



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:33 am GMT

PDB ID : 4Q4F
Title : Crystal structure of LIMP-2 (space group C2)
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Deposited on : 2014-04-14
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

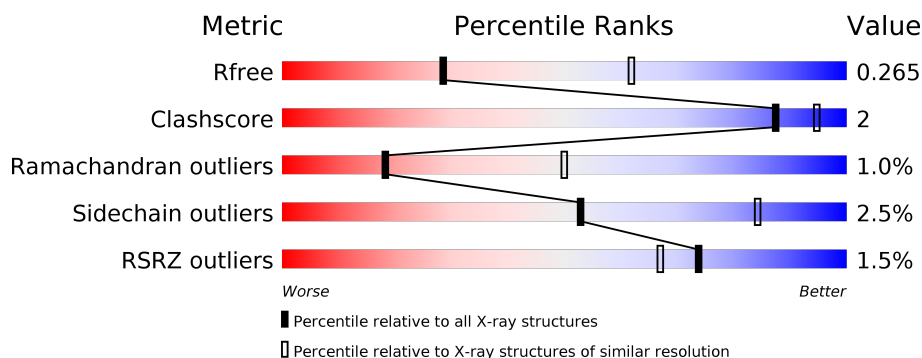
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	416	<div> <div></div> <div>86%</div> <div>8%</div> <div>5%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3568 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 Lysosome membrane protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3191	2059	517	603	12			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLU	-	EXPRESSION TAG	UNP Q14108
A	26	THR	-	EXPRESSION TAG	UNP Q14108
A	27	GLY	-	EXPRESSION TAG	UNP Q14108
A	433	GLY	-	EXPRESSION TAG	UNP Q14108
A	434	LYS	-	EXPRESSION TAG	UNP Q14108
A	435	HIS	-	EXPRESSION TAG	UNP Q14108
A	436	HIS	-	EXPRESSION TAG	UNP Q14108
A	437	HIS	-	EXPRESSION TAG	UNP Q14108
A	438	HIS	-	EXPRESSION TAG	UNP Q14108
A	439	HIS	-	EXPRESSION TAG	UNP Q14108
A	440	HIS	-	EXPRESSION TAG	UNP Q14108

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	6	Total	C	N	O	0	0
			72	40	2	30		
4	A	6	Total	C	N	O	0	0
			72	40	2	30		

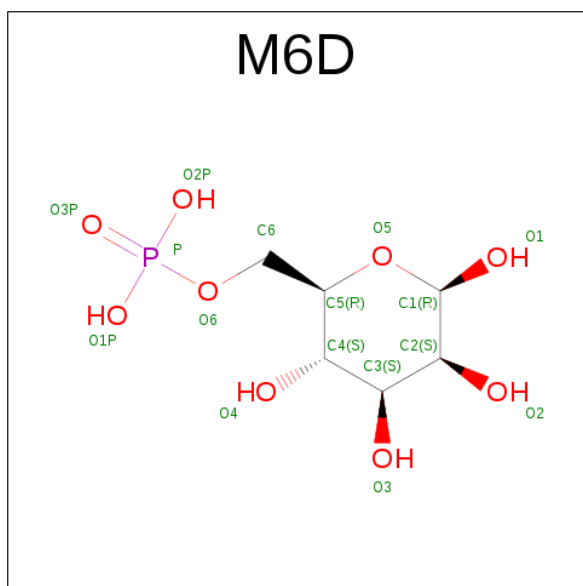
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is 6-O-PHOSPHONO-BETA-D-MANNOPYRANOSE (three-letter code: M6D) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			15	6	8	1		

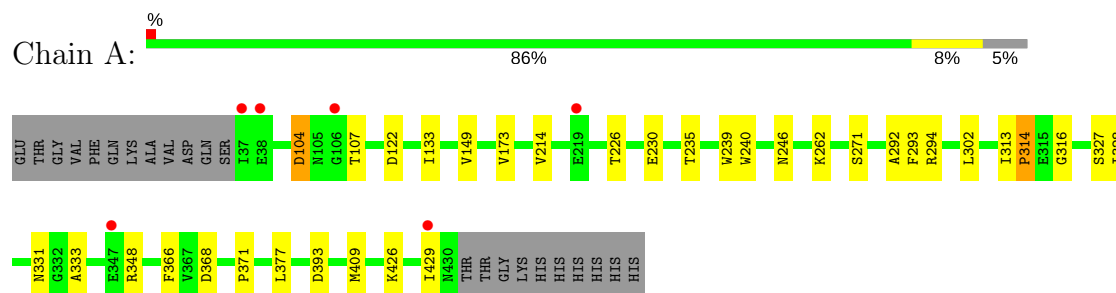
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lysosome membrane protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.69Å 63.39Å 114.38Å 90.00° 102.27° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.04 – 2.77	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-2.80) 93.9 (49.04-2.77)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.217 , 0.270 0.218 , 0.265	Depositor DCC
R_{free} test set	757 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3568	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, BMA, M6D, NAG, MAN

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	0.33	0/3274	0.53	0/4450

There are no bond length outliers.

