



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:21 PM UTC

PDB ID : 2RH1 / pdb_00002rh1
Title : High resolution crystal structure of human B2-adrenergic G protein-coupled receptor.
Authors : Cherezov, V.; Rosenbaum, D.M.; Hanson, M.A.; Rasmussen, S.G.F.; Thian, F.S.; Kobilka, T.S.; Choi, H.J.; Kuhn, P.; Weis, W.I.; Kobilka, B.K.; Stevens, R.C.; Accelerated Technologies Center for Gene to 3D Structure (ATCG3D); GPCR Network (GPCR)
Deposited on : 2007-10-05
Resolution : 2.40 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

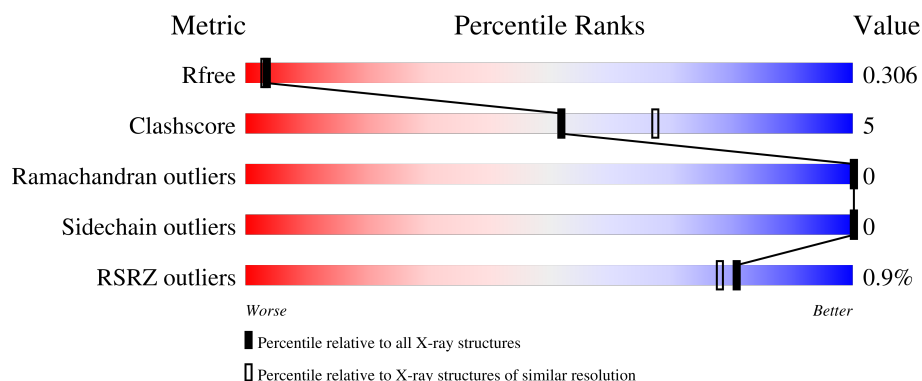
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

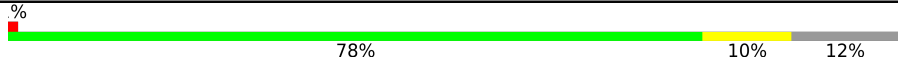
The reported resolution of this entry is 2.40 Å.

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. 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	500	
2	B	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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
2	GLC	B	1	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 3804 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 beta-2-adrenergic receptor/T4-lysozyme chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3543	2315	590	614	24			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	expression tag	UNP P07550
A	-5	TYR	-	expression tag	UNP P07550
A	-4	LYS	-	expression tag	UNP P07550
A	-3	ASP	-	expression tag	UNP P07550
A	-2	ASP	-	expression tag	UNP P07550
A	-1	ASP	-	expression tag	UNP P07550
A	0	ALA	-	expression tag	UNP P07550
A	187	GLU	ASN	engineered mutation	UNP P07550
A	1054	THR	CYS	engineered mutation	UNP P00720
A	1097	ALA	CYS	engineered mutation	UNP P00720

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



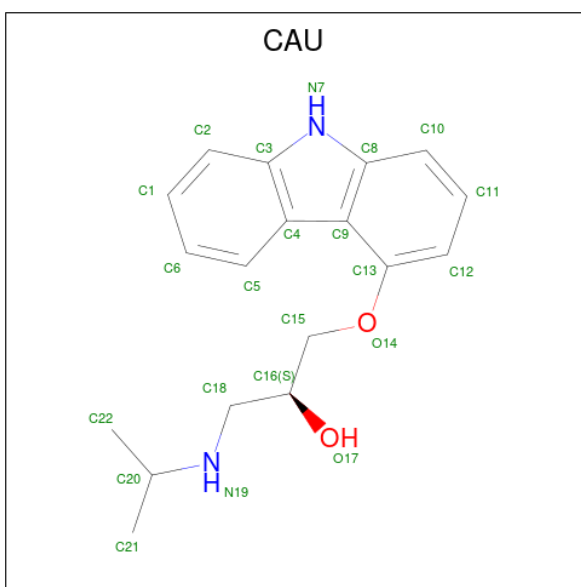
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



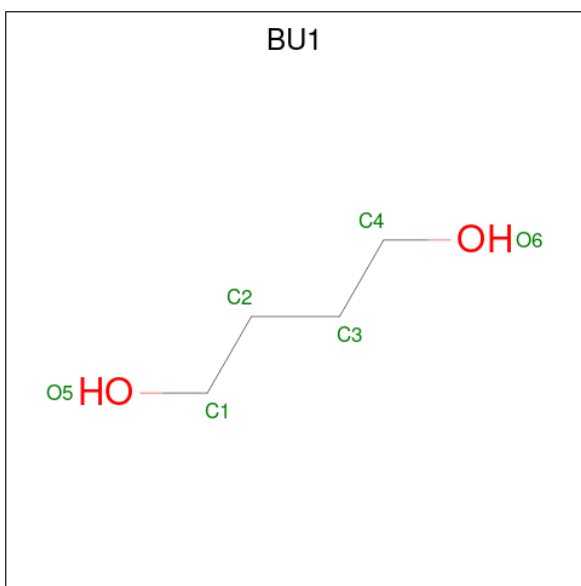
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (2S)-1-(9H-Carbazol-4-yloxy)-3-(isopropylamino)propan-2-ol (CCD ID: CAU) (formula: C₁₈H₂₂N₂O₂).



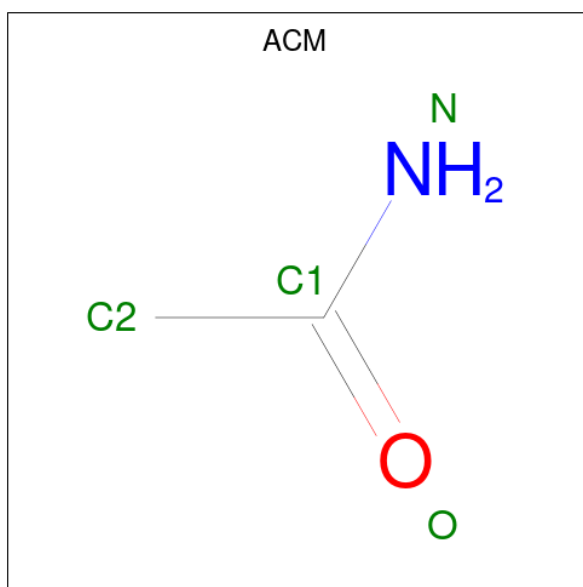
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	18	2	2		

- Molecule 5 is 1,4-BUTANEDIOL (CCD ID: BU1) (formula: $C_4H_{10}O_2$).



