



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 01:31 PM BST

PDB ID : 5LGD
Title : The CIDRa domain from MCvar1 PfEMP1 bound to CD36
Authors : Hsieh, F.L.; Higgins, M.K.
Deposited on : 2016-07-06
Resolution : 2.07 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

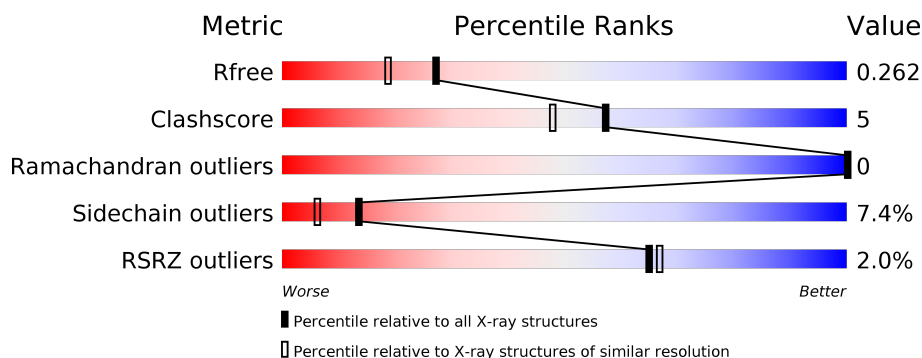
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 respectively. 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	472	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 70%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 70% 14% • 15% </div> </div>
2	B	179	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 10%, green 72%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 3% 72% 10% • 16% </div> </div>
3	C	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 33%, yellow 67%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 33% 67% </div> </div>

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
5	PLM	A	512	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4875 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 Platelet glycoprotein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3218	2071	533	602	12			

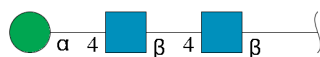
- Molecule 2 is a protein called PfEMP1 variant 1 of strain MC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	151	Total	C	N	O	S	0	2	0
			1272	805	220	237	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	626	SER	CYS	conflict	UNP Q25733

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



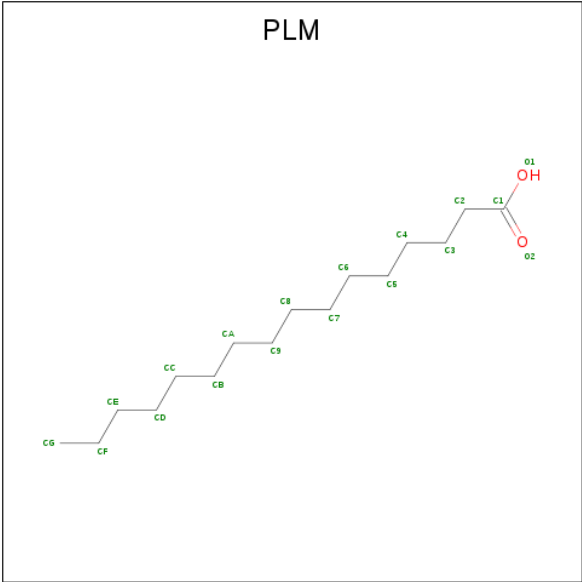
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



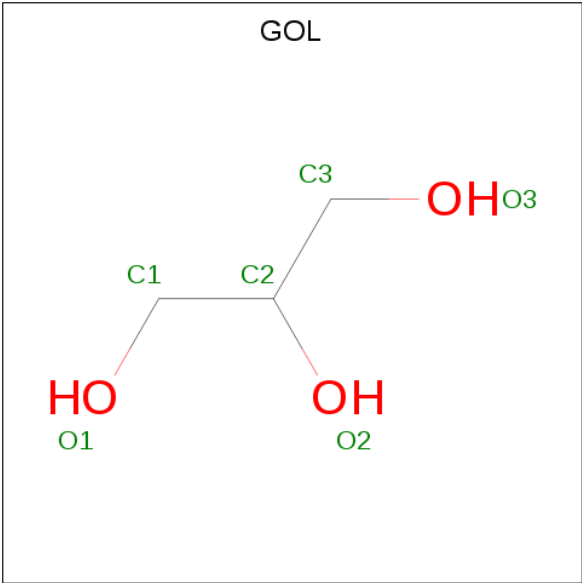
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			18	16	2		
5	A	1	Total	C	O	0	0
			18	16	2		

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



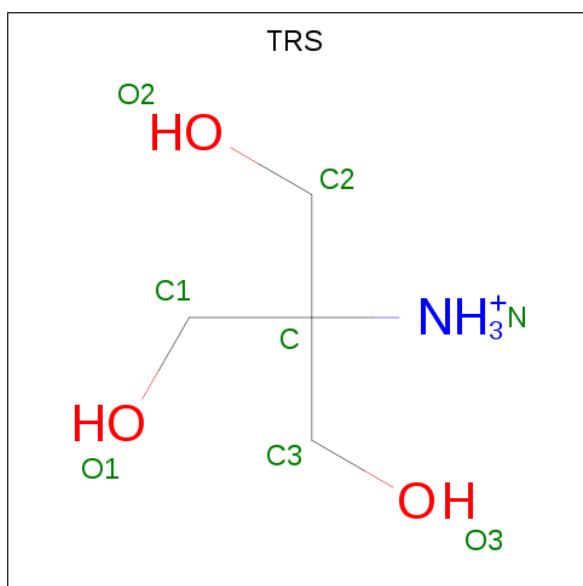
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		

