



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:58 pm BST

PDB ID : 4OR2
Title : Human class C G protein-coupled metabotropic glutamate receptor 1 in complex with a negative allosteric modulator
Authors : Wu, H.; Wang, C.; Gregory, K.J.; Han, G.W.; Cho, H.P.; Xia, Y.; Niswender, C.M.; Katritch, V.; Cherezov, V.; Conn, P.J.; Stevens, R.C.; GPCR Network (GPCR)
Deposited on : 2014-02-10
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

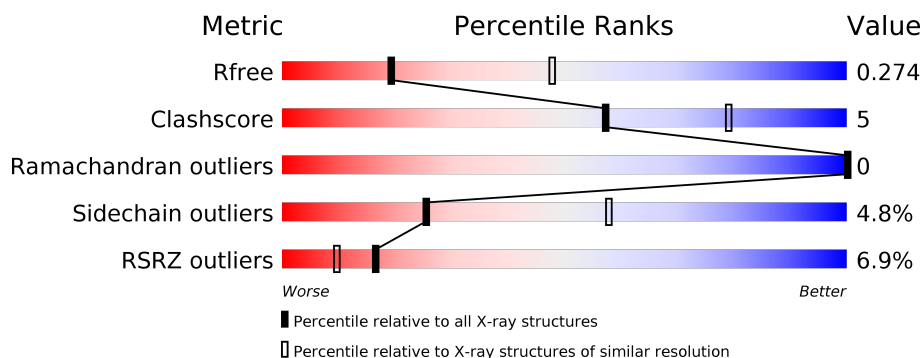
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	389	
1	B	389	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5906 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.

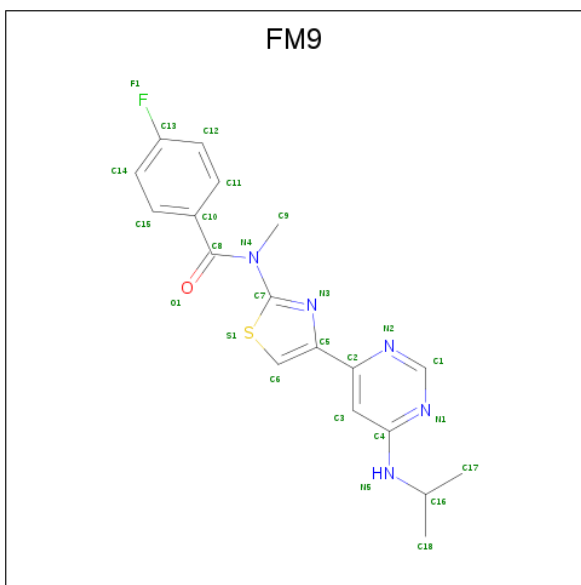
- Molecule 1 is a protein called Soluble cytochrome b562, Metabotropic glutamate receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	1	0
			2786	1821	443	502	20			
1	B	366	Total	C	N	O	S	0	0	0
			2817	1837	451	509	20			

There are 12 discrepancies between the modelled and reference sequences:

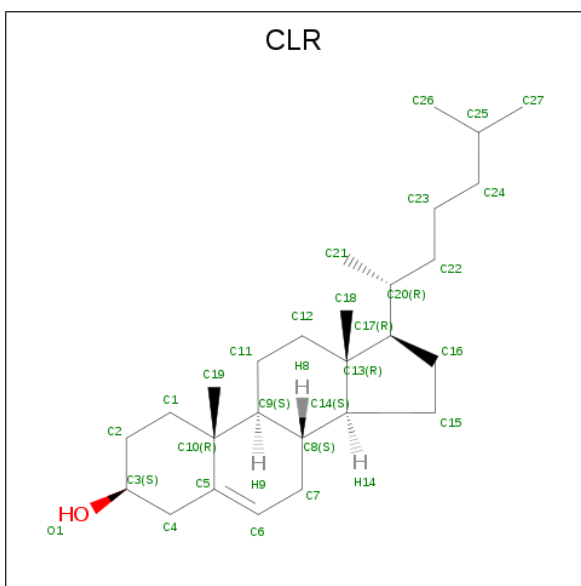
Chain	Residue	Modelled	Actual	Comment	Reference
A	998	GLY	-	EXPRESSION TAG	UNP P0ABE7
A	999	GLY	-	EXPRESSION TAG	UNP P0ABE7
A	1000	THR	-	EXPRESSION TAG	UNP P0ABE7
A	1007	TRP	MET	ENGINEERED MUTATION	UNP P0ABE7
A	1102	ILE	HIS	ENGINEERED MUTATION	UNP P0ABE7
A	1106	LEU	ARG	ENGINEERED MUTATION	UNP P0ABE7
B	998	GLY	-	EXPRESSION TAG	UNP P0ABE7
B	999	GLY	-	EXPRESSION TAG	UNP P0ABE7
B	1000	THR	-	EXPRESSION TAG	UNP P0ABE7
B	1007	TRP	MET	ENGINEERED MUTATION	UNP P0ABE7
B	1102	ILE	HIS	ENGINEERED MUTATION	UNP P0ABE7
B	1106	LEU	ARG	ENGINEERED MUTATION	UNP P0ABE7

- Molecule 2 is 4-fluoro-N-methyl-N-{4-[6-(propan-2-ylamino)pyrimidin-4-yl]-1,3-thiazol-2-yl} benzamide (three-letter code: FM9) (formula: C₁₈H₁₈FN₅OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			26	18	1	5	1	1		
2	B	1	Total	C	F	N	O	S	0	0
			26	18	1	5	1	1		

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



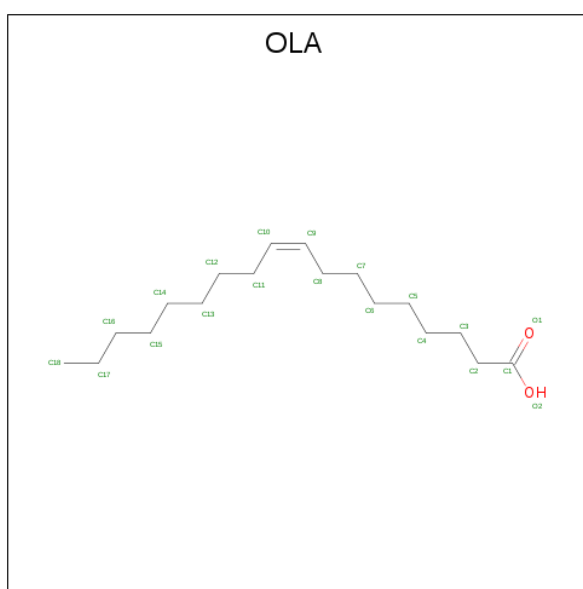
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		

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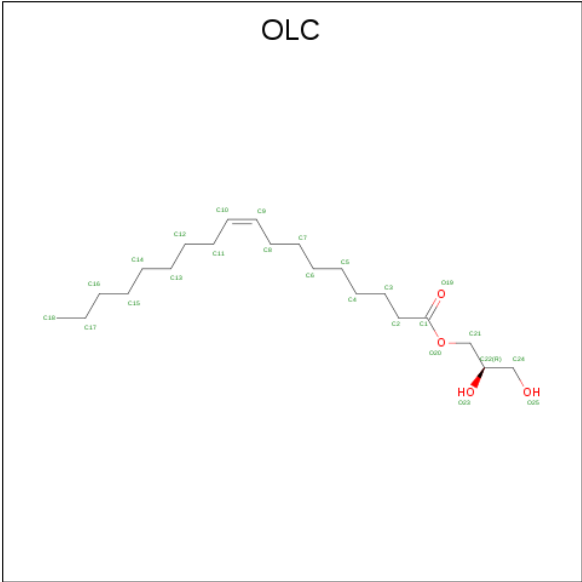
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		
3	A	1	Total	C	O	0	0
			28	27	1		
3	B	1	Total	C	O	0	0
			28	27	1		
3	B	1	Total	C	O	0	0
			28	27	1		

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



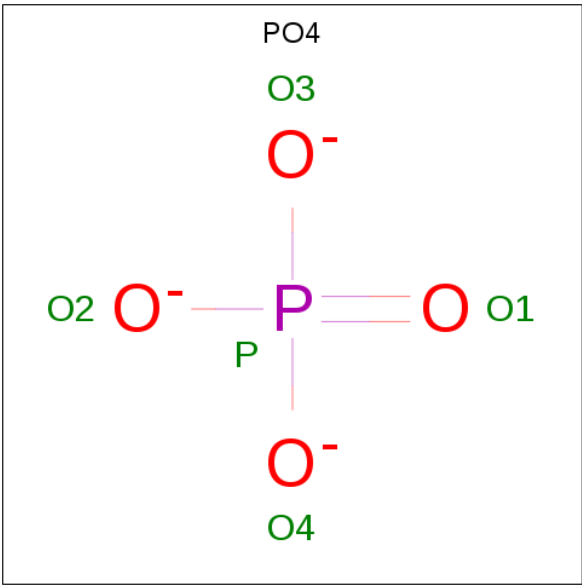
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	15	2		

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	12	4		
5	A	1	Total	C	O	0	0
			12	8	4		
5	B	1	Total	C	O	0	0
			15	11	4		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		

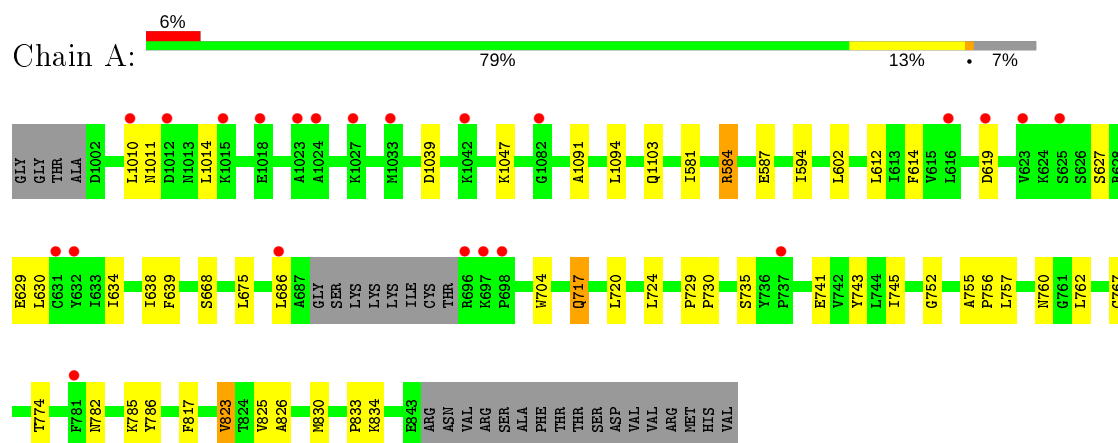
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	O	0	0
			6	6		
7	B	7	Total	O	0	0
			7	7		