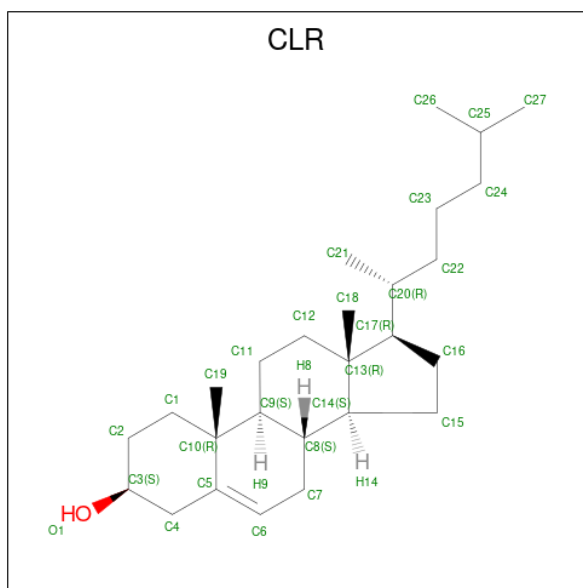
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		
5	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is ACETAMIDE (CCD ID: ACM) (formula: C_2H_5NO).



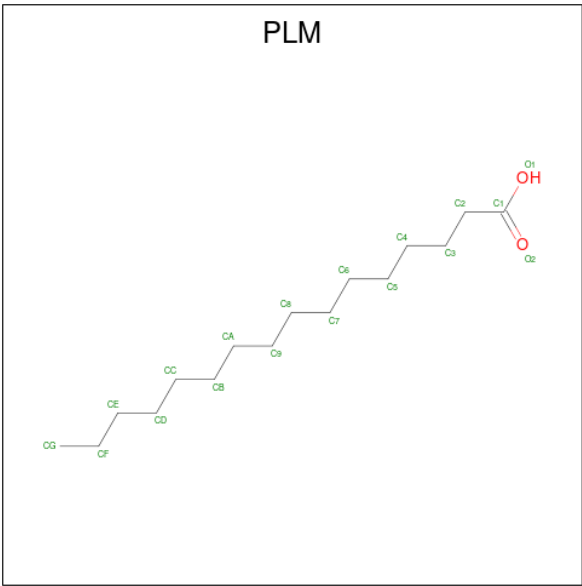
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



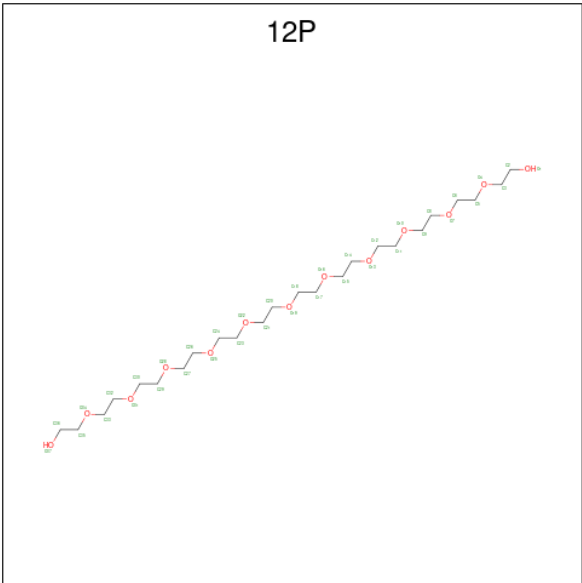
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			28	27	1		
7	A	1	Total	C	O	0	0
			28	27	1		
7	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 8 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			17	16	1		

- Molecule 9 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: C₂₄H₅₀O₁₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			21	14	7		

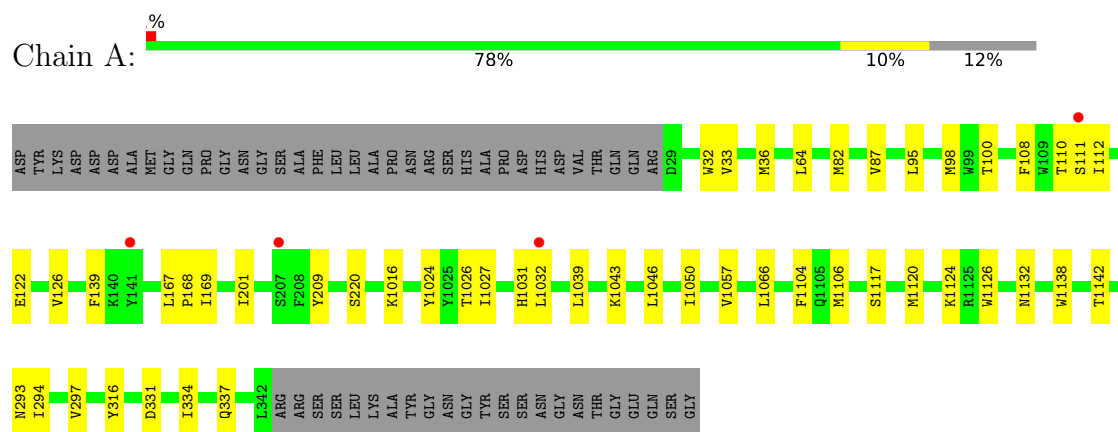
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	48	Total 48	O 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: beta-2-adrenergic receptor/T4-lysozyme chimera



