W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:58 PM GMT

|		
PDB ID	:	1MYR
Title	:	MYROSINASE FROM SINAPIS ALBA
Authors	:	Burmeister, W.P.; Iori, R.; Palmieri, S.; Henrissat, B.
Deposited on	:	1997-03-23
Resolution	:	1.64 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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.
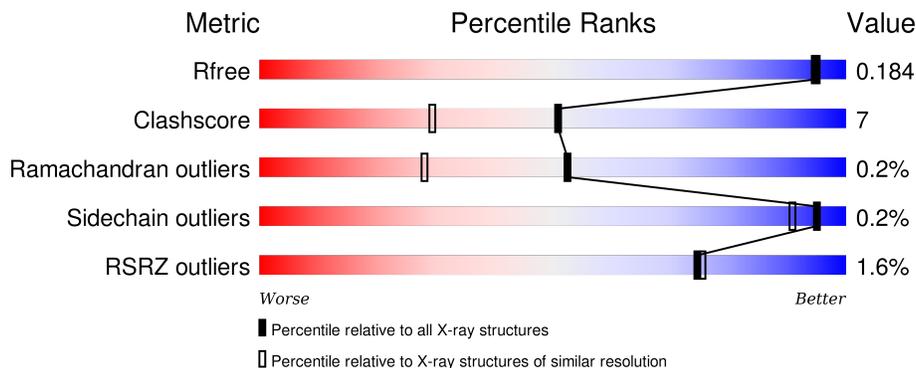
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1953 (1.66-1.62)
Clashscore	102246	2091 (1.66-1.62)
Ramachandran outliers	100387	2052 (1.66-1.62)
Sidechain outliers	100360	2052 (1.66-1.62)
RSRZ outliers	91569	1955 (1.66-1.62)

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. 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 <=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	501	

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
8	SO4	A	1000	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SO4	A	1001	-	-	-	X
8	SO4	A	993	-	-	-	X
8	SO4	A	995	-	-	X	X
9	GOL	A	1004	-	-	-	X
9	GOL	A	1005	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 5014 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 MYROSINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4003	2562	660	765	16			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
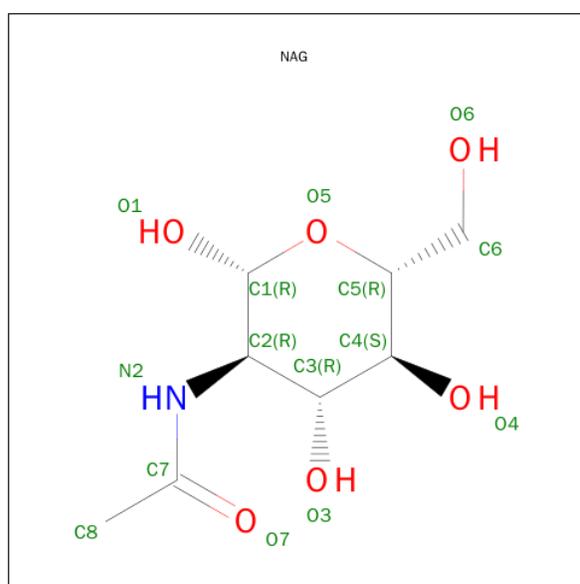
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

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

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

- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	7	Total 80	C 45	N 2	O 33	0	0

- Molecule 6 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).
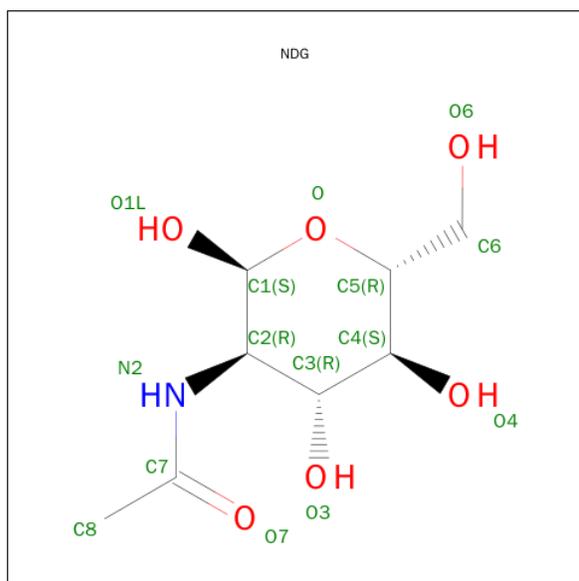
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 14	C 8	N 1	O 5	0	0