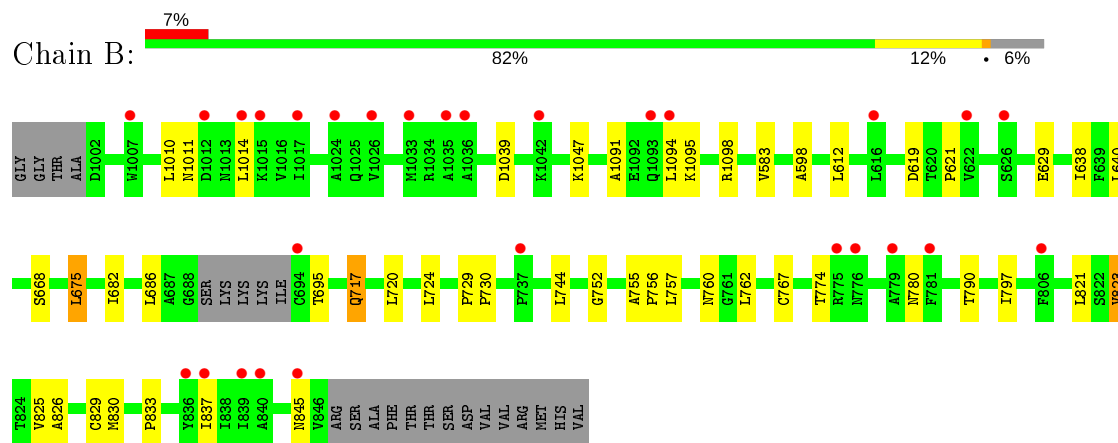
3 Residue-property plots [i](#)

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

- Molecule 1: Soluble cytochrome b562, Metabotropic glutamate receptor 1



- Molecule 1: Soluble cytochrome b562, Metabotropic glutamate receptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.36Å 86.55Å 168.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.68 – 2.80 35.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (35.68-2.80) 98.6 (35.59-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.227 , 0.268 0.239 , 0.274	Depositor DCC
R_{free} test set	1247 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5906	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, PO4, OLC, CLR, FM9

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	0.48	0/2844	0.62	0/3876
1	B	0.48	0/2875	0.60	0/3920
All	All	0.48	0/5719	0.61	0/7796

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	2786	0	2847	26	0
1	B	2817	0	2871	27	0
2	A	26	0	18	3	0
2	B	26	0	18	6	0
3	A	112	0	184	7	0
3	B	56	0	91	5	0
4	A	17	0	24	1	0
5	A	28	0	34	1	0
5	B	15	0	19	0	0
6	B	10	0	0	0	0
7	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	7	0	0	0	0
All	All	5906	0	6106	59	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 (59) 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:760:ASN:HD22	2:B:1901:FM9:H17	1.40	0.85
1:A:757:LEU:HA	2:A:1901:FM9:H18	1.69	0.74
1:A:612:LEU:HD23	1:B:612:LEU:HD23	1.69	0.73
1:A:1047:LYS:HA	1:B:1047:LYS:HA	1.71	0.72
1:A:602:LEU:HB2	3:A:1903:CLR:H262	1.73	0.71
2:B:1901:FM9:C15	2:B:1901:FM9:H16	2.25	0.67
1:A:782:ASN:HB3	1:A:785:LYS:HD3	1.80	0.61
1:A:584:ARG:HD2	1:A:743:TYR:CE1	2.36	0.61
1:B:797:ILE:HG22	2:B:1901:FM9:H3	1.84	0.59
1:B:821:LEU:O	1:B:825:VAL:HG23	2.03	0.58
1:A:638:ILE:HG23	1:A:823:VAL:HG13	1.84	0.58
1:B:1095:LYS:HG2	1:B:1098:ARG:HH21	1.70	0.56
1:B:668:SER:HB2	1:B:760:ASN:ND2	2.21	0.56
1:A:786:TYR:CE1	1:A:833:PRO:HG2	2.40	0.56
1:A:614:PHE:HZ	1:A:834:LYS:HD3	1.72	0.54
1:B:757:LEU:HA	2:B:1901:FM9:H18	1.88	0.54
1:B:760:ASN:ND2	2:B:1901:FM9:H17	2.17	0.54
1:B:682:ILE:HG22	1:B:774:THR:HG21	1.89	0.54
1:A:1103:GLN:HG2	1:A:581:ILE:HG12	1.90	0.53
1:B:638:ILE:HG23	1:B:823:VAL:HG13	1.91	0.53
2:A:1901:FM9:H16	2:A:1901:FM9:C11	2.38	0.52
1:B:717:GLN:HA	1:B:717:GLN:HE21	1.74	0.52
1:B:686:LEU:HD12	1:B:774:THR:HG22	1.92	0.51
1:A:717:GLN:HE21	1:A:717:GLN:HA	1.74	0.51
3:A:1905:CLR:H3	3:B:1905:CLR:H21	1.94	0.50
1:A:686:LEU:HD12	1:A:774:THR:HG22	1.94	0.50
1:B:583:VAL:HG11	1:B:744:LEU:HB2	1.92	0.50
1:A:717:GLN:HE22	1:A:756:PRO:HA	1.78	0.49
1:B:717:GLN:HE22	1:B:756:PRO:HA	1.78	0.49
1:B:833:PRO:O	1:B:837:ILE:HG12	2.14	0.47
3:A:1902:CLR:H241	3:A:1904:CLR:H231	1.97	0.47
1:A:1091:ALA:HA	1:A:1094:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1091:ALA:HA	1:B:1094:LEU:HD12	1.96	0.46
1:B:826:ALA:O	1:B:830:MET:HB2	2.16	0.45
1:A:729:PRO:HA	1:A:730:PRO:HD3	1.91	0.45
1:A:826:ALA:O	1:A:830:MET:HB2	2.17	0.44
1:B:621:PRO:HG2	1:B:845:ASN:O	2.17	0.44
1:A:760:ASN:OD1	2:A:1901:FM9:H17	2.17	0.44
1:A:634:ILE:HD12	1:A:675:LEU:HG	1.99	0.44
1:A:639:PHE:HZ	3:A:1904:CLR:H271	1.83	0.43
1:A:594:ILE:HG21	5:A:1908:OLC:H2	1.99	0.43
1:A:668:SER:HB2	1:A:760:ASN:OD1	2.18	0.43
1:A:735:SER:HB2	1:A:745:ILE:HD11	1.99	0.43
1:B:720:LEU:HD11	1:B:755:ALA:HB1	2.01	0.43
1:A:817:PHE:HB2	4:A:1906:OLA:H111	2.01	0.43
1:B:757:LEU:HD12	2:B:1901:FM9:H18	2.02	0.42
1:B:729:PRO:HA	1:B:730:PRO:HD3	1.92	0.42
1:A:720:LEU:HD11	1:A:755:ALA:HB1	2.01	0.42
1:B:598:ALA:HA	3:B:1905:CLR:H162	2.01	0.42
1:B:724:LEU:HD13	1:B:752:GLY:HA2	2.00	0.42
3:B:1906:CLR:H212	3:B:1906:CLR:H183	2.02	0.42
1:A:630:LEU:O	1:A:634:ILE:HG12	2.19	0.41
1:B:675:LEU:HB3	1:B:767:CYS:SG	2.61	0.41
1:B:790:THR:OG1	1:B:829:CYS:HB2	2.21	0.41
3:A:1902:CLR:H193	3:B:1906:CLR:H112	2.02	0.41
1:B:583:VAL:CG1	1:B:744:LEU:HB2	2.51	0.41
3:A:1903:CLR:H213	3:B:1906:CLR:H222	2.03	0.41
3:A:1904:CLR:H273	3:A:1905:CLR:H221	2.03	0.40
1:A:724:LEU:HD13	1:A:752:GLY:HA2	2.02	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	357/389 (92%)	349 (98%)	8 (2%)	0	100	100
1	B	362/389 (93%)	353 (98%)	9 (2%)	0	100	100
All	All	719/778 (92%)	702 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	300/336 (89%)	284 (95%)	16 (5%)	22	54
1	B	303/336 (90%)	290 (96%)	13 (4%)	29	62
All	All	603/672 (90%)	574 (95%)	29 (5%)	25	58

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1010	LEU
1	A	1011	ASN
1	A	1014	LEU
1	A	1039	ASP
1	A	584	ARG
1	A	587	GLU
1	A	619	ASP
1	A	627	SER
1	A	629	GLU
1	A	704	TRP
1	A	717	GLN
1	A	741	GLU
1	A	762	LEU
1	A	767	CYS
1	A	823	VAL
1	A	825	VAL
1	B	1010	LEU
1	B	1011	ASN

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Mol	Chain	Res	Type
1	B	1014	LEU
1	B	1039	ASP
1	B	619	ASP
1	B	629	GLU
1	B	640	LEU
1	B	675	LEU
1	B	695	THR
1	B	717	GLN
1	B	762	LEU
1	B	780	ASN
1	B	823	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1011	ASN
1	A	1013	ASN
1	A	706	GLN
1	A	717	GLN
1	B	1011	ASN
1	B	1013	ASN
1	B	717	GLN
1	B	760	ASN
1	B	782	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 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	CLR	A	1905	-	31,31,31	0.62	0	48,48,48	1.97	12 (25%)
3	CLR	B	1905	-	31,31,31	0.58	0	48,48,48	1.72	13 (27%)
6	PO4	B	1903	-	4,4,4	1.29	1 (25%)	6,6,6	0.63	0
3	CLR	B	1906	-	31,31,31	0.59	0	48,48,48	1.66	13 (27%)
3	CLR	A	1903	-	31,31,31	0.64	0	48,48,48	1.54	8 (16%)
3	CLR	A	1904	-	31,31,31	0.54	0	48,48,48	1.54	11 (22%)
5	OLC	B	1904	-	14,14,24	1.28	1 (7%)	15,15,25	1.08	1 (6%)
5	OLC	A	1908	-	11,11,24	1.44	1 (9%)	12,12,25	0.98	1 (8%)
5	OLC	A	1907	-	15,15,24	1.20	1 (6%)	16,16,25	0.96	1 (6%)
3	CLR	A	1902	-	31,31,31	0.60	0	48,48,48	1.72	13 (27%)
4	OLA	A	1906	-	13,16,19	0.34	0	12,16,19	0.48	0
6	PO4	B	1902	-	4,4,4	1.24	1 (25%)	6,6,6	0.58	0
2	FM9	B	1901	-	24,28,28	2.92	12 (50%)	29,39,39	1.62	6 (20%)
2	FM9	A	1901	-	24,28,28	2.96	12 (50%)	29,39,39	1.43	4 (13%)