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-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	106.32Å 169.24Å 40.15Å 90.00° 105.62° 90.00°	Depositor
Resolution (Å)	19.95 – 2.40 19.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.95-2.40) 99.6 (19.95-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.232 (Not available) , 0.306	Depositor DCC
R_{free} test set	1310 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 86.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for 1/2*h+1/2*k+l,3/2*h-1/2*k+l,-l 0.015 for 1/2*h-1/2*k+l,-3/2*h-1/2*k-l,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3804	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, ACM, BU1, CAU, GLC, SO4, 12P, 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	0.82	1/3624 (0.0%)	1.00	4/4920 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	VAL	CA-CB	6.55	1.58	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	PHE	N-CA-C	-7.20	101.58	110.65
1	A	220	SER	N-CA-C	-5.42	105.45	111.36
1	A	1142	THR	CA-C-N	5.06	124.23	118.97
1	A	1142	THR	C-N-CA	5.06	124.23	118.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3543	0	3610	30	0
2	B	23	0	21	1	0
3	A	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	22	0	22	0	0
5	A	12	0	20	0	0
6	A	4	0	3	0	0
7	A	84	0	138	9	0
8	A	17	0	31	0	0
9	A	21	0	24	0	0
10	A	48	0	0	0	0
All	All	3804	0	3869	39	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 (39) 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:1124:LYS:HD3	1:A:1126:TRP:CZ2	2.22	0.74
1:A:82:MET:HE1	1:A:316:TYR:CD2	2.30	0.66
1:A:334:ILE:HA	1:A:337:GLN:HE21	1.65	0.62
1:A:1106:MET:HE2	1:A:1138:TRP:CD1	2.35	0.61
7:A:412:CLR:H272	7:A:414:CLR:H262	1.84	0.60
7:A:412:CLR:H272	7:A:414:CLR:C26	2.32	0.59
1:A:82:MET:HE1	1:A:316:TYR:HD2	1.68	0.58
7:A:413:CLR:H212	7:A:413:CLR:H183	1.86	0.57
1:A:201:ILE:HD11	1:A:297:VAL:HG11	1.87	0.57
1:A:110:THR:HG22	1:A:169:ILE:HD13	1.86	0.56
1:A:209:TYR:CE1	1:A:294:ILE:HD11	2.42	0.55
7:A:414:CLR:H212	7:A:414:CLR:H121	1.90	0.54
1:A:98:MET:SD	1:A:100:THR:HG22	2.48	0.53
1:A:1124:LYS:HD3	1:A:1126:TRP:CH2	2.45	0.52
1:A:1117:SER:HA	1:A:1120:MET:HE3	1.93	0.51
1:A:108:PHE:HE2	1:A:112:ILE:HD11	1.76	0.51
1:A:108:PHE:CE2	1:A:112:ILE:HD11	2.46	0.51
1:A:32:TRP:CZ2	1:A:36:MET:HE3	2.47	0.49
1:A:1039:LEU:HD21	1:A:1043:LYS:HZ3	1.77	0.49
1:A:1104:PHE:O	2:B:1:GLC:H4	2.13	0.48
1:A:1026:THR:HG23	1:A:1031:HIS:O	2.14	0.47
1:A:1024:TYR:HB3	1:A:1032:LEU:HD11	1.97	0.47
1:A:122:GLU:O	1:A:126:VAL:HG23	2.15	0.46
1:A:1016:LYS:HG2	1:A:1057:VAL:HG22	1.97	0.46
1:A:64:LEU:HD21	1:A:331:ASP:HB3	1.98	0.45
7:A:414:CLR:C22	7:A:414:CLR:H263	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:VAL:HG13	1:A:95:LEU:HD22	1.99	0.44
1:A:1120:MET:HE1	1:A:1132:ASN:CG	2.42	0.44
7:A:412:CLR:H193	7:A:414:CLR:C6	2.46	0.44
7:A:412:CLR:H182	7:A:414:CLR:H71	2.00	0.44
7:A:412:CLR:C19	7:A:414:CLR:C6	2.96	0.43
1:A:201:ILE:CD1	1:A:297:VAL:HG11	2.48	0.43
1:A:1050:ILE:HD11	1:A:1066:LEU:HD11	2.02	0.42
1:A:293:ASN:O	1:A:297:VAL:HG23	2.20	0.42
1:A:1027:ILE:HG21	1:A:1046:LEU:HD13	2.02	0.42
1:A:111:SER:HA	1:A:169:ILE:HD12	2.02	0.41
1:A:167:LEU:HB2	1:A:168:PRO:HD3	2.02	0.41
7:A:414:CLR:H263	7:A:414:CLR:H222	2.03	0.41
1:A:82:MET:HE3	1:A:82:MET:HB3	1.91	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	440/500 (88%)	431 (98%)	9 (2%)	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	382/428 (89%)	382 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	1053	ASN
1	A	1123	GLN
1	A	1132	ASN
1	A	1141	GLN
1	A	296	HIS
1	A	337	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	B	1	2	12,12,12	0.96	1 (8%)	17,17,17	1.39	2 (11%)
2	GLC	B	2	2	11,11,12	1.45	2 (18%)	15,15,17	2.86	6 (40%)

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	2	1/1/5/5	2/2/22/22	0/1/1/1
2	GLC	B	2	2	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GLC	O2-C2	3.61	1.50	1.43
2	B	2	GLC	O5-C5	2.24	1.47	1.43
2	B	1	GLC	O4-C4	2.20	1.48	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GLC	C2-C3-C4	-6.95	98.64	110.86
2	B	2	GLC	O5-C1-C2	-5.19	98.41	110.79
2	B	2	GLC	C1-O5-C5	4.21	117.83	112.19
2	B	1	GLC	O3-C3-C2	-3.58	101.93	110.38
2	B	2	GLC	O2-C2-C1	2.64	115.27	109.22
2	B	2	GLC	C1-C2-C3	2.42	113.17	109.64
2	B	2	GLC	O5-C5-C4	2.11	115.95	110.83
2	B	1	GLC	C1-C2-C3	2.07	114.58	110.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	GLC	C1

All (4) torsion outliers are listed below:

