Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 12:17 PM EDT

PDB ID	:	4KPP
Title	:	Crystal Structure of H+/Ca2+ Exchanger CAX
Authors	:	Nishizawa, T.; Ishitani, R.; Nureki, O.
Deposited on	:	2013-05-14
Resolution	:	2.30 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

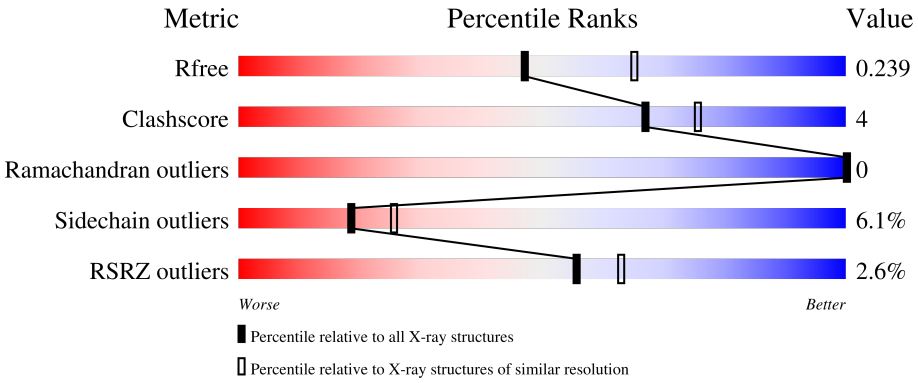
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of 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 <=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	405	3% 85% 11%
1	B	405	2% 82% 13% 5%
2	C	2	50% 50%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6108 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			2990	1988	462	535	5			
1	B	386	Total	C	N	O	S	0	0	0
			2952	1973	454	521	4			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	395	LEU	-	expression tag	UNP O29988
A	396	GLU	-	expression tag	UNP O29988
A	397	SER	-	expression tag	UNP O29988
A	398	SER	-	expression tag	UNP O29988
A	399	GLY	-	expression tag	UNP O29988
A	400	GLU	-	expression tag	UNP O29988
A	401	ASN	-	expression tag	UNP O29988
A	402	LEU	-	expression tag	UNP O29988
A	403	TYR	-	expression tag	UNP O29988
A	404	PHE	-	expression tag	UNP O29988
A	405	GLN	-	expression tag	UNP O29988
B	395	LEU	-	expression tag	UNP O29988
B	396	GLU	-	expression tag	UNP O29988
B	397	SER	-	expression tag	UNP O29988
B	398	SER	-	expression tag	UNP O29988
B	399	GLY	-	expression tag	UNP O29988
B	400	GLU	-	expression tag	UNP O29988
B	401	ASN	-	expression tag	UNP O29988
B	402	LEU	-	expression tag	UNP O29988
B	403	TYR	-	expression tag	UNP O29988
B	404	PHE	-	expression tag	UNP O29988
B	405	GLN	-	expression tag	UNP O29988

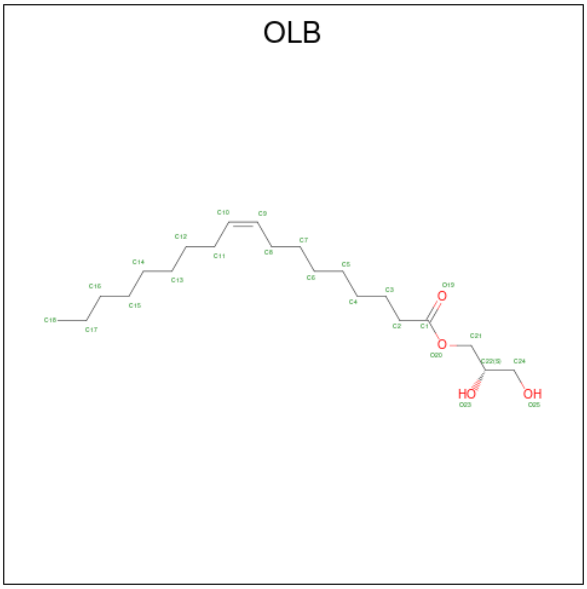
- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	2	Total C O 13 7 6	0	0	1

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

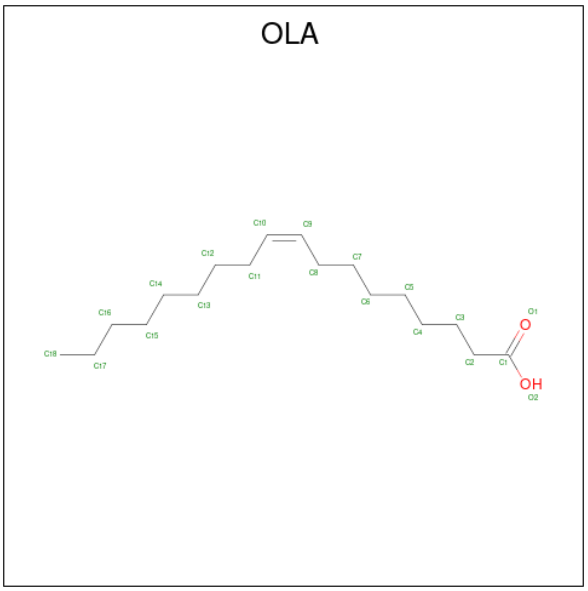
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is (2S)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLB) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 24 21 3	0	0

- Molecule 5 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 6 6	0	0
5	B	1	Total C O 13 11 2	0	0
5	B	1	Total C 13 13	0	0
5	B	1	Total C 7 7	0	0
5	B	1	Total C 11 11	0	0

- Molecule 6 is water.

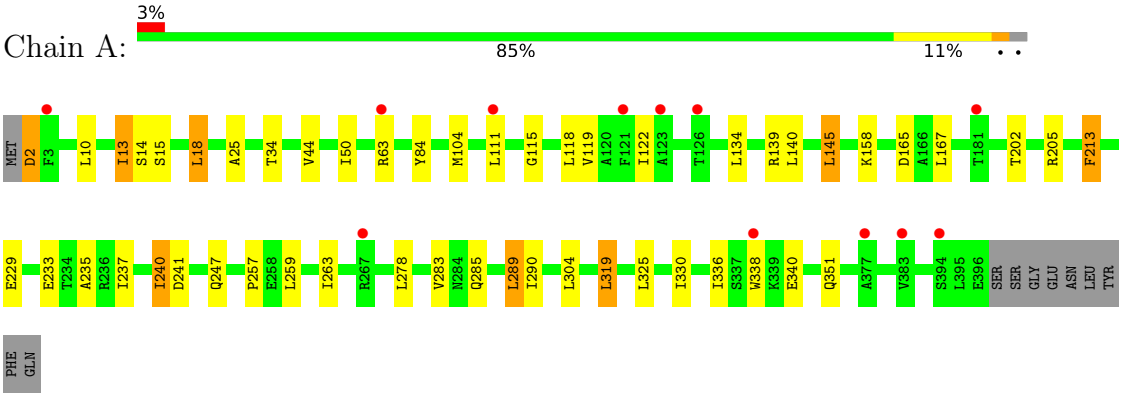
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	29	Total O 29 29	0	0
6	B	48	Total O 48 48	0	0

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.