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	CLR	A	1905	-	-	7/10/68/68	0/4/4/4
3	CLR	B	1905	-	-	7/10/68/68	0/4/4/4
3	CLR	B	1906	-	-	5/10/68/68	0/4/4/4
3	CLR	A	1903	-	-	2/10/68/68	0/4/4/4
3	CLR	A	1904	-	-	3/10/68/68	0/4/4/4
5	OLC	B	1904	-	-	6/14/14/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OLC	A	1908	-	-	5/11/11/24	-
5	OLC	A	1907	-	-	8/15/15/24	-
3	CLR	A	1902	-	-	5/10/68/68	0/4/4/4
4	OLA	A	1906	-	-	7/12/14/17	-
2	FM9	B	1901	-	-	4/14/20/20	0/3/3/3
2	FM9	A	1901	-	-	4/14/20/20	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1901	FM9	C15-C10	7.35	1.51	1.39
2	A	1901	FM9	C15-C10	6.61	1.50	1.39
2	B	1901	FM9	C14-C13	5.68	1.48	1.37
2	A	1901	FM9	C14-C13	5.50	1.47	1.37
2	A	1901	FM9	C8-N4	5.15	1.46	1.36
2	A	1901	FM9	C12-C11	5.04	1.47	1.38
2	B	1901	FM9	C12-C11	4.75	1.47	1.38
5	B	1904	OLC	O20-C1	4.62	1.46	1.33
5	A	1908	OLC	O20-C1	4.61	1.46	1.33
2	B	1901	FM9	C8-N4	4.49	1.44	1.36
5	A	1907	OLC	O20-C1	4.46	1.46	1.33
2	A	1901	FM9	C4-N5	3.72	1.45	1.37
2	A	1901	FM9	C9-N4	-3.54	1.40	1.46
2	B	1901	FM9	C9-N4	-3.48	1.40	1.46
2	B	1901	FM9	C4-N5	3.42	1.44	1.37
2	A	1901	FM9	C4-N1	3.33	1.40	1.34
2	B	1901	FM9	C4-N1	3.12	1.40	1.34
2	A	1901	FM9	C3-C4	3.10	1.47	1.39
2	B	1901	FM9	C3-C4	2.96	1.47	1.39
2	A	1901	FM9	C1-N2	2.86	1.39	1.33
2	B	1901	FM9	C1-N2	2.80	1.39	1.33
2	A	1901	FM9	C6-S1	2.64	1.74	1.70
6	B	1903	PO4	P-O1	2.32	1.56	1.50
6	B	1902	PO4	P-O1	2.26	1.56	1.50
2	A	1901	FM9	C2-N2	2.24	1.39	1.35
2	B	1901	FM9	C11-C10	-2.17	1.35	1.39
2	B	1901	FM9	C2-N2	2.10	1.39	1.35
2	B	1901	FM9	C10-C8	2.09	1.53	1.50
2	A	1901	FM9	C15-C14	-2.08	1.35	1.38

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1905	CLR	C1-C2-C3	6.97	119.41	110.47
3	A	1902	CLR	C4-C5-C10	4.98	123.04	116.42
3	A	1905	CLR	C2-C3-C4	4.19	116.05	110.31
3	A	1904	CLR	C4-C5-C10	3.91	121.61	116.42
3	B	1905	CLR	C4-C5-C10	3.91	121.61	116.42
3	B	1905	CLR	C13-C14-C8	3.86	120.10	114.38
2	A	1901	FM9	C1-N2-C2	3.86	120.97	115.74
3	A	1903	CLR	C4-C5-C6	-3.78	115.16	120.61
3	B	1905	CLR	C4-C5-C6	-3.77	115.18	120.61
3	A	1905	CLR	C15-C14-C13	3.73	108.34	103.84
2	B	1901	FM9	C1-N2-C2	3.71	120.77	115.74
3	B	1906	CLR	C15-C14-C13	3.71	108.31	103.84
3	A	1903	CLR	C4-C5-C10	3.63	121.24	116.42
2	A	1901	FM9	N2-C1-N1	-3.60	122.96	128.60
3	A	1902	CLR	C4-C5-C6	-3.58	115.45	120.61
3	A	1902	CLR	C15-C14-C13	3.54	108.11	103.84
3	A	1904	CLR	C15-C14-C13	3.49	108.05	103.84
3	A	1905	CLR	C4-C5-C10	3.49	121.06	116.42
2	B	1901	FM9	N2-C1-N1	-3.35	123.36	128.60
3	A	1903	CLR	C15-C14-C13	3.34	107.87	103.84
3	B	1906	CLR	C7-C8-C14	3.33	115.73	110.91
3	A	1904	CLR	C21-C20-C22	-3.24	105.28	110.36
3	B	1906	CLR	C11-C9-C8	3.24	116.42	111.75
3	B	1906	CLR	C14-C8-C9	3.09	113.23	109.09
3	A	1904	CLR	C4-C5-C6	-3.03	116.24	120.61
3	B	1905	CLR	C15-C14-C13	3.02	107.48	103.84
3	B	1906	CLR	C4-C5-C6	-2.97	116.32	120.61
3	B	1905	CLR	C11-C9-C10	2.95	116.96	113.08
3	B	1905	CLR	C14-C8-C9	2.92	113.00	109.09
3	A	1902	CLR	C21-C20-C22	-2.90	105.82	110.36
3	A	1905	CLR	C4-C5-C6	-2.90	116.44	120.61
3	A	1904	CLR	C11-C9-C10	2.89	116.88	113.08
3	A	1903	CLR	C14-C8-C9	2.83	112.88	109.09
3	B	1906	CLR	C4-C5-C10	2.80	120.14	116.42
3	B	1905	CLR	C8-C7-C6	-2.77	108.75	112.73
3	A	1905	CLR	C2-C1-C10	2.75	118.70	112.74
5	B	1904	OLC	O20-C1-C2	2.75	120.52	111.91
3	B	1905	CLR	C16-C17-C13	2.74	107.14	103.84
3	A	1902	CLR	C13-C14-C8	2.70	118.39	114.38
3	A	1905	CLR	C16-C17-C13	2.69	107.09	103.84
2	B	1901	FM9	C5-C6-S1	-2.65	108.53	111.79
3	A	1902	CLR	C13-C17-C20	2.61	123.57	119.49
3	B	1906	CLR	C8-C7-C6	-2.59	109.02	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1905	CLR	C22-C20-C17	2.58	115.62	110.28
3	A	1902	CLR	C3-C4-C5	2.56	116.37	112.03
3	B	1906	CLR	C12-C11-C9	2.55	117.54	113.11
3	A	1904	CLR	C13-C17-C20	2.54	123.46	119.49
5	A	1907	OLC	O20-C1-C2	2.53	119.84	111.91
3	A	1902	CLR	C11-C9-C10	2.50	116.38	113.08
3	B	1906	CLR	C13-C17-C20	2.50	123.41	119.49
3	B	1905	CLR	C11-C9-C8	2.49	115.35	111.75
3	A	1903	CLR	C11-C9-C10	2.49	116.36	113.08
2	B	1901	FM9	O1-C8-N4	-2.48	117.69	121.47
3	A	1904	CLR	C13-C14-C8	2.48	118.05	114.38
3	B	1906	CLR	C21-C20-C17	2.47	116.71	112.92
3	A	1905	CLR	C11-C9-C10	2.47	116.33	113.08
3	A	1903	CLR	C23-C22-C20	-2.43	108.06	115.03
3	A	1902	CLR	C12-C13-C14	-2.31	103.69	107.27
3	A	1903	CLR	C22-C20-C17	2.30	115.03	110.28
3	B	1906	CLR	C1-C2-C3	2.28	113.39	110.47
5	A	1908	OLC	O20-C1-C2	2.26	119.01	111.91
3	B	1905	CLR	C7-C8-C9	-2.26	106.98	109.71
3	A	1905	CLR	C11-C9-C8	2.25	115.00	111.75
3	A	1904	CLR	C11-C9-C8	2.25	114.99	111.75
3	B	1906	CLR	C12-C13-C17	-2.25	113.21	116.57
3	B	1905	CLR	C21-C20-C22	-2.21	106.89	110.36
3	A	1904	CLR	C16-C17-C13	2.20	106.49	103.84
3	A	1904	CLR	C1-C10-C9	2.20	111.80	108.73
2	B	1901	FM9	C11-C12-C13	2.17	120.61	118.36
3	A	1904	CLR	C14-C8-C9	2.16	111.99	109.09
3	B	1906	CLR	C16-C17-C13	2.15	106.43	103.84
3	A	1905	CLR	C12-C11-C9	2.14	116.82	113.11
3	A	1905	CLR	C7-C8-C14	2.14	114.00	110.91
3	A	1902	CLR	C12-C11-C9	2.12	116.79	113.11
3	A	1903	CLR	C13-C14-C8	2.11	117.51	114.38
3	A	1902	CLR	C16-C17-C13	2.09	106.36	103.84
2	B	1901	FM9	C14-C13-C12	-2.09	120.05	122.83
2	A	1901	FM9	C15-C14-C13	2.08	120.51	118.36
3	B	1905	CLR	C3-C4-C5	-2.07	108.51	112.03
3	A	1902	CLR	C11-C9-C8	2.04	114.70	111.75
3	B	1905	CLR	C17-C13-C14	-2.02	97.68	100.07
3	A	1902	CLR	C7-C8-C14	2.02	113.83	110.91
2	A	1901	FM9	C3-C2-N2	-2.02	119.54	122.16