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

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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
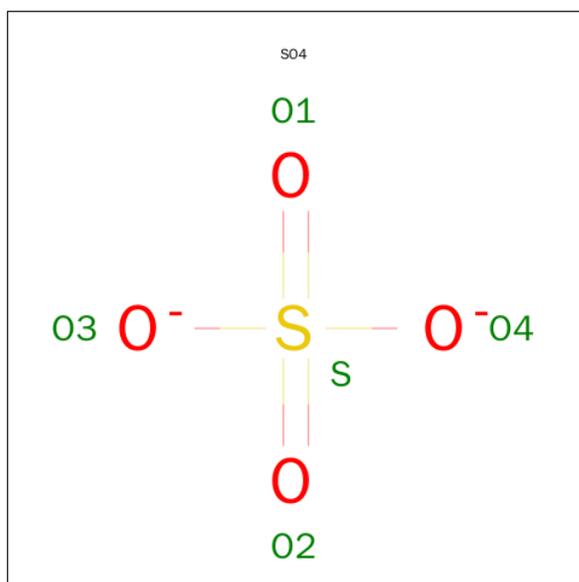
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total O S 5 4 1			0	0
8	A	1	Total O S 5 4 1			0	0
8	A	1	Total O S 5 4 1			0	0
8	A	1	Total O S 5 4 1			0	0
8	A	1	Total O S 5 4 1			0	0
8	A	1	Total O S 5 4 1			0	0
8	A	1	Total O S 5 4 1			0	0
8	A	1	Total O S 5 4 1			0	0
8	A	1	Total O S 5 4 1			0	0
8	A	1	Total O S 5 4 1			0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
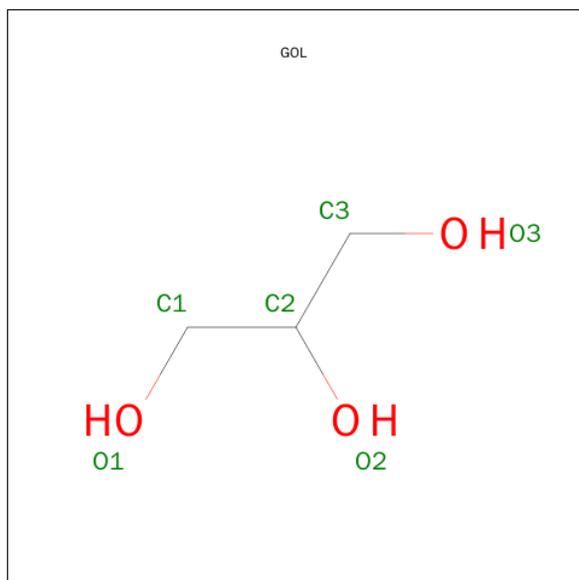
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 6	C 3	O 3	0	0
9	A	1	Total 6	C 3	O 3	0	0
9	A	1	Total 6	C 3	O 3	0	0
9	A	1	Total 6	C 3	O 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	672	Total 672	O 672	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 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
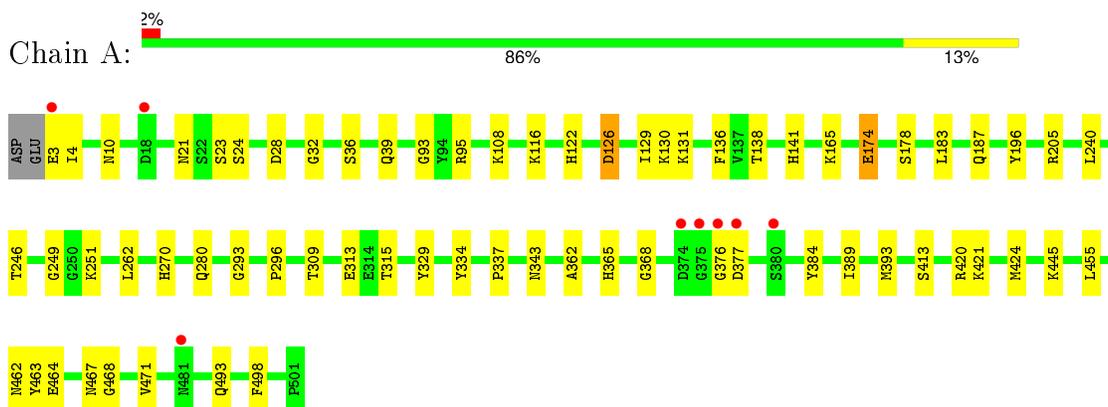
4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	134.30Å 136.40Å 80.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.40 – 1.64 17.38 – 1.64	Depositor EDS
% Data completeness (in resolution range)	98.3 (17.40-1.64) 98.3 (17.38-1.64)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.152 , 0.187 0.151 , 0.184	Depositor DCC
R_{free} test set	4533 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	12.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.2	EDS
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
L-test for twinning[1]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 88612 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5014	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: XYP, GOL, ZN, BMA, NAG, NDG, 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	A	1.01	1/4124 (0.0%)	0.89	0/5607

