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Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 10:22 PM EDT

PDB ID	:	2ZFE
Title	:	Crystal structure of bacteriorhodopsin-xenon complex
Authors	:	Kouyama, T.
Deposited on	:	2007-12-31
Resolution	:	2.50 Å(reported)

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

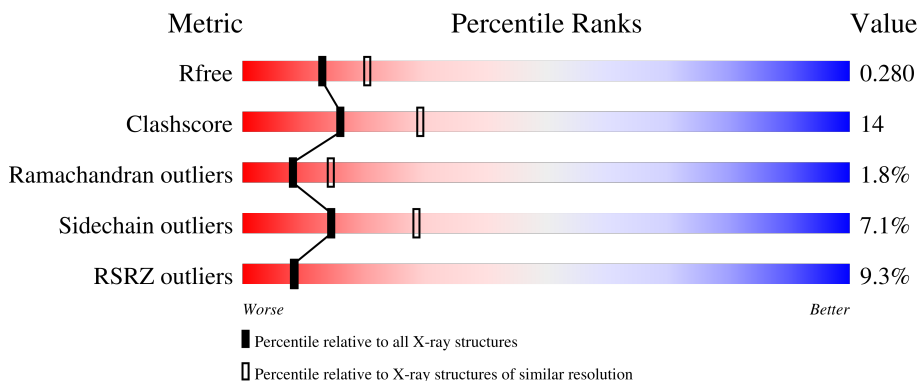|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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		0.280
Clashscore		14
Ramachandran outliers		1.8%
Sidechain outliers		7.1%
RSRZ outliers		9.3%

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	262	8% / 60% / 23% / • / 13%
2	B	3	67% / 33%

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:

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| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SGA	B	3	-	-	-	X
4	L3P	A	260	-	-	-	X
5	L2P	A	270	-	-	-	X
6	L1P	A	280	-	-	-	X
6	L1P	A	290	-	-	-	X
6	L1P	A	300	-	-	-	X
7	XE	A	638	-	-	X	-

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 2099 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 Bacteriorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total 1756	C 1180	N 268	O 299	S 9	0	0	0

- Molecule 2 is an oligosaccharide called 3-O-sulfo-beta-D-galactopyranose-(1-6)-alpha-D-mannopyranose-(1-2)-alpha-D-glucopyranose.
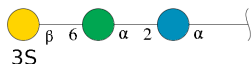
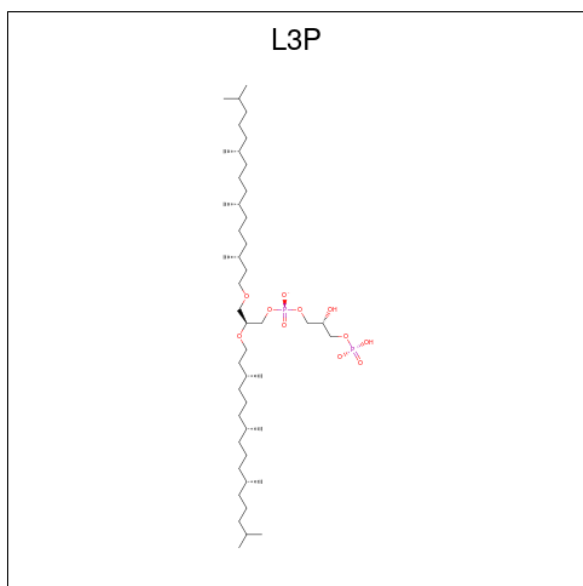| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total 37	C 18	O 18	S 1	0	0	0

- Molecule 3 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).
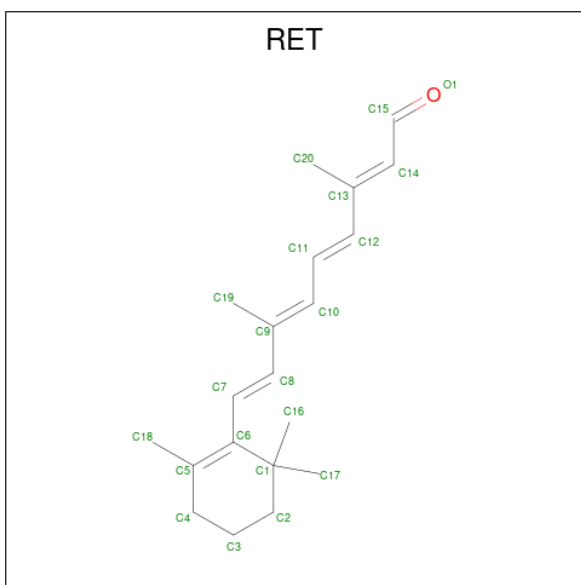
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 20	C 20	0	0

- Molecule 4 is 2,3-DI-O-PHYTANLY-3-SN-GLYCERO-1-PHOSPHORYL-3'-SN-GLYCEROL-1'-PHOSPHATE (three-letter code: L3P) (formula: $C_{46}H_{94}O_{11}P_2$).

L3P

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 59	C 46	O 11	P 2	0	0

- Molecule 5 is 2,3-DI-PHYTANYL-GLYCEROL (three-letter code: L2P) (formula: $C_{43}H_{88}O_3$).

L2P
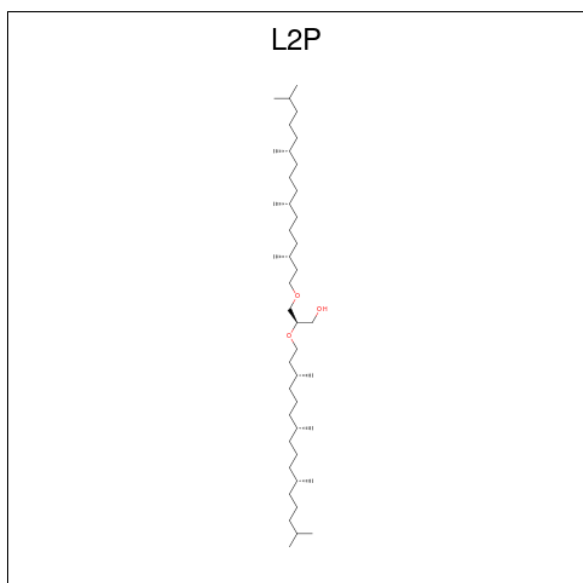
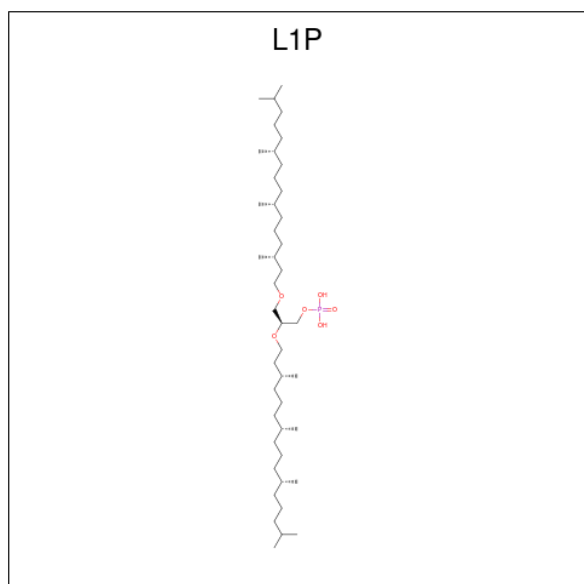| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 46	C 43	O 3	0	0

- Molecule 6 is 3-PHOSPHORYL-[1,2-DI-PHYTANYL]GLYCEROL (three-letter code: L1P) (formula: $C_{43}H_{89}O_6P$).

L1P

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 40	C 33	O 6	P 1	0	0
6	A	1	Total 50	C 43	O 6	P 1	0	0
6	A	1	Total 50	C 43	O 6	P 1	0	0

- Molecule 7 is XENON (three-letter code: XE) (formula: Xe).

