



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:37 AM GMT

PDB ID : 3FBX
Title : Crystal structure of the lysosomal 66.3 kDa protein from mouse solved by S-SAD
Authors : Lakomek, K.; Dickmanns, A.; Mueller, U.; Ficner, R.
Deposited on : 2008-11-20
Resolution : 2.40 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>

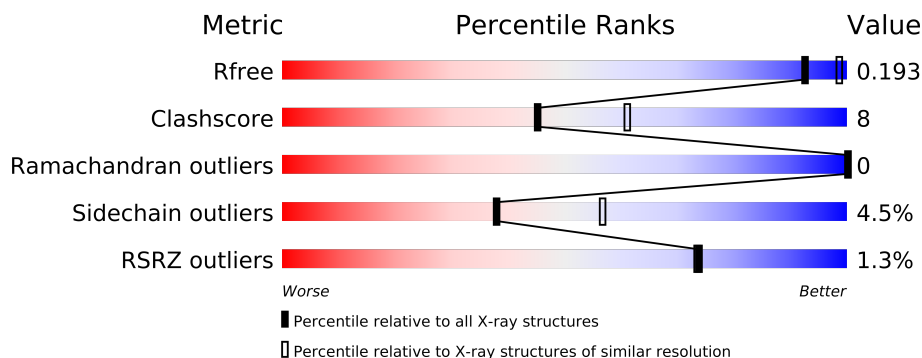
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	A	559	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	21	-	X
4	PG4	A	23	-	X
4	PG4	A	606	-	X
5	XE	A	607	-	X
6	GOL	A	1	-	X
6	GOL	A	2	-	X
6	GOL	A	3	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
8	PGE	A	22	-	X
9	NA	A	609	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4616 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 Putative phospholipase B-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	520	4192	2694	702	774	22	0	5	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	595	GLY	-	EXPRESSION TAG	UNP Q3TCN2
A	596	ARG	-	EXPRESSION TAG	UNP Q3TCN2
A	597	GLY	-	EXPRESSION TAG	UNP Q3TCN2
A	598	SER	-	EXPRESSION TAG	UNP Q3TCN2
A	599	HIS	-	EXPRESSION TAG	UNP Q3TCN2
A	600	HIS	-	EXPRESSION TAG	UNP Q3TCN2
A	601	HIS	-	EXPRESSION TAG	UNP Q3TCN2
A	602	HIS	-	EXPRESSION TAG	UNP Q3TCN2
A	603	HIS	-	EXPRESSION TAG	UNP Q3TCN2
A	604	HIS	-	EXPRESSION TAG	UNP Q3TCN2
A	605	GLY	-	EXPRESSION TAG	UNP Q3TCN2

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

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

There are 11 discrepancies between the modelled and reference sequences:

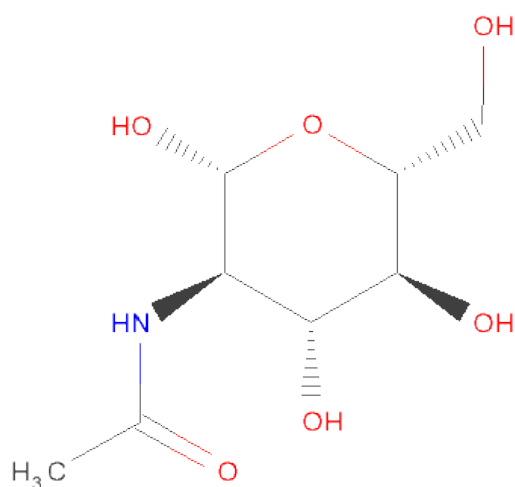
Chain	Residue	Modelled	Actual	Comment	Reference
A	595	GLY	-	EXPRESSION TAG	UNP Q3TCN2
A	596	ARG	-	EXPRESSION TAG	UNP Q3TCN2
A	597	GLY	-	EXPRESSION TAG	UNP Q3TCN2
A	598	SER	-	EXPRESSION TAG	UNP Q3TCN2
A	599	HIS	-	EXPRESSION TAG	UNP Q3TCN2