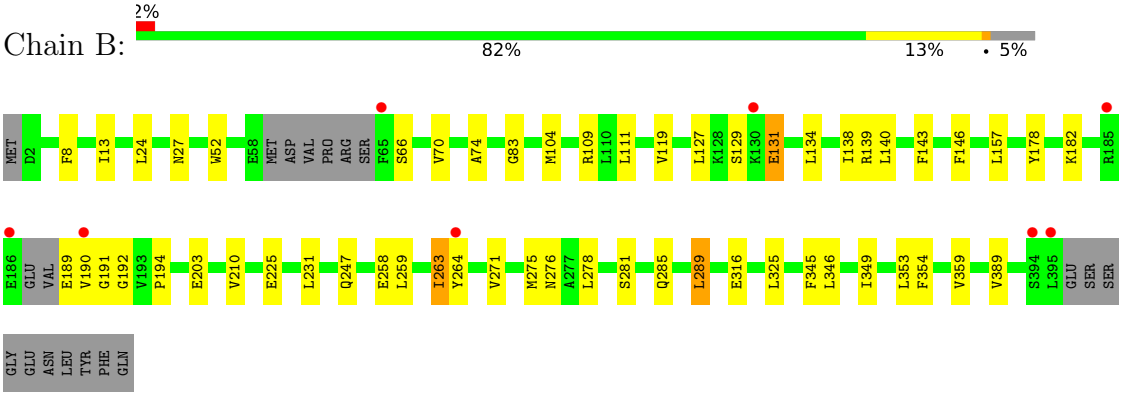
• Molecule 1: Putative uncharacterized protein

Chain A:



• Molecule 1: Putative uncharacterized protein

Chain B:



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.95Å 97.39Å 71.23Å 90.00° 99.37° 90.00°	Depositor
Resolution (Å)	30.71 – 2.30 30.71 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.6 (30.71-2.30) 87.6 (30.71-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.32 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.202 , 0.238 0.200 , 0.239	Depositor DCC
R_{free} test set	1678 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6108	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: OLA, OLB, CA, GLC

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	0.24	0/3056	0.40	0/4179
1	B	0.24	0/3018	0.39	0/4120
All	All	0.24	0/6074	0.39	0/8299

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	2990	0	3016	24	0
1	B	2952	0	3014	25	0
2	C	13	0	10	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	24	0	37	0	0
5	A	6	0	8	0	0
5	B	44	0	62	3	0
6	A	29	0	0	2	0
6	B	48	0	0	1	0
All	All	6108	0	6147	48	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 4.

All (48) 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:B:111:LEU:HD23	5:B:503:OLA:H122	1.74	0.68
1:A:247:GLN:NE2	6:A:617:HOH:O	2.29	0.63
1:B:225:GLU:HB3	2:C:2:GLC:H3	1.80	0.62
1:A:122:ILE:HD12	1:A:263:ILE:HD12	1.82	0.61
1:A:134:LEU:HD21	1:A:336:ILE:HG13	1.83	0.60
1:A:158:LYS:NZ	1:A:165:ASP:OD2	2.34	0.59
1:A:119:VAL:HG21	1:A:278:LEU:HD11	1.84	0.59
1:B:285:GLN:HA	1:B:289:LEU:HB2	1.86	0.57
1:A:2:ASP:N	1:A:2:ASP:OD1	2.37	0.57
1:B:259:LEU:HB2	5:B:503:OLA:H132	1.88	0.56
1:B:354:PHE:HB3	1:B:359:VAL:HG21	1.88	0.55
1:A:145:LEU:HD13	1:A:283:VAL:HG22	1.89	0.54
1:B:109:ARG:NH2	1:B:316:GLU:OE2	2.40	0.54
1:A:115:GLY:HA2	1:A:259:LEU:HD11	1.90	0.53
1:A:139:ARG:NH2	6:A:609:HOH:O	2.43	0.51
1:B:83:GLY:HA3	5:B:502:OLA:H9	1.91	0.50
1:A:44:VAL:HG13	1:A:257:PRO:HG3	1.93	0.50
1:A:285:GLN:HA	1:A:289:LEU:HB2	1.92	0.50
1:A:104:MET:SD	1:A:290:ILE:HG12	2.51	0.49
1:B:129:SER:OG	1:B:131:GLU:OE1	2.31	0.49
1:B:189:GLU:HA	1:B:190:VAL:HA	1.56	0.48
1:A:25:ALA:HB1	1:B:210:VAL:HG21	1.96	0.47
1:A:330:ILE:HD13	1:A:340:GLU:HB3	1.96	0.47
1:A:84:TYR:OH	1:A:229:GLU:OE2	2.28	0.47
1:A:202:THR:HG22	1:A:205:ARG:HH22	1.79	0.47
1:B:247:GLN:NE2	6:B:611:HOH:O	2.48	0.46
1:A:104:MET:HE2	1:A:104:MET:C	2.35	0.46
1:A:259:LEU:O	1:A:263:ILE:HG12	2.16	0.45
1:B:281:SER:OG	1:B:285:GLN:NE2	2.50	0.45
1:B:191:GLY:HA2	1:B:192:GLY:HA2	1.61	0.44
1:B:263:ILE:HG13	1:B:264:TYR:N	2.32	0.44
1:B:13:ILE:HD12	1:B:52:TRP:CH2	2.52	0.44
1:B:271:VAL:O	1:B:275:MET:HG2	2.18	0.44
1:B:119:VAL:HG21	1:B:278:LEU:HD11	1.99	0.43
1:B:190:VAL:HG13	1:B:194:PRO:HB2	1.99	0.43
1:B:178:TYR:OH	1:B:182:LYS:NZ	2.50	0.43
1:B:66:SER:O	1:B:70:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:PHE:CD2	1:B:389:VAL:HG21	2.54	0.42
1:A:240:ILE:HG13	1:A:241:ASP:N	2.32	0.42
1:B:345:PHE:CE2	1:B:349:ILE:HD13	2.55	0.42
1:A:235:ALA:HA	1:A:240:ILE:HG23	2.01	0.42
1:A:13:ILE:HG13	1:A:14:SER:N	2.35	0.42
1:B:346:LEU:HD23	1:B:349:ILE:HD11	2.02	0.42
1:A:319:LEU:HD11	1:A:351:GLN:HG3	2.02	0.41
1:A:15:SER:O	1:A:18:LEU:HB2	2.21	0.41
1:B:74:ALA:O	1:B:258:GLU:HG3	2.21	0.41
1:A:50:ILE:HG23	1:A:213:PHE:HE1	1.86	0.41
1:B:138:ILE:HD11	1:B:276:ASN:OD1	2.21	0.41