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	40	Total 40	O 40	0	0

3 Residue-property plots ⓘ

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: Bacteriorhodopsin
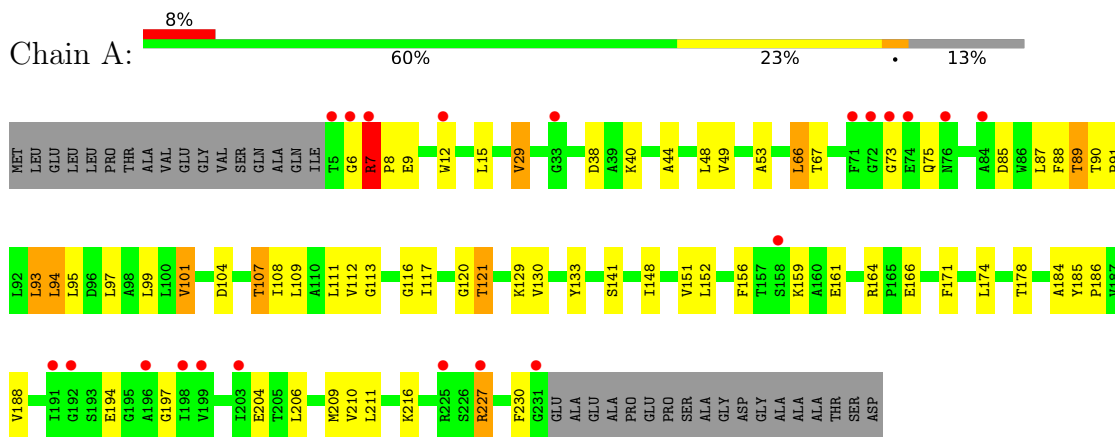
• Molecule 2: 3-O-sulfo-beta-D-galactopyranose-(1-6)-alpha-D-mannopyranose-(1-2)-alpha-D-glucopyranose
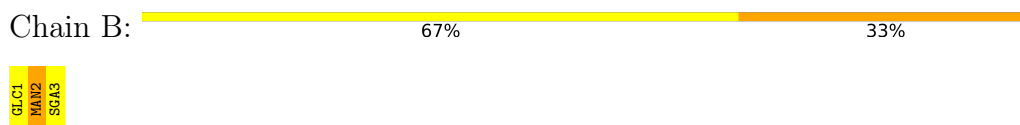
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α, β, γ	102.41Å 102.41Å 112.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 37.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-2.50) 98.7 (37.86-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.75 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.279 0.249 , 0.280	Depositor DCC
R_{free} test set	627 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	45.0	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.2	EDS
L-test for twinning[2]	$< |L| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2099	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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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: L1P, L2P, L3P, MAN, XE, RET, GLC, SGA

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	0.41	0/1804	0.56	0/2464

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	1756	0	1813	62	0
2	B	37	0	28	1	0
3	A	20	0	27	4	0
4	A	59	0	93	5	0
5	A	46	0	87	7	0
6	A	140	0	238	0	0
7	A	1	0	0	3	0
8	A	40	0	0	2	0
All	All	2099	0	2286	63	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 14.

All (63) 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:87:LEU:HD11	5:A:270:L2P:H271	1.32	1.11
1:A:121:THR:HG22	1:A:141:SER:HB2	1.43	0.99
1:A:108:ILE:HG23	7:A:638:XE:XE	2.48	0.91
1:A:87:LEU:HD21	5:A:270:L2P:H262	1.55	0.88
1:A:29:VAL:HG12	1:A:29:VAL:O	1.80	0.81
1:A:174:LEU:O	1:A:178:THR:HG23	1.84	0.77
1:A:121:THR:CG2	1:A:141:SER:HB2	2.15	0.74
1:A:111:LEU:HD21	1:A:151:VAL:HG11	1.69	0.74
1:A:15:LEU:HB3	1:A:209:MET:HE2	1.70	0.72
1:A:117:ILE:O	1:A:121:THR:HB	1.90	0.71
1:A:44:ALA:HA	4:A:260:L3P:H111	1.76	0.67
1:A:6:GLY:HA2	1:A:9:GLU:OE1	1.95	0.67
1:A:94:LEU:HB3	7:A:638:XE:XE	2.74	0.65
1:A:107:THR:O	1:A:111:LEU:HD23	1.97	0.65
1:A:40:LYS:HZ1	4:A:260:L3P:H42	1.63	0.63
1:A:227:ARG:HH11	1:A:227:ARG:HB3	1.62	0.63
1:A:104:ASP:HB2	1:A:107:THR:HG22	1.81	0.62
1:A:101:VAL:HG22	1:A:159:LYS:HB3	1.82	0.61
1:A:116:GLY:HA3	5:A:270:L2P:H541	1.82	0.61
1:A:104:ASP:HB2	1:A:107:THR:CG2	2.32	0.60
1:A:49:VAL:HG21	1:A:93:LEU:HD13	1.83	0.60
1:A:164:ARG:NH2	1:A:230:PHE:O	2.35	0.60
1:A:85:ASP:O	1:A:89:THR:HB	2.03	0.58
1:A:90:THR:OG1	1:A:91:PRO:HD3	2.06	0.55
1:A:15:LEU:HD23	1:A:209:MET:CE	2.36	0.55
1:A:164:ARG:NH1	1:A:166:GLU:OE2	2.40	0.54
1:A:152:LEU:O	1:A:156:PHE:HB2	2.09	0.53
1:A:186:PRO:HB3	3:A:250:RET:H183	1.91	0.52
1:A:12:TRP:CE3	1:A:206:LEU:HD23	2.44	0.52
1:A:141:SER:HB3	3:A:250:RET:H41	1.91	0.51
1:A:53:ALA:HB2	1:A:216:LYS:HE2	1.93	0.51
1:A:129:LYS:HE2	2:B:2:MAN:H61	1.94	0.50
1:A:40:LYS:HZ2	4:A:260:L3P:P1	2.36	0.49
1:A:66:LEU:HD23	1:A:67:THR:N	2.28	0.49
1:A:87:LEU:CD1	5:A:270:L2P:H271	2.24	0.48
1:A:194:GLU:OE1	1:A:204:GLU:OE2	2.30	0.48
1:A:29:VAL:O	1:A:29:VAL:CG1	2.53	0.48
1:A:112:VAL:HG23	7:A:638:XE:XE	2.92	0.47
1:A:109:LEU:HD11	5:A:270:L2P:H592	1.97	0.47
1:A:166:GLU:HG3	8:A:630:HOH:O	2.14	0.46
1:A:120:GLY:HA3	5:A:270:L2P:H491	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HG	4:A:260:L3P:H143	1.98	0.46
1:A:130:VAL:HB	1:A:133:TYR:CD2	2.52	0.45
1:A:15:LEU:HD23	1:A:209:MET:HE1	1.98	0.45
1:A:185:TYR:N	1:A:186:PRO:HD2	2.32	0.45
1:A:7:ARG:H	1:A:8:PRO:HD2	1.83	0.44
1:A:90:THR:N	1:A:91:PRO:CD	2.80	0.44
1:A:113:GLY:HA2	5:A:270:L2P:H543	2.00	0.44
3:A:250:RET:H7	3:A:250:RET:H181	1.84	0.43
1:A:107:THR:HG21	8:A:629:HOH:O	2.18	0.43
1:A:75:GLN:HA	1:A:75:GLN:OE1	2.18	0.43
1:A:88:PHE:C	1:A:91:PRO:HD2	2.40	0.42
1:A:95:LEU:O	1:A:99:LEU:HG	2.18	0.42
1:A:12:TRP:CD2	1:A:206:LEU:HD23	2.55	0.42
1:A:206:LEU:O	1:A:210:VAL:HG23	2.19	0.42
1:A:156:PHE:HB3	1:A:171:PHE:CZ	2.55	0.42
1:A:15:LEU:HD23	1:A:209:MET:HE2	2.01	0.41
1:A:184:ALA:O	1:A:188:VAL:HG23	2.21	0.41
1:A:7:ARG:N	1:A:8:PRO:HD2	2.36	0.41
1:A:53:ALA:HA	1:A:85:ASP:OD2	2.21	0.41
1:A:111:LEU:HD12	1:A:148:ILE:HG23	2.03	0.41
1:A:141:SER:CB	3:A:250:RET:H41	2.51	0.41
1:A:44:ALA:HA	4:A:260:L3P:H142	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/262 (86%)	209 (93%)	12 (5%)	4 (2%)	8	14

All (4) Ramachandran outliers are listed below:

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Mol	Chain	Res	Type
1	A	7	ARG
1	A	29	VAL
1	A	197	GLY
1	A	73	GLY

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	182/206 (88%)	169 (93%)	13 (7%)	14	28

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	38	ASP
1	A	66	LEU
1	A	89	THR
1	A	93	LEU
1	A	94	LEU
1	A	97	LEU
1	A	101	VAL
1	A	107	THR
1	A	121	THR
1	A	161	GLU
1	A	211	LEU
1	A	227	ARG

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

Mol	Chain	Res	Type
1	A	105	GLN

5.3.3   RNA   ⓘ

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)

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	#$|Z| > 2$
2	GLC	B	1	5,2	11,11,12	3.16	5 (45%)	15,15,17	1.19	1 (6%)
2	MAN	B	2	2	11,11,12	2.36	5 (45%)	15,15,17	3.64	7 (46%)
2	SGA	B	3	2	15,15,16	1.86	6 (40%)	17,22,24	3.59	7 (41%)