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1908	OLC	C21-C22-C24-O25
2	B	1901	FM9	N2-C2-C5-C6
2	B	1901	FM9	C3-C2-C5-C6
2	A	1901	FM9	C3-C2-C5-C6
5	B	1904	OLC	O19-C1-O20-C21
3	B	1906	CLR	C13-C17-C20-C21
3	B	1905	CLR	C21-C20-C22-C23
3	A	1905	CLR	C17-C20-C22-C23
3	B	1905	CLR	C17-C20-C22-C23
3	A	1902	CLR	C17-C20-C22-C23
5	B	1904	OLC	C2-C1-O20-C21
5	A	1907	OLC	C2-C1-O20-C21
3	A	1904	CLR	C17-C20-C22-C23
3	A	1905	CLR	C21-C20-C22-C23
3	A	1902	CLR	C21-C20-C22-C23
3	A	1902	CLR	C22-C23-C24-C25
5	A	1907	OLC	O20-C21-C22-O23
3	A	1904	CLR	C21-C20-C22-C23
5	A	1907	OLC	O19-C1-O20-C21
3	A	1905	CLR	C22-C23-C24-C25
3	B	1905	CLR	C20-C22-C23-C24
5	A	1907	OLC	O20-C21-C22-C24
3	A	1903	CLR	C17-C20-C22-C23
3	A	1902	CLR	C23-C24-C25-C27
5	A	1907	OLC	C4-C5-C6-C7
5	A	1907	OLC	C1-C2-C3-C4
5	B	1904	OLC	C3-C4-C5-C6
5	B	1904	OLC	C21-C22-C24-O25
4	A	1906	OLA	C3-C4-C5-C6
4	A	1906	OLA	C11-C12-C13-C14
5	A	1908	OLC	O23-C22-C24-O25
3	B	1905	CLR	C23-C24-C25-C27
3	A	1905	CLR	C20-C22-C23-C24
5	A	1908	OLC	C1-C2-C3-C4
3	B	1905	CLR	C23-C24-C25-C26
3	A	1902	CLR	C23-C24-C25-C26
4	A	1906	OLA	C2-C3-C4-C5
3	A	1905	CLR	C23-C24-C25-C26
4	A	1906	OLA	C12-C13-C14-C15
5	A	1908	OLC	C2-C3-C4-C5
4	A	1906	OLA	C10-C11-C12-C13
3	B	1906	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
3	A	1905	CLR	C23-C24-C25-C27
4	A	1906	OLA	C5-C6-C7-C8
3	B	1906	CLR	C13-C17-C20-C22
3	B	1906	CLR	C23-C24-C25-C27
3	B	1906	CLR	C23-C24-C25-C26
3	A	1905	CLR	C16-C17-C20-C22
3	B	1905	CLR	C16-C17-C20-C22
3	B	1905	CLR	C16-C17-C20-C21
3	A	1904	CLR	C22-C23-C24-C25
5	A	1907	OLC	C6-C7-C8-C9
2	A	1901	FM9	N2-C2-C5-C6
2	B	1901	FM9	N1-C4-N5-C16
2	A	1901	FM9	C10-C8-N4-C9
3	A	1903	CLR	C21-C20-C22-C23
4	A	1906	OLA	C7-C8-C9-C10
2	B	1901	FM9	C10-C8-N4-C9
5	B	1904	OLC	C5-C6-C7-C8
5	A	1907	OLC	O20-C1-C2-C3
5	B	1904	OLC	C4-C5-C6-C7
2	A	1901	FM9	O1-C8-N4-C9
5	A	1908	OLC	C2-C1-O20-C21

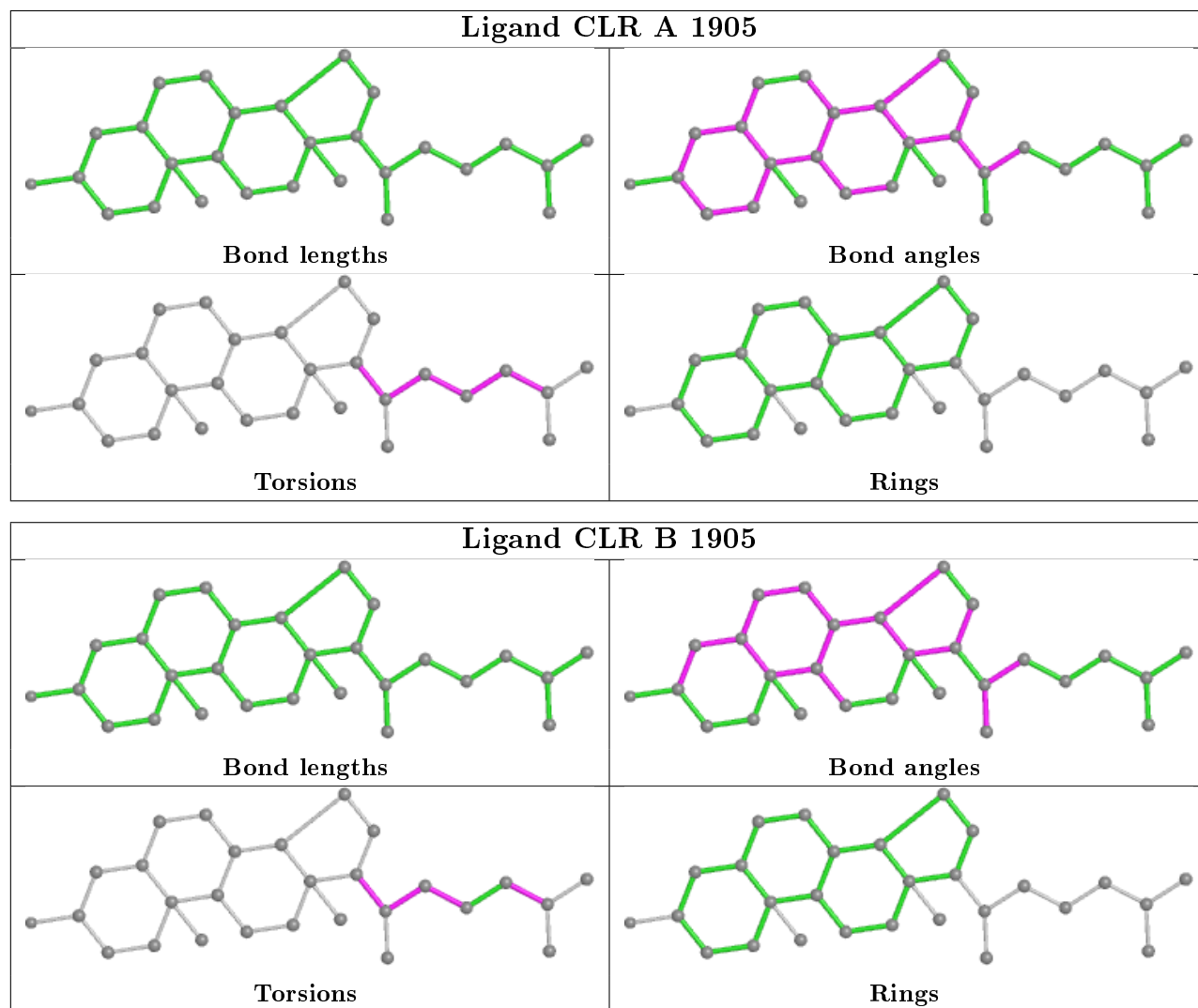
There are no ring outliers.

10 monomers are involved in 20 short contacts:

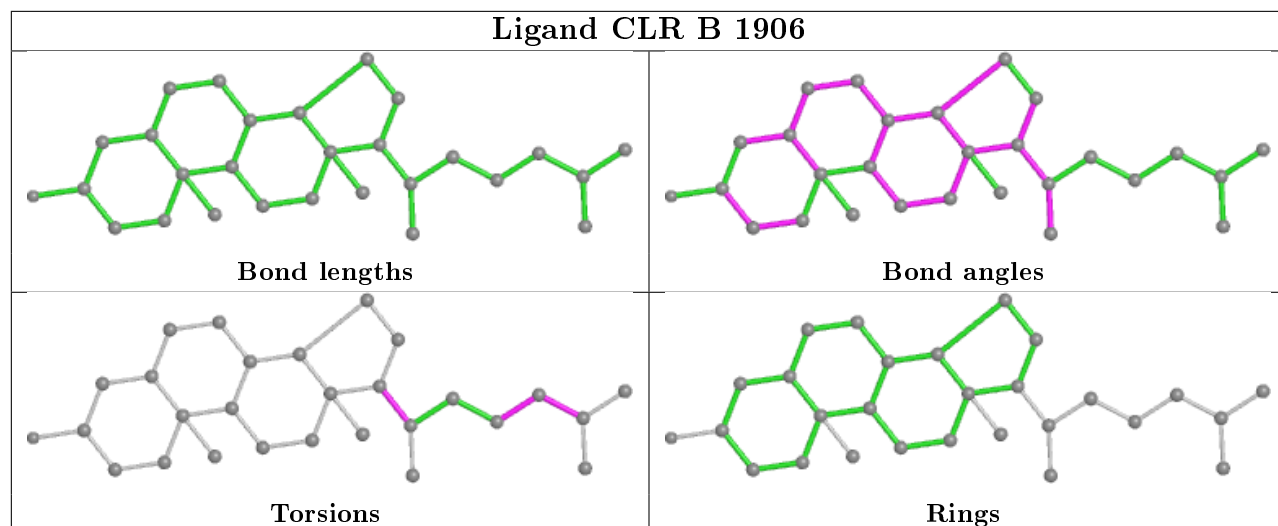
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1905	CLR	2	0
3	B	1905	CLR	2	0
3	B	1906	CLR	3	0
3	A	1903	CLR	2	0
3	A	1904	CLR	3	0
5	A	1908	OLC	1	0
3	A	1902	CLR	2	0
4	A	1906	OLA	1	0
2	B	1901	FM9	6	0
2	A	1901	FM9	3	0

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.

