9	GOL	M	1513	X	X
9	GOL	M	1514	-	X

2 Entry composition i

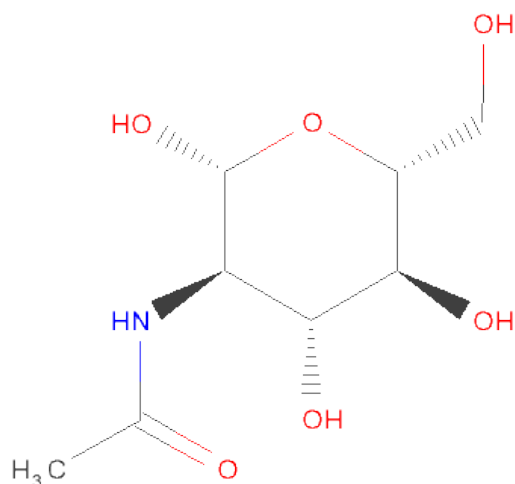
There are 10 unique types of molecules in this entry. The entry contains 5203 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MYROSINASE MA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	499	Total	C	N	O	S	0	21	0
			4082	2618	660	788	16			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	M	2	Total	C	N	O	0	0
			28	16	2	10		

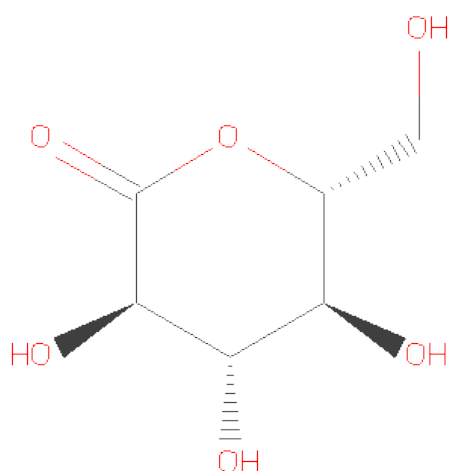
- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	M	5	Total	C	N	O	0	0
			58	33	2	23		

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	6	Total	C	N	O	0	0
			69	39	2	28		

- Molecule 6 is SUGAR ((3S,4R,5R,6S)-3,4,5-TRIHIDROXY-6-(HYDROXYMETHYL)TETRAHYDRO-2H-PYRAN-2-ONE) (three-letter code: LGC) (formula: C₆H₁₀O₆).

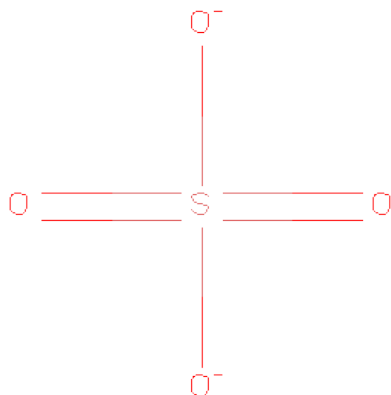


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

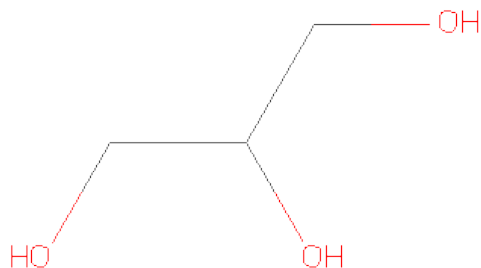
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Zn	0	0
			1	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			6	3	3		
9	M	1	Total	C	O	0	1
			7	3	4		
9	M	1	Total	C	O	0	0
			6	3	3		
9	M	1	Total	C	O	0	0
			6	3	3		