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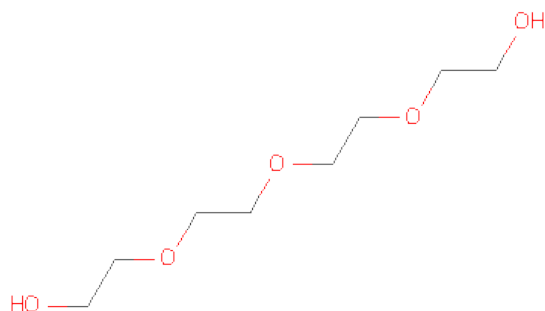
Chain	Residue	Modelled	Actual	Comment	Reference
A	600	HIS	-	EXPRESSION TAG	UNP Q3TCN2
A	601	HIS	-	EXPRESSION TAG	UNP Q3TCN2
A	602	HIS	-	EXPRESSION TAG	UNP Q3TCN2
A	603	HIS	-	EXPRESSION TAG	UNP Q3TCN2
A	604	HIS	-	EXPRESSION TAG	UNP Q3TCN2
A	605	GLY	-	EXPRESSION TAG	UNP Q3TCN2

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

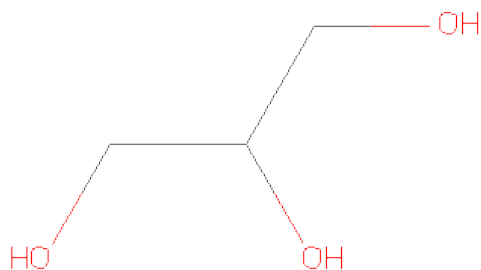


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is XENON (three-letter code: XE) (formula: Xe).

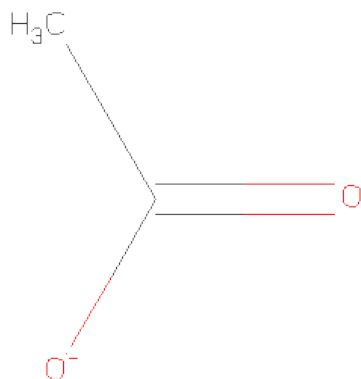
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Xe	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



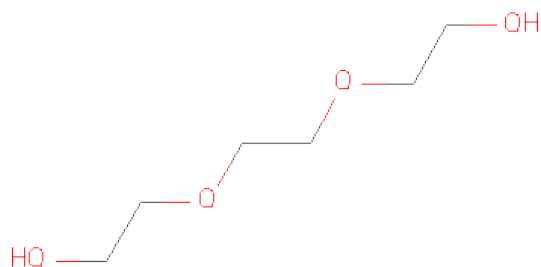
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Na	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	294	Total	O	0	0
			294	294		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.80Å 89.67Å 64.95Å 90.00° 98.67° 90.00°	Depositor
Resolution (Å)	32.11 – 2.40 32.11 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (32.11-2.40) 98.1 (32.11-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.93 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.156 , 0.198 0.156 , 0.193	Depositor DCC
R_{free} test set	1620 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 26.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 32415 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4616	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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: GOL, PGE, NAG, NA, XE, PG4, ACT, OCS

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	0.62	0/4317	0.68	0/5880

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	GLU	Peptide
1	A	154	VAL	Peptide

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	A	4192	0	4064	70	0
2	A	28	0	25	0	0
3	A	42	0	39	1	0
4	A	26	0	36	7	0
5	A	1	0	0	5	0
6	A	18	0	24	0	0
7	A	4	0	3	0	0
8	A	10	0	14	10	0
9	A	1	0	0	0	0
10	A	294	0	0	6	0
All	All	4616	0	4205	72	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 8.