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	393/405 (97%)	387 (98%)	6 (2%)	0	100	100
1	B	380/405 (94%)	377 (99%)	3 (1%)	0	100	100
All	All	773/810 (95%)	764 (99%)	9 (1%)	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	305/341 (89%)	285 (93%)	20 (7%)	16 22
1	B	305/341 (89%)	288 (94%)	17 (6%)	21 29
All	All	610/682 (89%)	573 (94%)	37 (6%)	18 25

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

Mol	Chain	Res	Type
1	A	2	ASP
1	A	10	LEU
1	A	13	ILE
1	A	18	LEU
1	A	34	THR
1	A	63	ARG
1	A	111	LEU
1	A	118	LEU
1	A	140	LEU
1	A	145	LEU
1	A	167	LEU
1	A	213	PHE
1	A	233	GLU
1	A	237	ILE
1	A	240	ILE
1	A	289	LEU
1	A	304	LEU
1	A	319	LEU
1	A	325	LEU
1	A	338	TRP
1	B	8	PHE
1	B	24	LEU
1	B	27	ASN
1	B	104	MET
1	B	127	LEU
1	B	131	GLU
1	B	134	LEU
1	B	139	ARG
1	B	140	LEU
1	B	146	PHE
1	B	157	LEU
1	B	203	GLU
1	B	231	LEU
1	B	263	ILE
1	B	289	LEU

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Mol	Chain	Res	Type
1	B	325	LEU
1	B	353	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	285	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

2 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	$\#\|Z\| > 2$
2	GLC	C	1	2	1,1,12	0.08	0	-		
2	GLC	C	2	2	11,11,12	0.60	0	15,15,17	0.73	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
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

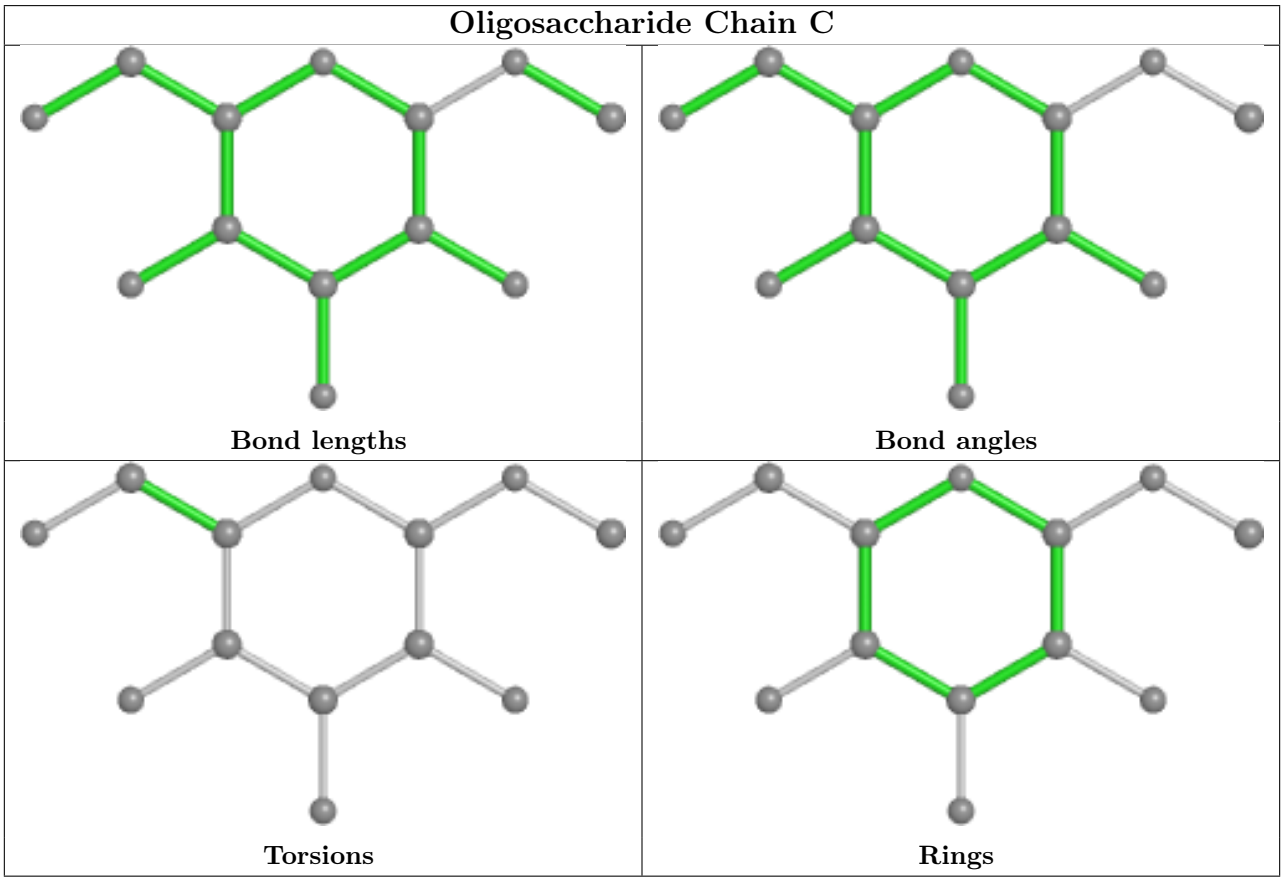
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	GLC	1	0