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	B	1	5,2	-	2/2/19/22	0/1/1/1
2	MAN	B	2	2	-	2/2/19/22	0/1/1/1
2	SGA	B	3	2	-	2/7/24/27	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	GLC	O5-C1	5.61	1.52	1.43
2	B	1	GLC	O5-C5	5.14	1.53	1.43
2	B	1	GLC	C1-C2	4.97	1.63	1.52
2	B	2	MAN	C2-C3	4.54	1.59	1.52
2	B	1	GLC	C2-C3	4.28	1.58	1.52
2	B	2	MAN	O2-C2	3.82	1.51	1.43
2	B	3	SGA	O1S-S	3.05	1.58	1.45
2	B	3	SGA	O2S-S	3.01	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	MAN	C1-C2	2.79	1.58	1.52
2	B	3	SGA	C2-C3	2.73	1.58	1.52
2	B	3	SGA	O5-C5	2.67	1.48	1.43
2	B	2	MAN	O5-C1	2.66	1.48	1.43
2	B	3	SGA	O3-C3	-2.50	1.41	1.46
2	B	2	MAN	O5-C5	2.28	1.48	1.43
2	B	3	SGA	C1-C2	2.08	1.56	1.52
2	B	1	GLC	C4-C5	2.06	1.57	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	SGA	C3-O3-S	10.86	139.86	118.88
2	B	2	MAN	O6-C6-C5	9.73	144.67	111.29
2	B	2	MAN	C1-O5-C5	5.77	120.00	112.19
2	B	2	MAN	O5-C1-C2	-5.30	102.60	110.77
2	B	3	SGA	O2S-S-O1S	-5.08	91.84	112.22
2	B	3	SGA	O3S-S-O1S	-4.88	91.54	108.49
2	B	3	SGA	C1-C2-C3	-4.72	103.47	109.17
2	B	2	MAN	C2-C3-C4	-3.64	104.59	110.89
2	B	2	MAN	C6-C5-C4	-3.40	105.04	113.00
2	B	3	SGA	O5-C5-C6	3.33	112.42	107.20
2	B	3	SGA	O3S-S-O2S	-2.37	100.26	108.49
2	B	1	GLC	O5-C1-C2	-2.20	107.37	110.77
2	B	2	MAN	C1-C2-C3	2.17	112.33	109.67
2	B	3	SGA	C6-C5-C4	-2.16	107.94	113.00
2	B	2	MAN	O2-C2-C3	2.12	114.38	110.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	SGA	C2-C3-O3-S
2	B	2	MAN	O5-C5-C6-O6
2	B	3	SGA	O5-C5-C6-O6
2	B	2	MAN	C4-C5-C6-O6
2	B	1	GLC	C4-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	MAN	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.
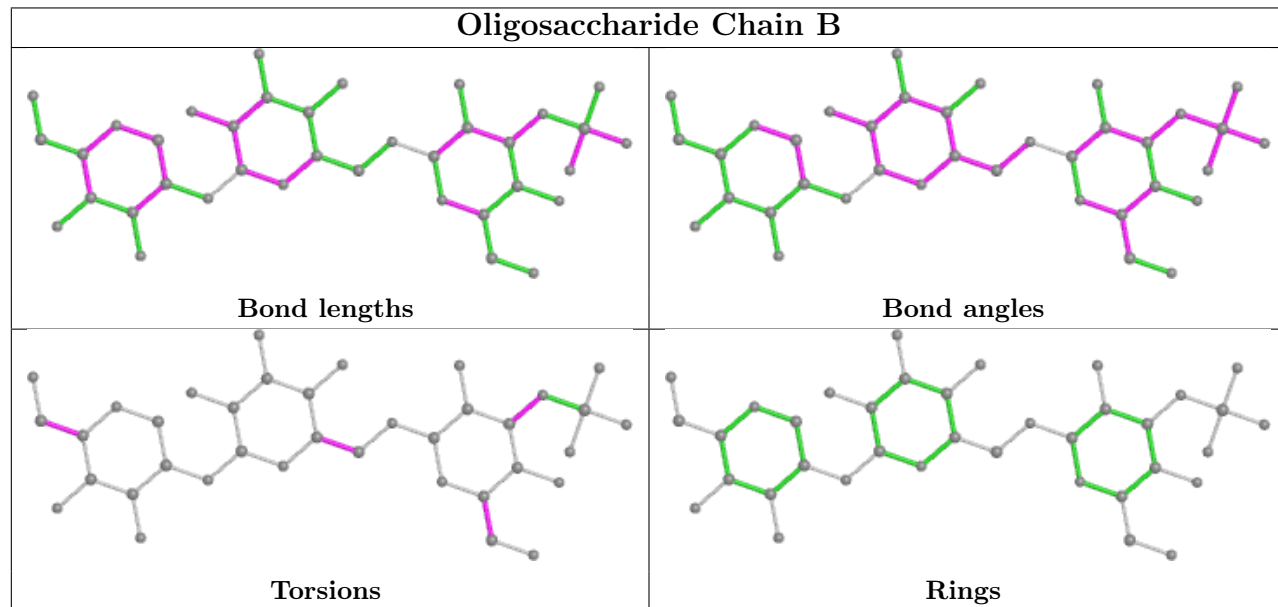
5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 1 is 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	$\#|Z| > 2$
3	RET	A	250	1	20,20,21	2.27	5 (25%)	27,27,28	1.74	8 (29%)
6	L1P	A	290	-	49,49,49	1.77	15 (30%)	57,60,60	1.24	6 (10%)
4	L3P	A	260	-	58,58,58	1.22	8 (13%)	67,73,73	1.28	7 (10%)
5	L2P	A	270	2	45,45,45	1.75	12 (26%)	51,53,53	1.26	5 (9%)
6	L1P	A	300	-	49,49,49	1.66	13 (26%)	57,60,60	1.13	6 (10%)
6	L1P	A	280	-	39,39,49	1.92	12 (30%)	45,48,60	1.03	2 (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
3	RET	A	250	1	-	0/13/30/31	0/1/1/1
6	L1P	A	290	-	-	26/55/55/55	-
4	L3P	A	260	-	-	33/67/67/67	-
5	L2P	A	270	2	-	18/51/51/51	-
6	L1P	A	300	-	-	30/55/55/55	-
6	L1P	A	280	-	-	18/43/43/55	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	250	RET	C1-C6	6.19	1.62	1.53
6	A	280	L1P	O2-C2	5.01	1.57	1.43
3	A	250	RET	C14-C13	4.56	1.37	1.33
3	A	250	RET	C5-C6	4.53	1.42	1.34
6	A	290	L1P	P-O3	4.42	1.74	1.60
6	A	300	L1P	P-O3	4.30	1.74	1.60
6	A	280	L1P	P-O3P	4.06	1.70	1.54
5	A	270	L2P	C26-C25	3.98	1.69	1.52
6	A	280	L1P	C3-C2	3.80	1.62	1.50
5	A	270	L2P	C3-C2	3.52	1.59	1.51
6	A	280	L1P	C1-C2	3.47	1.61	1.50
5	A	270	L2P	C42-C41	3.21	1.61	1.50
6	A	290	L1P	C3-C2	3.17	1.60	1.50
4	A	260	L3P	O2-C41	3.14	1.51	1.43
5	A	270	L2P	C47-C48	3.13	1.69	1.52
6	A	290	L1P	C12-C11	3.10	1.61	1.50
5	A	270	L2P	O2-C41	3.09	1.51	1.43
6	A	300	L1P	C12-C11	3.05	1.61	1.50
4	A	260	L3P	P1-O3	2.95	1.71	1.59
6	A	300	L1P	C3-C2	2.93	1.59	1.50
6	A	290	L1P	P-O3P	2.92	1.66	1.54
6	A	300	L1P	P-O3P	2.85	1.65	1.54
5	A	270	L2P	C24-C23	2.82	1.61	1.52
6	A	280	L1P	O2-C41	2.82	1.50	1.43
3	A	250	RET	C7-C6	2.79	1.55	1.45
6	A	290	L1P	C15-C13	2.71	1.66	1.52
3	A	250	RET	C2-C3	-2.70	1.45	1.52
4	A	260	L3P	O2-C2	2.63	1.51	1.43
6	A	280	L1P	C56-C55	2.59	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	300	L1P	C15-C13	2.57	1.66	1.52
6	A	280	L1P	O1-C1	2.56	1.49	1.42
6	A	290	L1P	O1-C11	2.55	1.53	1.42
4	A	260	L3P	C42-C41	2.51	1.59	1.50
6	A	290	L1P	C55-C53	2.50	1.65	1.52
6	A	290	L1P	C14-C13	2.49	1.60	1.52
6	A	290	L1P	C19-C18	2.47	1.60	1.52
6	A	280	L1P	P-O3	2.45	1.68	1.60
4	A	260	L3P	C6-C5	2.44	1.59	1.51
6	A	290	L1P	C26-C27	2.44	1.62	1.52
6	A	300	L1P	C26-C27	2.41	1.62	1.52
6	A	290	L1P	C17-C18	2.39	1.65	1.52
6	A	300	L1P	C17-C18	2.37	1.65	1.52
5	A	270	L2P	C50-C48	2.36	1.65	1.52
6	A	300	L1P	C55-C53	2.36	1.65	1.52
6	A	290	L1P	C56-C55	2.34	1.62	1.52
6	A	300	L1P	C19-C18	2.32	1.60	1.52
6	A	300	L1P	C14-C13	2.32	1.60	1.52
5	A	270	L2P	O2-C2	2.31	1.50	1.43
6	A	300	L1P	O1-C11	2.31	1.52	1.42
5	A	270	L2P	C25-C23	2.31	1.64	1.52
5	A	270	L2P	C22-C23	2.30	1.64	1.52
6	A	280	L1P	C42-C41	2.30	1.58	1.50
6	A	280	L1P	C52-C53	2.24	1.64	1.52
4	A	260	L3P	P1-O4	2.20	1.68	1.59
4	A	260	L3P	P2-O6	2.19	1.67	1.60
6	A	290	L1P	C54-C53	2.19	1.59	1.52
6	A	290	L1P	C25-C23	2.16	1.63	1.52
6	A	280	L1P	C56-C57	2.12	1.61	1.52
4	A	260	L3P	P1-O2P	-2.08	1.45	1.55
6	A	300	L1P	C56-C55	2.08	1.61	1.52
6	A	290	L1P	C26-C25	2.05	1.60	1.52
5	A	270	L2P	C1-C2	2.04	1.57	1.50
5	A	270	L2P	C56-C57	2.01	1.60	1.52
6	A	300	L1P	C26-C25	2.00	1.60	1.52
6	A	280	L1P	C12-C11	2.00	1.57	1.50