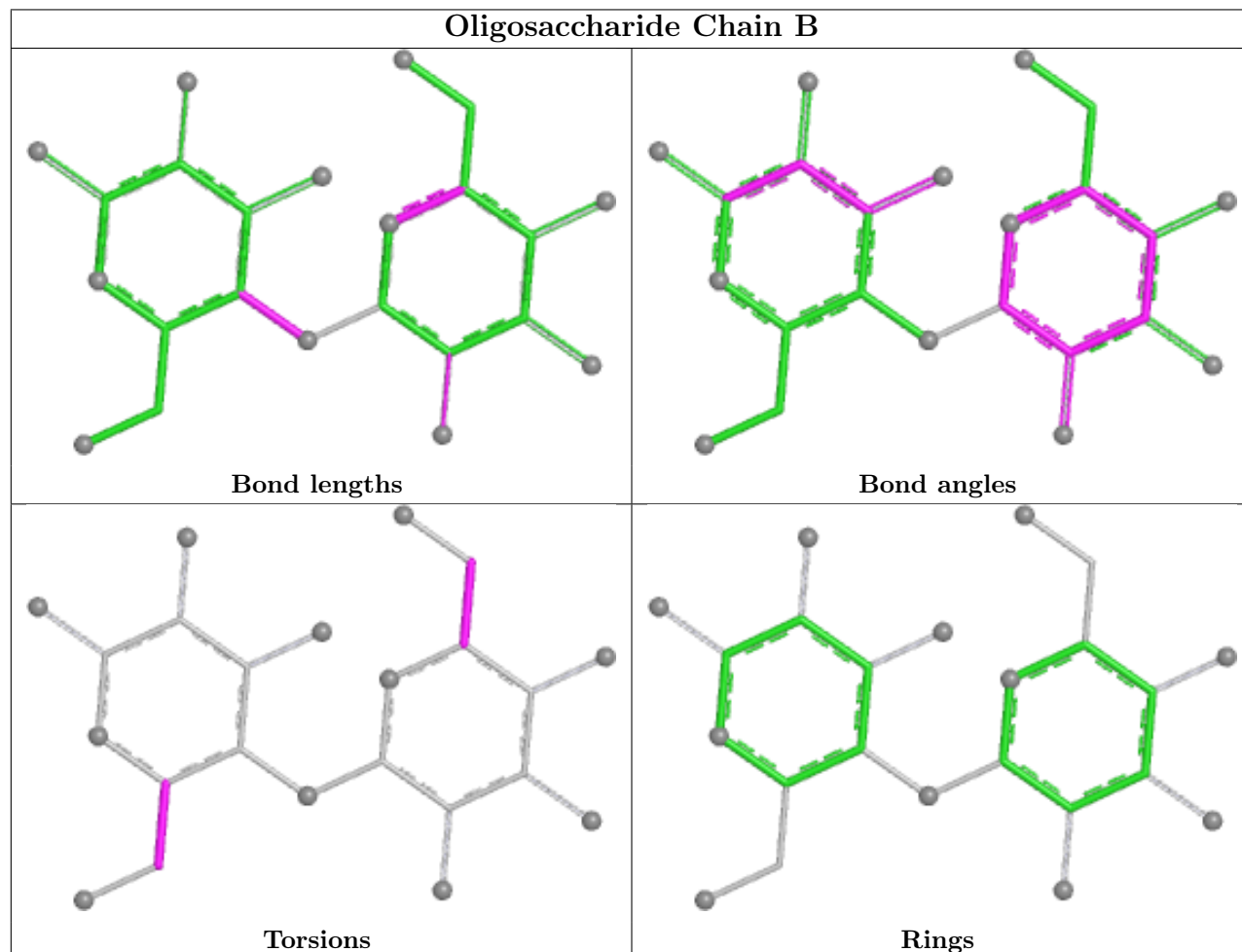
Mol	Chain	Res	Type	Atoms
2	B	2	GLC	O5-C5-C6-O6
2	B	1	GLC	O5-C5-C6-O6
2	B	1	GLC	C4-C5-C6-O6
2	B	2	GLC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	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 [i](#)

15 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
3	SO4	A	407	-	4,4,4	0.28	0	6,6,6	0.11	0
3	SO4	A	406	-	4,4,4	0.26	0	6,6,6	0.20	0
7	CLR	A	412	-	31,31,31	0.92	1 (3%)	48,48,48	1.30	5 (10%)
3	SO4	A	403	-	4,4,4	0.36	0	6,6,6	0.54	0
9	12P	A	416	-	20,20,36	0.61	0	19,19,35	0.53	0
3	SO4	A	404	-	4,4,4	0.23	0	6,6,6	0.34	0
5	BU1	A	409	-	5,5,5	0.18	0	4,4,4	0.39	0
4	CAU	A	408	-	24,24,24	1.56	3 (12%)	33,33,33	1.86	10 (30%)
6	ACM	A	411	1	3,3,3	0.77	0	3,3,3	0.46	0
7	CLR	A	413	-	31,31,31	0.70	0	48,48,48	1.18	5 (10%)
8	PLM	A	415	1	15,16,17	0.45	0	14,15,17	0.49	0
7	CLR	A	414	-	31,31,31	0.64	0	48,48,48	1.02	3 (6%)
5	BU1	A	410	-	5,5,5	0.45	0	4,4,4	0.22	0
3	SO4	A	405	-	4,4,4	0.24	0	6,6,6	0.25	0
3	SO4	A	402	-	4,4,4	0.29	0	6,6,6	0.45	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
7	CLR	A	412	-	-	4/10/68/68	0/4/4/4
9	12P	A	416	-	-	8/18/18/34	-
7	CLR	A	413	-	-	4/10/68/68	0/4/4/4
5	BU1	A	409	-	-	1/3/3/3	-
4	CAU	A	408	-	-	0/10/10/10	0/3/3/3
7	CLR	A	414	-	-	0/10/68/68	0/4/4/4
5	BU1	A	410	-	-	2/3/3/3	-
8	PLM	A	415	1	-	8/14/14/15	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	408	CAU	C4-C9	-4.50	1.36	1.46
4	A	408	CAU	C9-C8	4.24	1.46	1.41
4	A	408	CAU	C4-C3	3.23	1.46	1.41
7	A	412	CLR	C19-C10	-2.66	1.50	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	412	CLR	C19-C10-C5	-4.30	101.81	108.38
7	A	413	CLR	C3-C4-C5	-4.14	105.45	112.05
4	A	408	CAU	C2-C3-N7	3.97	134.74	129.07
4	A	408	CAU	C10-C8-N7	3.54	134.12	129.07
4	A	408	CAU	O14-C13-C9	3.51	121.05	115.52
4	A	408	CAU	C2-C3-C4	-3.40	118.14	121.68
4	A	408	CAU	C10-C8-C9	-3.36	118.31	122.37
7	A	412	CLR	C2-C3-C4	3.35	115.00	110.29
4	A	408	CAU	C8-C9-C13	2.90	121.43	118.64
7	A	412	CLR	C4-C5-C10	2.72	119.91	116.42
4	A	408	CAU	C15-O14-C13	2.69	124.19	118.21
7	A	412	CLR	C17-C13-C14	2.54	103.01	100.10
7	A	413	CLR	O1-C3-C2	2.51	116.74	110.17
4	A	408	CAU	C12-C13-C9	-2.47	117.51	121.10
7	A	414	CLR	C19-C10-C5	-2.47	104.61	108.38
7	A	414	CLR	C4-C5-C10	2.28	119.34	116.42
4	A	408	CAU	C18-N19-C20	2.27	121.32	114.38
7	A	413	CLR	C19-C10-C5	-2.24	104.96	108.38
7	A	413	CLR	C21-C20-C17	2.22	116.22	112.88
7	A	413	CLR	C7-C8-C9	2.22	112.28	109.72
7	A	412	CLR	C1-C10-C9	2.19	111.64	108.74
7	A	414	CLR	C16-C17-C20	2.13	115.40	112.18
4	A	408	CAU	C9-C4-C3	2.01	108.15	106.21