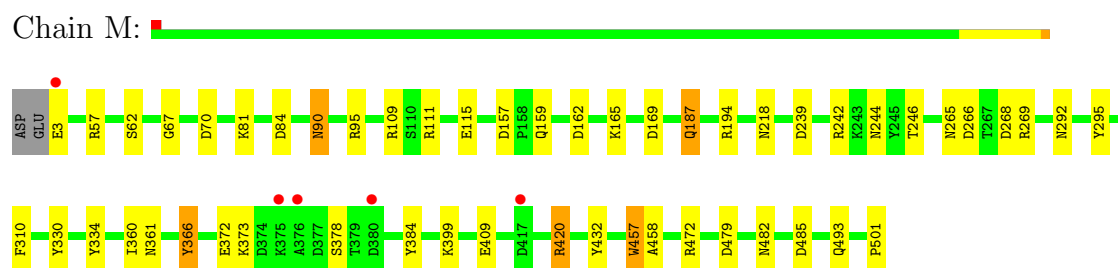
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	804	Total	O	0	0
			804	804		

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 ($RSRZ > 2$). 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: MYROSINASE MA1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	135.30Å 137.20Å 80.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.60 9.98 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.7 (10.00-1.60) 96.0 (9.98-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.138 , 0.178 0.151 , 0.181	Depositor DCC
R_{free} test set	4817 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , 60.2	EDS
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 94406 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5203	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, GOL, ZN, BMA, NAG, LGC, SO4, MAN, FUC

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	M	0.79	1/4290 (0.0%)	1.43	42/5833 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1
3	M	1	0
5	M	1	0
All	All	2	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	501	PRO	N-CD	6.03	1.56	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	70	ASP	CB-CG-OD2	-18.31	101.82	118.30
1	M	109	ARG	NE-CZ-NH2	-15.30	112.65	120.30
1	M	70	ASP	CB-CG-OD1	13.54	130.49	118.30
1	M	242	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	M	109	ARG	NH1-CZ-NH2	11.24	131.77	119.40
1	M	109	ARG	NE-CZ-NH1	-9.44	115.58	120.30
1	M	334	TYR	CB-CG-CD2	9.27	126.56	121.00
1	M	115	GLU	OE1-CD-OE2	-8.99	112.52	123.30
1	M	295	TYR	CB-CG-CD1	-8.51	115.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	162	ASP	CB-CG-OD1	8.35	125.81	118.30
1	M	90	ASN	CB-CG-OD1	7.59	136.78	121.60
1	M	239	ASP	CB-CG-OD1	7.46	125.01	118.30
1	M	95	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	M	482	ASN	CB-CG-OD1	7.29	136.18	121.60
1	M	162	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	M	295	TYR	CB-CG-CD2	6.98	125.19	121.00
1	M	366[A]	TYR	CB-CG-CD2	-6.89	116.86	121.00
1	M	366[B]	TYR	CB-CG-CD2	-6.89	116.86	121.00
1	M	420	ARG	CD-NE-CZ	6.84	133.18	123.60
1	M	472	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	M	479	ASP	CB-CG-OD1	6.57	124.21	118.30
1	M	372	GLU	OE1-CD-OE2	-6.41	115.61	123.30
1	M	269	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	M	457	TRP	O-C-N	-6.17	112.83	122.70
1	M	269	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	M	111	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	M	361	ASN	CB-CG-OD1	5.92	133.44	121.60
1	M	482	ASN	CA-CB-CG	-5.92	100.38	113.40
1	M	458	ALA	N-CA-CB	5.74	118.13	110.10
1	M	432	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	M	485	ASP	CB-CG-OD1	5.59	123.33	118.30
1	M	384	TYR	CA-CB-CG	5.57	123.98	113.40
1	M	157	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	M	57	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	M	169[A]	ASP	CB-CG-OD1	5.36	123.13	118.30
1	M	169[B]	ASP	CB-CG-OD1	5.36	123.13	118.30
1	M	84	ASP	CB-CG-OD1	5.32	123.08	118.30
1	M	268	ASP	CB-CG-OD1	5.31	123.08	118.30
1	M	330	TYR	CB-CG-CD1	-5.24	117.85	121.00
1	M	310	PHE	CB-CG-CD1	-5.21	117.15	120.80
1	M	266	ASP	CB-CG-OD1	5.10	122.89	118.30
1	M	334	TYR	CB-CG-CD1	-5.09	117.94	121.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	M	923	NAG	C4
5	M	954	BMA	C4