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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	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	B	1	Total	C	N	O	0	0
			8	4	1	3		

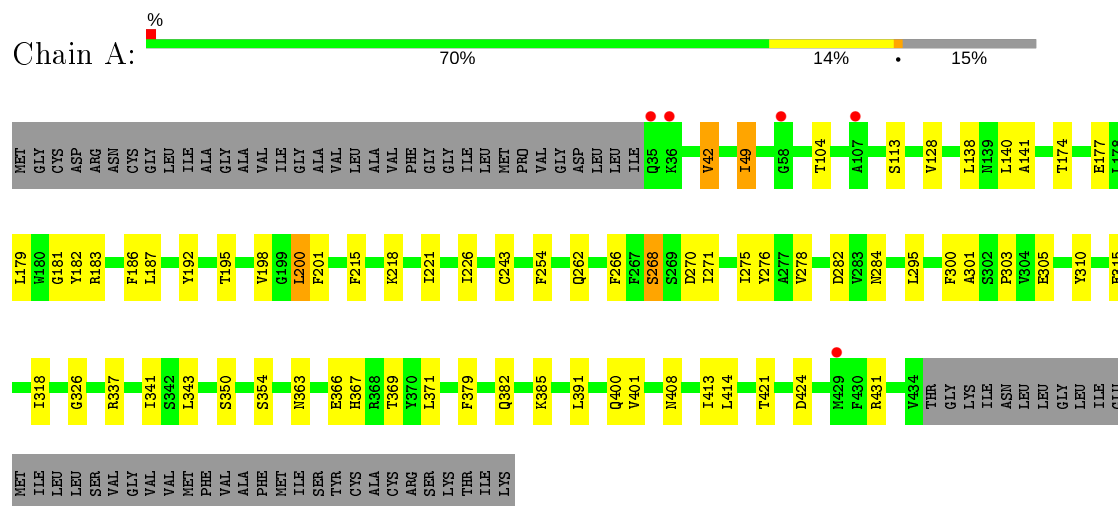
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	119	Total	O	0	0
			119	119		
8	B	33	Total	O	0	0
			33	33		

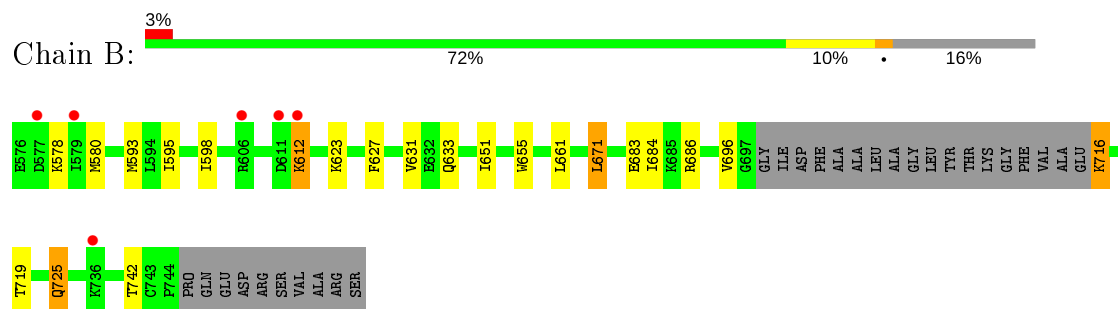
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Platelet glycoprotein 4



• Molecule 2: PfEMP1 variant 1 of strain MC



• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	129.83 Å 40.73 Å 138.84 Å 90.00° 114.85° 90.00°	Depositor
Resolution (Å)	62.99 – 2.07 58.90 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.2 (62.99-2.07) 99.3 (58.90-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.07 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.212 , 0.253 0.219 , 0.262	Depositor DCC
R_{free} test set	2057 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4875	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, TRS, MAN, NAG, PLM

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	0.53	0/3296	0.73	0/4478
2	B	0.52	0/1300	0.68	0/1741
All	All	0.53	0/4596	0.72	0/6219

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

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	3218	0	3180	38	0
2	B	1272	0	1257	9	0
3	C	39	0	34	0	0
4	A	112	0	104	1	0
5	A	36	0	62	10	0
6	A	24	0	32	1	0
6	B	6	0	8	0	0
7	A	8	0	12	2	0
7	B	8	0	12	0	0
8	A	119	0	0	1	0
8	B	33	0	0	1	0
All	All	4875	0	4701	46	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 5.