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	A	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	GLU	CG-CD	5.61	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ASN	Sidechain
1	A	126	ASP	Mainchain
1	A	329	TYR	Sidechain

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	4003	0	3757	55	0
2	A	56	0	52	6	0
3	A	56	0	50	1	0
4	A	58	0	50	0	0
5	A	80	0	68	1	0
6	A	14	0	13	0	0
7	A	1	0	0	0	0
8	A	50	0	0	2	0
9	A	24	0	32	1	0
10	A	672	0	0	18	0
All	All	5014	0	4022	58	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 7.

All (58) 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:A:246:THR:HG22	10:A:1342:HOH:O	1.64	0.97
1:A:108:LYS:HD2	10:A:1126:HOH:O	1.83	0.79
1:A:293:GLY:HA3	1:A:315:THR:HG23	1.67	0.76
1:A:464:GLU:HG2	1:A:467:ASN:HD22	1.51	0.74
8:A:995:SO4:S	8:A:1000:SO4:O3	2.52	0.68
1:A:116:LYS:HG2	10:A:1048:HOH:O	1.94	0.68
1:A:493:GLN:NE2	10:A:1628:HOH:O	2.29	0.65
1:A:421:LYS:HD2	10:A:1627:HOH:O	1.99	0.62
1:A:249:GLY:HA3	9:A:1004:GOL:H31	1.83	0.60
1:A:95:ARG:HB2	1:A:455:LEU:HD13	1.85	0.58
1:A:251:LYS:HE2	10:A:1425:HOH:O	2.03	0.58
1:A:365:HIS:HD2	10:A:1288:HOH:O	1.86	0.57
1:A:4:ILE:HD11	1:A:445:LYS:HD2	1.86	0.57
1:A:280:GLN:NE2	1:A:296:PRO:HB3	2.20	0.56
1:A:365:HIS:HE1	10:A:1330:HOH:O	1.88	0.56
1:A:462:ASN:ND2	10:A:1491:HOH:O	2.38	0.56
1:A:293:GLY:CA	1:A:315:THR:HG23	2.36	0.55
1:A:126:ASP:O	1:A:130:LYS:HG2	2.08	0.53
1:A:463:TYR:CE1	1:A:468:GLY:HA2	2.45	0.52
1:A:165:LYS:NZ	2:A:931:NAG:H81	2.25	0.52
1:A:467:ASN:ND2	10:A:1098:HOH:O	2.42	0.51
1:A:28:ASP:HB3	10:A:1632:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LYS:NZ	2:A:931:NAG:C8	2.73	0.51
1:A:240:LEU:HD13	2:A:931:NAG:H83	1.92	0.51
1:A:130:LYS:HD3	10:A:1347:HOH:O	2.10	0.50
1:A:389:ILE:O	1:A:393:MET:HG2	2.13	0.49
1:A:129:ILE:CD1	1:A:178:SER:HB3	2.43	0.49
1:A:130:LYS:NZ	10:A:1350:HOH:O	2.31	0.48
1:A:413:SER:HB2	1:A:471:VAL:HB	1.96	0.48
1:A:122:HIS:HE1	1:A:174:GLU:O	1.97	0.48
1:A:343:ASN:HB2	10:A:1303:HOH:O	2.13	0.47
1:A:270:HIS:HB3	1:A:337:PRO:HG3	1.97	0.46
1:A:464:GLU:CG	1:A:467:ASN:HD22	2.24	0.45
1:A:95:ARG:HA	1:A:136:PHE:O	2.16	0.45
1:A:376:GLY:O	1:A:377:ASP:HB2	2.17	0.44
1:A:24:SER:O	1:A:445:LYS:NZ	2.50	0.44
1:A:309:THR:HG23	10:A:1084:HOH:O	2.18	0.44