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	290	L1P	O1-C1-C2	5.17	121.60	109.44
4	A	260	L3P	C41-O2-C2	5.03	126.96	115.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	270	L2P	C24-C23-C22	-3.93	97.05	111.29
5	A	270	L2P	C22-C21-C20	-3.62	96.62	113.24
6	A	280	L1P	C51-C50-C48	3.61	127.59	115.92
3	A	250	RET	C1-C6-C7	3.16	124.72	115.78
4	A	260	L3P	O2-C41-C42	3.12	115.31	108.77
5	A	270	L2P	C21-C22-C23	3.02	125.69	115.92
4	A	260	L3P	C46-C45-C43	-3.00	106.22	115.92
6	A	290	L1P	O3P-P-O3	2.89	114.42	106.73
6	A	300	L1P	O3P-P-O3	2.82	114.23	106.73
5	A	270	L2P	C26-C25-C23	-2.78	106.92	115.92
6	A	300	L1P	O1-C1-C2	2.75	115.89	109.44
3	A	250	RET	C8-C9-C10	-2.74	114.74	118.94
4	A	260	L3P	C26-C25-C23	-2.73	107.09	115.92
3	A	250	RET	C2-C3-C4	2.73	117.47	111.38
6	A	300	L1P	C47-C46-C45	-2.67	100.97	113.24
6	A	290	L1P	C47-C46-C45	-2.64	101.11	113.24
3	A	250	RET	C2-C1-C6	2.60	114.48	110.48
3	A	250	RET	C1-C6-C5	-2.54	119.03	122.61
4	A	260	L3P	C51-C50-C48	-2.51	107.81	115.92
6	A	280	L1P	O2-C41-C42	2.45	113.91	108.77
4	A	260	L3P	C11-O1-C1	2.42	124.42	113.61
5	A	270	L2P	C21-C20-C18	2.41	123.70	115.92
6	A	290	L1P	O3-P-O1P	2.36	113.11	106.47
4	A	260	L3P	P2-O6-C6	2.32	124.68	118.30
6	A	300	L1P	O3-P-O1P	2.29	112.89	106.47
6	A	300	L1P	C16-C17-C18	2.25	123.21	115.92
6	A	300	L1P	C21-C20-C18	2.24	123.15	115.92
3	A	250	RET	C19-C9-C8	2.23	121.59	118.08
3	A	250	RET	C16-C1-C6	2.19	113.85	110.30
6	A	290	L1P	C21-C20-C18	2.17	122.92	115.92
3	A	250	RET	C7-C6-C5	-2.16	116.24	121.46
6	A	290	L1P	C16-C17-C18	2.08	122.64	115.92

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	260	L3P	O4-C4-C5-C6
4	A	260	L3P	C4-O4-P1-O1P
4	A	260	L3P	C4-O4-P1-O2P
4	A	260	L3P	C41-C42-C43-C44
5	A	270	L2P	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
6	A	280	L1P	C49-C48-C50-C51
6	A	290	L1P	C3-O3-P-O1P
6	A	290	L1P	C3-O3-P-O2P
6	A	290	L1P	C3-O3-P-O3P
6	A	300	L1P	C3-O3-P-O1P
6	A	300	L1P	C3-O3-P-O2P
6	A	300	L1P	C3-O3-P-O3P
6	A	300	L1P	C16-C17-C18-C19
6	A	290	L1P	C53-C55-C56-C57
4	A	260	L3P	O4-C4-C5-O5
6	A	290	L1P	C48-C50-C51-C52
6	A	300	L1P	C23-C25-C26-C27
5	A	270	L2P	C11-C12-C13-C15
6	A	280	L1P	C45-C46-C47-C48
6	A	280	L1P	C55-C56-C57-C58
4	A	260	L3P	C52-C53-C55-C56
4	A	260	L3P	C25-C26-C27-C28
6	A	290	L1P	C25-C26-C27-C28
6	A	290	L1P	C50-C51-C52-C53
4	A	260	L3P	C23-C25-C26-C27
6	A	300	L1P	C55-C56-C57-C58
4	A	260	L3P	C48-C50-C51-C52
6	A	300	L1P	C43-C45-C46-C47
4	A	260	L3P	C4-O4-P1-O3
6	A	280	L1P	C56-C57-C58-C59
6	A	280	L1P	C16-C17-C18-C19
6	A	290	L1P	C26-C27-C28-C30
6	A	290	L1P	C56-C57-C58-C60
6	A	280	L1P	C44-C43-C45-C46
6	A	280	L1P	C42-C41-O2-C2
6	A	280	L1P	C16-C17-C18-C20
6	A	280	L1P	C56-C57-C58-C60
6	A	290	L1P	C13-C15-C16-C17
6	A	290	L1P	C15-C16-C17-C18
6	A	300	L1P	C15-C16-C17-C18
6	A	290	L1P	C26-C27-C28-C29
6	A	290	L1P	C56-C57-C58-C59
6	A	300	L1P	C2-C3-O3-P
6	A	300	L1P	C45-C46-C47-C48
6	A	280	L1P	O2-C41-C42-C43
4	A	260	L3P	C20-C21-C22-C23
6	A	290	L1P	C45-C46-C47-C48

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Mol	Chain	Res	Type	Atoms
5	A	270	L2P	C17-C18-C20-C21
6	A	280	L1P	C42-C43-C45-C46
5	A	270	L2P	C25-C26-C27-C28
4	A	260	L3P	C21-C22-C23-C24
4	A	260	L3P	C49-C48-C50-C51
4	A	260	L3P	C54-C53-C55-C56
5	A	270	L2P	C19-C18-C20-C21
6	A	300	L1P	C44-C43-C45-C46
4	A	260	L3P	C18-C20-C21-C22
6	A	300	L1P	C26-C27-C28-C30
6	A	300	L1P	C26-C27-C28-C29
6	A	300	L1P	O1-C11-C12-C13
4	A	260	L3P	C53-C55-C56-C57
6	A	300	L1P	C50-C51-C52-C53
6	A	300	L1P	C56-C57-C58-C59
4	A	260	L3P	C21-C22-C23-C25
4	A	260	L3P	C22-C23-C25-C26
4	A	260	L3P	C47-C48-C50-C51
6	A	280	L1P	C12-C13-C15-C16
6	A	290	L1P	C52-C53-C55-C56
6	A	300	L1P	C16-C17-C18-C20
6	A	300	L1P	C42-C43-C45-C46
4	A	260	L3P	C19-C18-C20-C21
4	A	260	L3P	C24-C23-C25-C26
4	A	260	L3P	C44-C43-C45-C46
5	A	270	L2P	C16-C17-C18-C19
6	A	280	L1P	C14-C13-C15-C16
6	A	300	L1P	C51-C52-C53-C54
4	A	260	L3P	C42-C41-O2-C2
6	A	280	L1P	C43-C45-C46-C47
4	A	260	L3P	C1-C2-C3-O3
6	A	290	L1P	C1-C2-C3-O3
5	A	270	L2P	O1-C1-C2-C3
6	A	290	L1P	O1-C1-C2-C3
6	A	300	L1P	C46-C47-C48-C49
6	A	300	L1P	C56-C57-C58-C60
4	A	260	L3P	C17-C18-C20-C21
4	A	260	L3P	C42-C43-C45-C46
6	A	280	L1P	C47-C48-C50-C51
6	A	300	L1P	C2-C1-O1-C11
4	A	260	L3P	O2-C2-C3-O3
6	A	280	L1P	C12-C11-O1-C1