All (46) 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:337:ARG:HD3	5:A:512:PLM:H31	1.70	0.74
1:A:141:ALA:HA	5:A:512:PLM:H42	1.70	0.73
2:B:716:LYS:HA	2:B:725:GLN:HE22	1.61	0.66
2:B:595:ILE:HD11	2:B:683:GLU:HG3	1.79	0.65
1:A:42:VAL:HG12	1:A:221:ILE:HD11	1.81	0.63
2:B:598:ILE:HG21	2:B:686[A]:ARG:HE	1.64	0.62
1:A:198:VAL:HG11	5:A:512:PLM:H41	1.85	0.58
1:A:266:PHE:HZ	1:A:295:LEU:HD11	1.67	0.57
1:A:301:ALA:HB1	1:A:305:GLU:HB2	1.87	0.57
2:B:612:LYS:HE3	2:B:612:LYS:H	1.70	0.57
1:A:363:ASN:H	1:A:367:HIS:HD2	1.52	0.56
1:A:187:LEU:HD11	5:A:512:PLM:H21	1.86	0.56
1:A:408:ASN:HB2	7:A:518:TRS:H21	1.87	0.55
1:A:303:PRO:HG3	1:A:310:TYR:HA	1.89	0.54
1:A:201:PHE:HE1	5:A:512:PLM:HG3	1.71	0.54
1:A:382:GLN:HE21	1:A:421:THR:HB	1.75	0.52
1:A:104:THR:HG23	1:A:113:SER:HB2	1.92	0.51
1:A:181:GLY:HA2	1:A:198:VAL:O	2.11	0.50
1:A:243:CYS:HA	4:A:504:NAG:H83	1.93	0.50
1:A:49:ILE:HD11	1:A:379:PHE:HE2	1.76	0.50
1:A:200:LEU:HD23	1:A:414:LEU:HD21	1.95	0.49
1:A:182:TYR:CZ	1:A:198:VAL:HG23	2.49	0.48
1:A:200:LEU:HD23	1:A:414:LEU:CD2	2.45	0.46
1:A:192:TYR:HB3	2:B:655:TRP:CD2	2.51	0.46
2:B:627:PHE:O	2:B:631:VAL:HG23	2.16	0.46
1:A:363:ASN:HB3	1:A:366:GLU:HB3	1.99	0.45
1:A:198:VAL:CG1	5:A:512:PLM:H41	2.46	0.44
1:A:337:ARG:CD	5:A:512:PLM:H31	2.43	0.44
1:A:215:PHE:HB3	8:A:632:HOH:O	2.17	0.44
1:A:270:ASP:O	5:A:512:PLM:HF2	2.18	0.44
1:A:363:ASN:H	1:A:367:HIS:CD2	2.35	0.43
1:A:271:ILE:HG22	1:A:341:ILE:HG21	2.00	0.43
1:A:337:ARG:HD2	5:A:512:PLM:H52	2.01	0.43
1:A:200:LEU:HD21	1:A:413:ILE:HG21	2.00	0.43
1:A:300:PHE:HB3	1:A:326:GLY:HA2	2.01	0.43
2:B:696:VAL:HG11	2:B:719:THR:HG23	2.01	0.42
1:A:254:PHE:HD1	6:A:517:GOL:H32	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:671:LEU:HG	2:B:684:ILE:HG23	2.02	0.42
2:B:580:MET:HB2	8:B:916:HOH:O	2.19	0.42
1:A:318:ILE:HG23	7:A:518:TRS:H22	2.01	0.41
1:A:140:LEU:HB3	5:A:512:PLM:H51	2.03	0.41
1:A:268:SER:HB3	1:A:271:ILE:HG12	2.03	0.41
1:A:369:THR:HG23	1:A:385:LYS:HA	2.02	0.41
1:A:275:ILE:HG12	1:A:276:TYR:H	1.86	0.41
1:A:174:THR:OG1	1:A:177:GLU:HG3	2.21	0.40
1:A:200:LEU:HD21	1:A:413:ILE:CG2	2.51	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	398/472 (84%)	385 (97%)	13 (3%)	0	100	100
2	B	149/179 (83%)	146 (98%)	3 (2%)	0	100	100
All	All	547/651 (84%)	531 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	363/419 (87%)	337 (93%)	26 (7%)	14	7
2	B	141/159 (89%)	130 (92%)	11 (8%)	12	5
All	All	504/578 (87%)	467 (93%)	37 (7%)	13	6

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	49	ILE
1	A	128	VAL
1	A	138	LEU
1	A	179	LEU
1	A	183	ARG
1	A	186	PHE
1	A	195	THR
1	A	200	LEU
1	A	218	LYS
1	A	226	ILE
1	A	262	GLN
1	A	268	SER
1	A	278	VAL
1	A	282	ASP
1	A	284	ASN
1	A	315	GLU
1	A	343	LEU
1	A	350	SER
1	A	354	SER
1	A	371	LEU
1	A	391	LEU
1	A	400	GLN
1	A	401	VAL
1	A	424	ASP
1	A	431	ARG
2	B	578	LYS
2	B	593	MET
2	B	612	LYS
2	B	623	LYS
2	B	633	GLN
2	B	651	ILE
2	B	661	LEU
2	B	671	LEU
2	B	716	LYS

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Mol	Chain	Res	Type
2	B	725	GLN
2	B	742	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	HIS
1	A	382	GLN
2	B	693	GLN
2	B	725	GLN
2	B	726	HIS