1:A:362:ALA:HB3	3:A:981:NAG:H82	1.99	0.44
1:A:21:ASN:OD1	1:A:23:SER:HB2	2.18	0.44
8:A:995:SO4:O1	8:A:1000:SO4:O3	2.36	0.43
1:A:368:GLY:HA3	1:A:384:TYR:O	2.18	0.43
1:A:262:LEU:O	1:A:334:TYR:HA	2.19	0.43
1:A:421:LYS:NZ	10:A:1627:HOH:O	2.52	0.43
1:A:293:GLY:O	1:A:315:THR:HG23	2.20	0.42
1:A:21:ASN:HA	1:A:498:PHE:CD2	2.54	0.42
1:A:165:LYS:CE	2:A:931:NAG:H81	2.50	0.42
1:A:313:GLU:HG3	10:A:1458:HOH:O	2.19	0.42
1:A:165:LYS:HZ3	2:A:931:NAG:H82	1.85	0.41
1:A:39:GLN:O	1:A:462:ASN:HB2	2.20	0.41
1:A:131:LYS:HA	1:A:131:LYS:HD3	1.78	0.41
1:A:293:GLY:HA3	1:A:315:THR:CG2	2.44	0.41
5:A:956:MAN:H61	10:A:1631:HOH:O	2.20	0.41
1:A:138:THR:HA	1:A:183:LEU:HB2	2.03	0.41
1:A:32:GLY:HA3	1:A:93:GLY:O	2.21	0.41
1:A:420:ARG:O	1:A:424:MET:HG2	2.20	0.40
1:A:196:TYR:CE2	1:A:205:ARG:HD3	2.56	0.40
1:A:165:LYS:HE2	2:A:931:NAG:H81	2.03	0.40
1:A:36:SER:HB2	1:A:141:HIS:CG	2.56	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	497/501 (99%)	481 (97%)	15 (3%)	1 (0%)	52	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLN

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	430/432 (100%)	429 (100%)	1 (0%)	95	91

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

Mol	Chain	Res	Type
1	A	3	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	365	HIS
1	A	462	ASN
1	A	467	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)

16 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	A	921	1,3	14,14,15	0.85	0	15,19,21	0.91	0
3	NAG	A	923	3	14,14,15	1.13	1 (7%)	15,19,21	0.87	1 (6%)
4	NAG	A	941	1,4	14,14,15	0.69	0	15,19,21	0.83	0
4	FUC	A	942	4	10,10,11	0.62	0	14,14,16	1.11	1 (7%)
4	NAG	A	943	4	14,14,15	0.96	1 (7%)	15,19,21	0.77	0
4	BMA	A	944	4	11,11,12	1.48	3 (27%)	14,15,17	0.98	0
4	XYP	A	945	4	9,9,10	1.44	2 (22%)	12,12,14	1.13	1 (8%)
5	NAG	A	951	1,5	14,14,15	0.74	0	15,19,21	0.81	0
5	FUC	A	952	5	10,10,11	1.12	1 (10%)	14,14,16	1.01	1 (7%)
5	NAG	A	953	5	14,14,15	0.94	0	15,19,21	1.06	0
5	BMA	A	954	5	11,11,12	1.65	2 (18%)	14,15,17	1.04	0
5	XYP	A	955	5	9,9,10	0.63	0	12,12,14	0.77	0
5	MAN	A	956	5	11,11,12	0.95	0	14,15,17	1.06	1 (7%)
5	MAN	A	957	5	11,11,12	1.70	3 (27%)	14,15,17	1.85	3 (21%)
3	NAG	A	981	1,3	14,14,15	0.87	1 (7%)	15,19,21	0.51	0
3	NAG	A	983	3	14,14,15	1.63	4 (28%)	15,19,21	0.91	1 (6%)