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	415	PLM	O2-C1-C2-C3
9	A	416	12P	O31-C32-C33-O34
7	A	412	CLR	C21-C20-C22-C23
7	A	412	CLR	C22-C23-C24-C25
7	A	413	CLR	C22-C23-C24-C25
7	A	413	CLR	C17-C20-C22-C23
8	A	415	PLM	CA-CB-CC-CD
8	A	415	PLM	C9-CA-CB-CC
8	A	415	PLM	C5-C6-C7-C8
9	A	416	12P	O16-C17-C18-O19
8	A	415	PLM	C2-C3-C4-C5
5	A	410	BU1	C2-C3-C4-O6
8	A	415	PLM	C7-C8-C9-CA
9	A	416	12P	C20-C21-O22-C23
7	A	413	CLR	C21-C20-C22-C23

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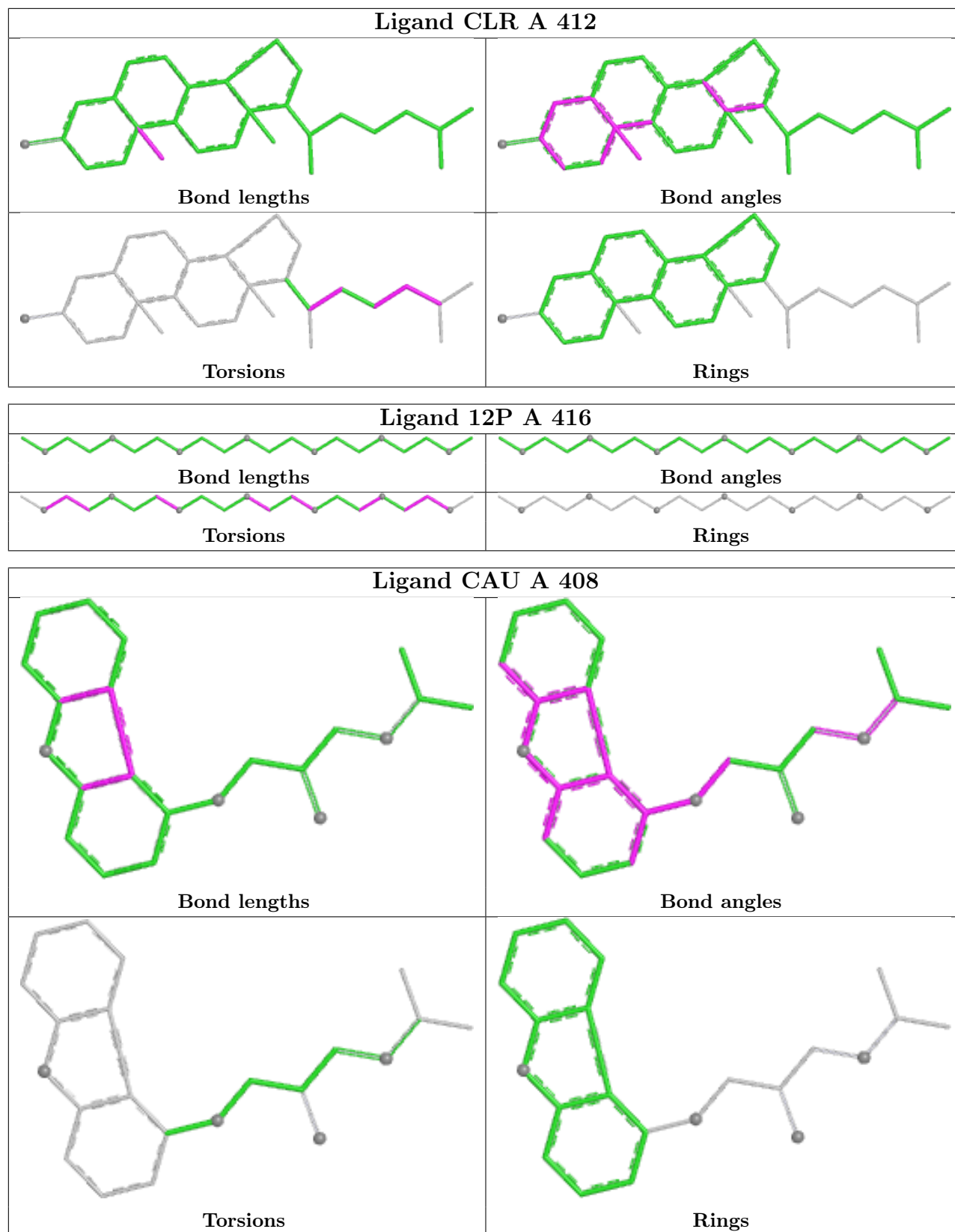
Mol	Chain	Res	Type	Atoms
7	A	412	CLR	C23-C24-C25-C26
7	A	412	CLR	C23-C24-C25-C27
8	A	415	PLM	C1-C2-C3-C4
9	A	416	12P	C27-C26-O25-C24
5	A	410	BU1	C1-C2-C3-C4
8	A	415	PLM	C8-C9-CA-CB
5	A	409	BU1	C1-C2-C3-C4
9	A	416	12P	C18-C17-O16-C15
9	A	416	12P	C32-C33-O34-C35
9	A	416	12P	C29-C30-O31-C32
9	A	416	12P	C26-C27-O28-C29
7	A	413	CLR	C16-C17-C20-C22