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 ⓘ

3 monosaccharides 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	C	1	1,3	14,14,15	0.34	0	17,19,21	0.85	0
3	NAG	C	2	3	14,14,15	0.34	0	17,19,21	1.06	1 (5%)
3	MAN	C	3	3	11,11,12	0.49	0	15,15,17	2.12	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	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	MAN	C	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	MAN	C1-O5-C5	7.60	122.50	112.19
3	C	2	NAG	C1-O5-C5	3.74	117.25	112.19

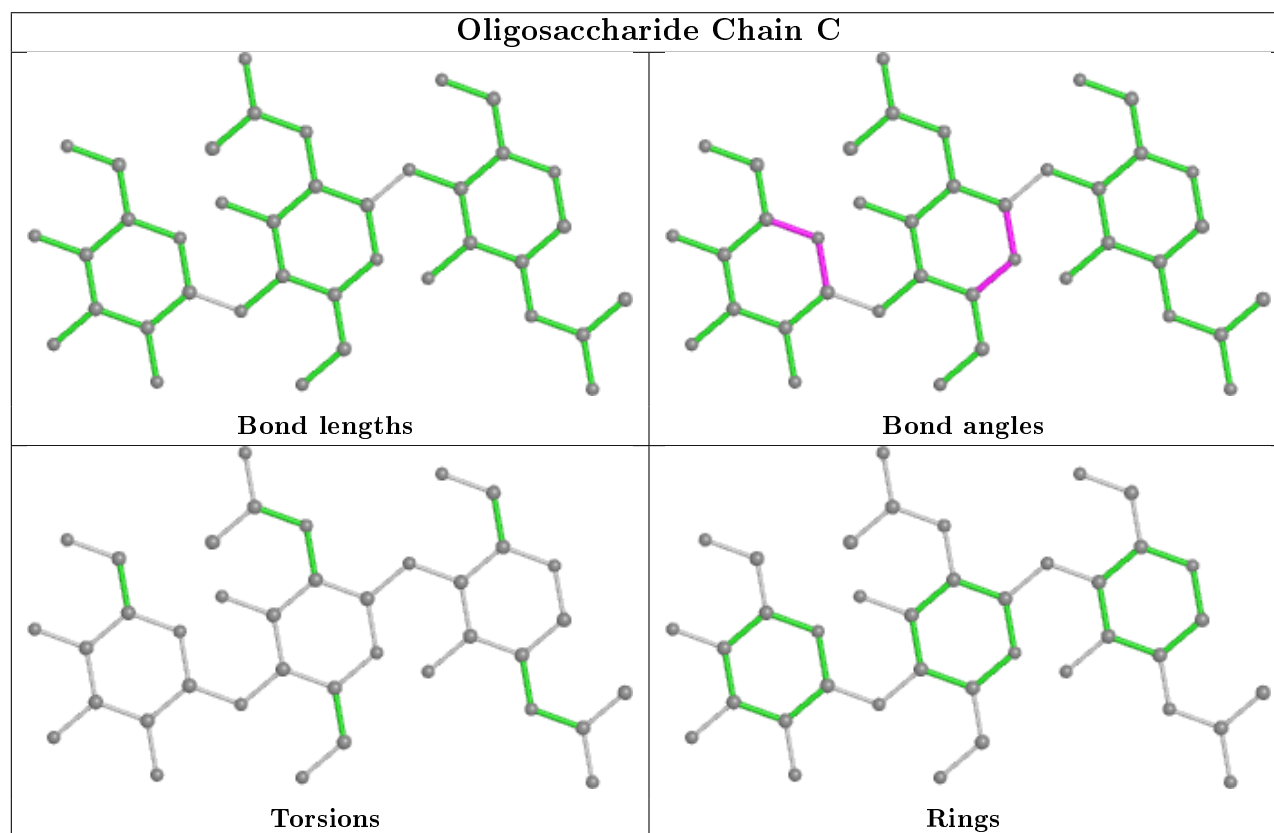
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry

17 ligands 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$
4	NAG	A	505	1	14,14,15	0.32	0	17,19,21	1.26	1 (5%)
5	PLM	A	513	-	14,17,17	0.17	0	13,17,17	0.49	0
4	NAG	A	509	1	14,14,15	0.31	0	17,19,21	1.14	1 (5%)
5	PLM	A	512	-	14,17,17	0.58	0	13,17,17	0.59	0
4	NAG	A	511	1	14,14,15	0.34	0	17,19,21	0.59	0
4	NAG	A	504	1	14,14,15	0.30	0	17,19,21	0.74	0
6	GOL	A	517	-	5,5,5	0.07	0	5,5,5	0.14	0
4	NAG	A	508	1	14,14,15	0.27	0	17,19,21	0.92	1 (5%)
4	NAG	A	510	1	14,14,15	0.32	0	17,19,21	0.78	1 (5%)
4	NAG	A	506	1	14,14,15	0.33	0	17,19,21	0.72	0
6	GOL	A	516	-	5,5,5	0.08	0	5,5,5	0.27	0
6	GOL	A	514	-	5,5,5	0.09	0	5,5,5	0.22	0
6	GOL	B	801	-	5,5,5	0.08	0	5,5,5	0.49	0
6	GOL	A	515	-	5,5,5	0.17	0	5,5,5	0.25	0
7	TRS	A	518	-	7,7,7	0.21	0	9,9,9	0.26	0
7	TRS	B	802	-	7,7,7	0.18	0	9,9,9	0.17	0
4	NAG	A	507	1	14,14,15	0.28	0	17,19,21	0.69	1 (5%)