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

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
5	OLA	B	504	-	6,6,19	0.27	0	5,5,19	0.45	0
4	OLB	A	502	-	22,23,24	1.07	2 (9%)	22,24,25	1.02	1 (4%)
5	OLA	A	503	-	5,5,19	0.27	0	4,4,19	0.39	0
5	OLA	B	503	-	12,12,19	0.83	1 (8%)	11,11,19	0.49	0
5	OLA	B	502	-	12,12,19	0.94	1 (8%)	12,12,19	1.15	0
5	OLA	B	505	-	10,10,19	0.94	1 (10%)	9,9,19	0.51	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
5	OLA	B	504	-	-	2/4/4/17	-
4	OLB	A	502	-	-	8/22/22/24	-
5	OLA	A	503	-	-	2/3/3/17	-
5	OLA	B	503	-	-	5/10/10/17	-
5	OLA	B	502	-	-	8/10/10/17	-
5	OLA	B	505	-	-	4/8/8/17	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	OLB	C10-C9	3.06	1.49	1.31
4	A	502	OLB	O20-C21	-3.05	1.38	1.45
5	B	505	OLA	C10-C9	2.82	1.48	1.31
5	B	503	OLA	C10-C9	2.74	1.47	1.31
5	B	502	OLA	C9-C10	2.49	1.48	1.29

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	OLB	O20-C1-C2	2.77	120.61	111.91

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	OLB	O20-C21-C22-O23
5	B	502	OLA	C1-C2-C3-C4
4	A	502	OLB	C2-C3-C4-C5
5	B	502	OLA	C3-C4-C5-C6
4	A	502	OLB	C11-C10-C9-C8
5	B	505	OLA	C11-C12-C13-C14
5	B	505	OLA	C12-C13-C14-C15
5	A	503	OLA	C4-C5-C6-C7
4	A	502	OLB	O20-C21-C22-C24
5	B	504	OLA	C3-C4-C5-C6
5	A	503	OLA	C3-C4-C5-C6
5	B	502	OLA	C2-C3-C4-C5
4	A	502	OLB	C15-C16-C17-C18
4	A	502	OLB	C1-C2-C3-C4
5	B	504	OLA	C4-C5-C6-C7
5	B	503	OLA	C11-C10-C9-C8
5	B	502	OLA	C6-C7-C8-C9
5	B	502	OLA	C11-C10-C9-C8
5	B	503	OLA	C4-C5-C6-C7
5	B	503	OLA	C3-C4-C5-C6
5	B	502	OLA	C4-C5-C6-C7
5	B	505	OLA	C9-C10-C11-C12
5	B	502	OLA	C5-C6-C7-C8
5	B	503	OLA	C7-C8-C9-C10
4	A	502	OLB	C3-C4-C5-C6
4	A	502	OLB	C9-C10-C11-C12
5	B	503	OLA	C9-C10-C11-C12
5	B	505	OLA	C13-C14-C15-C16
5	B	502	OLA	O2-C1-C2-C3

There are no ring outliers.

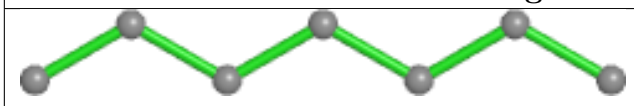
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	503	OLA	2	0
5	B	502	OLA	1	0

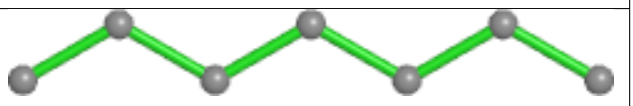
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