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	457	TRP	Mainchain

5.2 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 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	M	4082	0	0	25	0
2	M	84	0	76	3	0
3	M	28	0	24	3	0
4	M	58	0	50	2	0
5	M	69	0	57	6	0
6	M	12	0	10	2	0
7	M	1	0	0	0	0
8	M	40	0	0	6	0
9	M	25	0	0	7	0
10	M	804	0	0	19	0
All	All	5203	0	217	43	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 11.

All (43) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CZ	2.04	1.39
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:CE1	2.23	1.21
9:M:1513:GOL:C1	10:M:2801:HOH:O	1.95	1.14
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CE1	2.32	1.12
9:M:1513:GOL:C2	10:M:2801:HOH:O	1.98	1.05
9:M:1513:GOL:O1	10:M:2801:HOH:O	1.75	1.03
1:M:360[B]:ILE:CD1	1:M:366[B]:TYR:OH	2.12	0.95
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CD1	2.65	0.78
5:M:954:BMA:C5	10:M:2750:HOH:O	2.34	0.75
1:M:165:LYS:NZ	2:M:931:NAG:H82	2.03	0.73
5:M:954:BMA:C4	10:M:2750:HOH:O	2.38	0.69
8:M:1505:SO4:O2	8:M:1510:SO4:S	2.54	0.66
5:M:954:BMA:C6	10:M:2750:HOH:O	2.46	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:M:1513:GOL:C3	10:M:2801:HOH:O	2.40	0.62
1:M:244:ASN:ND2	2:M:931:NAG:O5	2.32	0.62
8:M:1505:SO4:S	8:M:1510:SO4:O3	2.59	0.61
8:M:1510:SO4:O1	10:M:2794:HOH:O	2.16	0.59
1:M:218:ASN:ND2	3:M:921:NAG:C2	2.64	0.59
1:M:292:ASN:ND2	5:M:951:NAG:O5	2.37	0.56
1:M:265:ASN:ND2	4:M:941:NAG:C2	2.64	0.55
8:M:1505:SO4:O1	8:M:1510:SO4:O3	2.25	0.54
9:M:1513:GOL:O2	10:M:2801:HOH:O	2.12	0.53
9:M:1511:GOL:C1	10:M:2795:HOH:O	2.56	0.53
1:M:265:ASN:ND2	4:M:941:NAG:O5	2.37	0.53
1:M:90:ASN:ND2	2:M:911:NAG:C2	2.68	0.52
1:M:360[B]:ILE:CG1	1:M:366[B]:TYR:CZ	2.72	0.52
1:M:493:GLN:NE2	10:M:2703:HOH:O	2.43	0.51
1:M:187:GLN:OE1	6:M:999:LGC:O1	2.29	0.50
5:M:954:BMA:H61	10:M:2750:HOH:O	2.08	0.50
1:M:246:THR:CG2	10:M:2398:HOH:O	2.61	0.49
1:M:399:LYS:NZ	10:M:2607:HOH:O	2.48	0.47
1:M:218:ASN:ND2	3:M:921:NAG:O5	2.43	0.45
1:M:159:GLN:NE2	10:M:2315:HOH:O	2.49	0.45
5:M:956:MAN:H61	10:M:2455:HOH:O	2.17	0.45
1:M:62[B]:SER:OG	1:M:67:GLY:O	2.36	0.43
1:M:373:LYS:NZ	1:M:378:SER:OG	2.52	0.43
1:M:194:ARG:NH1	8:M:1510:SO4:O4	2.51	0.42
9:M:1511:GOL:C1	10:M:2798:HOH:O	2.67	0.42
8:M:1505:SO4:O2	8:M:1510:SO4:O3	2.38	0.42
1:M:81:LYS:NZ	10:M:2168:HOH:O	2.53	0.42
1:M:409:GLU:OE1	6:M:999:LGC:C1	2.68	0.41
3:M:923:NAG:O6	3:M:923:NAG:O4	2.35	0.41
1:M:420:ARG:NE	10:M:2631:HOH:O	2.53	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	M	518/501 (103%)	503 (97%)	14 (3%)	1 (0%)	56 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	187	GLN