There are no bond angle outliers.

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	3191	0	3096	17	0
2	A	28	0	26	0	0
3	A	122	0	104	0	0
4	A	144	0	121	0	0
5	A	39	0	34	0	0
6	A	28	0	25	1	0
7	A	15	0	9	0	0
8	A	1	0	0	0	0
All	All	3568	0	3415	17	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 2.

All (17) 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:104:ASP:HB2	1:A:107:THR:HG22	1.77	0.64
1:A:292:ALA:HB2	1:A:377:LEU:HD12	1.85	0.59
1:A:426:LYS:O	1:A:429:ILE:HG22	2.03	0.58
1:A:294:ARG:NE	1:A:368:ASP:OD1	2.34	0.56
1:A:149:VAL:O	1:A:149:VAL:HG12	2.07	0.55
1:A:104:ASP:HB2	1:A:107:THR:CG2	2.37	0.54
1:A:348:ARG:NH2	6:A:517:NAG:H81	2.25	0.52
1:A:313:ILE:HG23	1:A:314:PRO:HA	1.92	0.51
1:A:293:PHE:CE2	1:A:371:PRO:HB3	2.47	0.50
1:A:240:TRP:O	1:A:246:ASN:ND2	2.43	0.49
1:A:327:SER:HA	1:A:333:ALA:O	2.14	0.48
1:A:230:GLU:HG2	1:A:235:THR:HG22	1.97	0.46
1:A:214:VAL:HG12	1:A:230:GLU:HB2	1.98	0.45
1:A:133:ILE:HD13	1:A:173:VAL:CG2	2.48	0.44
1:A:294:ARG:HD2	1:A:366:PHE:HB2	2.02	0.42
1:A:133:ILE:HD13	1:A:173:VAL:HG22	2.00	0.42
1:A:313:ILE:CG2	1:A:314:PRO:HA	2.50	0.41

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	392/416 (94%)	367 (94%)	21 (5%)	4 (1%)	18	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	THR
1	A	316	GLY
1	A	262	LYS

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Mol	Chain	Res	Type
1	A	314	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	355/374 (95%)	346 (98%)	9 (2%)	53 84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ASP
1	A	122	ASP
1	A	239	TRP
1	A	271	SER
1	A	302	LEU
1	A	328	ILE
1	A	331	ASN
1	A	393	ASP
1	A	409	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	257	HIS
1	A	331	ASN
1	A	360	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 ⓘ