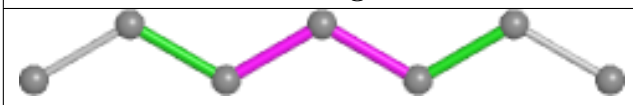
Ligand OLA B 504



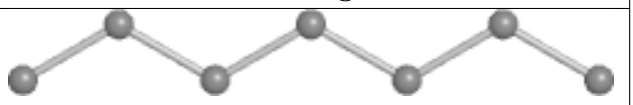
Bond lengths



Bond angles

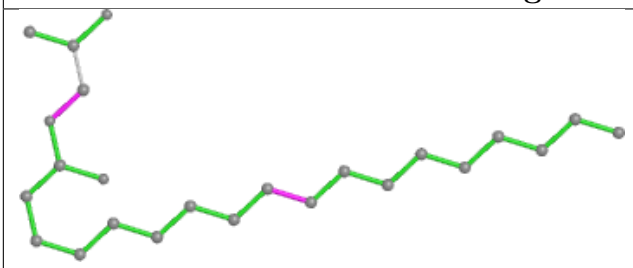


Torsions

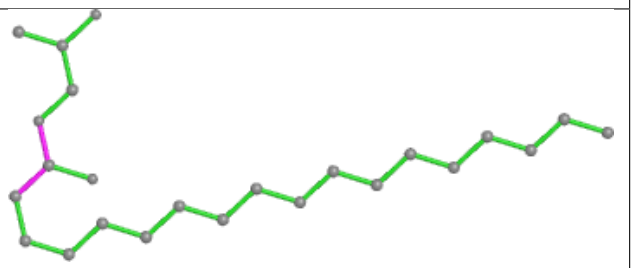


Rings

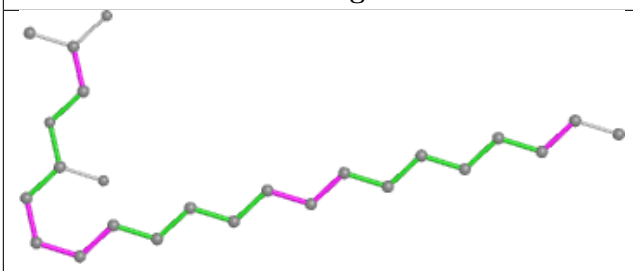
Ligand OLB A 502



Bond lengths



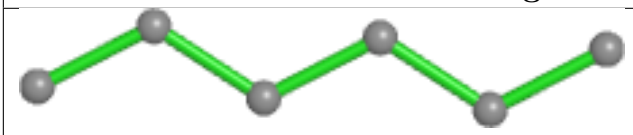
Bond angles



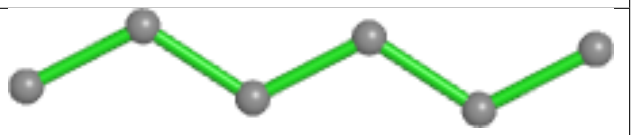
Torsions

Rings

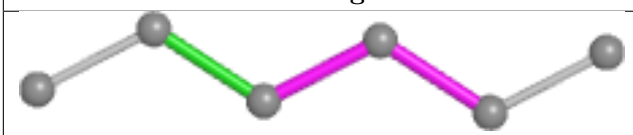
Ligand OLA A 503



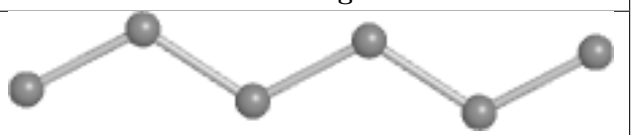
Bond lengths



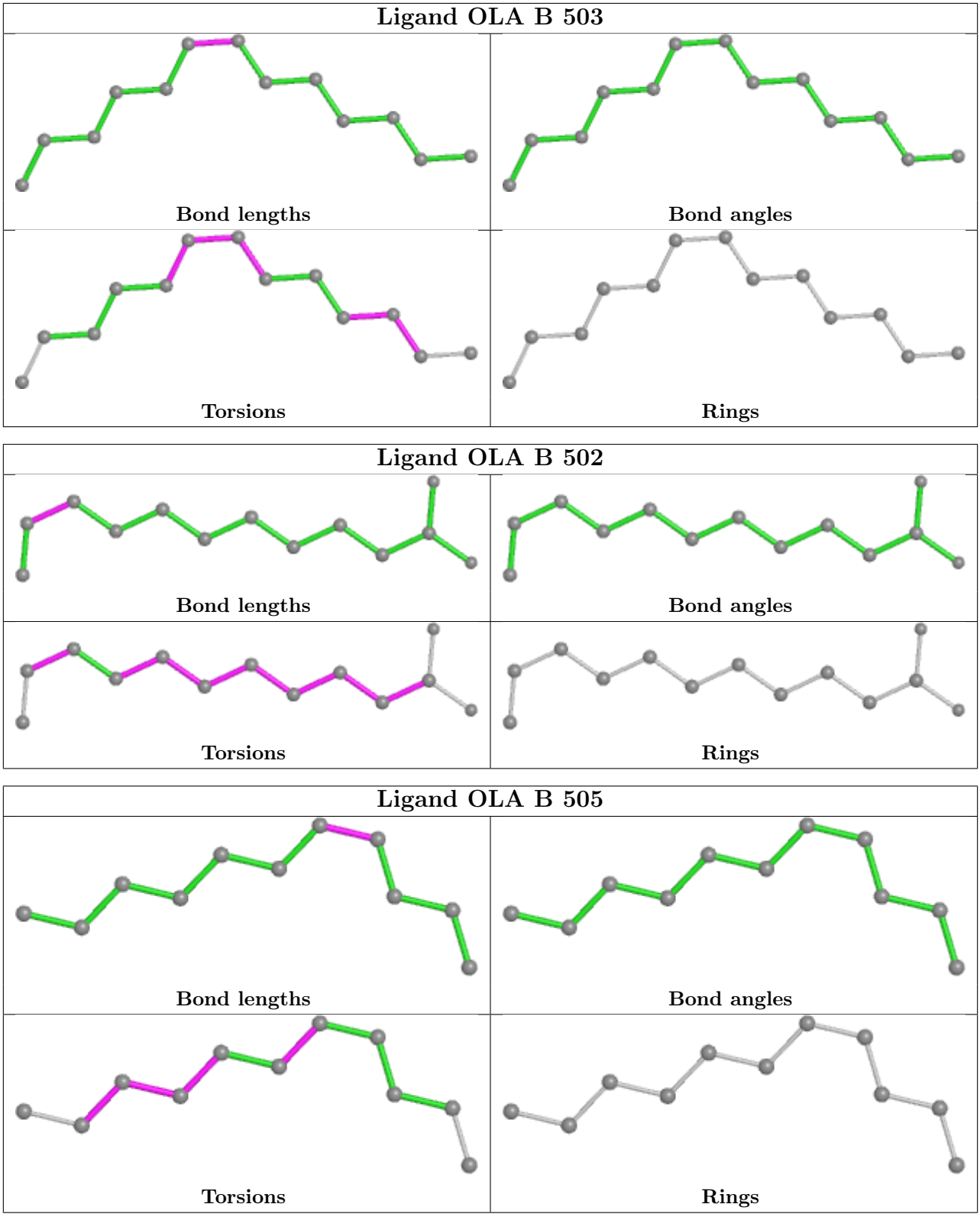
Bond angles



Torsions



Rings



5.7 Other polymers

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

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, 95^{th} 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	395/405 (97%)	-0.11	12 (3%) 50 57	19, 35, 65, 87	0
1	B	386/405 (95%)	-0.16	8 (2%) 63 70	16, 31, 58, 97	0
All	All	781/810 (96%)	-0.13	20 (2%) 56 63	16, 33, 62, 97	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	THR	3.0
1	A	338	TRP	3.0
1	A	394	SER	2.9
1	A	181	THR	2.7
1	A	267	ARG	2.6
1	A	63	ARG	2.6
1	A	123	ALA	2.6
1	A	3	PHE	2.5
1	B	65	PHE	2.4
1	A	111	LEU	2.4
1	B	394	SER	2.3
1	B	264	TYR	2.3
1	B	186	GLU	2.3
1	B	185	ARG	2.2
1	A	377	ALA	2.2
1	A	383	VAL	2.2
1	B	190	VAL	2.2
1	A	121	PHE	2.1
1	B	395	LEU	2.0
1	B	130	LYS	2.0

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)