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	M	456/437 (104%)	455 (100%)	1 (0%)	96 92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	3	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

13 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
3	NAG	M	921	1,3	12,14,15	2.20	5 (41%)	15,19,21	1.50	2 (13%)
3	NAG	M	923	3	12,14,15	1.48	3 (25%)	15,19,21	3.74	6 (40%)
4	NAG	M	941	1,4	12,14,15	1.14	1 (8%)	15,19,21	2.82	10 (66%)
4	FUC	M	942	4	9,10,11	1.04	0	10,14,16	1.76	3 (30%)
4	NAG	M	943	4	12,14,15	0.96	1 (8%)	15,19,21	1.11	1 (6%)
4	BMA	M	944	4	10,11,12	1.58	2 (20%)	11,15,17	2.71	3 (27%)
4	XYP	M	945	4	8,9,10	0.95	0	8,12,14	1.54	2 (25%)
5	NAG	M	951	1,5	12,14,15	1.25	1 (8%)	15,19,21	1.78	4 (26%)
5	FUC	M	952	5	9,10,11	1.45	1 (11%)	10,14,16	2.30	5 (50%)
5	NAG	M	953	5	12,14,15	1.32	2 (16%)	15,19,21	2.94	8 (53%)
5	BMA	M	954	5	10,11,12	1.41	2 (20%)	11,15,17	7.46	8 (72%)
5	XYP	M	955	5	8,9,10	1.10	0	8,12,14	2.16	3 (37%)
5	MAN	M	956	5	10,11,12	1.04	0	11,15,17	2.16	6 (54%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	921	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	923	3	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	M	941	1,4	-	0/6/23/26	0/1/1/1
4	FUC	M	942	4	-	0/0/17/20	0/1/1/1
4	NAG	M	943	4	-	0/6/23/26	0/1/1/1
4	BMA	M	944	4	-	0/2/19/22	0/1/1/1
4	XYP	M	945	4	-	0/0/14/17	0/1/1/1
5	NAG	M	951	1,5	-	0/6/23/26	0/1/1/1
5	FUC	M	952	5	-	0/0/17/20	0/1/1/1
5	NAG	M	953	5	-	0/6/23/26	0/1/1/1
5	BMA	M	954	5	1/1/4/5	0/2/19/22	0/1/1/1
5	XYP	M	955	5	-	0/0/14/17	0/1/1/1
5	MAN	M	956	5	-	0/2/19/22	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	921	NAG	C4-C5	4.55	1.63	1.53
3	M	921	NAG	O7-C7	3.83	1.31	1.23
4	M	944	BMA	C3-C2	-3.48	1.45	1.52
5	M	954	BMA	C3-C2	-3.28	1.45	1.52
4	M	944	BMA	C4-C5	2.93	1.59	1.53
5	M	953	NAG	C3-C2	-2.74	1.47	1.52
5	M	952	FUC	C6-C5	2.69	1.58	1.51
5	M	951	NAG	C2-N2	-2.65	1.43	1.46
3	M	921	NAG	O5-C5	2.57	1.50	1.45
3	M	923	NAG	C4-C5	-2.50	1.47	1.53
3	M	921	NAG	O4-C4	2.50	1.49	1.43
3	M	923	NAG	C3-C2	-2.40	1.47	1.52
4	M	941	NAG	C3-C2	2.31	1.57	1.52
3	M	921	NAG	C3-C2	2.17	1.57	1.52
3	M	923	NAG	C6-C5	-2.17	1.44	1.52
5	M	953	NAG	O5-C5	-2.10	1.41	1.45
5	M	954	BMA	O3-C3	2.05	1.47	1.43
4	M	943	NAG	O7-C7	2.03	1.27	1.23