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Mol	Chain	Res	Type	Atoms
5	A	270	L2P	O1-C1-C2-O2
5	A	270	L2P	C12-C13-C15-C16
5	A	270	L2P	C16-C17-C18-C20
6	A	290	L1P	O2-C2-C3-O3
6	A	300	L1P	C46-C47-C48-C50
6	A	300	L1P	C51-C52-C53-C55
4	A	260	L3P	C41-C42-C43-C45
4	A	260	L3P	C26-C27-C28-C29
5	A	270	L2P	C26-C27-C28-C30
6	A	290	L1P	O1-C1-C2-O2
5	A	270	L2P	C26-C27-C28-C29
6	A	290	L1P	C54-C53-C55-C56
4	A	260	L3P	C26-C27-C28-C30
4	A	260	L3P	C3-O3-P1-O4
6	A	300	L1P	C12-C11-O1-C1
5	A	270	L2P	C14-C13-C15-C16
4	A	260	L3P	C12-C11-O1-C1
4	A	260	L3P	C50-C51-C52-C53
6	A	290	L1P	C42-C43-C45-C46
5	A	270	L2P	C45-C46-C47-C48
5	A	270	L2P	C55-C56-C57-C58
6	A	290	L1P	C55-C56-C57-C58
6	A	290	L1P	C42-C41-O2-C2
5	A	270	L2P	O2-C2-C3-O3
5	A	270	L2P	C50-C51-C52-C53
6	A	290	L1P	C44-C43-C45-C46
6	A	300	L1P	C49-C48-C50-C51
6	A	300	L1P	C41-C42-C43-C45
5	A	270	L2P	C51-C52-C53-C54
6	A	290	L1P	C12-C11-O1-C1
6	A	280	L1P	O1-C11-C12-C13
6	A	300	L1P	C21-C22-C23-C24
6	A	290	L1P	C23-C25-C26-C27
6	A	300	L1P	C21-C22-C23-C25
6	A	300	L1P	C47-C48-C50-C51
6	A	280	L1P	C50-C51-C52-C53

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	250	RET	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	260	L3P	5	0
5	A	270	L2P	7	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 RET A 250