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	A	921	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	923	3	-	0/6/23/26	0/1/1/1
4	NAG	A	941	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	942	4	-	0/0/17/20	0/1/1/1
4	NAG	A	943	4	-	0/6/23/26	0/1/1/1
4	BMA	A	944	4	-	0/2/19/22	0/1/1/1
4	XYP	A	945	4	-	0/0/14/17	0/1/1/1
5	NAG	A	951	1,5	-	0/6/23/26	0/1/1/1
5	FUC	A	952	5	-	0/0/17/20	0/1/1/1
5	NAG	A	953	5	-	0/6/23/26	0/1/1/1
5	BMA	A	954	5	-	0/2/19/22	0/1/1/1
5	XYP	A	955	5	-	0/0/14/17	0/1/1/1
5	MAN	A	956	5	-	0/2/19/22	0/1/1/1
5	MAN	A	957	5	-	0/2/19/22	0/1/1/1
3	NAG	A	981	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	983	3	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	954	BMA	C2-C3	-4.21	1.46	1.52
4	A	943	NAG	C1-C2	-2.63	1.48	1.52
4	A	945	XYP	C1B-C2B	2.03	1.57	1.52
4	A	944	BMA	O5-C5	2.03	1.47	1.43
5	A	952	FUC	C1-C2	2.03	1.57	1.52
5	A	957	MAN	O5-C5	2.17	1.48	1.43
3	A	923	NAG	C4-C5	2.18	1.57	1.53
3	A	983	NAG	O5-C5	2.20	1.48	1.43
5	A	957	MAN	C4-C5	2.22	1.57	1.53
5	A	954	BMA	C4-C5	2.31	1.58	1.53
4	A	944	BMA	C4-C3	2.42	1.58	1.52
4	A	945	XYP	C2B-C3B	2.43	1.55	1.52
3	A	983	NAG	C8-C7	2.58	1.55	1.50
3	A	981	NAG	C1-C2	3.01	1.56	1.52
3	A	983	NAG	C4-C5	3.03	1.59	1.53
3	A	983	NAG	C1-C2	3.09	1.56	1.52
4	A	944	BMA	C4-C5	3.21	1.59	1.53
5	A	957	MAN	C2-C3	4.03	1.58	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	945	XYP	C4B-C3B-C2B	-3.23	108.05	111.24
3	A	923	NAG	C8-C7-N2	-2.20	111.90	116.11
3	A	983	NAG	C1-O5-C5	2.10	114.91	112.25
5	A	952	FUC	C1-O5-C5	2.12	115.65	112.38
5	A	956	MAN	C1-C2-C3	2.22	112.17	109.54
5	A	957	MAN	C3-C4-C5	2.63	114.79	110.20
4	A	942	FUC	C1-O5-C5	3.05	117.09	112.38
5	A	957	MAN	C1-C2-C3	3.88	114.13	109.54
5	A	957	MAN	C1-O5-C5	4.50	117.96	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	956	MAN	1	0
3	A	981	NAG	1	0