All (72) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:382:GLN:NE2	1:A:407:GLU:OE2	2.03	0.90
1:A:432:ASN:HD22	1:A:463:ARG:HH22	1.17	0.90
1:A:334:LYS:HD3	1:A:448:LEU:HD11	1.63	0.80
1:A:84:PHE:CZ	1:A:86:PRO:HG3	2.18	0.79
1:A:279:ILE:HG21	1:A:591:VAL:HG11	1.67	0.77
1:A:254:LYS:HG2	1:A:474:VAL:HG22	1.67	0.77
1:A:358:ASN:HB2	8:A:22:PGE:H12	1.67	0.76
1:A:72:ASP:O	1:A:76:GLY:HA2	1.86	0.76
1:A:355:VAL:HG13	8:A:22:PGE:H2	1.67	0.75
1:A:362:LEU:HD13	10:A:762:HOH:O	1.84	0.75
1:A:359:ARG:HG2	8:A:22:PGE:H42	1.70	0.74
1:A:75:SER:HB3	1:A:77:GLN:H	1.52	0.73
1:A:349:LEU:HD23	5:A:607:XE:XE	2.67	0.73
1:A:359:ARG:CG	8:A:22:PGE:H42	2.19	0.72
1:A:349:LEU:CD2	5:A:607:XE:XE	3.15	0.71
1:A:254:LYS:NZ	1:A:471:GLN:HE22	1.88	0.70
1:A:65:ARG:NH1	10:A:791:HOH:O	2.27	0.69
1:A:477:MET:HE1	1:A:545:LEU:HD12	1.75	0.68
1:A:334:LYS:HD3	1:A:448:LEU:CD1	2.25	0.67
1:A:358:ASN:CB	8:A:22:PGE:H12	2.24	0.66
1:A:358:ASN:ND2	1:A:367:TRP:HE1	1.93	0.66
8:A:22:PGE:H52	8:A:22:PGE:H22	1.77	0.66
1:A:279:ILE:HD13	1:A:591:VAL:HG21	1.80	0.63
1:A:344:PRO:HD3	4:A:606:PG4:H41	1.81	0.62
1:A:75:SER:HB3	1:A:77:GLN:N	2.16	0.61
1:A:365:ALA:O	4:A:23:PG4:H71	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:249:OCS:OD1	1:A:249:OCS:N	2.32	0.60
1:A:567:TRP:HE1	1:A:580:GLN:NE2	1.98	0.60
1:A:254:LYS:HZ3	1:A:471:GLN:HE22	1.50	0.59
1:A:358:ASN:HD22	1:A:367:TRP:HE1	1.49	0.59
1:A:268:THR:HG23	1:A:537:ASP:OD2	2.04	0.58
3:A:21:NAG:H82	4:A:606:PG4:H52	1.85	0.58
1:A:268:THR:HG22	1:A:539:LYS:NZ	2.18	0.57
1:A:477:MET:CE	1:A:545:LEU:HD12	2.35	0.56
1:A:268:THR:HG21	1:A:315:ASP:CG	2.27	0.55
1:A:70:LEU:HD13	1:A:81:GLU:HG3	1.91	0.53
1:A:165:GLU:HG3	1:A:216:PRO:HG3	1.92	0.51