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
4	NAG	A	505	1	-	3/6/23/26	0/1/1/1
5	PLM	A	513	-	-	5/13/15/15	-
4	NAG	A	509	1	-	2/6/23/26	0/1/1/1
5	PLM	A	512	-	-	5/13/15/15	-
4	NAG	A	511	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	504	1	-	0/6/23/26	0/1/1/1
6	GOL	A	517	-	-	0/4/4/4	-
4	NAG	A	508	1	-	0/6/23/26	0/1/1/1
4	NAG	A	510	1	-	0/6/23/26	0/1/1/1
4	NAG	A	506	1	-	0/6/23/26	0/1/1/1
6	GOL	A	516	-	-	0/4/4/4	-
6	GOL	A	514	-	-	1/4/4/4	-
6	GOL	B	801	-	-	3/4/4/4	-
6	GOL	A	515	-	-	2/4/4/4	-
7	TRS	A	518	-	-	0/9/9/9	-
7	TRS	B	802	-	-	0/9/9/9	-
4	NAG	A	507	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	NAG	C1-O5-C5	4.73	118.60	112.19
4	A	509	NAG	O5-C1-C2	3.66	117.07	111.29
4	A	508	NAG	C1-O5-C5	3.20	116.53	112.19
4	A	510	NAG	C1-O5-C5	2.76	115.94	112.19
4	A	507	NAG	O5-C1-C2	-2.00	108.13	111.29

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	NAG	C4-C5-C6-O6
4	A	505	NAG	O5-C5-C6-O6
4	A	509	NAG	O5-C5-C6-O6
5	A	512	PLM	C5-C6-C7-C8
6	B	801	GOL	O1-C1-C2-C3
5	A	513	PLM	C4-C5-C6-C7
5	A	513	PLM	C2-C3-C4-C5
5	A	512	PLM	C2-C3-C4-C5
5	A	513	PLM	CC-CD-CE-CF
5	A	512	PLM	CD-CE-CF-CG
6	A	515	GOL	O2-C2-C3-O3
4	A	509	NAG	C4-C5-C6-O6
6	B	801	GOL	O2-C2-C3-O3
5	A	512	PLM	C1-C2-C3-C4

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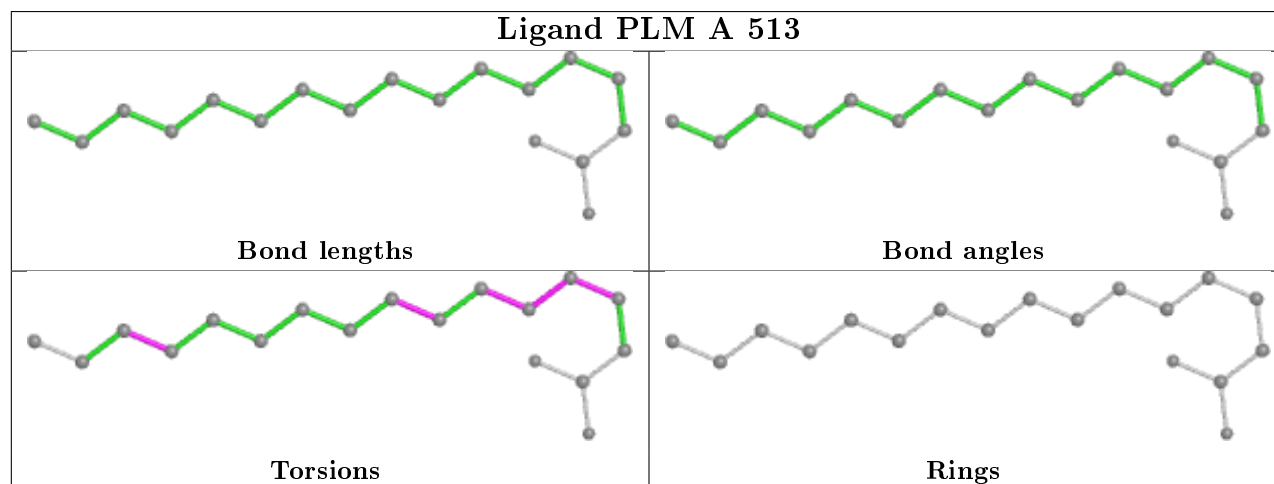
Mol	Chain	Res	Type	Atoms
5	A	513	PLM	C3-C4-C5-C6
5	A	512	PLM	C7-C8-C9-CA
4	A	505	NAG	C8-C7-N2-C2
5	A	513	PLM	C6-C7-C8-C9
6	A	514	GOL	O1-C1-C2-C3
6	B	801	GOL	C1-C2-C3-O3
6	A	515	GOL	C1-C2-C3-O3