Bond lengths

Bond angles

Torsions

Rings

Ligand L1P A 290

Bond lengths

Bond angles

Torsions

Rings

Ligand L3P A 260

Bond lengths

Bond angles

Torsions

Rings

Ligand L2P A 270

Bond lengths

Bond angles

Torsions

Rings

Ligand L1P A 300

Bond lengths

Bond angles

Torsions

Rings

Ligand L1P A 280

Bond lengths

Bond angles

Torsions

Rings
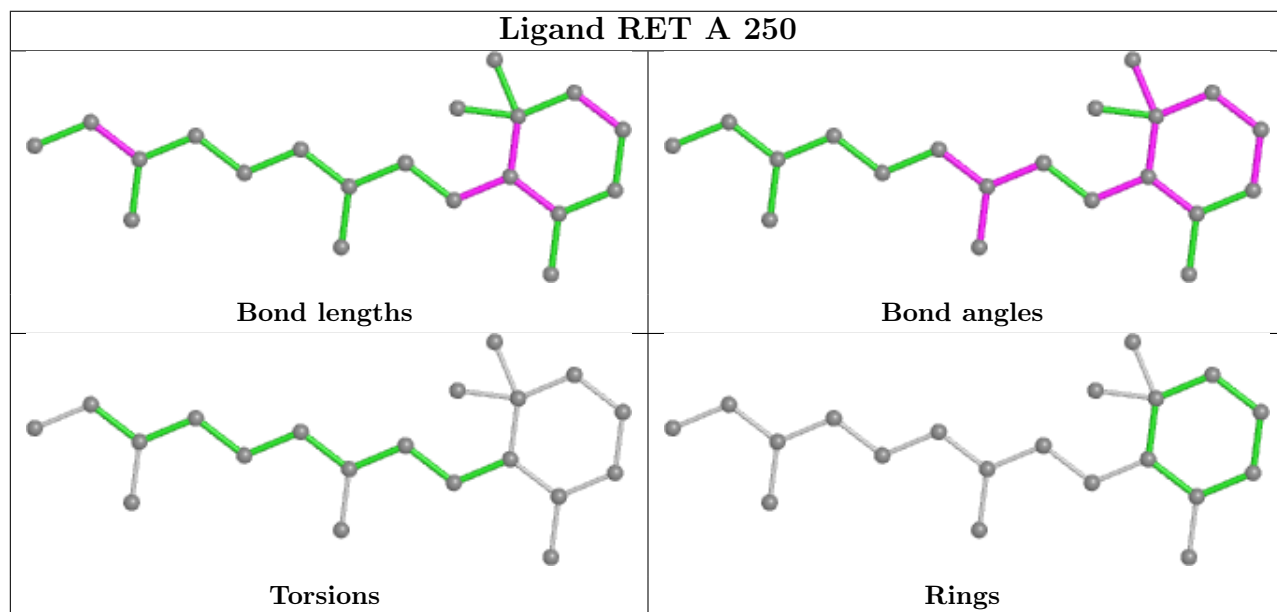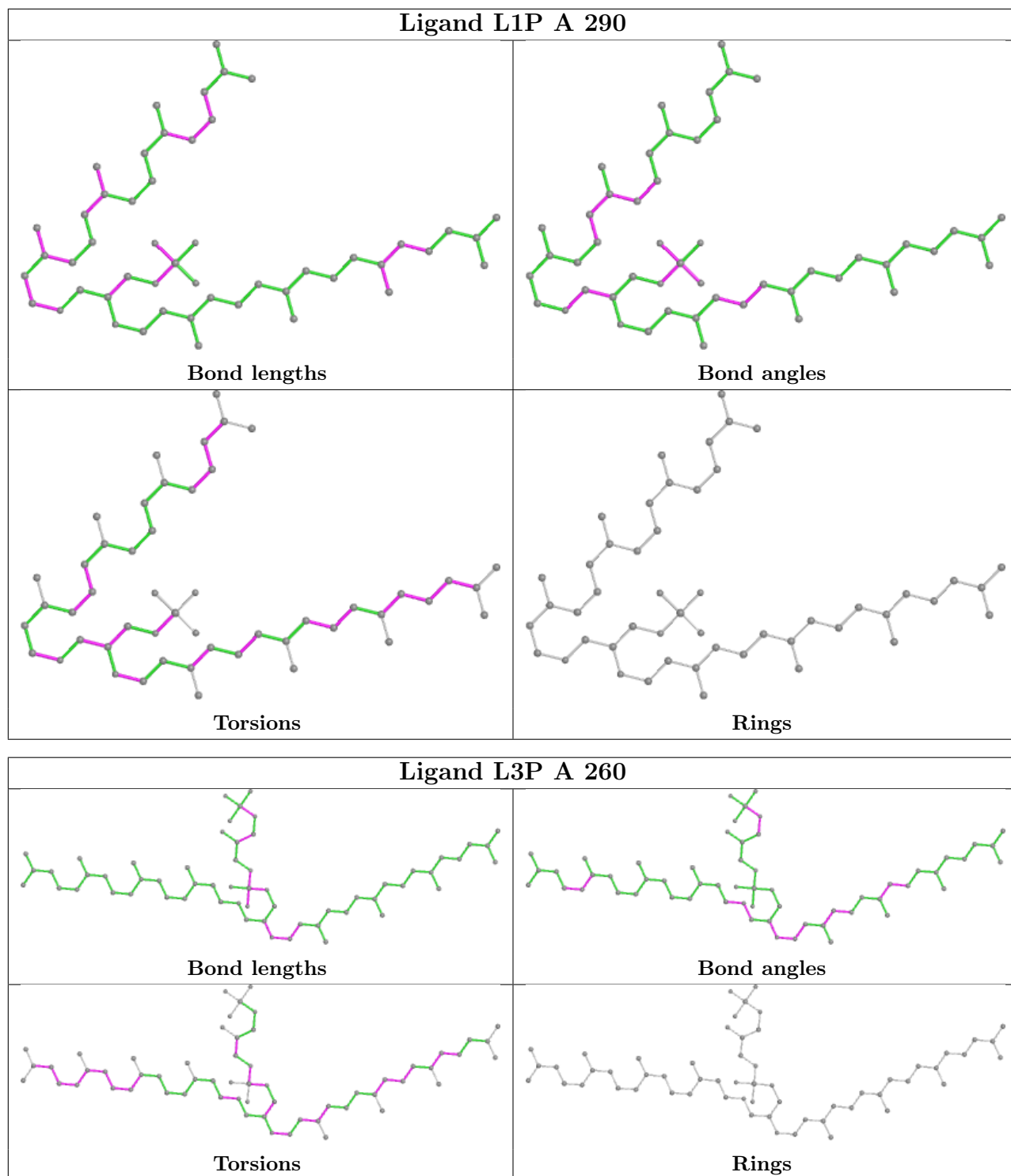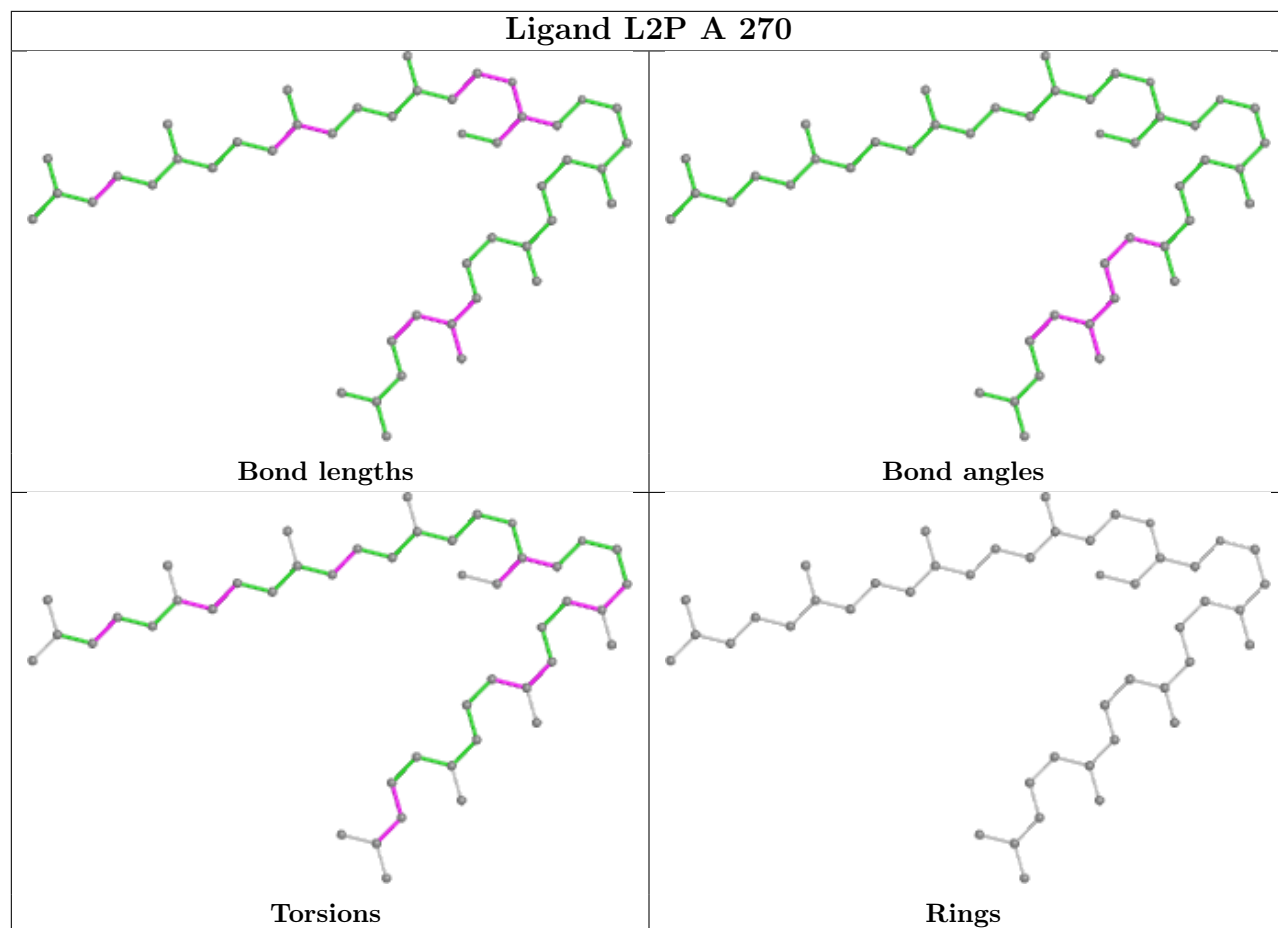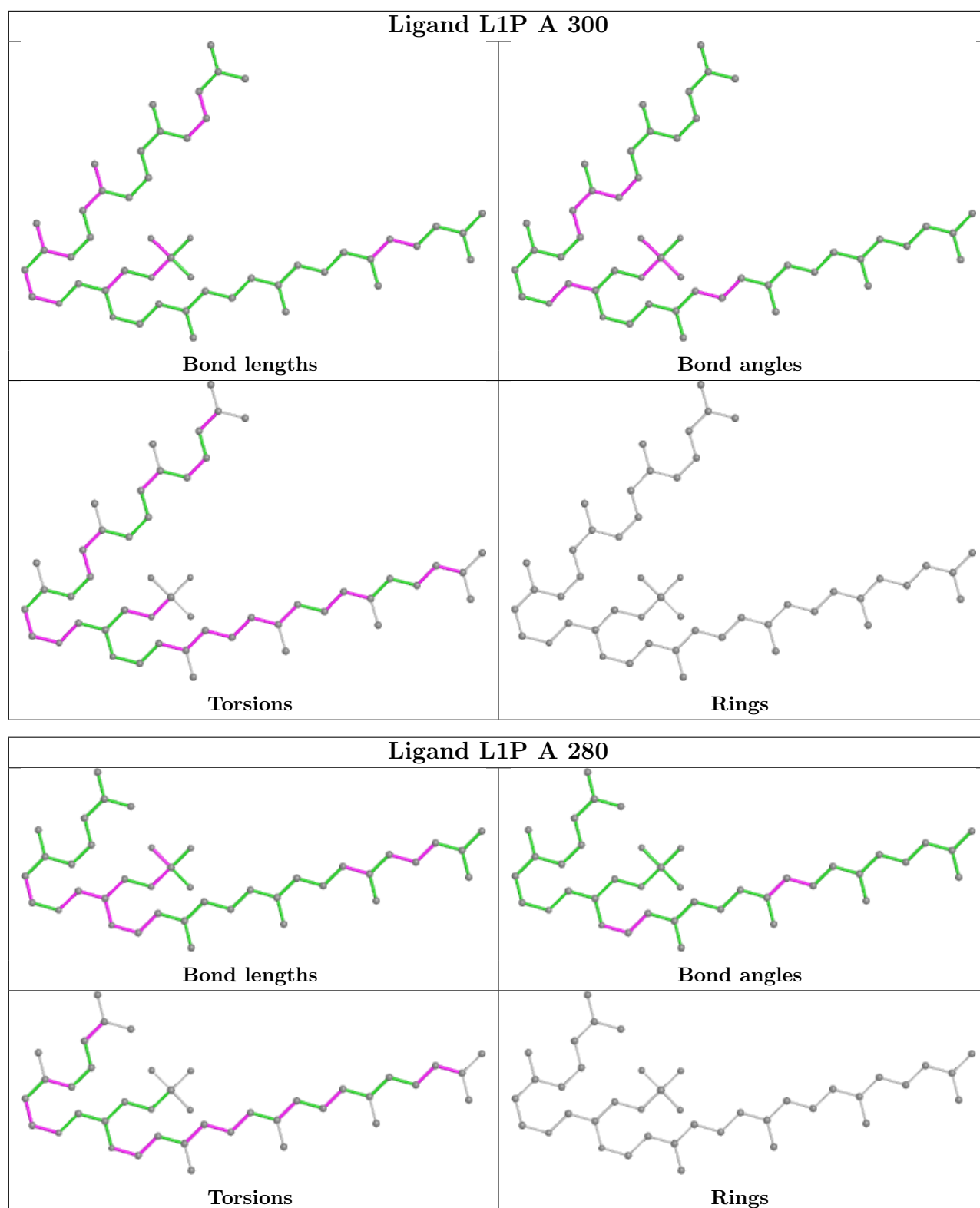
5.7 Other polymers ⓘ

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, 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	227/262 (86%)	0.36	21 (9%)	8	8	33, 44, 66, 88	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	THR	11.9
1	A	72	GLY	5.6
1	A	74	GLU	4.4
1	A	196	ALA	4.0
1	A	6	GLY	3.5
1	A	73	GLY	3.5
1	A	203	ILE	3.1
1	A	198	ILE	2.6
1	A	71	PHE	2.6
1	A	12	TRP	2.5
1	A	227	ARG	2.5
1	A	158	SER	2.3
1	A	192	GLY	2.3
1	A	7	ARG	2.3
1	A	231	GLY	2.2
1	A	84	ALA	2.2
1	A	33	GLY	2.1
1	A	191	ILE	2.1
1	A	76	ASN	2.1
1	A	199	VAL	2.1
1	A	225	ARG	2.0