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	954	BMA	C6-C5-C4	12.75	143.80	113.00
5	M	954	BMA	O5-C5-C6	-12.25	94.13	106.98
3	M	923	NAG	C3-C4-C5	10.54	129.03	110.20
5	M	954	BMA	O4-C4-C5	10.02	135.68	109.28
5	M	954	BMA	C3-C4-C5	9.35	126.90	110.20
5	M	954	BMA	C4-C3-C2	-6.96	101.17	110.50
4	M	944	BMA	O3-C3-C2	6.27	121.41	109.94
5	M	954	BMA	O4-C4-C3	-6.03	96.84	110.35
4	M	941	NAG	O5-C5-C4	-5.12	104.16	110.65
5	M	953	NAG	C2-N2-C7	-4.90	114.85	123.09
3	M	923	NAG	O5-C5-C6	-4.84	101.91	106.98
3	M	923	NAG	C3-C2-N2	-4.78	104.48	111.76
5	M	953	NAG	O5-C5-C6	4.53	111.74	106.98
3	M	923	NAG	O5-C5-C4	-4.49	104.95	110.65
5	M	953	NAG	C3-C2-N2	-4.44	104.99	111.76
5	M	953	NAG	O4-C4-C3	-4.31	100.69	110.35
4	M	941	NAG	C8-C7-N2	-4.28	107.74	116.11
4	M	944	BMA	O5-C5-C4	-4.27	105.23	110.65
5	M	953	NAG	O4-C4-C5	-4.26	98.06	109.28
3	M	923	NAG	O3-C3-C4	4.25	119.88	110.35
5	M	955	XYP	C4B-C3B-C2B	-4.24	104.39	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	941	NAG	O3-C3-C2	-4.05	100.58	109.09
4	M	941	NAG	C2-N2-C7	-4.00	116.37	123.09
5	M	952	FUC	C4-C3-C2	3.85	115.68	110.50
5	M	953	NAG	O5-C5-C4	-3.66	106.01	110.65
5	M	956	MAN	O5-C5-C4	3.66	115.29	110.65
5	M	951	NAG	O5-C5-C6	-3.63	103.17	106.98
5	M	954	BMA	O3-C3-C2	-3.58	103.38	109.94
3	M	921	NAG	O4-C4-C5	-3.51	100.03	109.28
5	M	956	MAN	C4-C3-C2	-3.42	105.91	110.50
4	M	944	BMA	C4-C3-C2	3.33	114.97	110.50
4	M	942	FUC	O5-C5-C6	-3.24	102.83	108.03
4	M	942	FUC	O3-C3-C2	-3.10	104.27	109.94
5	M	952	FUC	O5-C5-C4	-3.08	105.57	110.22
5	M	952	FUC	C6-C5-C4	-3.04	108.12	113.06
5	M	951	NAG	C3-C2-N2	3.02	116.36	111.76
4	M	941	NAG	O7-C7-N2	3.01	128.19	121.90
5	M	955	XYP	O3B-C3B-C4B	2.98	115.41	110.03
5	M	954	BMA	O2-C2-C3	-2.94	103.84	110.18
5	M	951	NAG	C8-C7-N2	-2.85	110.54	116.11
5	M	953	NAG	C8-C7-N2	-2.78	110.68	116.11
5	M	951	NAG	O7-C7-C8	2.74	127.39	122.04
3	M	923	NAG	O6-C6-C5	-2.58	102.48	111.36
4	M	942	FUC	O2-C2-C3	-2.55	104.66	110.18
4	M	945	XYP	O2B-C2B-C3B	-2.49	104.81	110.18
5	M	952	FUC	O4-C4-C3	-2.48	104.78	110.35
5	M	956	MAN	O2-C2-C3	-2.47	104.85	110.18
4	M	945	XYP	C5B-C4B-C3B	-2.47	106.60	109.71
4	M	943	NAG	C3-C2-N2	-2.45	108.03	111.76
5	M	956	MAN	O3-C3-C4	-2.37	105.03	110.35
4	M	941	NAG	O5-C5-C6	-2.30	104.57	106.98
5	M	956	MAN	C3-C4-C5	-2.27	106.14	110.20
3	M	921	NAG	O5-C5-C4	-2.26	107.79	110.65
5	M	953	NAG	O7-C7-C8	2.25	126.44	122.04
4	M	941	NAG	C4-C3-C2	-2.20	105.94	111.32
4	M	941	NAG	O4-C4-C5	-2.20	103.50	109.28
4	M	941	NAG	C3-C2-N2	-2.17	108.45	111.76
5	M	952	FUC	O3-C3-C2	-2.16	105.99	109.94
5	M	955	XYP	C5B-C4B-C3B	-2.15	107.00	109.71
5	M	956	MAN	O6-C6-C5	-2.10	104.15	111.36
4	M	941	NAG	O4-C4-C3	-2.03	105.81	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	954	BMA	C4
3	M	923	NAG	C4