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	A	1000	-	4,4,4	4.25	3 (75%)	6,6,6	0.44	0
8	SO4	A	1001	-	4,4,4	1.63	1 (25%)	6,6,6	0.37	0
8	SO4	A	1002	-	4,4,4	1.23	1 (25%)	6,6,6	0.23	0
9	GOL	A	1003	-	5,5,5	0.63	0	5,5,5	0.52	0
9	GOL	A	1004	-	5,5,5	0.31	0	5,5,5	0.47	0
9	GOL	A	1005	-	5,5,5	0.25	0	5,5,5	0.26	0
9	GOL	A	1006	-	5,5,5	0.59	0	5,5,5	0.68	0
2	NAG	A	901	1	14,14,15	0.90	1 (7%)	15,19,21	0.94	1 (6%)
2	NAG	A	911	1	14,14,15	0.81	0	15,19,21	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NAG	A	931	1	14,14,15	0.99	1 (7%)	15,19,21	1.70	2 (13%)
6	NDG	A	971	1	14,14,15	2.07	4 (28%)	15,19,21	1.27	2 (13%)
2	NAG	A	991	1	14,14,15	1.93	4 (28%)	15,19,21	1.77	3 (20%)
8	SO4	A	993	-	4,4,4	2.49	3 (75%)	6,6,6	0.36	0
8	SO4	A	994	-	4,4,4	0.62	0	6,6,6	0.28	0
8	SO4	A	995	-	4,4,4	2.31	2 (50%)	6,6,6	0.68	0
8	SO4	A	996	-	4,4,4	1.91	1 (25%)	6,6,6	0.41	0
8	SO4	A	997	-	4,4,4	1.47	1 (25%)	6,6,6	0.30	0
8	SO4	A	998	-	4,4,4	0.63	0	6,6,6	0.28	0
8	SO4	A	999	-	4,4,4	1.97	2 (50%)	6,6,6	0.29	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
8	SO4	A	1000	-	-	0/0/0/0	0/0/0/0
8	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
8	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
9	GOL	A	1003	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1004	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1005	-	-	0/4/4/4	0/0/0/0
9	GOL	A	1006	-	-	0/4/4/4	0/0/0/0
2	NAG	A	901	1	-	0/6/23/26	0/1/1/1
2	NAG	A	911	1	-	0/6/23/26	0/1/1/1
2	NAG	A	931	1	-	0/6/23/26	0/1/1/1
6	NDG	A	971	1	-	0/6/23/26	0/1/1/1
2	NAG	A	991	1	-	0/6/23/26	0/1/1/1
8	SO4	A	993	-	-	0/0/0/0	0/0/0/0
8	SO4	A	994	-	-	0/0/0/0	0/0/0/0
8	SO4	A	995	-	-	0/0/0/0	0/0/0/0
8	SO4	A	996	-	-	0/0/0/0	0/0/0/0
8	SO4	A	997	-	-	0/0/0/0	0/0/0/0
8	SO4	A	998	-	-	0/0/0/0	0/0/0/0
8	SO4	A	999	-	-	0/0/0/0	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1000	SO4	O3-S	-7.77	1.19	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	996	SO4	O3-S	-3.66	1.34	1.47
8	A	995	SO4	O3-S	-3.08	1.36	1.47
8	A	995	SO4	O2-S	-2.91	1.37	1.47
8	A	993	SO4	O3-S	-2.81	1.37	1.47
8	A	993	SO4	O1-S	-2.67	1.38	1.47
8	A	1000	SO4	O2-S	-2.59	1.38	1.47
8	A	993	SO4	O2-S	-2.50	1.38	1.47
8	A	1001	SO4	O2-S	-2.45	1.38	1.47
8	A	1000	SO4	O1-S	-2.24	1.39	1.47
8	A	997	SO4	O3-S	-2.03	1.40	1.47
6	A	971	NDG	C4-C3	2.02	1.57	1.52
8	A	999	SO4	O4-S	2.06	1.54	1.47
8	A	1002	SO4	O1-S	2.12	1.54	1.47
2	A	901	NAG	C4-C5	2.18	1.57	1.53
2	A	991	NAG	C3-C2	2.30	1.57	1.52
6	A	971	NDG	C3-C2	2.46	1.58	1.52
8	A	999	SO4	O1-S	2.51	1.55	1.47
2	A	991	NAG	C4-C3	2.53	1.59	1.52
2	A	931	NAG	C1-C2	2.53	1.56	1.52
2	A	991	NAG	C4-C5	2.65	1.58	1.53
6	A	971	NDG	C4-C5	3.61	1.60	1.53
2	A	991	NAG	C1-C2	4.40	1.58	1.52
6	A	971	NDG	C1-C2	5.50	1.60	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	991	NAG	C4-C3-C2	-4.31	104.52	111.23
2	A	931	NAG	C4-C3-C2	-3.95	105.08	111.23
2	A	931	NAG	C3-C4-C5	-3.42	104.23	110.20
6	A	971	NDG	O-C5-C6	-2.55	101.83	107.35
2	A	991	NAG	C8-C7-N2	-2.21	111.88	116.11
2	A	991	NAG	C3-C4-C5	-2.14	106.47	110.20
2	A	901	NAG	C3-C4-C5	-2.05	106.62	110.20
6	A	971	NDG	C1-O-C5	3.82	117.09	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1000	SO4	2	0
9	A	1004	GOL	1	0
2	A	931	NAG	6	0
8	A	995	SO4	2	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	499/501 (99%)	-0.52	8 (1%)	74	75	7, 11, 29, 50	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	GLY	7.9
1	A	375	GLY	5.0
1	A	3	GLU	3.7
1	A	374	ASP	2.9
1	A	377	ASP	2.7
1	A	18	ASP	2.7
1	A	481	ASN	2.3
1	A	380	SER	2.1