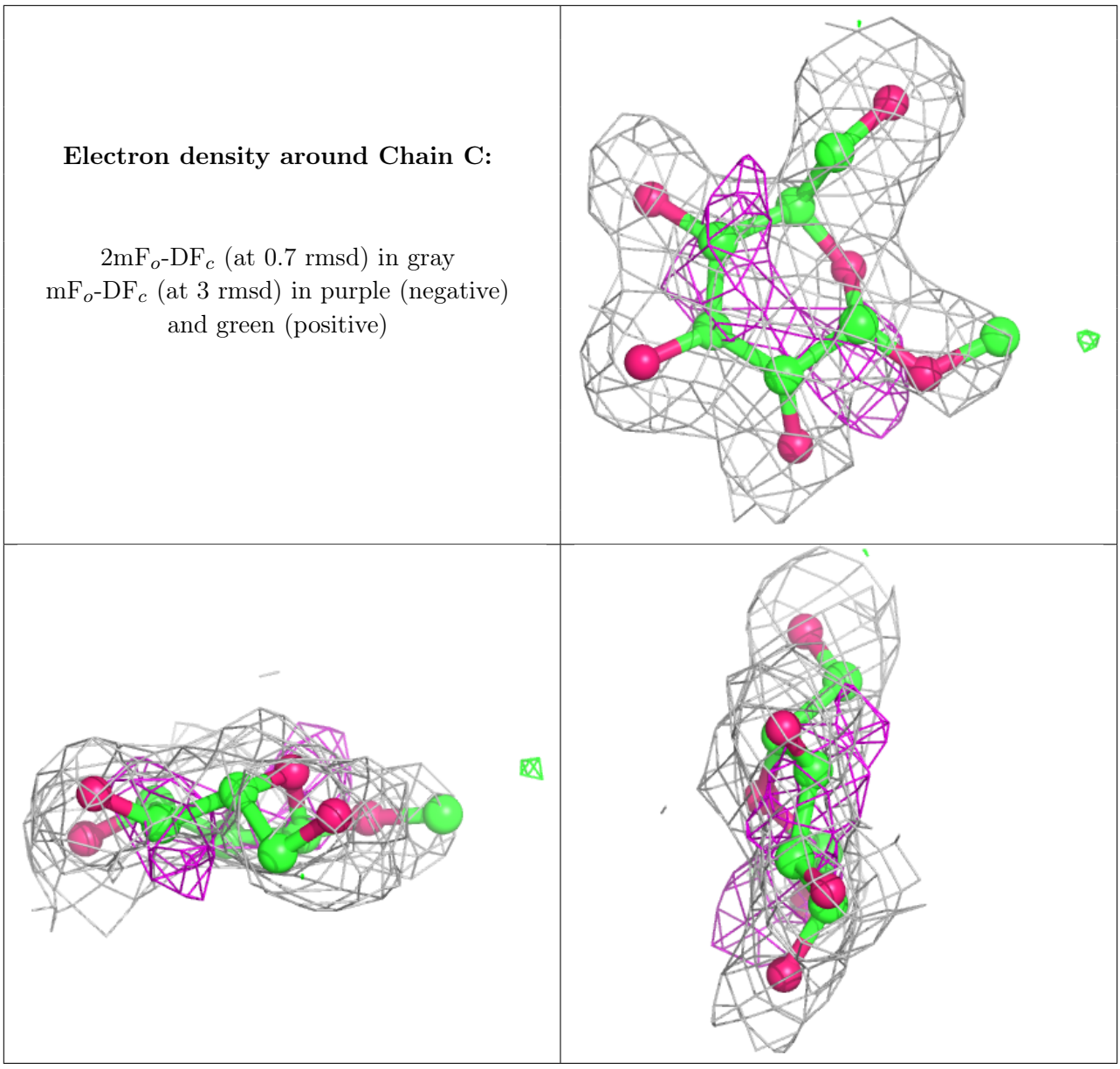
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	C	2	11/12	0.74	0.25	34,48,53,54	0
2	GLC	C	1	2/12	0.83	0.39	56,56,56,58	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.

Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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, 95^{th} 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(Å^2)	Q<0.9
5	OLA	B	503	13/20	0.83	0.26	43,45,47,48	0
5	OLA	B	505	11/20	0.85	0.21	47,52,54,55	0
5	OLA	B	504	7/20	0.88	0.15	57,58,58,59	0
4	OLB	A	502	24/25	0.89	0.17	44,58,73,75	0
5	OLA	B	502	13/20	0.91	0.21	43,50,63,66	0

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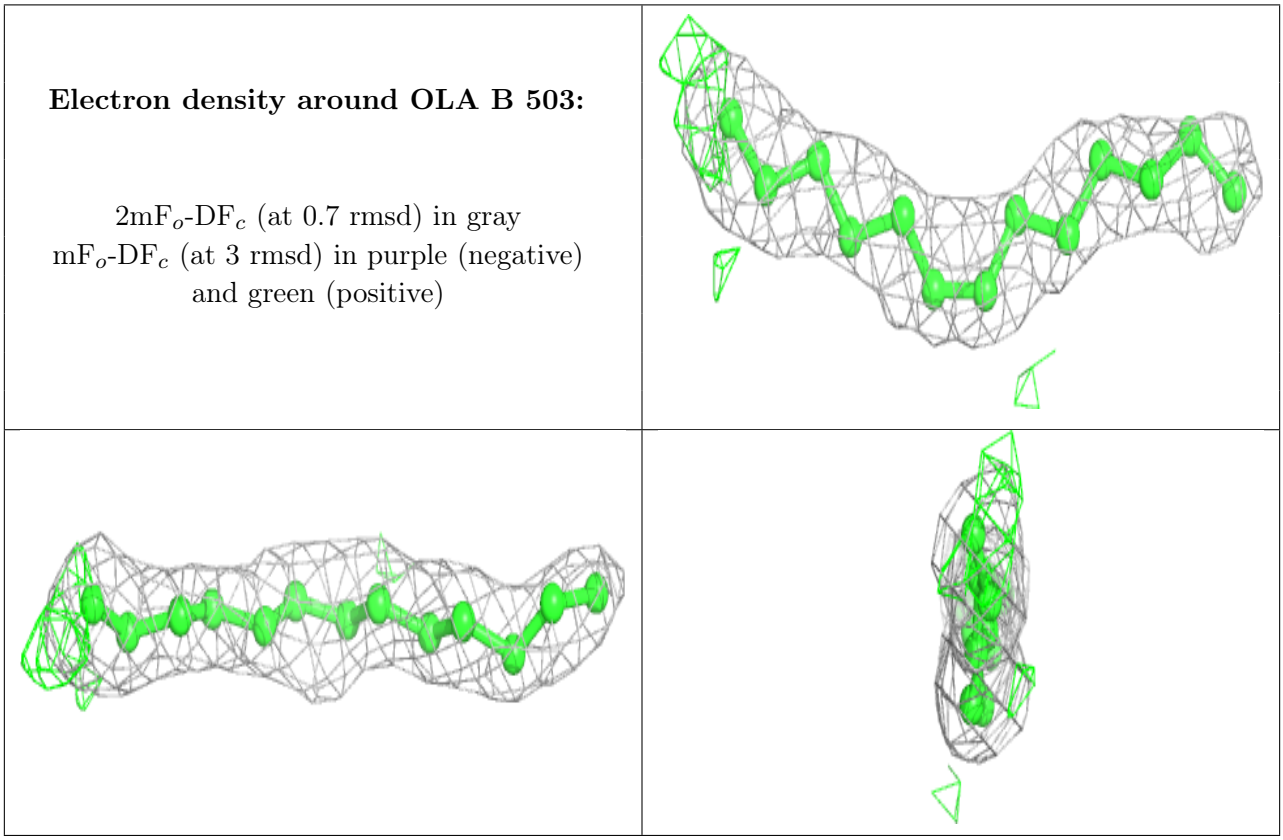
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	B	501	1/1	0.91	0.10	61,61,61,61	0
5	OLA	A	503	6/20	0.92	0.11	52,54,55,55	0
3	CA	A	501	1/1	0.97	0.15	63,63,63,63	0

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.