1:A:154:VAL:N	1:A:155:GLY:HA3	2.25	0.51
1:A:432:ASN:HD22	1:A:463:ARG:NH2	1.98	0.51
1:A:151:GLU:HG2	10:A:650:HOH:O	2.12	0.50
1:A:583:LEU:HD21	1:A:585:MET:HE3	1.93	0.49
1:A:359:ARG:CG	8:A:22:PGE:C4	2.89	0.49
1:A:432:ASN:ND2	1:A:463:ARG:HH22	1.99	0.49
1:A:401:ARG:HG2	4:A:23:PG4:H12	1.93	0.49
1:A:589:ILE:HD12	1:A:591:VAL:HG23	1.94	0.48
1:A:153:GLU:HG2	10:A:771:HOH:O	2.14	0.48
1:A:175:MET:CE	1:A:187:VAL:HG12	2.44	0.48
1:A:471:GLN:O	1:A:474:VAL:HG13	2.14	0.48
1:A:349:LEU:HD21	5:A:607:XE:XE	2.92	0.47
1:A:281:LYS:HD3	1:A:283:ARG:NH2	2.30	0.47
1:A:347:CYS:HB3	5:A:607:XE:XE	2.93	0.47
1:A:340:LYS:HA	4:A:606:PG4:H72	1.97	0.46
1:A:539:LYS:HB2	1:A:539:LYS:HE2	1.70	0.46
1:A:147:CYS:HA	1:A:151:GLU:HG3	1.98	0.46
1:A:268:THR:HG22	1:A:539:LYS:HZ2	1.81	0.44
1:A:173:ARG:NH1	1:A:177:LEU:HD21	2.32	0.44
1:A:358:ASN:CB	8:A:22:PGE:C1	2.95	0.44
1:A:125:VAL:HA	1:A:200:SER:HB2	2.00	0.43
1:A:119:GLN:HE22	1:A:285:GLN:HB2	1.83	0.43
1:A:345:GLN:HB2	1:A:345:GLN:HE21	1.69	0.43
1:A:268:THR:HG23	1:A:537:ASP:CG	2.39	0.43
1:A:285:GLN:NE2	10:A:646:HOH:O	2.51	0.43
1:A:401:ARG:HA	4:A:23:PG4:H21	2.01	0.42
1:A:254:LYS:HZ2	1:A:471:GLN:HE22	1.65	0.41
1:A:359:ARG:HG3	8:A:22:PGE:C4	2.50	0.41
1:A:404:THR:HG23	4:A:23:PG4:H31	2.02	0.41
1:A:485:ARG:NH1	10:A:751:HOH:O	2.20	0.41
1:A:514:SER:HB3	1:A:531:ARG:HG3	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:477:MET:CE	1:A:545:LEU:CD1	2.99	0.41
1:A:347:CYS:CB	5:A:607:XE:XE	3.47	0.40
1:A:82:ASP:O	1:A:85:HIS:HE1	2.04	0.40
1:A:358:ASN:OD1	8:A:22:PGE:H12	2.22	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	A	521/559 (93%)	507 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	450/477 (94%)	430 (96%)	20 (4%)	39	58