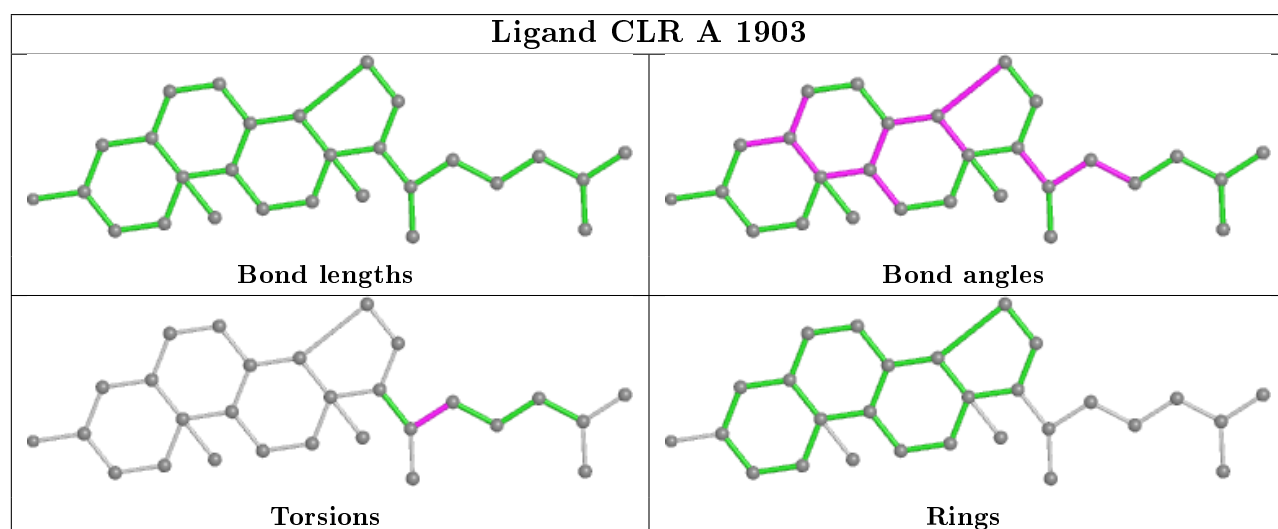
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