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 1 is monoatomic and 2 are modelled with single atom - leaving 18 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	$\# Z > 2$
8	SO4	M	1503	-	4,4,4	1.34	0	6,6,6	0.72	0
8	SO4	M	1504	-	4,4,4	1.21	0	6,6,6	0.54	0
8	SO4	M	1505	8	4,4,4	1.01	0	6,6,6	0.77	0
8	SO4	M	1506	-	4,4,4	0.66	0	6,6,6	0.35	0
8	SO4	M	1507	-	4,4,4	1.28	1 (25%)	6,6,6	0.84	0
8	SO4	M	1508	-	4,4,4	1.32	0	6,6,6	0.78	0
8	SO4	M	1509	-	4,4,4	1.04	0	6,6,6	0.11	0
8	SO4	M	1510	8	4,4,4	0.72	0	6,6,6	1.58	1 (16%)
9	GOL	M	1511	-	5,5,5	0.35	0	5,5,5	0.96	0
9	GOL	M	1513	-	5,5,5	2.94	3 (60%)	5,5,5	3.04	4 (80%)
9	GOL	M	1514	-	5,5,5	0.28	0	5,5,5	1.08	0
2	NAG	M	901	1	12,14,15	1.35	2 (16%)	15,19,21	1.50	2 (13%)
2	NAG	M	911	1	12,14,15	1.22	1 (8%)	15,19,21	1.77	2 (13%)
2	NAG	M	931	1	12,14,15	1.75	2 (16%)	15,19,21	5.40	7 (46%)
2	NAG	M	961	1	12,14,15	1.71	3 (25%)	15,19,21	1.23	2 (13%)
2	NAG	M	971	1	12,14,15	1.53	2 (16%)	15,19,21	2.25	3 (20%)
2	NAG	M	991	1	12,14,15	1.53	3 (25%)	15,19,21	1.48	3 (20%)
6	LGC	M	999	-	12,12,12	3.71	3 (25%)	17,17,17	3.40	9 (52%)

