W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 14, 2017 – 08:58 pm GMT

PDB ID	:	5EBB
Title	:	Structure of human sphingomyelinase phosphodiesterase like 3A (SMPDL3A) with Zn2+
Authors	:	Lim, S.M.; Yeung, K.; Tresaugues, L.; Teo, H.L.; Nordlund, P.
Deposited on	:	2015-10-19
Resolution	:	2.60 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.60 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	Percentile Ranks	Value
Rfree		0.252
Clashscore		15
Ramachandran outliers		0.3%
Sidechain outliers		5.4%
RSRZ outliers		8.1%

Worse ← → Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
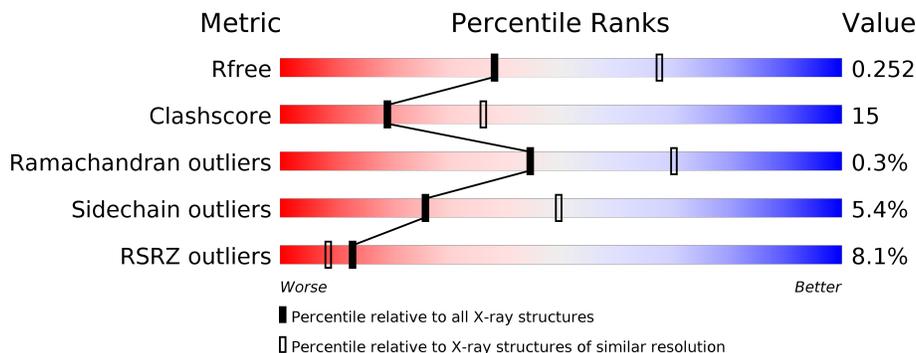
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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	410	82% 17%
1	B	410	66% 30%
1	C	410	68% 29%

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
3	NAG	A	703	-	-	-	X
3	NAG	A	704	-	-	-	X
3	NAG	C	704	X	-	-	-
4	MLI	A	706	-	-	-	X
4	MLI	B	706	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 10414 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 Acid sphingomyelinase-like phosphodiesterase 3a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	3	0
			3302	2127	529	633	13			
1	B	410	Total	C	N	O	S	0	7	0
			3327	2143	532	639	13			
1	C	410	Total	C	N	O	S	0	5	0
			3319	2139	532	635	13			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

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

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

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).
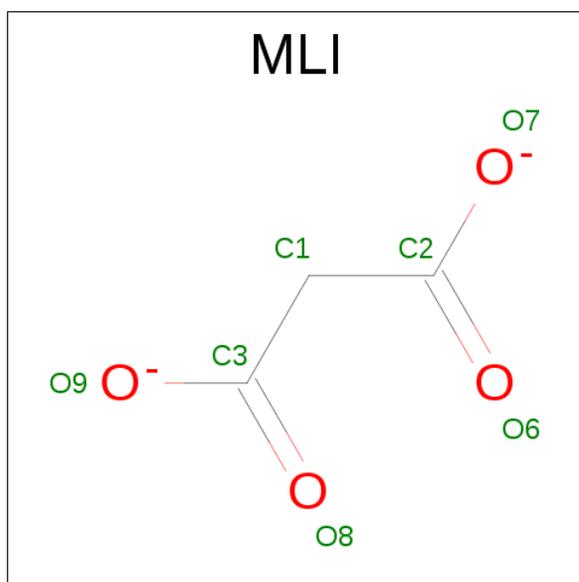
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 7	C 3	O 4	0	0
4	B	1	Total 7	C 3	O 4	0	0
4	C	1	Total 7	C 3	O 4	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
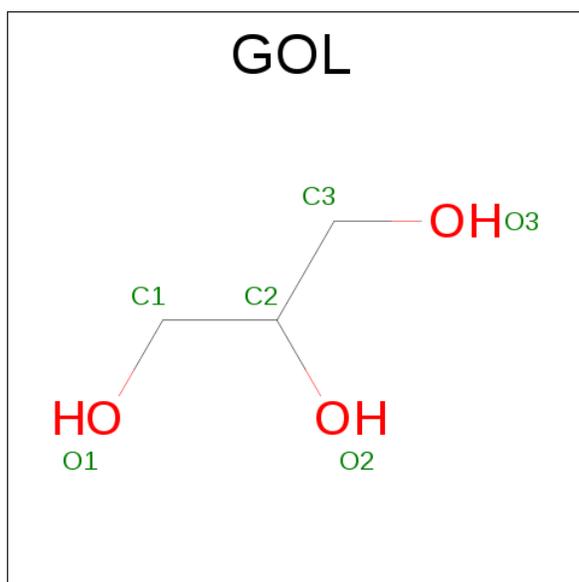
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 6	C 3	O 3	0	0