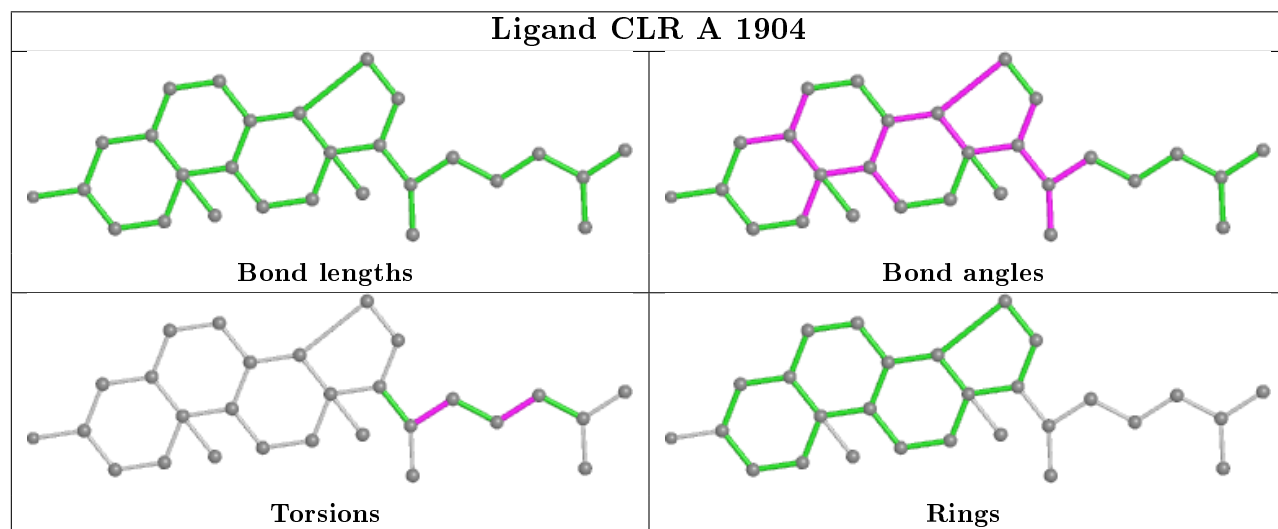
Ligand CLR B 1906

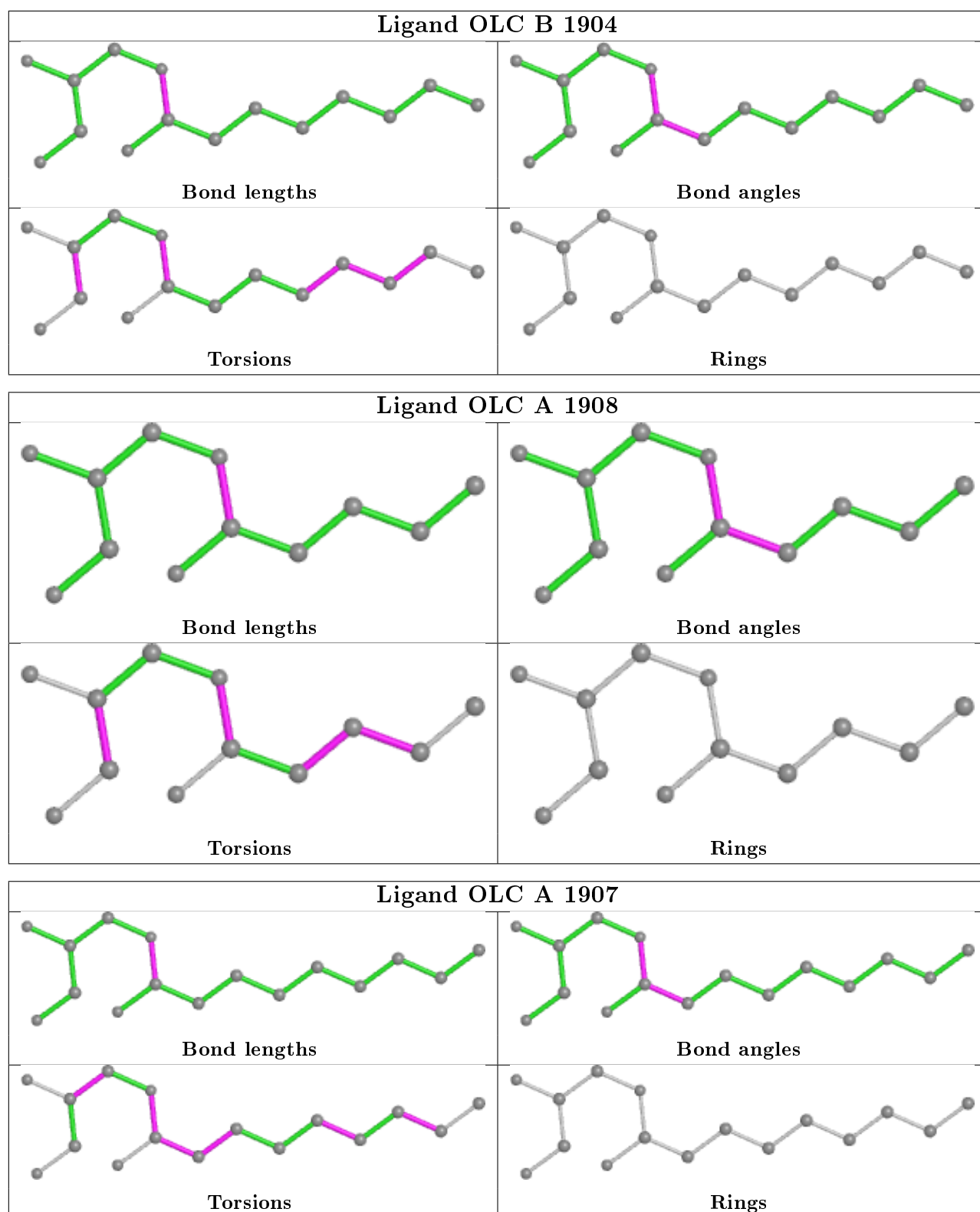


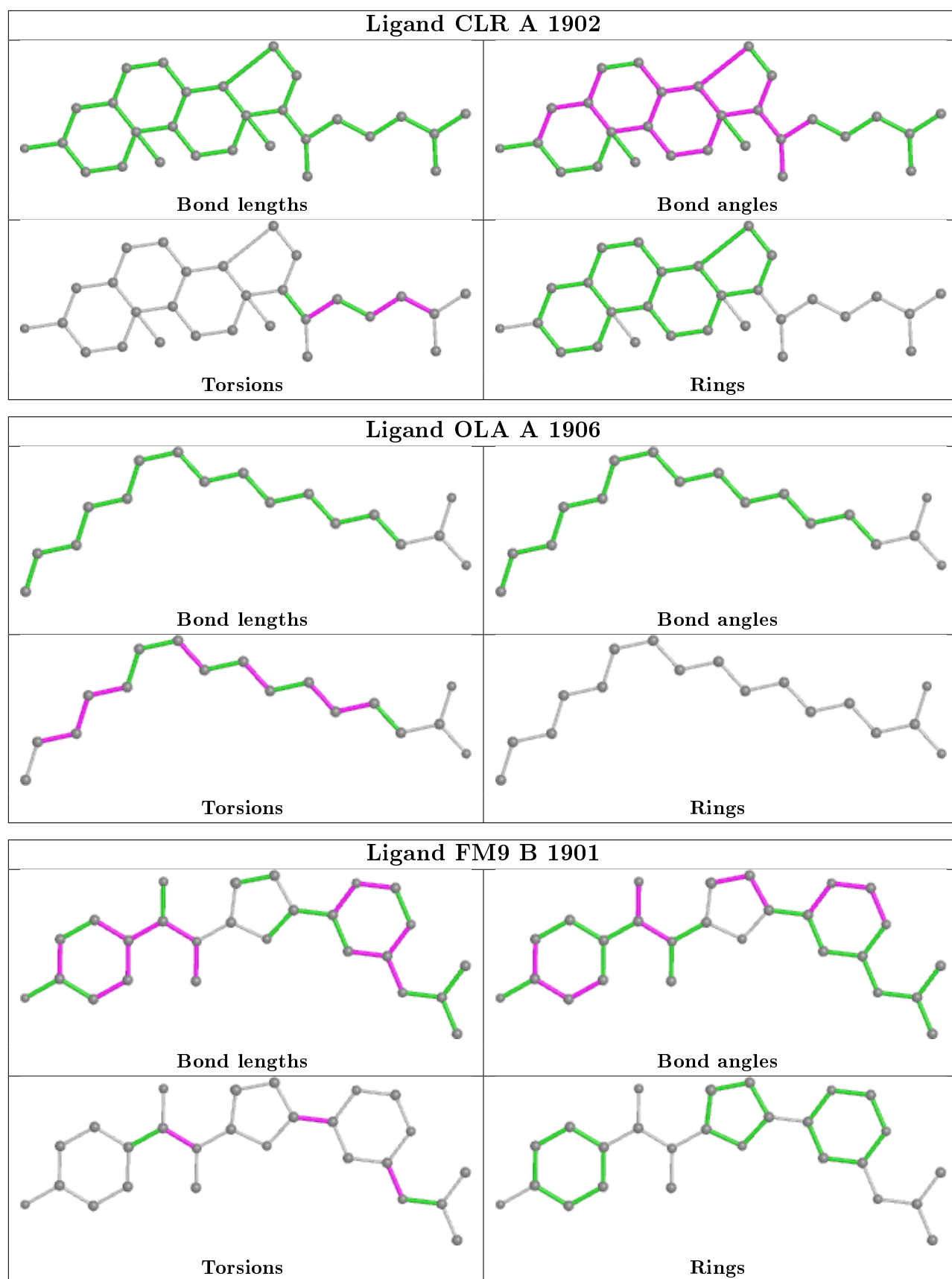
Ligand CLR A 1903

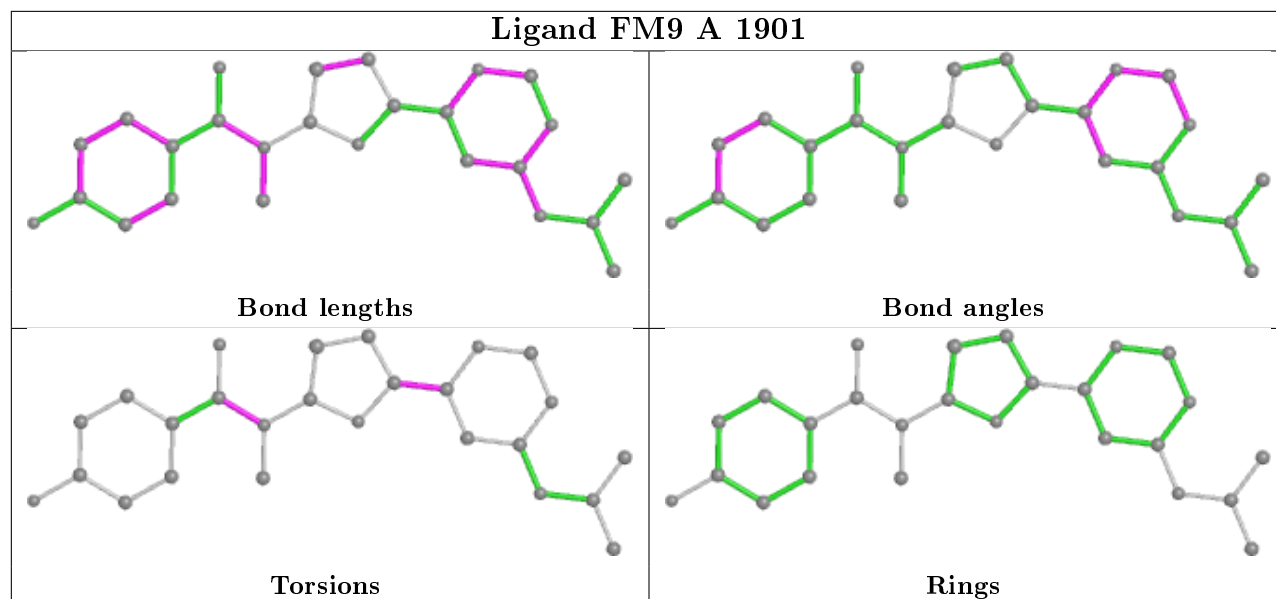


Ligand CLR A 1904









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	360/389 (92%)	0.41	22 (6%)	21 13	62, 88, 181, 218	0
1	B	366/389 (94%)	0.34	28 (7%)	13 7	57, 83, 162, 185	0
All	All	726/778 (93%)	0.38	50 (6%)	16 10	57, 85, 171, 218	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	694	CYS	6.3
1	A	737	PRO	6.0
1	A	698	PRO	5.8
1	B	1015	LYS	5.2
1	B	840	ALA	5.0
1	A	1024	ALA	4.6
1	A	625	SER	4.4
1	A	1082	GLY	4.0
1	A	1010	LEU	4.0
1	A	697	LYS	3.7
1	B	776	ASN	3.7
1	B	845	ASN	3.6
1	A	1018	GLU	3.5
1	A	1033	MET	3.4
1	A	1023	ALA	3.4
1	B	1033	MET	3.2
1	B	836	TYR	3.0
1	B	1093	GLN	3.0
1	A	623	VAL	3.0
1	B	616	LEU	2.9
1	B	839	ILE	2.9
1	B	779	ALA	2.8
1	A	1015	LYS	2.7
1	B	1036	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1094	LEU	2.7
1	B	737	PRO	2.7
1	B	1035	ALA	2.6
1	B	1007	TRP	2.6
1	B	1026	VAL	2.6
1	A	616	LEU	2.6
1	B	1012	ASP	2.5
1	B	626	SER	2.5
1	A	1012	ASP	2.5
1	A	686	LEU	2.5
1	A	1042	LYS	2.4
1	B	1042	LYS	2.4
1	B	1014	LEU	2.3
1	B	1024	ALA	2.3
1	B	775	ARG	2.3
1	A	696	ARG	2.2
1	A	1027	LYS	2.2
1	B	1017	ILE	2.1
1	A	631	CYS	2.1
1	B	837	ILE	2.1
1	B	781	PHE	2.1
1	B	622	VAL	2.1
1	A	781	PHE	2.1
1	B	806	PHE	2.1
1	A	619	ASP	2.0
1	A	632	TYR	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](#)

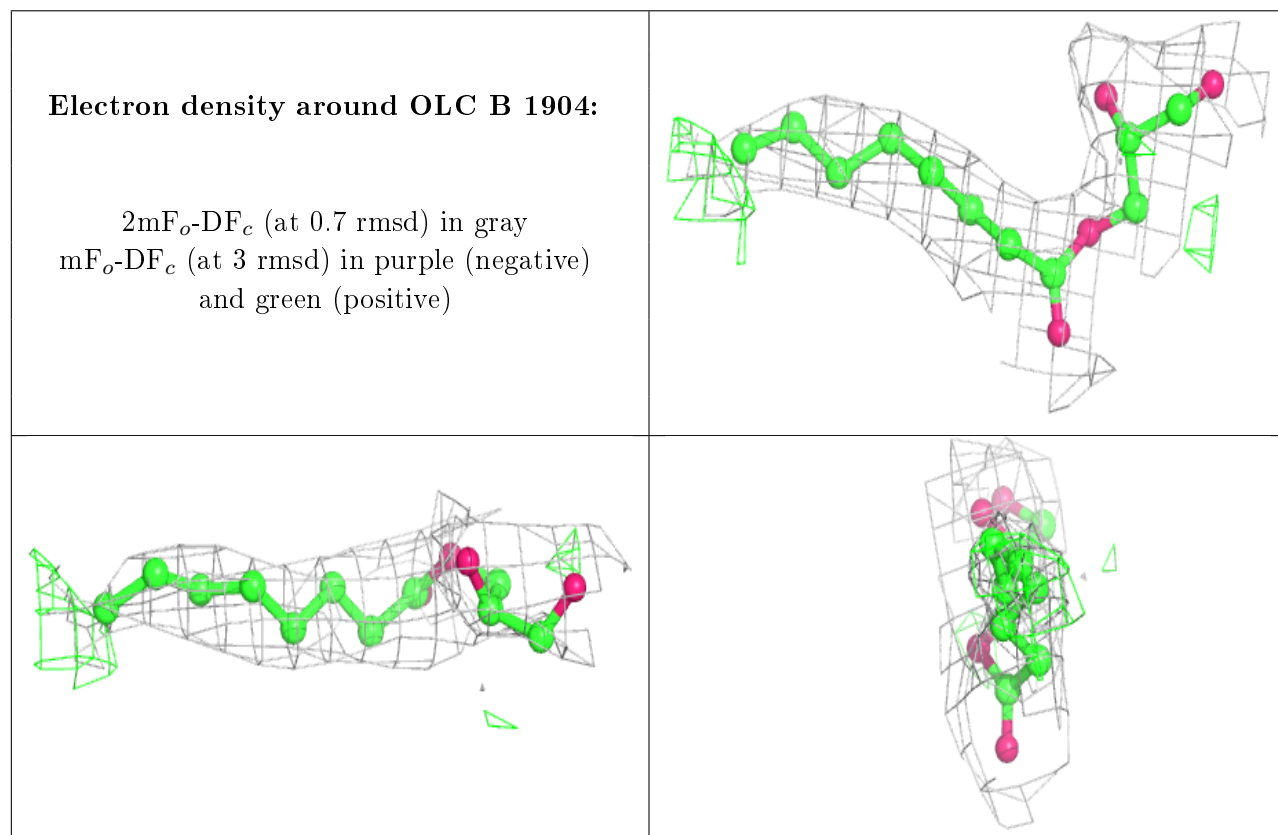
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