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
8	SO4	M	1503	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1504	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1505	8	-	0/0/0/0	0/0/0/0
8	SO4	M	1506	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1507	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1508	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1509	-	-	0/0/0/0	0/0/0/0
8	SO4	M	1510	8	-	0/0/0/0	0/0/0/0
9	GOL	M	1511	-	-	0/4/4/4	0/0/0/0
9	GOL	M	1513	-	-	0/4/4/4	0/0/0/0
9	GOL	M	1514	-	-	0/4/4/4	0/0/0/0
2	NAG	M	901	1	-	0/6/23/26	0/1/1/1
2	NAG	M	911	1	-	0/6/23/26	0/1/1/1
2	NAG	M	931	1	-	0/6/23/26	0/1/1/1
2	NAG	M	961	1	-	0/6/23/26	0/1/1/1
2	NAG	M	971	1	-	0/6/23/26	0/1/1/1
2	NAG	M	991	1	1/1/5/7	0/6/23/26	0/1/1/1
6	LGC	M	999	-	-	0/2/22/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	999	LGC	C2-C1	-11.50	1.40	1.51
9	M	1513	GOL	O1-C1	4.73	1.62	1.42
2	M	931	NAG	O7-C7	-4.43	1.13	1.23
2	M	971	NAG	O7-C7	-4.07	1.14	1.23
6	M	999	LGC	O5-C1	3.97	1.40	1.34
2	M	991	NAG	O7-C7	-3.68	1.15	1.23
9	M	1513	GOL	O2-C2	3.61	1.54	1.43
2	M	911	NAG	O7-C7	-3.61	1.15	1.23
2	M	961	NAG	O7-C7	-3.60	1.15	1.23
2	M	901	NAG	O7-C7	-3.12	1.16	1.23
2	M	961	NAG	C2-N2	3.11	1.50	1.46
2	M	931	NAG	C2-N2	-2.95	1.42	1.46
2	M	901	NAG	C2-N2	2.77	1.49	1.46
2	M	961	NAG	O5-C5	-2.75	1.40	1.45
6	M	999	LGC	O1-C1	2.46	1.27	1.21
2	M	971	NAG	O5-C5	-2.44	1.40	1.45
2	M	991	NAG	C2-N2	2.38	1.49	1.46
9	M	1513	GOL	C1-C2	2.34	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	1507	SO4	O2-S	2.30	1.54	1.47
2	M	991	NAG	O5-C5	-2.13	1.41	1.45

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	931	NAG	C2-N2-C7	17.49	152.45	123.09
2	M	931	NAG	C3-C2-N2	8.07	124.06	111.76
6	M	999	LGC	O5-C1-O1	-7.50	107.45	118.51
6	M	999	LGC	O5-C1-C2	7.11	130.45	119.08
2	M	971	NAG	O5-C5-C6	-6.10	100.58	106.98
6	M	999	LGC	O5-C5-C6	-5.32	101.05	106.52
2	M	911	NAG	O5-C5-C4	-5.17	104.09	110.65
2	M	971	NAG	O5-C5-C4	-5.15	104.12	110.65
9	M	1513	GOL	C3-C2-C1	5.08	133.68	111.26
2	M	901	NAG	O5-C5-C4	-4.60	104.81	110.65
6	M	999	LGC	C4-C3-C2	-4.26	104.94	110.62
2	M	931	NAG	O7-C7-N2	-4.12	113.31	121.90
2	M	931	NAG	O5-C5-C4	-3.94	105.65	110.65
6	M	999	LGC	O5-C5-C4	-3.78	103.28	109.97
2	M	991	NAG	O5-C5-C4	-3.78	105.86	110.65
2	M	931	NAG	C3-C4-C5	3.51	116.46	110.20
8	M	1510	SO4	O2-S-O1	-3.50	97.96	109.53
9	M	1513	GOL	O3-C3-C2	3.12	124.95	109.71
6	M	999	LGC	C6-C5-C4	3.11	120.52	113.00
2	M	911	NAG	O3-C3-C2	-2.62	103.58	109.09
2	M	991	NAG	C4-C3-C2	-2.35	105.57	111.32
2	M	961	NAG	C3-C4-C5	2.33	114.36	110.20
2	M	901	NAG	O3-C3-C2	-2.29	104.28	109.09
9	M	1513	GOL	O1-C1-C2	2.29	120.86	109.71
2	M	931	NAG	C8-C7-N2	2.27	120.55	116.11
6	M	999	LGC	C3-C4-C5	-2.27	106.15	110.20
6	M	999	LGC	O4-C4-C5	-2.23	103.41	109.28
6	M	999	LGC	O3-C3-C2	-2.20	106.03	109.36
2	M	991	NAG	O5-C5-C6	-2.16	104.72	106.98
2	M	961	NAG	O4-C4-C5	-2.12	103.69	109.28
2	M	931	NAG	O7-C7-C8	2.10	126.14	122.04
2	M	971	NAG	C3-C2-N2	-2.07	108.60	111.76
9	M	1513	GOL	O2-C2-C1	-2.00	99.09	108.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	M	991	NAG	C1