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)

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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	921	14/15	0.94	0.09	0.84	16,19,30,36	0
3	NAG	A	981	14/15	0.97	0.07	0.43	9,13,15,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
5	NAG	A	953	14/15	0.94	0.10	-	15,20,27,28	0
4	NAG	A	943	14/15	0.92	0.16	-	21,28,38,45	0
5	XYP	A	955	9/10	0.84	0.22	-	24,35,48,51	0
4	FUC	A	942	10/11	0.89	0.18	-	20,30,44,46	0
5	MAN	A	957	11/12	0.63	0.29	-	39,47,49,54	0
4	NAG	A	941	14/15	0.94	0.09	-	14,19,22,23	0
4	XYP	A	945	9/10	0.66	0.41	-	45,47,50,50	0
5	FUC	A	952	10/11	0.93	0.10	-	19,22,24,27	0
4	BMA	A	944	11/12	0.71	0.30	-	40,45,48,51	0
5	BMA	A	954	11/12	0.91	0.12	-	22,27,36,39	0
5	NAG	A	951	14/15	0.96	0.08	-	13,16,21,22	0
3	NAG	A	983	14/15	0.85	0.28	-	19,31,47,49	0
5	MAN	A	956	11/12	0.80	0.24	-	19,46,47,48	0
3	NAG	A	923	14/15	0.62	0.34	-	31,47,50,52	0

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. 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	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
8	SO4	A	1001	5/5	0.72	0.29	48.00	37,43,47,50	5
8	SO4	A	995	5/5	0.90	0.18	31.53	18,34,40,45	5
8	SO4	A	993	5/5	0.98	0.09	5.58	21,22,26,31	5
9	GOL	A	1005	6/6	0.95	0.12	5.51	10,13,22,23	0
9	GOL	A	1004	6/6	0.97	0.08	2.59	11,23,25,30	0
2	NAG	A	901	14/15	0.93	0.15	0.52	24,36,42,42	0
9	GOL	A	1003	6/6	0.98	0.06	0.10	11,13,15,16	0
8	SO4	A	999	5/5	0.71	0.26	-	35,38,47,53	5
8	SO4	A	1002	5/5	0.87	0.17	-	43,44,47,54	5
8	SO4	A	994	5/5	0.93	0.11	-	18,29,39,42	5
2	NAG	A	931	14/15	0.78	0.26	-	33,40,50,50	0
8	SO4	A	998	5/5	0.82	0.20	-	16,40,47,48	5
2	NAG	A	911	14/15	0.91	0.19	-	19,29,38,40	0
8	SO4	A	996	5/5	0.99	0.04	-	14,19,21,22	0
8	SO4	A	1000	5/5	0.89	0.21	-	25,40,45,45	5
2	NAG	A	991	14/15	0.56	0.50	-	42,48,51,58	0
6	NDG	A	971	14/15	0.63	0.53	-	45,50,54,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	ZN	A	992	1/1	1.00	0.04	-	9,9,9,9	1
8	SO4	A	997	5/5	0.91	0.13	-	28,29,38,44	5
9	GOL	A	1006	6/6	0.70	0.20	-	35,38,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.