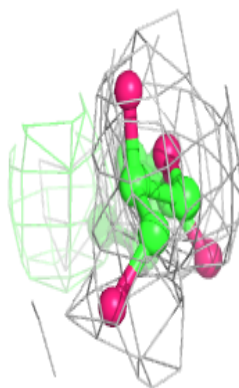
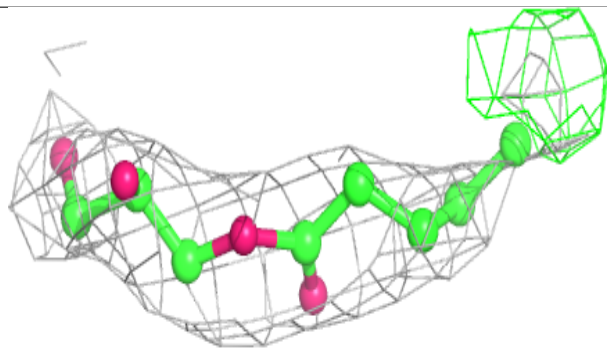
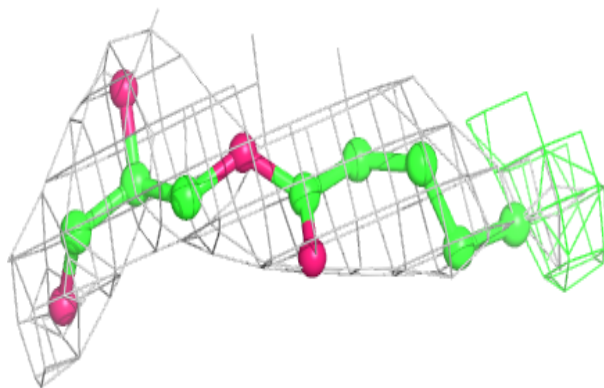
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PO4	B	1903	5/5	0.72	0.32	146,146,146,147	0
5	OLC	B	1904	15/25	0.72	0.27	87,100,119,119	0
5	OLC	A	1908	12/25	0.79	0.29	113,116,118,118	0
6	PO4	B	1902	5/5	0.79	0.32	144,145,146,146	0
5	OLC	A	1907	16/25	0.80	0.53	91,102,108,110	0
4	OLA	A	1906	17/20	0.84	0.31	63,70,96,98	0
3	CLR	A	1904	28/28	0.86	0.29	110,113,117,117	0
3	CLR	A	1905	28/28	0.88	0.33	109,110,114,115	0
3	CLR	A	1903	28/28	0.89	0.26	67,71,78,85	0
3	CLR	B	1905	28/28	0.91	0.31	97,101,108,108	0
3	CLR	A	1902	28/28	0.92	0.30	94,99,107,108	0
2	FM9	B	1901	26/26	0.94	0.22	62,71,74,77	0
2	FM9	A	1901	26/26	0.95	0.22	60,72,76,77	0
3	CLR	B	1906	28/28	0.96	0.26	73,83,89,90	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.

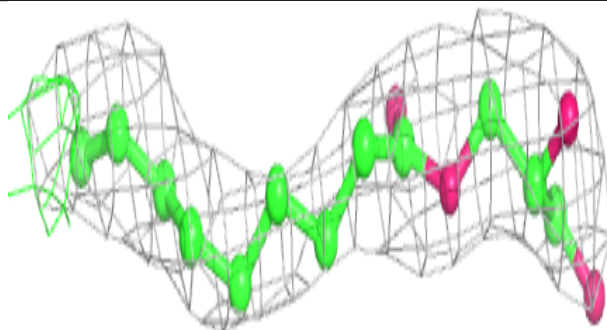
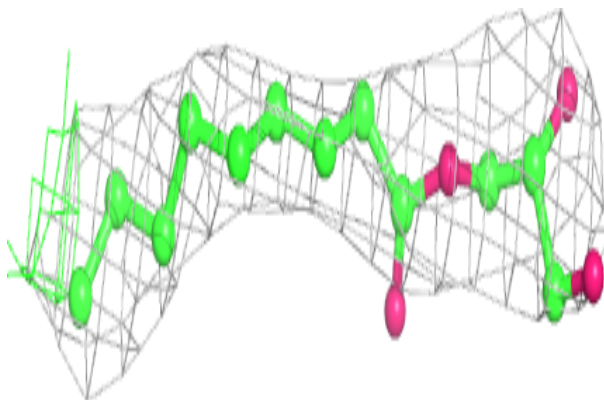


Electron density around OLC A 1908:

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

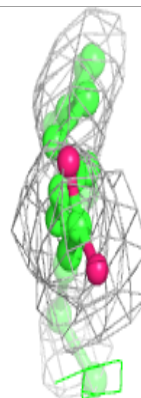
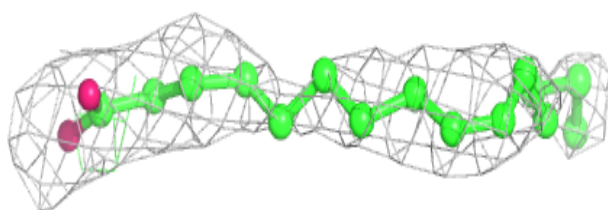
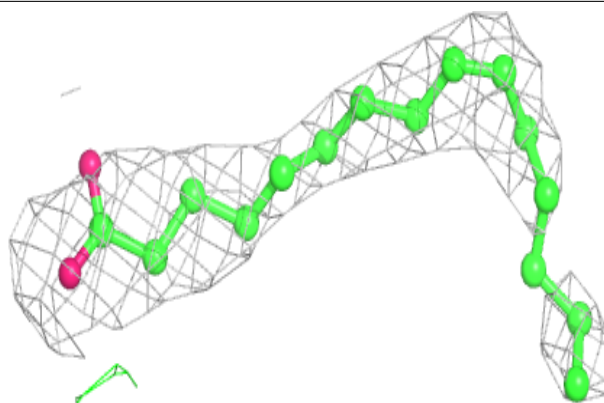
**Electron density around OLC A 1907:**

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

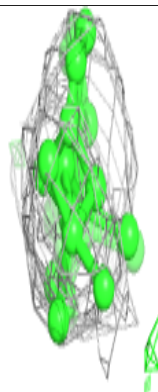
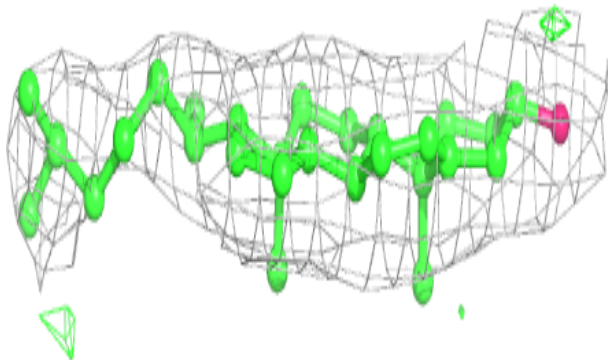
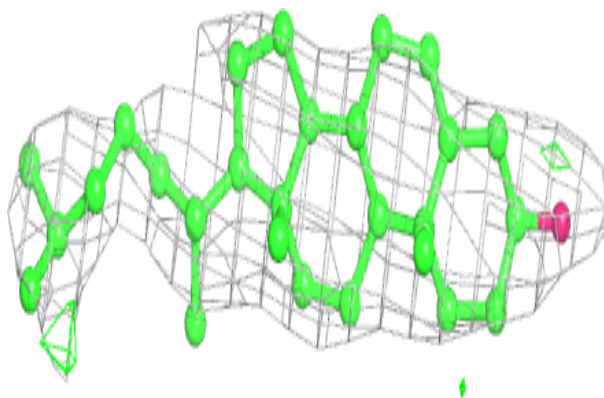


Electron density around OLA A 1906:

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

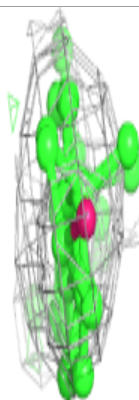
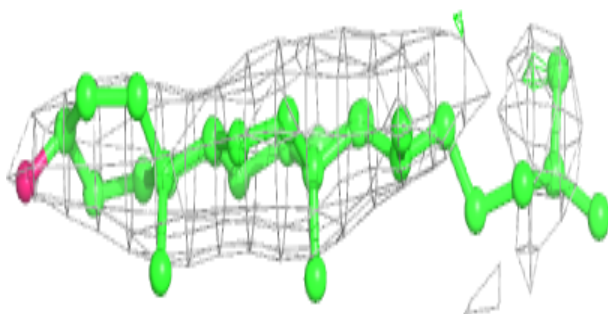
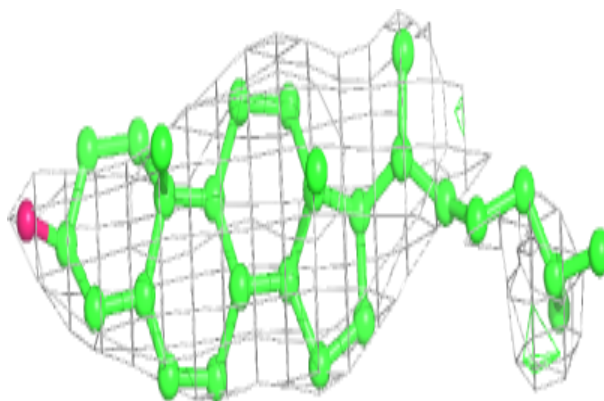
**Electron density around CLR A 1904:**

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

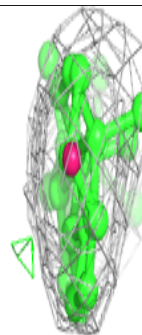
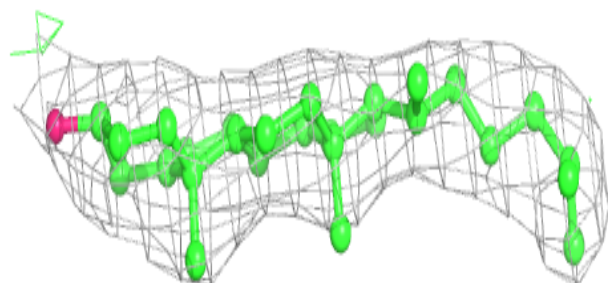
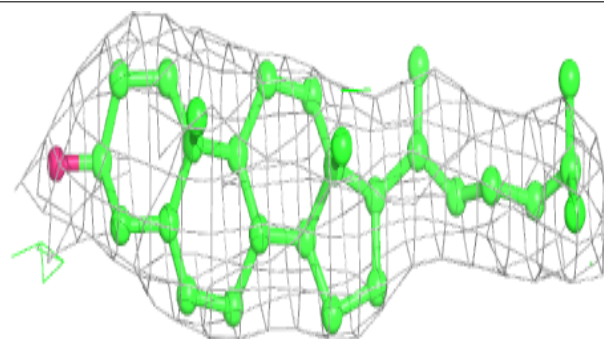