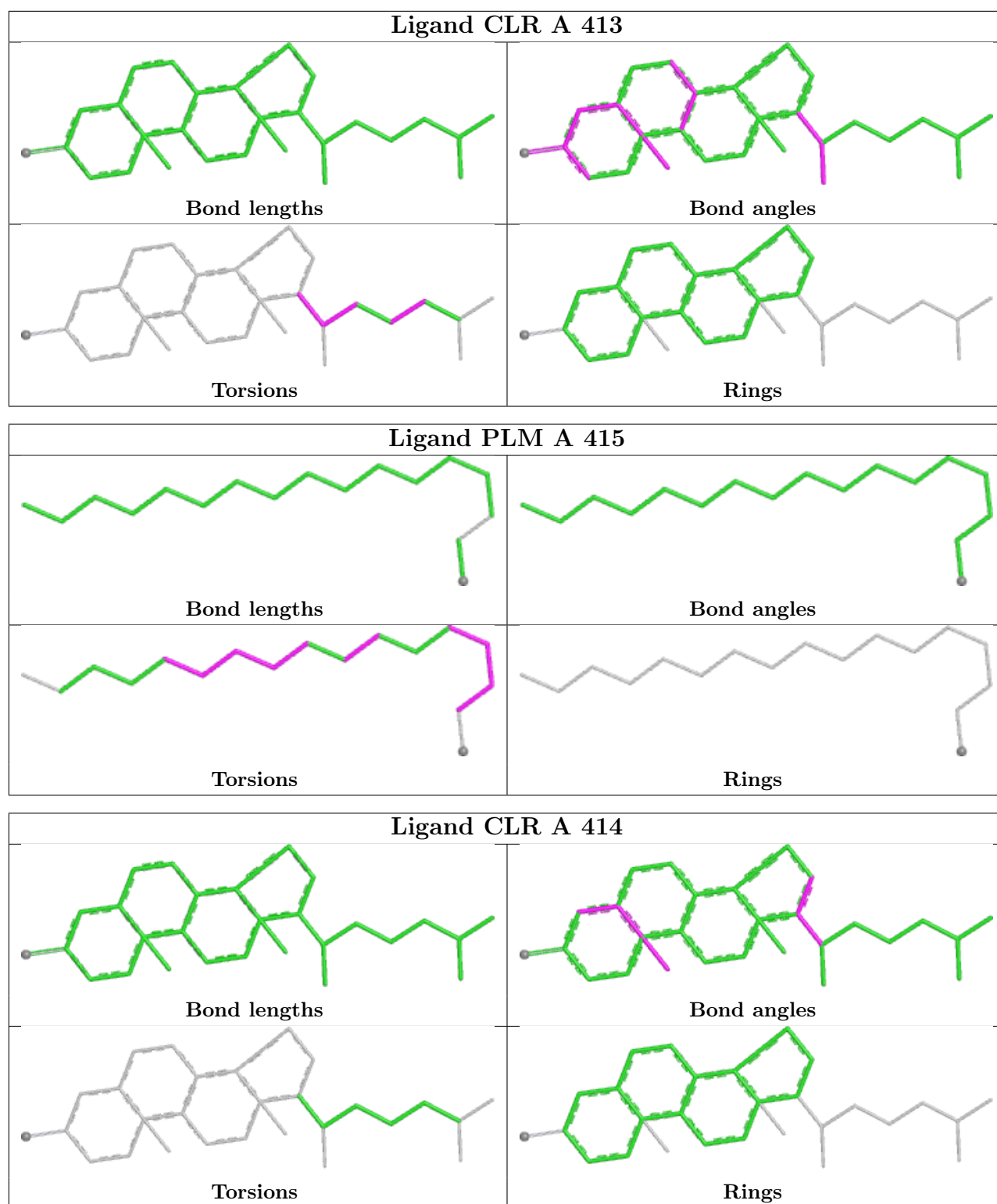
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	412	CLR	5	0
7	A	413	CLR	1	0
7	A	414	CLR	8	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	442/500 (88%)	0.54	4 (0%) 81 78	63, 75, 86, 99	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	TYR	3.5
1	A	111	SER	2.2
1	A	1032	LEU	2.1
1	A	207	SER	2.0