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

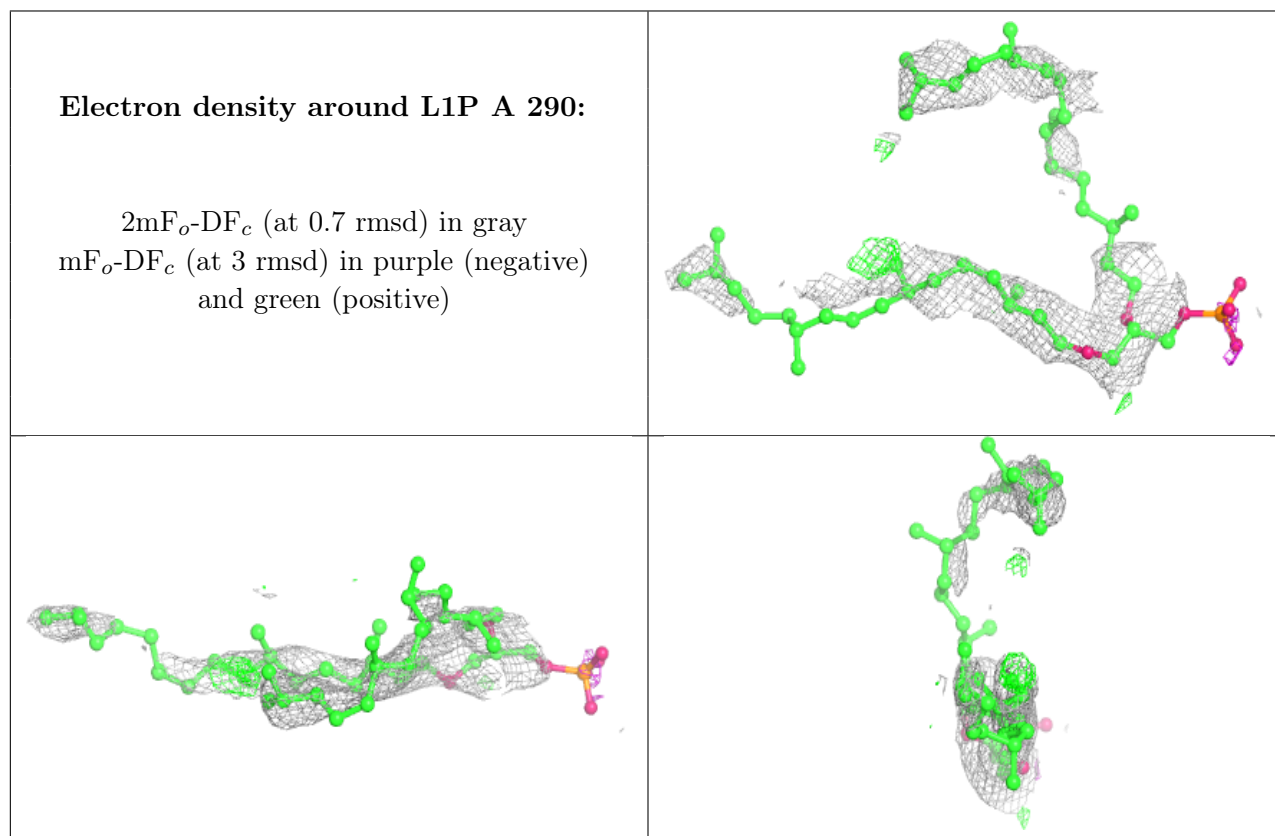There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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($Å^2$)	Q<0.9
2	SGA	B	3	15/16	0.09	0.79	106,107,113,113	0
2	MAN	B	2	11/12	0.80	0.26	95,97,101,104	0
2	GLC	B	1	11/12	0.81	0.29	89,90,91,92	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.
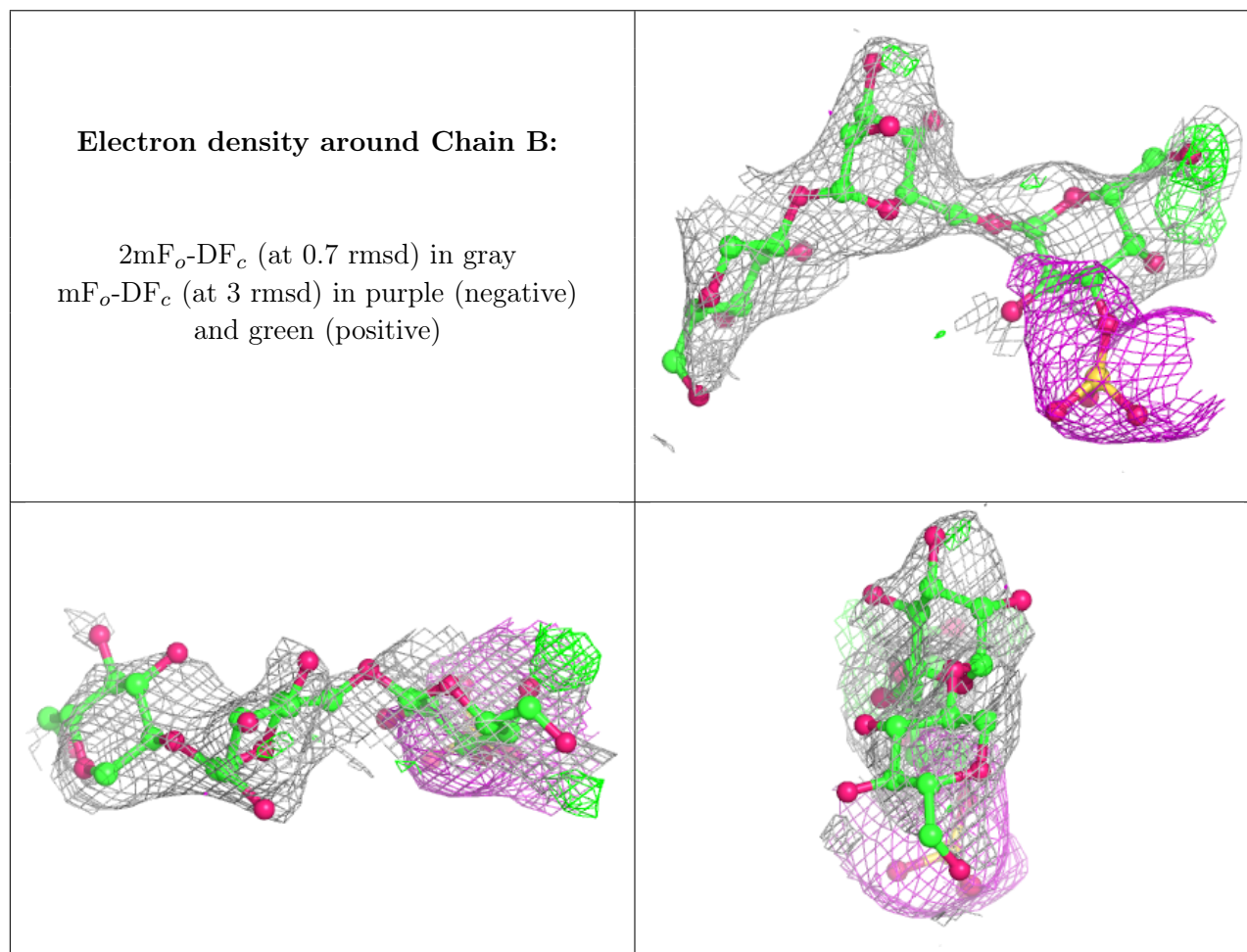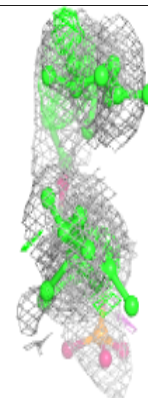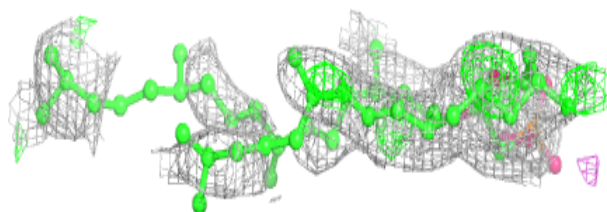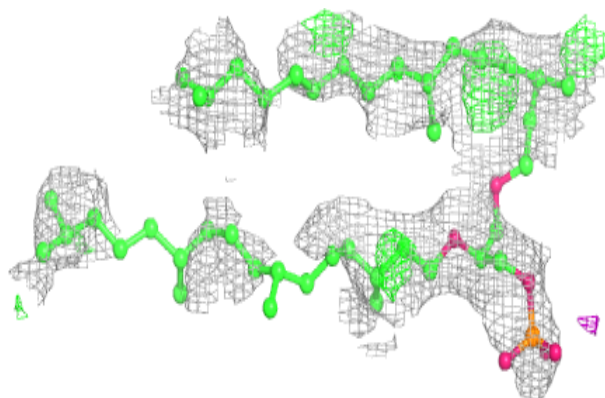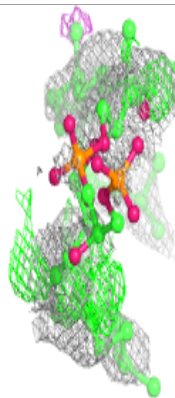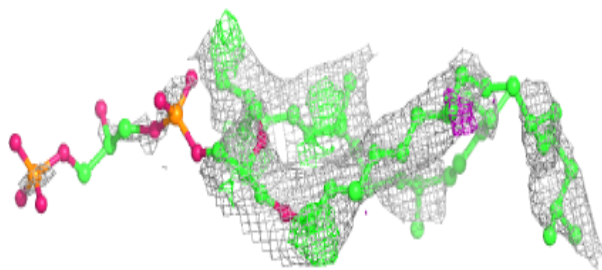