27 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	502	1,3	14,14,15	0.63	0	15,19,21	1.16	1 (6%)
3	NAG	A	503	3	14,14,15	0.67	0	15,19,21	0.94	1 (6%)
3	BMA	A	504	3	11,11,12	0.41	0	13,15,17	1.50	3 (23%)
3	MAN	A	505	3	11,11,12	0.58	0	13,15,17	1.15	1 (7%)
3	MAN	A	506	3	11,11,12	0.71	0	13,15,17	1.14	1 (7%)
4	NAG	A	507	1,4	14,14,15	0.51	0	15,19,21	0.61	0
4	NAG	A	508	4	14,14,15	0.58	0	15,19,21	0.66	0
4	BMA	A	509	4	11,11,12	0.33	0	13,15,17	0.55	0
4	MAN	A	510	4	11,11,12	0.52	0	13,15,17	0.95	1 (7%)
4	MAN	A	511	4	11,11,12	0.79	0	13,15,17	1.58	1 (7%)
4	MAN	A	512	4	11,11,12	0.55	0	13,15,17	0.94	1 (7%)
5	NAG	A	514	1,5	14,14,15	0.34	0	15,19,21	2.48	3 (20%)
5	NAG	A	515	5	14,14,15	0.35	0	15,19,21	2.01	4 (26%)
5	BMA	A	516	5	11,11,12	0.36	0	13,15,17	1.04	1 (7%)
6	NAG	A	517	1,6	14,14,15	0.67	0	15,19,21	1.20	1 (6%)
6	NAG	A	518	6	14,14,15	0.48	0	15,19,21	0.99	0
4	NAG	A	519	1,4	14,14,15	0.65	0	15,19,21	1.00	0
4	NAG	A	520	4	14,14,15	0.45	0	15,19,21	1.24	2 (13%)
4	BMA	A	521	4	11,11,12	0.37	0	13,15,17	0.95	0
4	MAN	A	522	4	11,11,12	0.64	0	13,15,17	0.65	0
4	MAN	A	523	4,7	11,11,12	0.54	0	13,15,17	1.41	3 (23%)
4	MAN	A	524	4	11,11,12	0.84	0	13,15,17	2.14	3 (23%)
3	NAG	A	526	1,3	14,14,15	0.46	0	15,19,21	2.07	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	527	3	14,14,15	0.52	0	15,19,21	0.97	1 (6%)
3	BMA	A	528	3	11,11,12	0.55	0	13,15,17	1.98	3 (23%)
3	MAN	A	529	3	11,11,12	0.59	0	13,15,17	0.80	1 (7%)
3	MAN	A	530	3	11,11,12	0.57	0	13,15,17	0.56	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	502	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	503	3	-	0/6/23/26	0/1/1/1
3	BMA	A	504	3	-	0/2/19/22	0/1/1/1
3	MAN	A	505	3	-	0/2/19/22	0/1/1/1
3	MAN	A	506	3	-	0/2/19/22	0/1/1/1
4	NAG	A	507	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	508	4	-	0/6/23/26	0/1/1/1
4	BMA	A	509	4	-	0/2/19/22	0/1/1/1
4	MAN	A	510	4	-	0/2/19/22	0/1/1/1
4	MAN	A	511	4	-	0/2/19/22	0/1/1/1
4	MAN	A	512	4	-	0/2/19/22	0/1/1/1
5	NAG	A	514	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	515	5	-	0/6/23/26	0/1/1/1
5	BMA	A	516	5	-	0/2/19/22	0/1/1/1
6	NAG	A	517	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	518	6	-	0/6/23/26	0/1/1/1
4	NAG	A	519	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	520	4	-	0/6/23/26	0/1/1/1
4	BMA	A	521	4	-	0/2/19/22	0/1/1/1
4	MAN	A	522	4	-	0/2/19/22	0/1/1/1
4	MAN	A	523	4,7	-	0/2/19/22	0/1/1/1
4	MAN	A	524	4	-	0/2/19/22	0/1/1/1
3	NAG	A	526	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	527	3	-	0/6/23/26	0/1/1/1
3	BMA	A	528	3	-	0/2/19/22	0/1/1/1
3	MAN	A	529	3	-	0/2/19/22	0/1/1/1
3	MAN	A	530	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	526	NAG	C4-C3-C2	-4.75	104.06	111.02
3	A	528	BMA	O5-C1-C2	-4.40	103.90	110.79
5	A	515	NAG	C4-C3-C2	-4.16	104.92	111.02
3	A	526	NAG	O5-C1-C2	-4.09	105.78	111.47
3	A	502	NAG	O5-C1-C2	-2.77	107.61	111.47
3	A	503	NAG	O7-C7-C8	-2.54	117.43	122.06
3	A	504	BMA	O3-C3-C4	-2.35	105.24	110.36
5	A	516	BMA	O5-C1-C2	-2.34	107.12	110.79
5	A	514	NAG	O4-C4-C3	-2.27	105.43	110.36
4	A	523	MAN	O5-C1-C2	-2.22	107.32	110.79
3	A	527	NAG	O5-C1-C2	-2.03	108.64	111.47
3	A	526	NAG	C2-N2-C7	2.04	125.91	122.94
4	A	523	MAN	C1-O5-C5	2.04	114.98	112.17
4	A	520	NAG	C3-C4-C5	2.07	113.87	110.22
3	A	529	MAN	C1-O5-C5	2.15	115.12	112.17
4	A	524	MAN	C2-C3-C4	2.19	114.70	110.88
5	A	515	NAG	C1-C2-N2	2.20	114.24	110.49
3	A	504	BMA	C3-C4-C5	2.24	114.17	110.22
3	A	528	BMA	C2-C3-C4	2.34	114.96	110.88
4	A	512	MAN	C1-O5-C5	2.34	115.39	112.17
5	A	514	NAG	O5-C1-C2	2.59	115.08	111.47
4	A	524	MAN	O5-C1-C2	2.76	115.12	110.79
3	A	526	NAG	C1-O5-C5	2.84	116.07	112.17
4	A	510	MAN	C1-O5-C5	2.87	116.12	112.17
4	A	523	MAN	C3-C4-C5	3.00	115.51	110.22
3	A	506	MAN	C1-C2-C3	3.01	113.47	109.65
3	A	505	MAN	C1-O5-C5	3.23	116.62	112.17
3	A	504	BMA	C1-C2-C3	3.32	113.86	109.65
6	A	517	NAG	C4-C3-C2	3.33	115.89	111.02
4	A	520	NAG	C1-O5-C5	3.43	116.89	112.17
5	A	515	NAG	O4-C4-C5	3.57	118.28	109.28
5	A	515	NAG	C1-O5-C5	3.58	117.10	112.17
3	A	528	BMA	C3-C4-C5	4.11	117.46	110.22
4	A	511	MAN	C1-C2-C3	4.34	115.16	109.65
4	A	524	MAN	C1-C2-C3	6.49	117.88	109.65
5	A	514	NAG	C1-O5-C5	8.69	124.14	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	517	NAG	1	0