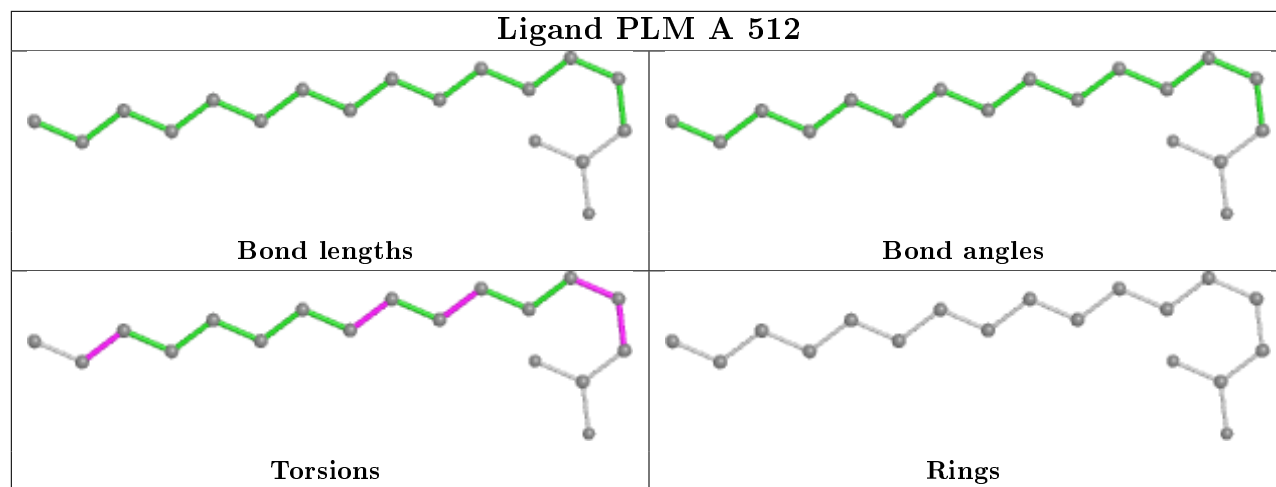
There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	512	PLM	10	0
4	A	504	NAG	1	0
6	A	517	GOL	1	0
7	A	518	TRS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	400/472 (84%)	-0.12	5 (1%) 77 78	25, 42, 72, 105	0
2	B	151/179 (84%)	0.17	6 (3%) 38 40	29, 51, 94, 115	0
All	All	551/651 (84%)	-0.04	11 (1%) 65 67	25, 44, 81, 115	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	579	ILE	4.8
2	B	612	LYS	4.5
1	A	35	GLN	3.7
1	A	36	LYS	3.1
1	A	58	GLY	2.6
2	B	736	LYS	2.5
2	B	606	ARG	2.5
2	B	611	ASP	2.3
1	A	107	ALA	2.2
1	A	429	MET	2.2
2	B	577	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

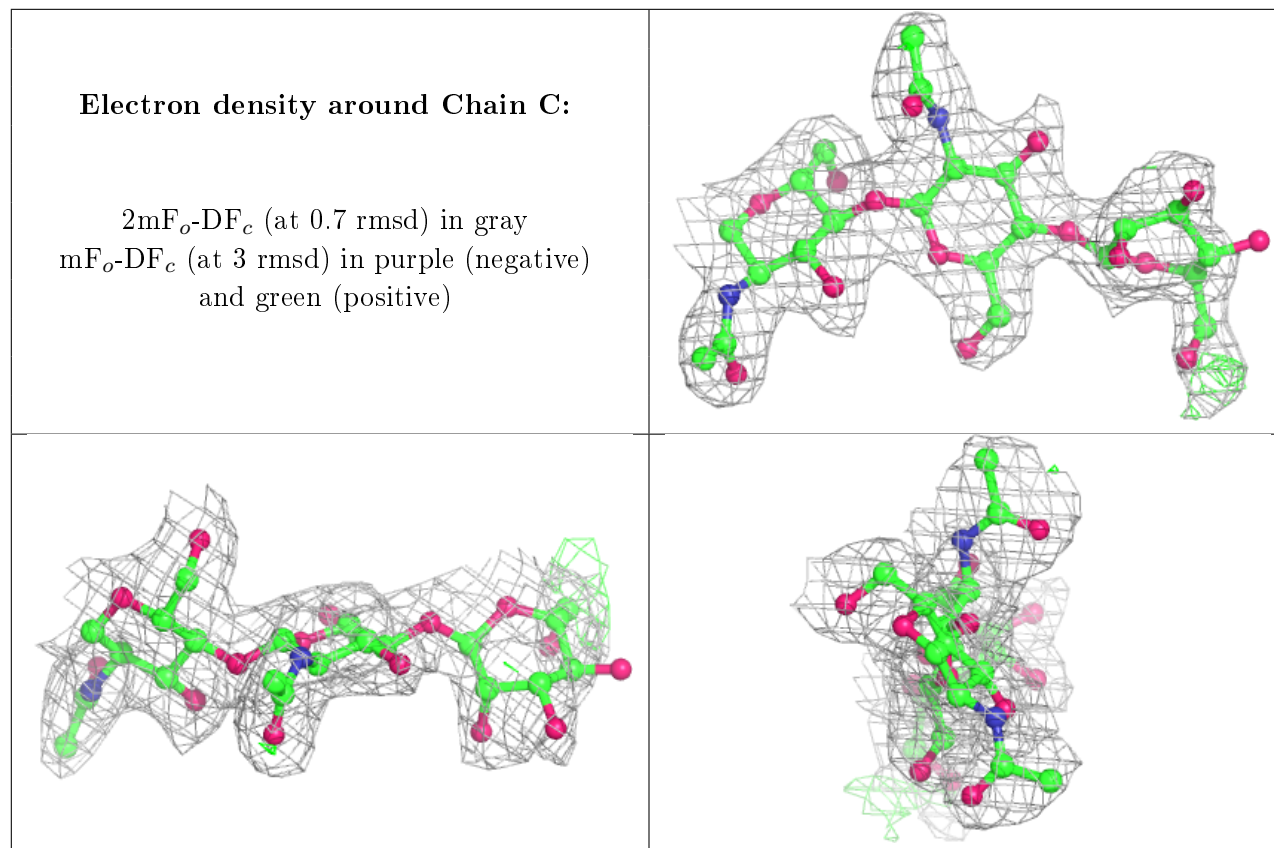
There are no non-standard protein/DNA/RNA residues in this entry.