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	56	Total 56	O 56	0	0
6	B	126	Total 126	O 126	0	0
6	C	119	Total 119	O 119	0	0

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 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: Acid sphingomyelinase-like phosphodiesterase 3a
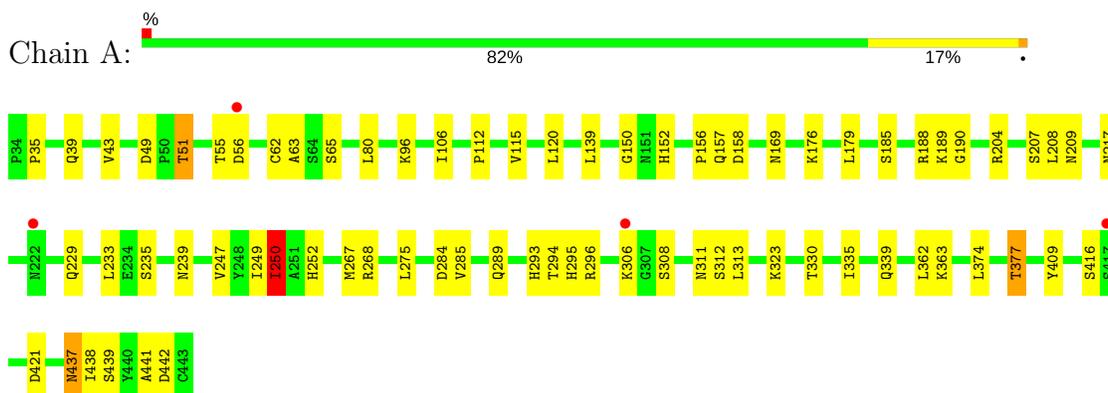
- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a
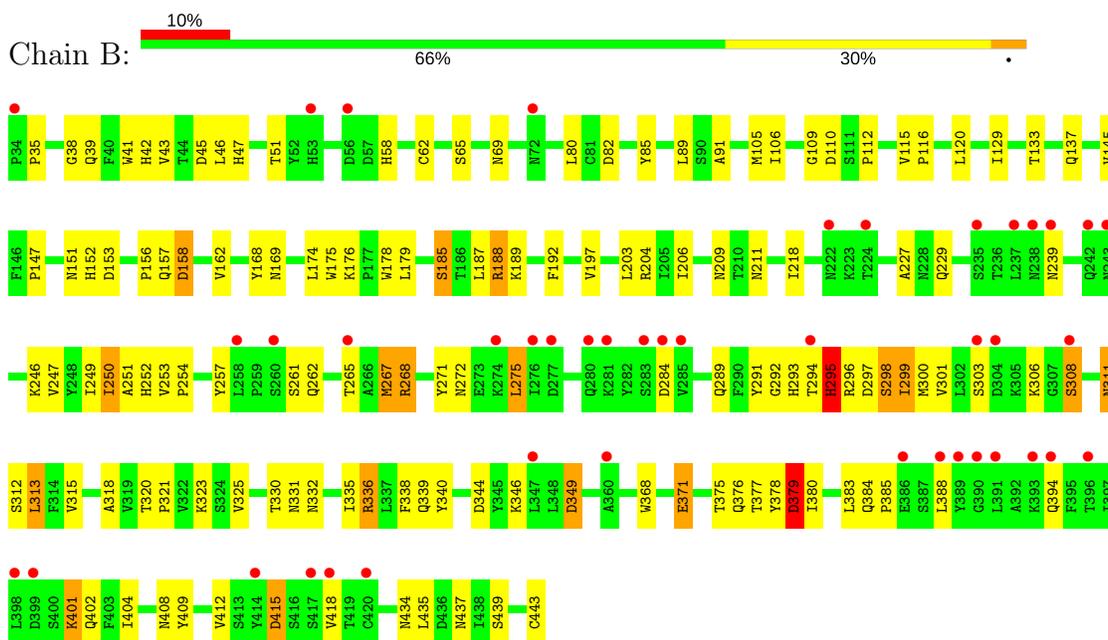
- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a
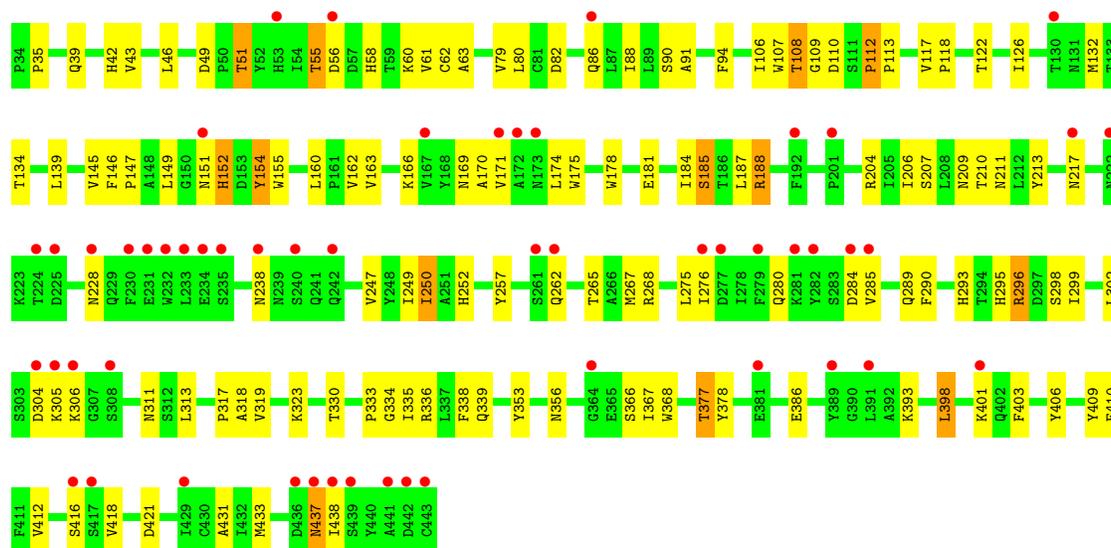
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.79Å 147.79Å 139.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.38 – 2.60 47.22 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.38-2.60) 99.4 (47.22-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.237 , 0.255 0.246 , 0.252	Depositor DCC
R_{free} test set	2658 reflections (5.15%)	DCC
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 61.7	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10414	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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 77.32 % 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 8.7055e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, ZN, MLI, NAG