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	75	SER
1	A	82	ASP
1	A	99	ARG
1	A	113	ARG
1	A	160	LEU

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Mol	Chain	Res	Type
1	A	161	LYS
1	A	204	ARG
1	A	267	ASN
1	A	268	THR
1	A	345	GLN
1	A	379	TYR
1	A	457	SER
1	A	469	ARG
1	A	471	GLN
1	A	474	VAL
1	A	477	MET
1	A	497	CYS
1	A	531	ARG
1	A	539	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	119	GLN
1	A	260	HIS
1	A	285	GLN
1	A	333	ASN
1	A	343	GLN
1	A	345	GLN
1	A	354	ASN
1	A	358	ASN
1	A	432	ASN
1	A	446	GLN
1	A	451	GLN
1	A	471	GLN
1	A	491	HIS
1	A	580	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	OCS	A	249	1,9	8,8,9	6.86	1 (12%)	9,11,13	1.81	2 (22%)

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
1	OCS	A	249	1,9	-	0/5/7/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	OCS	O-C	19.21	1.24	1.11

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	OCS	C-CA-N	-4.10	109.73	113.83
1	A	249	OCS	OD2-SG-CB	2.25	108.53	105.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

2 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	$\# Z > 2$
2	NAG	A	11	1,2	12,14,15	0.54	0	15,19,21	1.07	2 (13%)
2	NAG	A	12	2	12,14,15	0.49	0	15,19,21	1.31	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
2	NAG	A	11	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	12	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	12	NAG	O5-C5-C6	3.89	111.06	106.98
2	A	11	NAG	O5-C5-C6	2.15	109.24	106.98
2	A	11	NAG	C2-N2-C7	2.01	126.46	123.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
6	GOL	A	1	-	5,5,5	0.45	0	5,5,5	0.47	0
6	GOL	A	2	-	5,5,5	0.33	0	5,5,5	0.84	0
3	NAG	A	21	1	12,14,15	0.47	0	15,19,21	1.02	2 (13%)
8	PGE	A	22	-	9,9,9	0.56	0	8,8,8	0.81	0
4	PG4	A	23	-	12,12,12	0.60	0	11,11,11	0.29	0
6	GOL	A	3	-	5,5,5	0.39	0	5,5,5	0.64	0
3	NAG	A	31	1	12,14,15	0.52	0	15,19,21	1.07	1 (6%)
3	NAG	A	41	1	12,14,15	0.72	0	15,19,21	1.13	1 (6%)
4	PG4	A	606	-	12,12,12	0.67	0	11,11,11	0.46	0
7	ACT	A	608	-	1,3,3	1.21	0	0,3,3	0.00	-

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
6	GOL	A	1	-	-	0/4/4/4	0/0/0/0
6	GOL	A	2	-	-	0/4/4/4	0/0/0/0
3	NAG	A	21	1	-	0/6/23/26	0/1/1/1
8	PGE	A	22	-	-	0/7/7/7	0/0/0/0
4	PG4	A	23	-	-	0/10/10/10	0/0/0/0
6	GOL	A	3	-	-	0/4/4/4	0/0/0/0
3	NAG	A	31	1	-	0/6/23/26	0/1/1/1
3	NAG	A	41	1	-	0/6/23/26	0/1/1/1
4	PG4	A	606	-	-	0/10/10/10	0/0/0/0
7	ACT	A	608	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	31	NAG	O5-C5-C6	2.67	109.78	106.98
3	A	41	NAG	O5-C5-C4	-2.44	107.56	110.65
3	A	21	NAG	O5-C5-C6	2.37	109.47	106.98
3	A	21	NAG	C3-C2-N2	-2.19	108.43	111.76

There are no chirality outliers.

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	A	520/559 (93%)	-0.49	6 (1%) 75 75	12, 22, 41, 56	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	TYR	4.3
1	A	74	ALA	3.5
1	A	548	TYR	2.9
1	A	238	THR	2.6
1	A	63	VAL	2.4
1	A	154	VAL	2.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	OCS	A	249	9/10	0.17	0.83	20,24,29,29	3

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(\AA^2)	Q<0.9
2	NAG	A	12	14/15	0.12	0.00	38,41,43,44	0
2	NAG	A	11	14/15	0.09	-0.05	22,25,27,31	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
4	PG4	A	23	13/13	0.43	9.38	42,53,56,56	0
5	XE	A	607	1/1	0.28	7.91	25,25,25,25	1
6	GOL	A	3	6/6	0.31	6.47	53,54,54,54	0
8	PGE	A	22	10/10	0.26	5.18	30,37,44,44	0
4	PG4	A	606	13/13	0.27	4.15	40,55,59,59	0
3	NAG	A	21	14/15	0.27	2.70	61,65,67,68	0
6	GOL	A	1	6/6	0.21	2.69	53,55,55,55	0
6	GOL	A	2	6/6	0.22	2.55	47,50,52,54	0
9	NA	A	609	1/1	0.23	2.24	32,32,32,32	0
3	NAG	A	31	14/15	0.14	-0.07	38,41,43,44	0
7	ACT	A	608	4/4	0.14	-1.22	73,74,74,74	0
3	NAG	A	41	14/15	0.38	-	66,72,74,74	0

6.5 Other polymers

There are no such residues in this entry.