Electron density around Chain B:

$2mF_o$-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, 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(Å^2)	Q<0.9
6	L1P	A	290	50/50	0.27	0.53	120,130,140,141	0
6	L1P	A	280	40/50	0.37	0.49	108,124,128,129	0
6	L1P	A	300	50/50	0.43	0.47	112,122,126,126	0
4	L3P	A	260	59/59	0.59	0.49	67,92,104,105	13
5	L2P	A	270	46/46	0.69	0.65	67,86,114,114	0
3	RET	A	250	20/21	0.92	0.19	34,40,43,44	0
7	XE	A	638	1/1	0.97	0.09	44,44,44,44	1

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 L1P A 290:

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

Electron density around L1P A 280:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
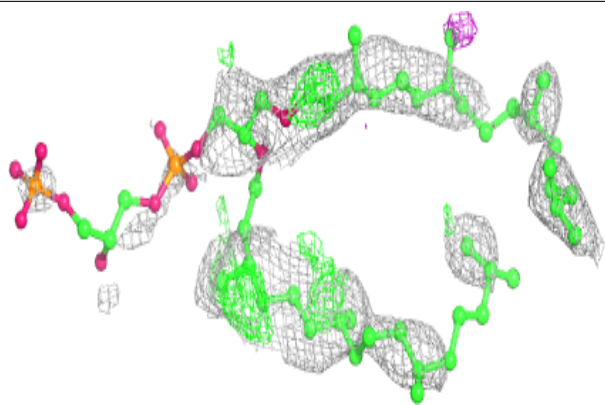and green (positive)
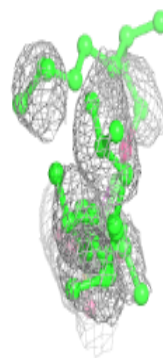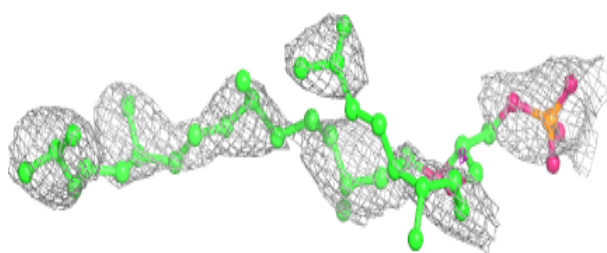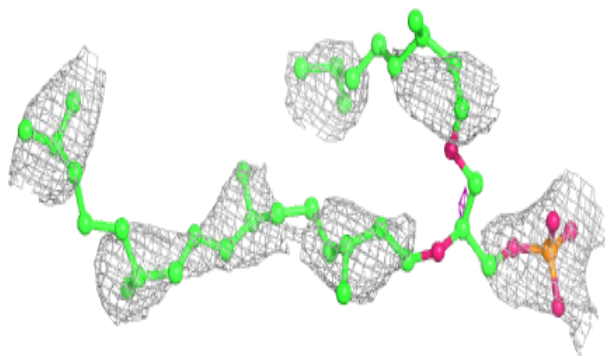
Electron density around L1P A 300:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
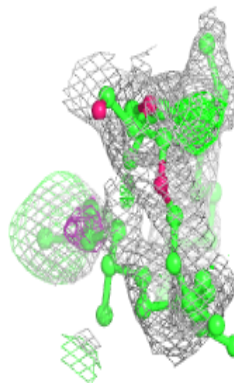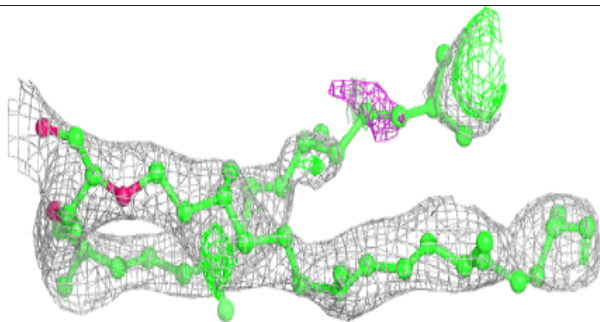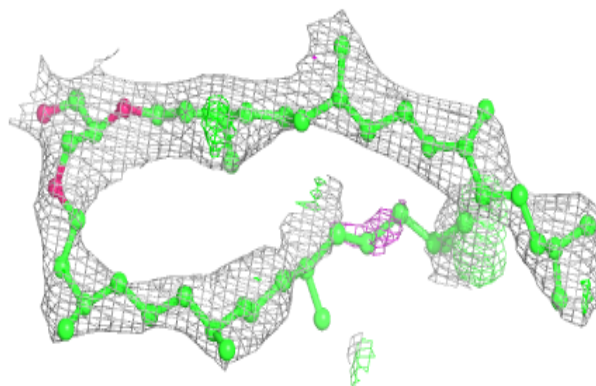mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
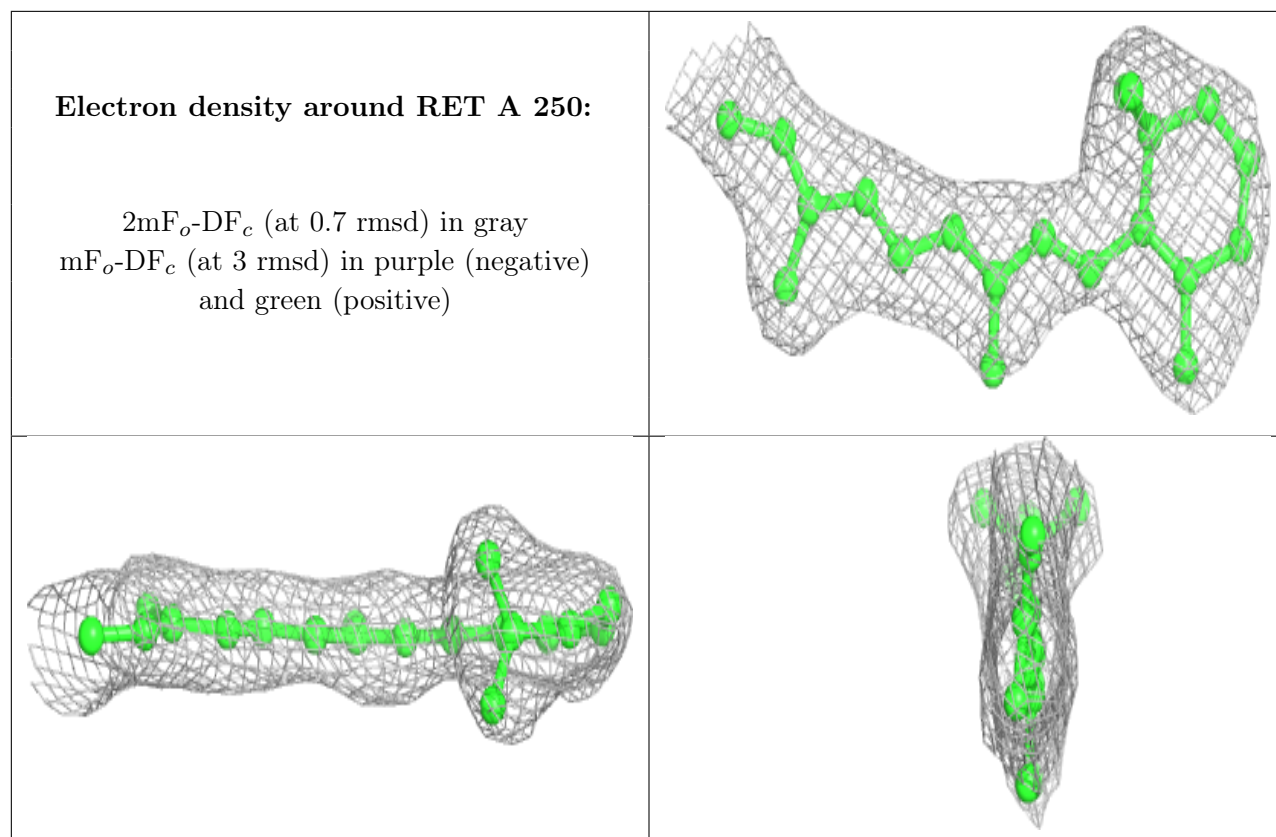and green (positive)

Electron density around L3P A 260:

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

Electron density around L2P A 270:

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

Electron density around RET A 250:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.