Electron density around OLA B 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OLA B 505:

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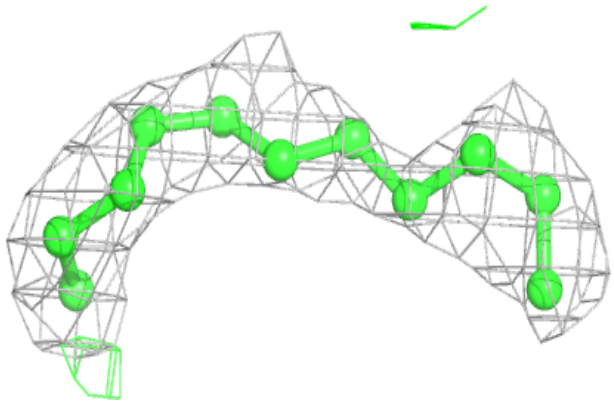
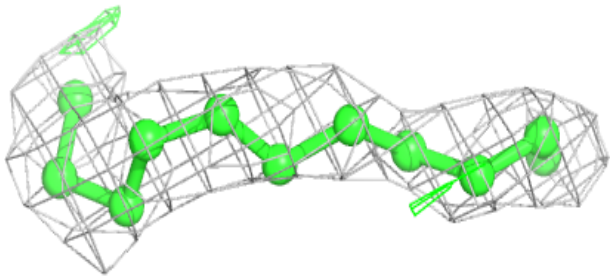
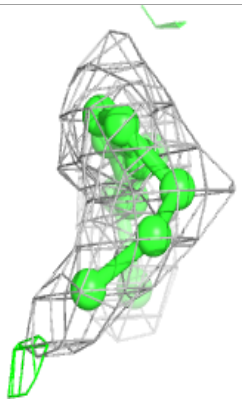
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

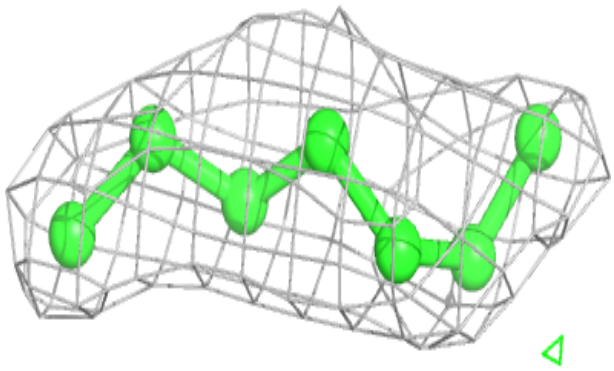


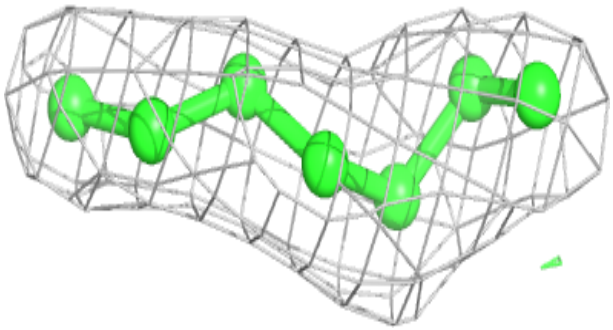


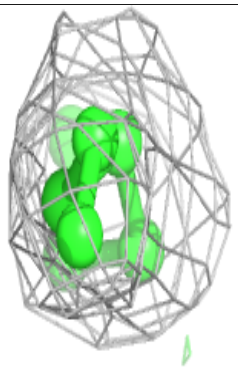


Electron density around OLA B 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