There are no torsion outliers.

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	M	499/501 (99%)	-0.65	5 (1%) 79 81	11, 16, 29, 54	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	376	ALA	7.9
1	M	3	GLU	3.3
1	M	417	ASP	3.0
1	M	380	ASP	2.9
1	M	375	LYS	2.5

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
4	XYP	M	945	9/10	0.29	14.85	44,45,46,48	0
5	MAN	M	956	11/12	0.36	6.38	32,45,48,48	0
5	NAG	M	953	14/15	0.12	5.67	24,27,32,35	0
4	NAG	M	941	14/15	0.09	2.34	20,22,25,26	0
3	NAG	M	923	14/15	0.36	2.24	41,45,51,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	M	951	14/15	0.08	2.13	22,23,26,27	0
3	NAG	M	921	14/15	0.08	1.94	21,26,30,34	0
5	FUC	M	952	10/11	0.14	1.83	27,28,31,33	0
4	FUC	M	942	10/11	0.17	-	29,33,36,38	0
5	BMA	M	954	11/12	0.16	-	28,32,38,42	0
4	NAG	M	943	14/15	0.08	-	26,30,34,35	0
5	XYP	M	955	9/10	0.30	-	42,45,47,48	0
4	BMA	M	944	11/12	0.28	-	39,41,44,46	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
8	SO4	M	1510	5/5	0.30	46.48	45,46,47,48	1
9	GOL	M	1514	6/6	0.26	33.02	42,43,44,45	6
2	NAG	M	971	14/15	0.37	32.24	58,64,66,67	0
8	SO4	M	1503	5/5	0.15	13.46	26,26,29,29	5
2	NAG	M	961	14/15	0.38	13.38	43,47,55,56	0
9	GOL	M	1513	6/6	0.28	13.22	16,24,26,28	6
8	SO4	M	1505	5/5	0.12	12.83	27,28,30,31	5
8	SO4	M	1507	5/5	0.18	11.70	34,35,36,37	5
9	GOL	M	1511	6/6	0.23	11.12	42,43,44,44	6
2	NAG	M	911	14/15	0.19	10.83	26,29,32,33	0
2	NAG	M	991	14/15	0.44	9.54	43,45,51,51	0
2	NAG	M	931	14/15	0.30	9.10	40,46,49,52	0
8	SO4	M	1508	5/5	0.26	7.42	31,35,36,37	5
8	SO4	M	1504	5/5	0.14	6.62	23,29,31,32	5
6	LGC	M	999	12/12	0.09	3.76	14,18,20,24	0
9	GOL	M	1512[B]	1/6	0.10	2.81	19,19,19,19	1
2	NAG	M	901	14/15	0.17	2.06	33,38,39,42	0
9	GOL	M	1512[A]	1/6	0.10	1.75	6,6,6,6	1
8	SO4	M	1506	5/5	0.04	-2.59	19,21,25,27	0
7	ZN	M	1502	1/1	0.02	-8.93	13,13,13,13	1
8	SO4	M	1509	5/5	0.25	-	42,42,42,43	5

6.5 Other polymers ⓘ

There are no such residues in this entry.