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. 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	B-factors(\AA^2)	Q<0.9
3	MAN	C	3	11/12	0.79	0.14	78,87,90,95	0
3	NAG	C	2	14/15	0.92	0.10	47,55,62,70	0
3	NAG	C	1	14/15	0.95	0.09	39,42,46,50	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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. 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.

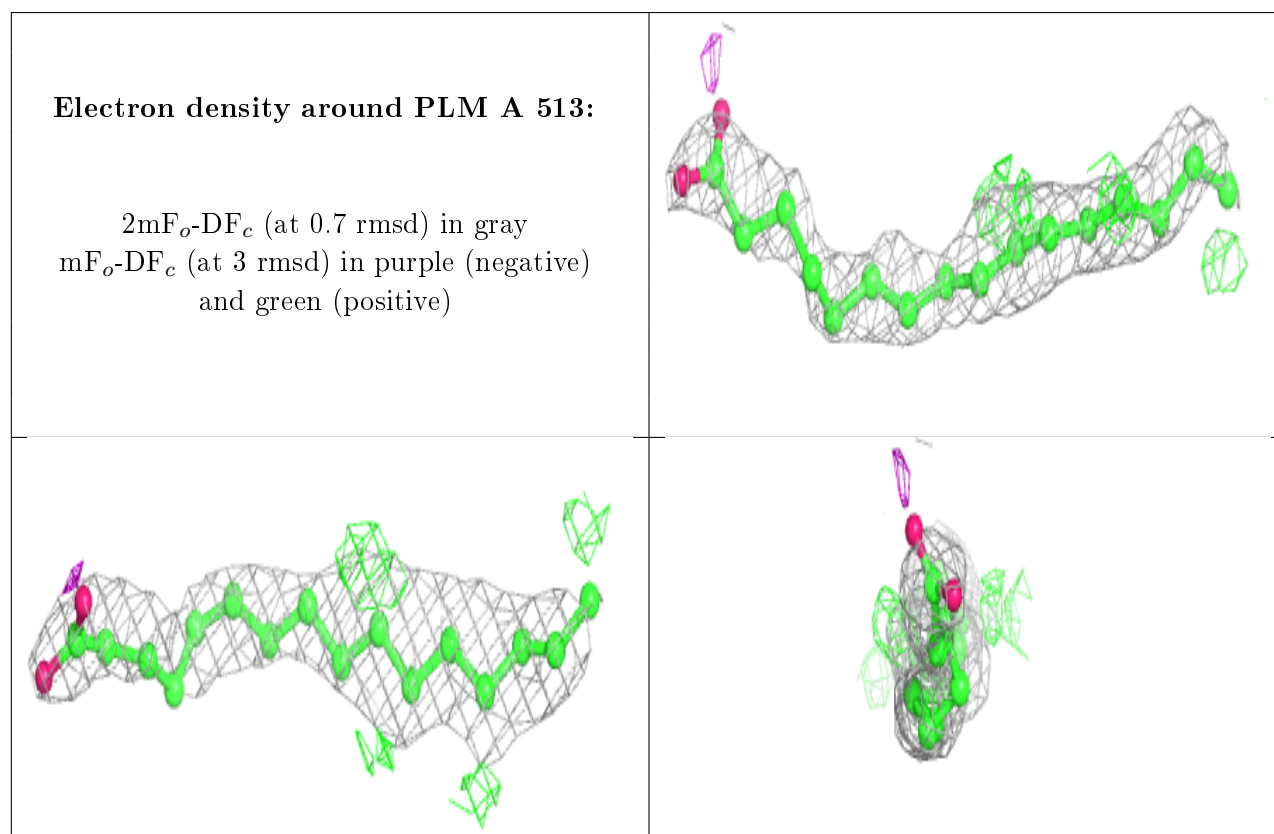
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	509	14/15	0.67	0.36	97,101,106,108	0
5	PLM	A	513	18/18	0.71	0.24	53,61,72,75	0
6	GOL	A	515	6/6	0.76	0.23	52,68,70,72	0
4	NAG	A	510	14/15	0.78	0.35	79,86,91,92	0
4	NAG	A	511	14/15	0.79	0.21	91,95,99,100	0
5	PLM	A	512	18/18	0.81	0.22	33,39,59,61	0