Electron density around CLR A 1905:

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

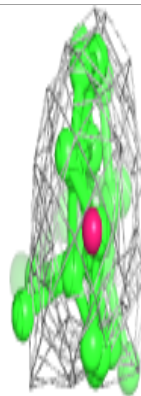
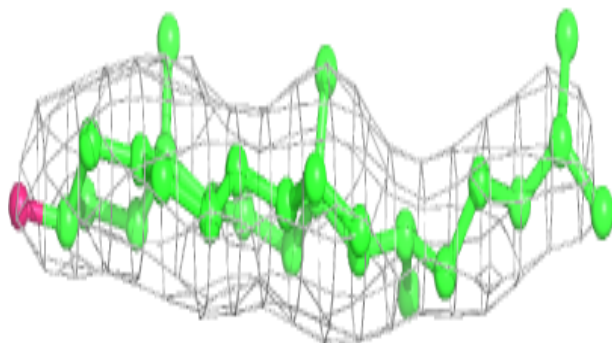
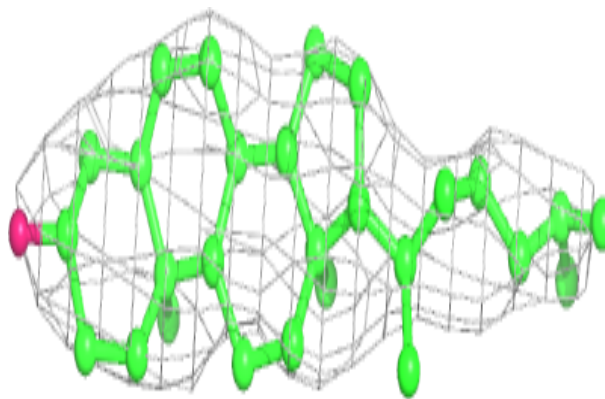
**Electron density around CLR A 1903:**

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

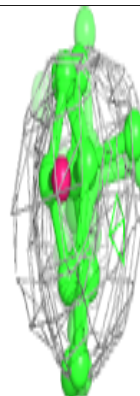
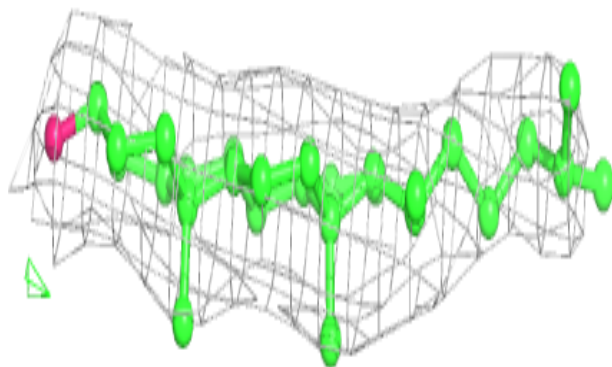
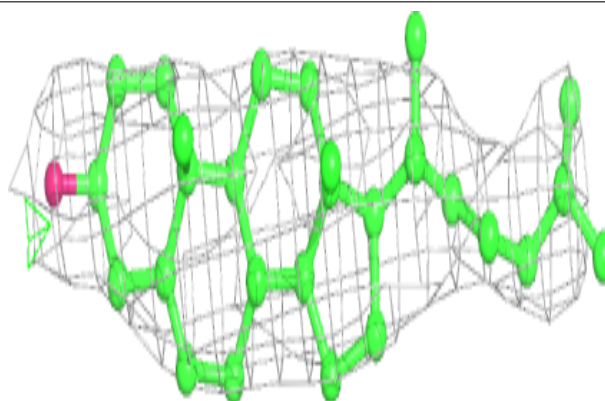


Electron density around CLR B 1905:

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

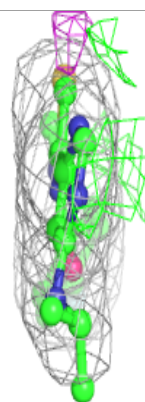
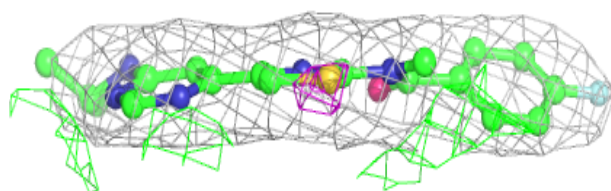
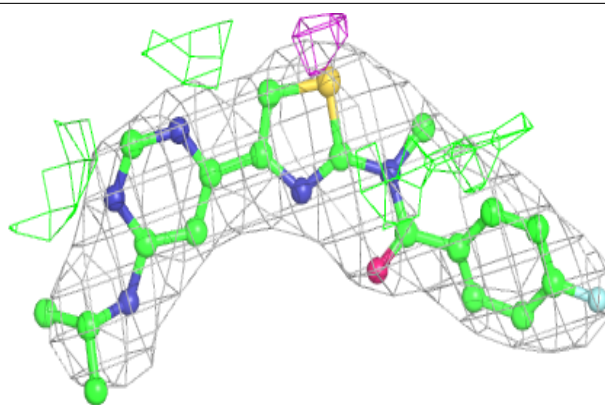
**Electron density around CLR A 1902:**

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

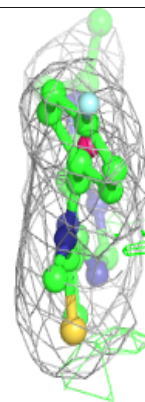
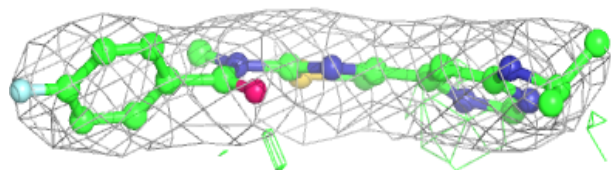
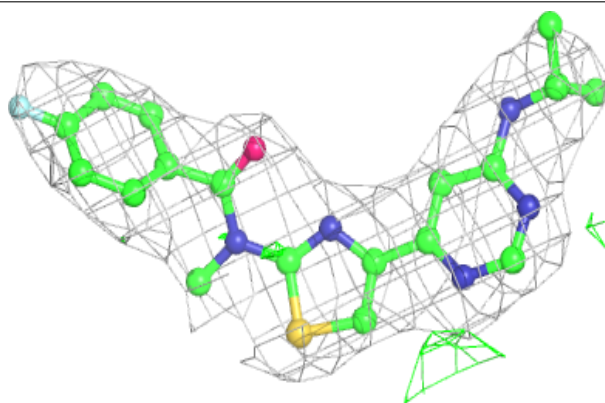


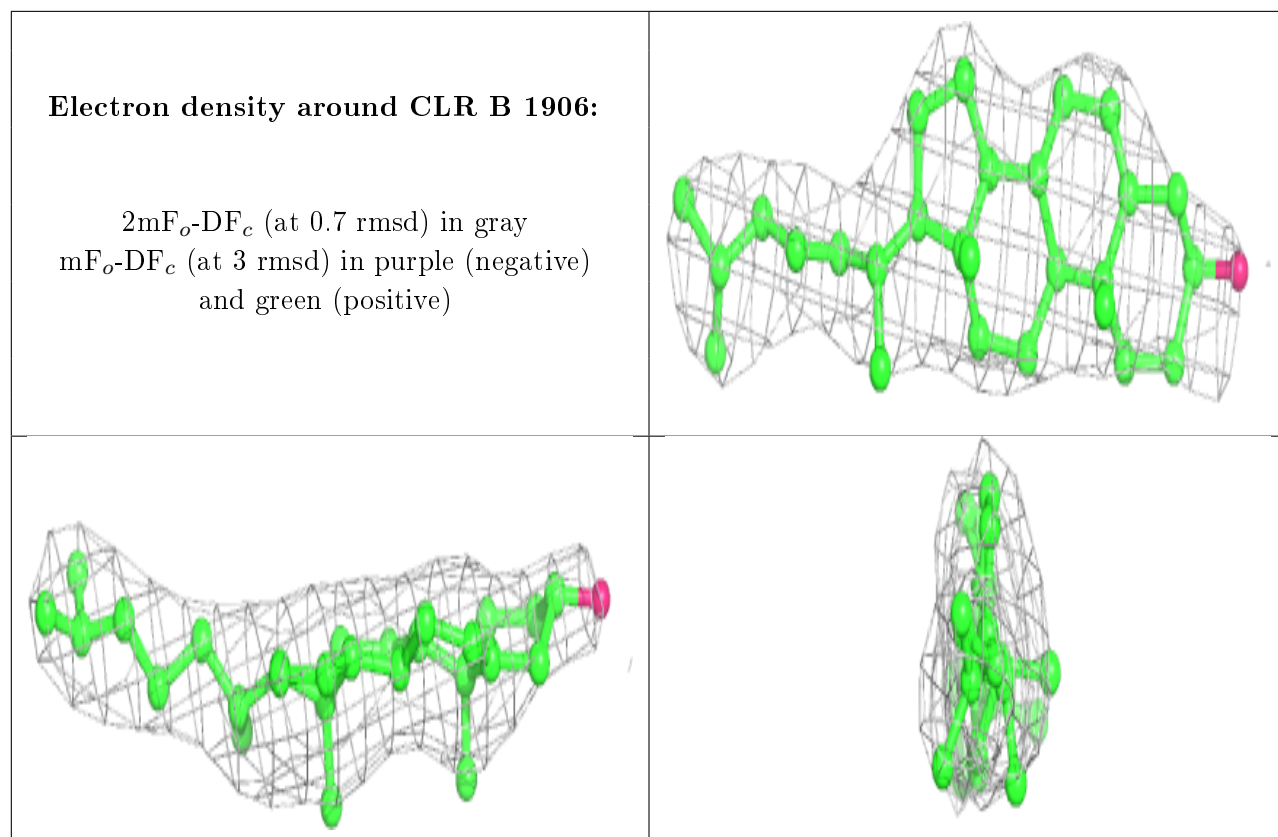
Electron density around FM9 B 1901:

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

**Electron density around FM9 A 1901:**

$2mF_o-DF_c$ (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.