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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$
2	NAG	A	501	1	14,14,15	0.48	0	15,19,21	1.03	1 (6%)
2	NAG	A	513	1	14,14,15	0.52	0	15,19,21	1.12	1 (6%)
7	M6D	A	525	4	15,15,16	0.42	0	21,22,24	1.22	1 (4%)

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	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	513	1	-	0/6/23/26	0/1/1/1
7	M6D	A	525	4	-	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	501	NAG	C1-O5-C5	2.78	116.00	112.17
2	A	513	NAG	C1-O5-C5	3.54	117.05	112.17
7	A	525	M6D	C1-O5-C5	4.35	118.16	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	394/416 (94%)	-0.07	6 (1%) 74 67	47, 67, 107, 135	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	GLY	4.5
1	A	38	GLU	3.1
1	A	37	ILE	3.0
1	A	429	ILE	2.6
1	A	219	GLU	2.5
1	A	347	GLU	2.3

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	526	14/15	0.94	0.20	1.83	63,65,68,72	0
5	NAG	A	514	14/15	0.95	0.18	0.71	86,92,96,99	0
6	NAG	A	517	14/15	0.77	0.21	0.16	92,102,109,114	0
4	MAN	A	523	11/12	0.92	0.16	-0.42	107,110,114,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	507	14/15	0.96	0.17	-0.80	61,70,78,79	0
4	NAG	A	519	14/15	0.96	0.17	-0.93	56,59,64,65	0
3	NAG	A	502	14/15	0.96	0.14	-1.23	52,54,56,58	0
4	NAG	A	520	14/15	0.92	0.16	-1.34	66,70,75,80	0
3	NAG	A	527	14/15	0.96	0.12	-2.18	59,65,69,75	0
4	MAN	A	522	11/12	0.91	0.22	-	88,94,97,102	0
3	MAN	A	506	11/12	0.85	0.16	-	92,94,100,103	0
5	NAG	A	515	14/15	0.88	0.12	-	103,106,112,112	0
3	BMA	A	504	11/12	0.94	0.10	-	75,83,87,88	0
6	NAG	A	518	14/15	0.80	0.29	-	108,118,124,126	0
3	BMA	A	528	11/12	0.88	0.12	-	79,86,93,102	0
4	BMA	A	521	11/12	0.84	0.15	-	84,86,92,97	0
5	BMA	A	516	11/12	0.81	0.16	-	113,115,118,119	0
4	NAG	A	508	14/15	0.91	0.18	-	85,87,94,98	0
3	MAN	A	505	11/12	0.91	0.16	-	92,94,97,97	0
4	MAN	A	512	11/12	0.89	0.18	-	124,125,130,132	0
4	MAN	A	511	11/12	0.90	0.18	-	115,120,125,126	0
4	MAN	A	510	11/12	0.88	0.18	-	100,105,107,109	0
4	BMA	A	509	11/12	0.88	0.13	-	100,103,106,111	0
3	MAN	A	529	11/12	0.93	0.15	-	83,89,92,93	0
3	MAN	A	530	11/12	0.69	0.30	-	107,111,113,118	0
4	MAN	A	524	11/12	0.88	0.16	-	97,103,109,110	0
3	NAG	A	503	14/15	0.96	0.13	-	54,59,65,70	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(\AA^2)	Q<0.9
7	M6D	A	525	15/16	0.86	0.17	-1.28	119,125,141,143	0
8	CL	A	531	1/1	0.96	0.17	-	62,62,62,62	0
2	NAG	A	501	14/15	0.75	0.31	-	113,122,125,125	0
2	NAG	A	513	14/15	0.77	0.39	-	114,119,120,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.