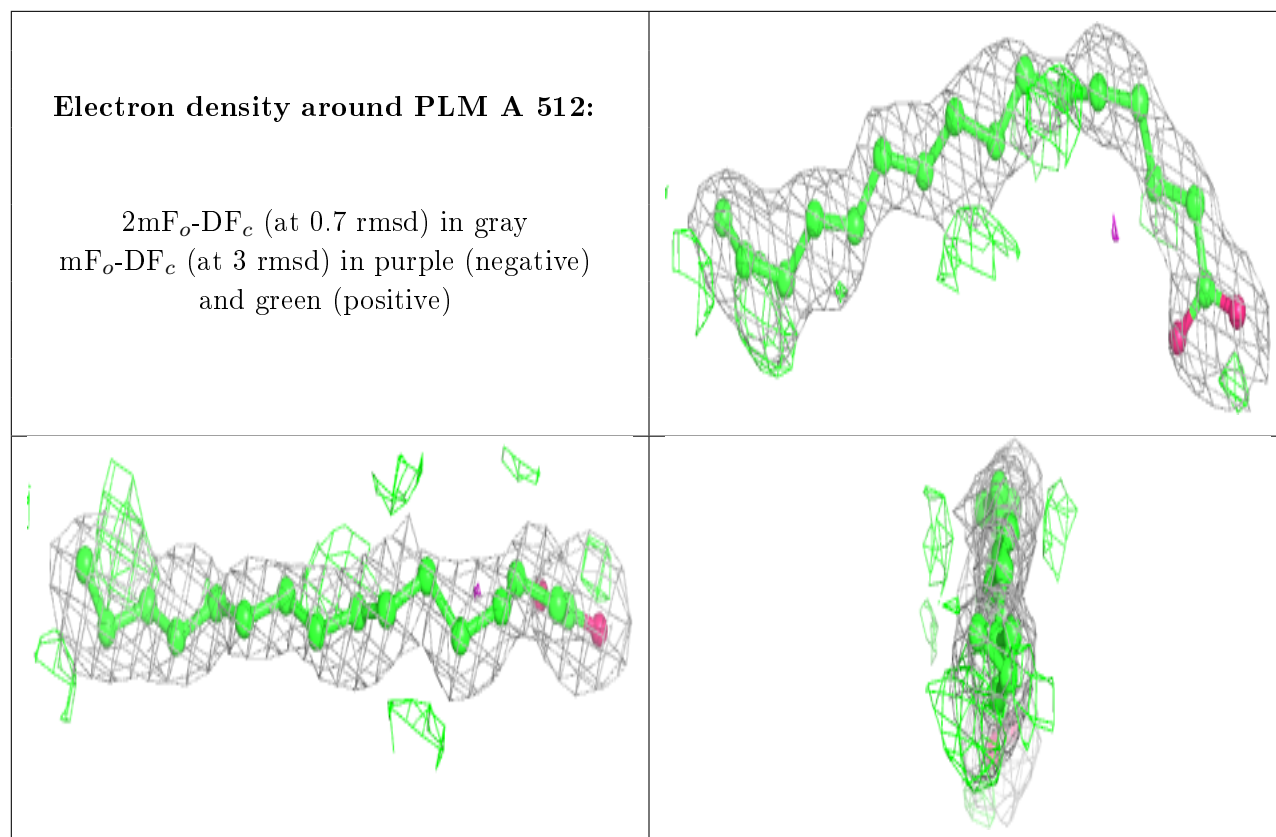
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	A	516	6/6	0.84	0.18	60,64,66,66	0
7	TRS	A	518	8/8	0.86	0.30	84,84,86,87	0
4	NAG	A	505	14/15	0.88	0.15	50,55,64,68	0
4	NAG	A	508	14/15	0.88	0.17	54,66,75,76	0
7	TRS	B	802	8/8	0.91	0.23	67,71,75,76	0
4	NAG	A	506	14/15	0.92	0.12	49,61,72,77	0
6	GOL	A	517	6/6	0.92	0.23	60,65,69,71	0
4	NAG	A	504	14/15	0.94	0.10	30,42,46,48	0
6	GOL	A	514	6/6	0.94	0.11	34,51,57,58	0
6	GOL	B	801	6/6	0.95	0.19	39,45,53,59	0
4	NAG	A	507	14/15	0.96	0.14	33,39,43,46	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.