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

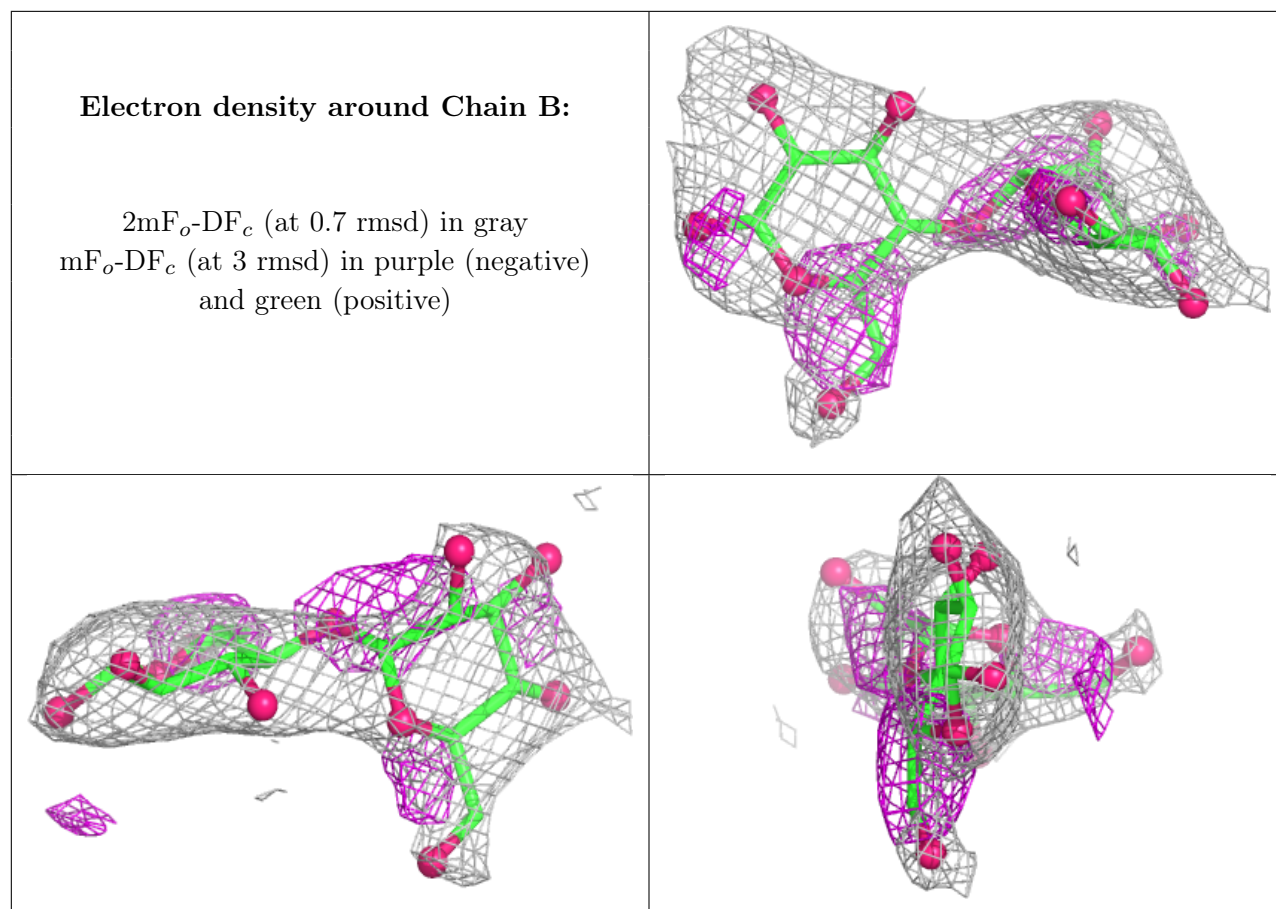
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	GLC	B	1	12/12	0.69	0.16	101,118,118,120	0
2	GLC	B	2	11/12	0.69	0.17	110,113,116,118	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(Å ²)	Q<0.9
3	SO4	A	406	5/5	0.47	0.15	129,131,133,137	0
9	12P	A	416	21/37	0.70	0.20	77,91,108,110	0
7	CLR	A	414	28/28	0.78	0.17	111,114,116,117	0
7	CLR	A	413	28/28	0.78	0.17	81,89,93,94	0
8	PLM	A	415	17/18	0.80	0.19	86,92,101,101	0
6	ACM	A	411	4/4	0.81	0.29	69,71,72,74	0
7	CLR	A	412	28/28	0.81	0.17	96,100,106,107	0
5	BU1	A	410	6/6	0.89	0.23	70,72,80,82	0
3	SO4	A	407	5/5	0.90	0.22	100,103,106,107	0
4	CAU	A	408	22/22	0.91	0.15	45,54,59,66	0
3	SO4	A	402	5/5	0.91	0.27	79,79,88,91	0
5	BU1	A	409	6/6	0.92	0.22	46,52,60,65	0
3	SO4	A	404	5/5	0.93	0.21	76,78,81,85	0

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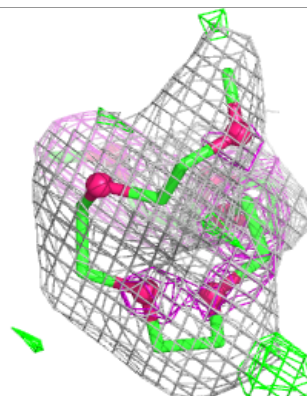
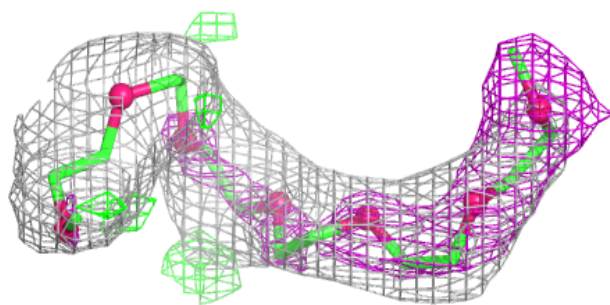
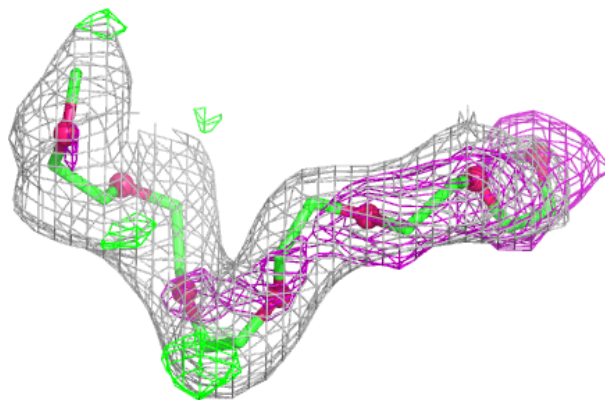
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	403	5/5	0.93	0.20	84,84,93,95	0
3	SO4	A	405	5/5	0.96	0.20	62,74,76,77	0

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.