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	0.96	0/3399	0.95	6/4641 (0.1%)
1	B	1.12	1/3430 (0.0%)	1.10	16/4684 (0.3%)
1	C	1.12	4/3416 (0.1%)	1.12	11/4663 (0.2%)
All	All	1.07	5/10245 (0.0%)	1.06	33/13988 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	GLY	C-O	-6.04	1.14	1.23
1	B	284	ASP	CB-CG	5.90	1.64	1.51
1	C	155	TRP	CB-CG	-5.57	1.40	1.50
1	C	154	TYR	CB-CG	5.19	1.59	1.51
1	C	152	HIS	C-O	-5.04	1.13	1.23

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	296	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	C	296	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	C	421	ASP	CB-CG-OD1	7.07	124.67	118.30
1	A	296	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	C	188	ARG	NE-CZ-NH1	6.62	123.61	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3302	0	3209	43	0
1	B	3327	0	3235	142	0
1	C	3319	0	3231	106	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	42	0	39	0	0
3	B	42	0	38	0	0
3	C	42	0	39	3	0
4	A	7	0	2	0	0
4	B	7	0	2	2	0
4	C	7	0	2	0	0
5	B	6	0	8	0	0
5	C	6	0	8	1	0
6	A	56	0	0	2	0
6	B	126	0	0	45	0
6	C	119	0	0	9	0
All	All	10414	0	9813	292	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 15.