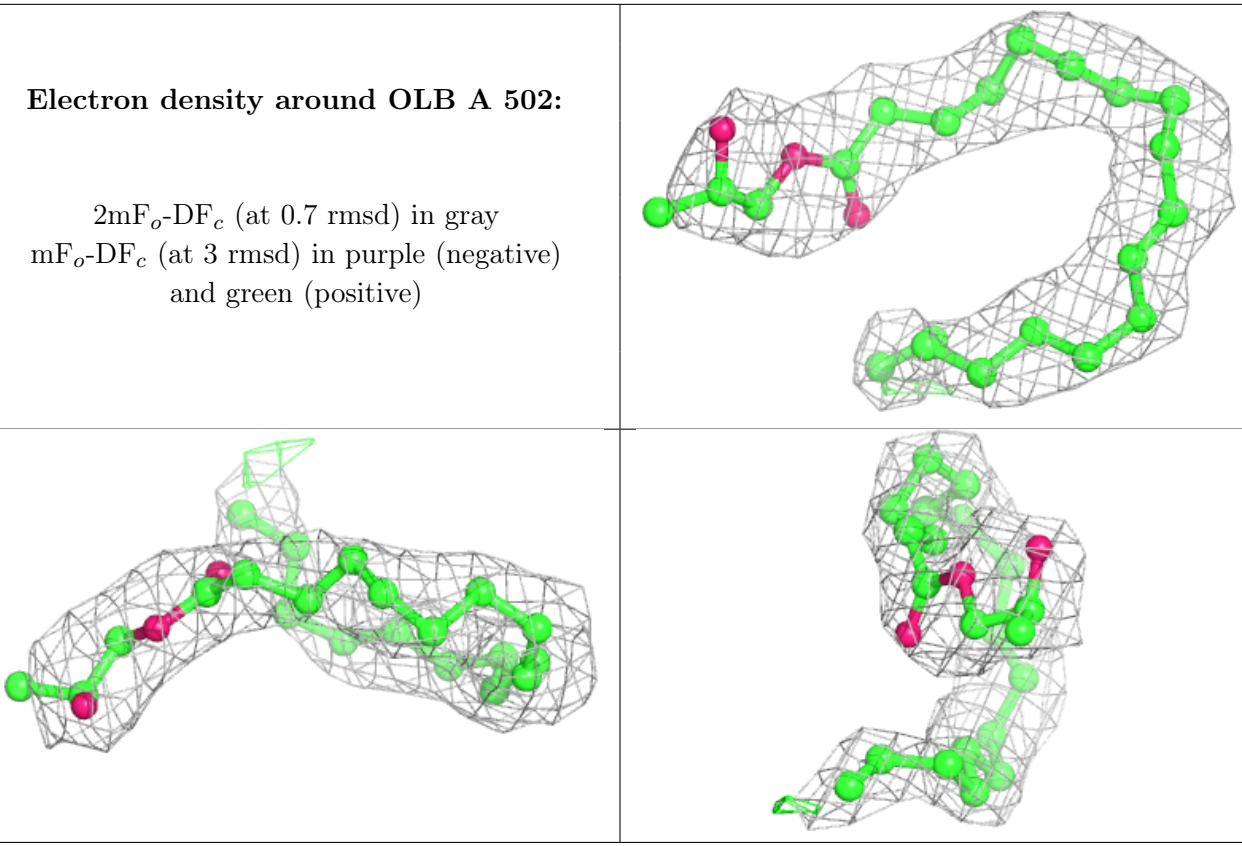






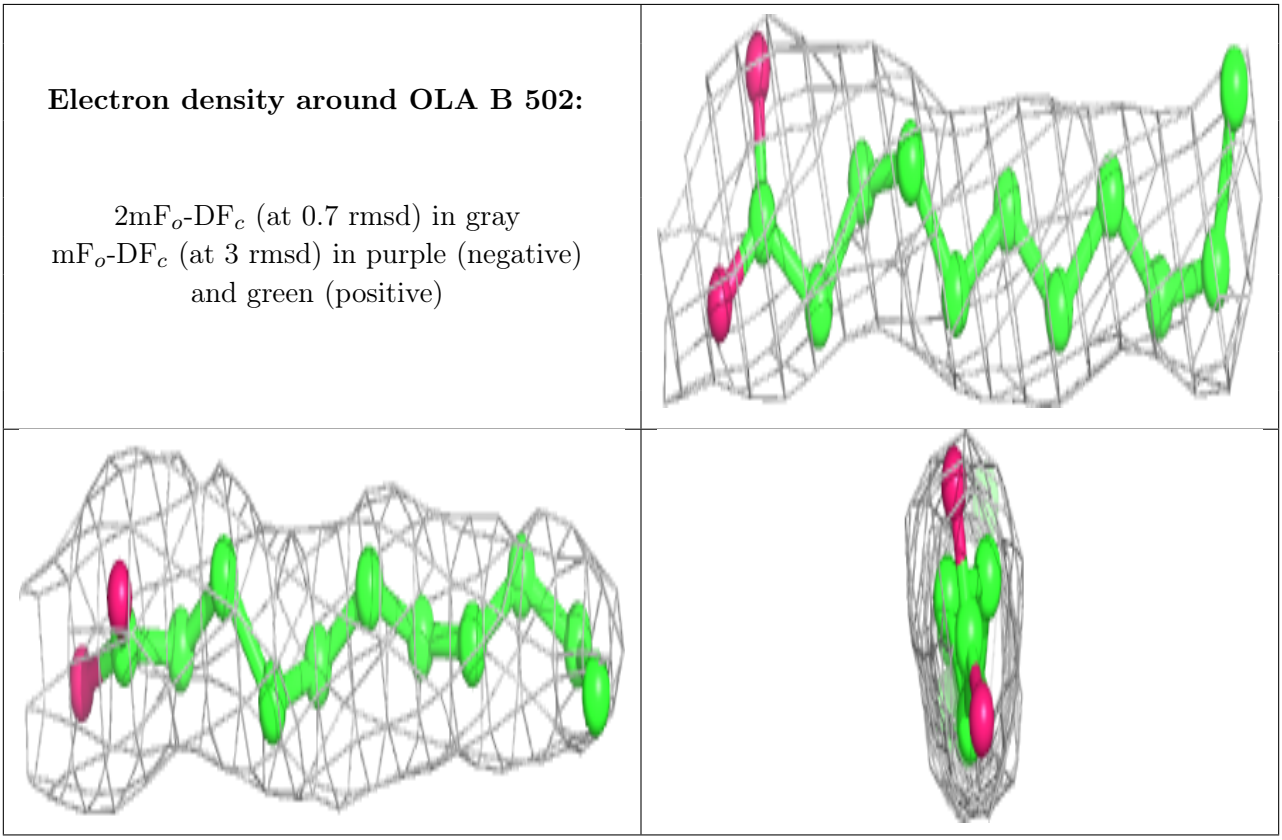
Electron density around OLB A 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OLA B 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OLA A 503:

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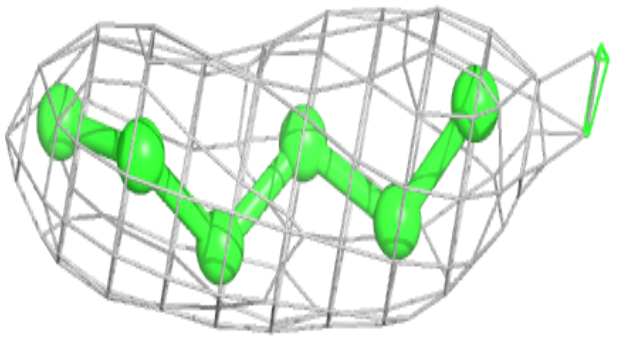
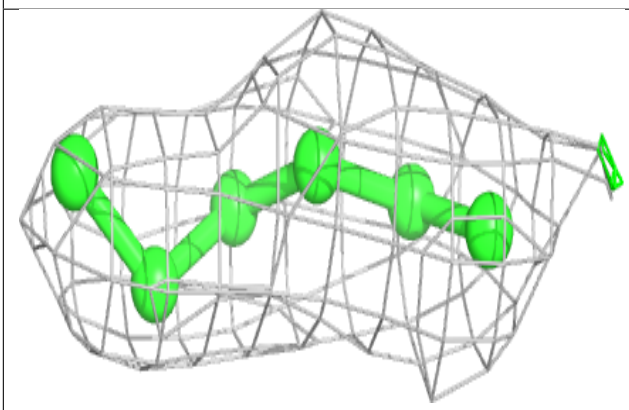
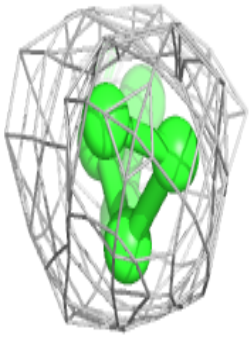
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.