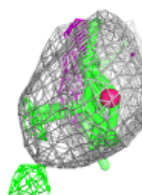
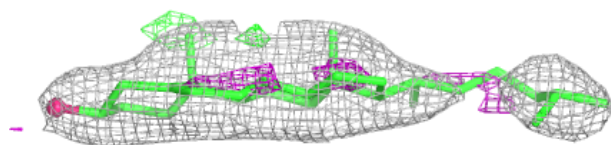
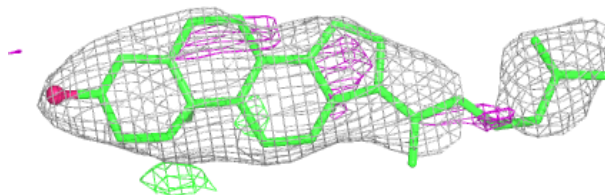
Electron density around 12P A 416:

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

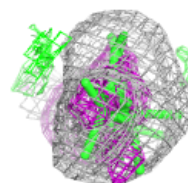
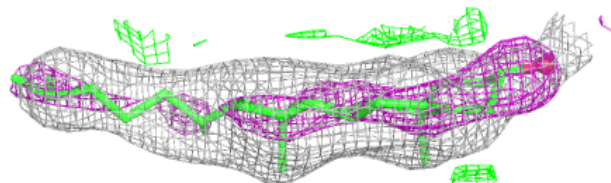
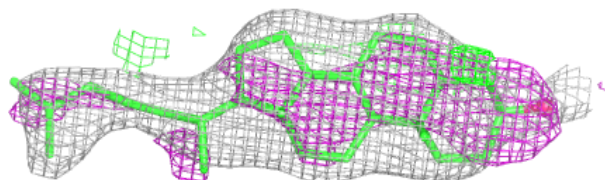


Electron density around CLR A 414:

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

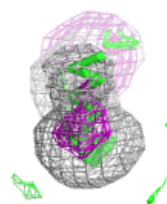
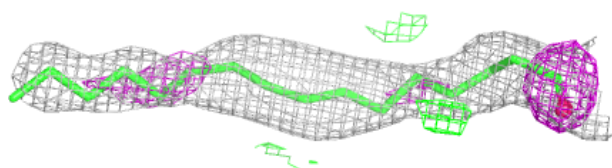
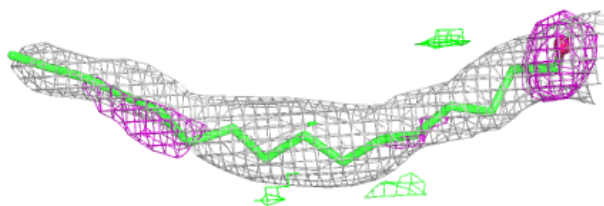
**Electron density around CLR A 413:**

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

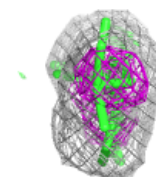
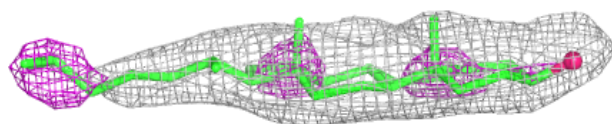
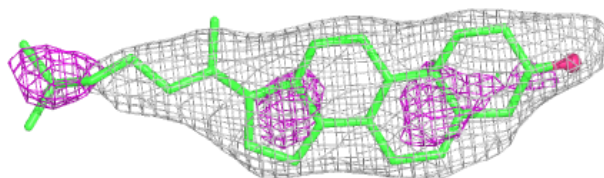


Electron density around PLM A 415:

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

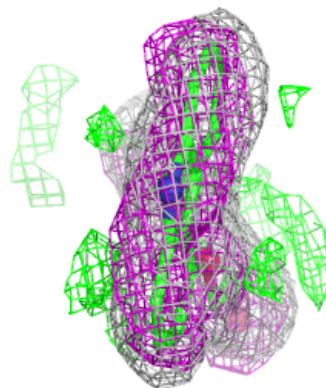
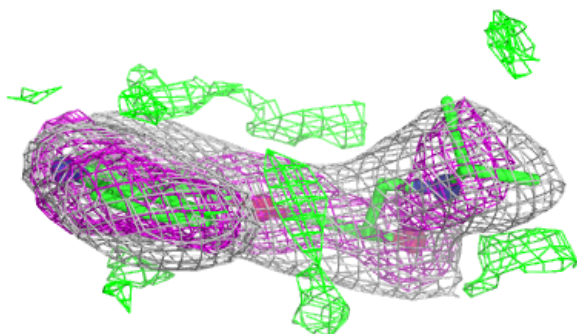
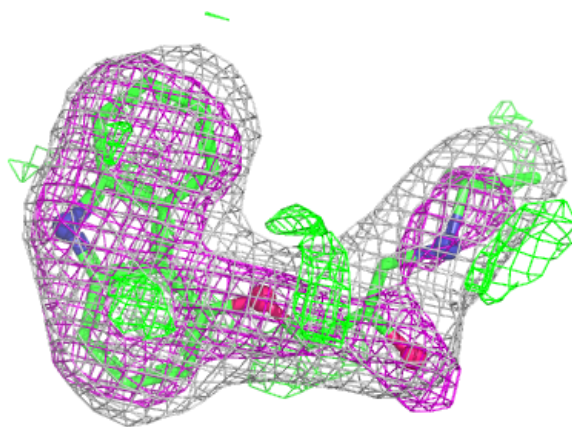
**Electron density around CLR A 412:**

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



Electron density around CAU A 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 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.