The worst 5 of 292 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)
3:C:704:NAG:C1	3:C:704:NAG:C2	1.77	1.60
1:C:151:ASN:HD21	1:C:152:HIS:CD2	1.39	1.40
1:B:254:PRO:HB2	6:B:876:HOH:O	1.30	1.26
1:B:69:ASN:O	6:B:801:HOH:O	1.54	1.21
1:C:151:ASN:ND2	1:C:152:HIS:CD2	2.11	1.19

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	411/410 (100%)	387 (94%)	23 (6%)	1 (0%)	51	76
1	B	415/410 (101%)	385 (93%)	26 (6%)	4 (1%)	18	37
1	C	413/410 (101%)	380 (92%)	33 (8%)	0	100	100
All	All	1239/1230 (101%)	1152 (93%)	82 (7%)	5 (0%)	44	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	295	HIS
1	B	379[A]	ASP
1	B	379[B]	ASP
1	A	190	GLY
1	B	321	PRO

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	375/372 (101%)	361 (96%)	14 (4%)	39	66
1	B	379/372 (102%)	357 (94%)	22 (6%)	23	46
1	C	377/372 (101%)	350 (93%)	27 (7%)	17	33
All	All	1131/1116 (101%)	1068 (94%)	63 (6%)	26	48

5 of 63 residues with a non-rotameric sidechain are listed below:

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Mol	Chain	Res	Type
1	B	313	LEU
1	B	437	ASN
1	C	401	LYS
1	B	349	ASP
1	B	379[B]	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	200	ASN
1	B	263	ASN
1	C	332	ASN
1	B	211	ASN
1	B	229	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 ⓘ

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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
3	NAG	A	703	1	14,14,15	1.92	5 (35%)	15,19,21	1.39	2 (13%)
3	NAG	A	704	1	14,14,15	1.71	3 (21%)	15,19,21	1.23	1 (6%)
3	NAG	A	705	1	14,14,15	2.27	2 (14%)	15,19,21	3.48	9 (60%)
4	MLI	A	706	2	0,6,6	0.00	-	0,7,7	0.00	-
3	NAG	B	703	1	14,14,15	2.47	5 (35%)	15,19,21	1.34	2 (13%)
3	NAG	B	704	1	14,14,15	1.68	3 (21%)	15,19,21	1.61	3 (20%)
3	NAG	B	705	1	14,14,15	2.40	4 (28%)	15,19,21	2.32	6 (40%)
4	MLI	B	706	2	0,6,6	0.00	-	0,7,7	0.00	-
5	GOL	B	707	-	5,5,5	0.62	0	5,5,5	0.37	0
3	NAG	C	703	1	14,14,15	2.00	4 (28%)	15,19,21	1.58	3 (20%)
3	NAG	C	704	1	14,14,15	5.85	6 (42%)	15,19,21	2.86	8 (53%)
3	NAG	C	705	1	14,14,15	2.44	4 (28%)	15,19,21	2.34	7 (46%)
4	MLI	C	706	2	0,6,6	0.00	-	0,7,7	0.00	-
5	GOL	C	707	-	5,5,5	0.47	0	5,5,5	0.94	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
3	NAG	A	703	1	-	0/6/23/26	0/1/1/1
3	NAG	A	704	1	-	0/6/23/26	0/1/1/1
3	NAG	A	705	1	-	0/6/23/26	0/1/1/1
4	MLI	A	706	2	-	0/0/4/4	0/0/0/0
3	NAG	B	703	1	-	0/6/23/26	0/1/1/1
3	NAG	B	704	1	-	0/6/23/26	0/1/1/1
3	NAG	B	705	1	-	0/6/23/26	0/1/1/1
4	MLI	B	706	2	-	0/0/4/4	0/0/0/0
5	GOL	B	707	-	-	0/4/4/4	0/0/0/0
3	NAG	C	703	1	-	0/6/23/26	0/1/1/1
3	NAG	C	704	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	705	1	-	0/6/23/26	0/1/1/1
4	MLI	C	706	2	-	0/0/4/4	0/0/0/0
5	GOL	C	707	-	-	0/4/4/4	0/0/0/0

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	705	NAG	O3-C3	-4.74	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	705	NAG	O5-C5	2.04	1.47	1.43
3	A	703	NAG	O5-C1	2.22	1.47	1.43
3	C	703	NAG	O4-C4	2.22	1.48	1.43
3	B	703	NAG	C4-C5	2.29	1.57	1.53

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	705	NAG	O5-C1-C2	-4.50	105.22	111.47
3	A	705	NAG	O3-C3-C2	-4.25	100.28	109.39
3	B	705	NAG	C3-C4-C5	-3.97	103.22	110.22
3	C	703	NAG	C1-O5-C5	-3.66	107.12	112.17
3	A	705	NAG	O6-C6-C5	-3.36	100.02	111.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	704	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	706	MLI	2	0
3	C	704	NAG	3	0
5	C	707	GOL	1	0

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   (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	410/410 (100%)	-0.26	4 (0%)	82	79	3, 13, 32, 56	0
1	B	410/410 (100%)	0.73	43 (10%)	7	4	7, 23, 42, 60	0
1	C	410/410 (100%)	0.82	53 (12%)	4	2	7, 23, 43, 65	0
All	All	1230/1230 (100%)	0.43	100 (8%)	13	8	3, 20, 41, 65	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	283	SER	5.0
1	B	396	THR	5.0
1	B	56	ASP	4.8
1	B	277	ASP	4.8
1	B	284	ASP	4.6

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)

There are no carbohydrates in this entry.

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(Å^2)	Q<0.9
3	NAG	A	704	14/15	0.89	0.20	5.95	26,31,39,44	0
4	MLI	A	706	7/7	0.97	0.19	3.39	22,35,41,41	0
3	NAG	A	703	14/15	0.89	0.26	2.62	25,30,38,43	0
3	NAG	B	703	14/15	0.79	0.33	1.36	35,43,53,56	0
3	NAG	B	704	14/15	0.83	0.23	1.35	34,44,49,54	0
4	MLI	C	706	7/7	0.94	0.29	0.99	38,49,50,54	0
4	MLI	B	706	7/7	0.94	0.20	0.62	21,28,35,35	0
3	NAG	C	703	14/15	0.80	0.28	0.39	29,41,51,58	0
3	NAG	A	705	14/15	0.93	0.17	0.07	16,18,20,21	0
3	NAG	C	705	14/15	0.89	0.18	-0.46	22,24,27,27	0
2	ZN	A	702	1/1	0.99	0.13	-0.83	7,7,7,7	0
2	ZN	C	701	1/1	0.99	0.10	-1.19	13,13,13,13	0
2	ZN	C	702	1/1	0.94	0.08	-1.51	23,23,23,23	0
3	NAG	B	705	14/15	0.87	0.19	-2.48	31,33,35,36	0
2	ZN	B	702	1/1	0.99	0.05	-4.52	23,23,23,23	0
2	ZN	B	701	1/1	0.99	0.05	-4.81	19,19,19,19	0
2	ZN	A	701	1/1	1.00	0.11	-4.95	14,14,14,14	0
3	NAG	C	704	14/15	0.62	0.32	-	40,47,55,56	0
5	GOL	B	707	6/6	0.89	0.23	-	32,36,37,41	0
5	GOL	C	707	6/6	0.78	0.20	-	43,49,51,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.