Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 07:09 AM JST

PDB ID	:	7F83
Title	:	Crystal Structure of a receptor in Complex with inverse agonist
Authors	:	Xu, Z.; Shao, Z.
Deposited on	:	2021-07-01
Resolution	:	2.94 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

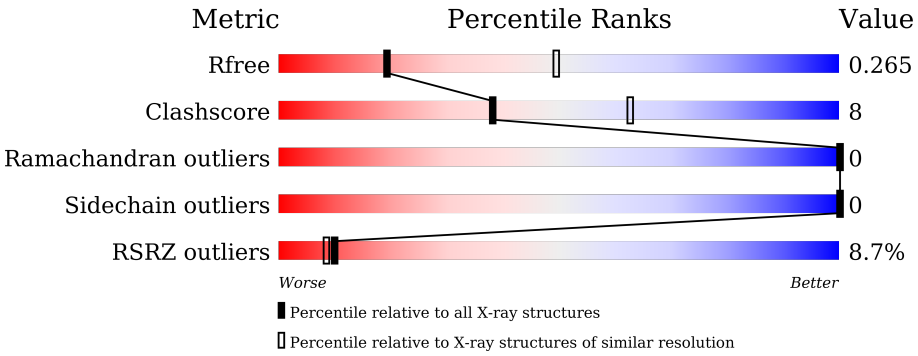
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	416	4% 73% 22% 5%
1	B	416	13% 78% 15% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6227 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 Growth hormone secretagogue receptor type 1,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3158	2074	525	540	19			
1	B	389	Total	C	N	O	S	0	0	0
			2867	1879	479	492	17			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	LYS	THR	engineered mutation	UNP Q92847
A	188	GLN	ASN	engineered mutation	UNP Q92847
A	1001	GLY	-	linker	UNP Q92847
A	1002	GLY	-	linker	UNP Q92847
A	1003	THR	-	linker	UNP Q92847
A	1004	THR	-	linker	UNP Q92847
A	1005	MET	-	linker	UNP Q92847
A	1012	TRP	MET	engineered mutation	UNP P0ABE7
A	1107	ILE	HIS	engineered mutation	UNP P0ABE7
A	1111	LEU	ARG	engineered mutation	UNP P0ABE7
A	343	GLU	-	expression tag	UNP Q92847
A	344	ASN	-	expression tag	UNP Q92847
A	345	LEU	-	expression tag	UNP Q92847
A	346	TYR	-	expression tag	UNP Q92847
A	347	PHE	-	expression tag	UNP Q92847
A	348	GLN	-	expression tag	UNP Q92847
B	130	LYS	THR	engineered mutation	UNP Q92847
B	188	GLN	ASN	engineered mutation	UNP Q92847
B	1001	GLY	-	linker	UNP Q92847
B	1002	GLY	-	linker	UNP Q92847
B	1003	THR	-	linker	UNP Q92847
B	1004	THR	-	linker	UNP Q92847
B	1005	MET	-	linker	UNP Q92847
B	1012	TRP	MET	engineered mutation	UNP P0ABE7

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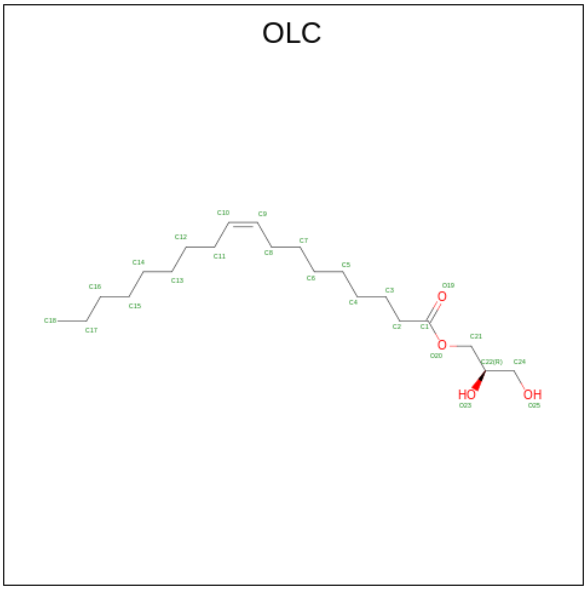
Chain	Residue	Modelled	Actual	Comment	Reference
B	1107	ILE	HIS	engineered mutation	UNP P0ABE7
B	1111	LEU	ARG	engineered mutation	UNP P0ABE7
B	343	GLU	-	expression tag	UNP Q92847
B	344	ASN	-	expression tag	UNP Q92847
B	345	LEU	-	expression tag	UNP Q92847
B	346	TYR	-	expression tag	UNP Q92847
B	347	PHE	-	expression tag	UNP Q92847
B	348	GLN	-	expression tag	UNP Q92847

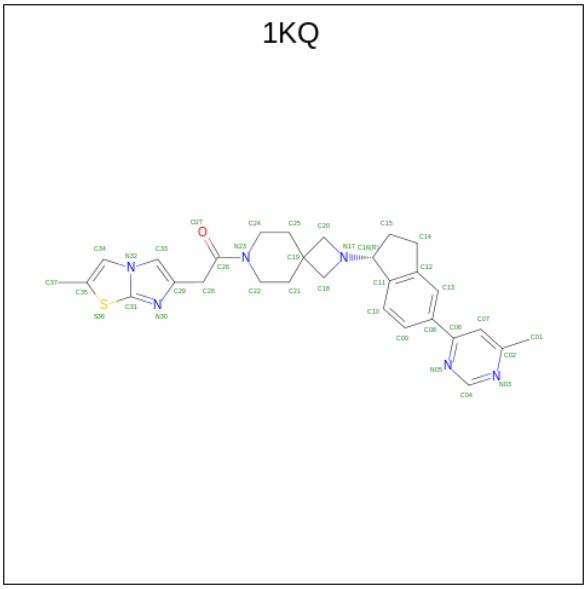
- Molecule 2 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 18 14 4	0	0
2	A	1	Total C O 25 21 4	0	0
2	B	1	Total C O 19 15 4	0	0
2	B	1	Total C O 16 12 4	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C O 25 21 4	0	0

- Molecule 3 is 2-(2-methylimidazo[2,1-b][1,3]thiazol-6-yl)-1-[2-[(1R)-5-(6-methylpyrimidin-

4-yl)-2,3-dihydro-1H-inden-1-yl]-2,7-diazaspiro[3.5]nonan-7-yl]ethanone (three-letter code: 1KQ) (formula: $C_{29}H_{32}N_6OS$).



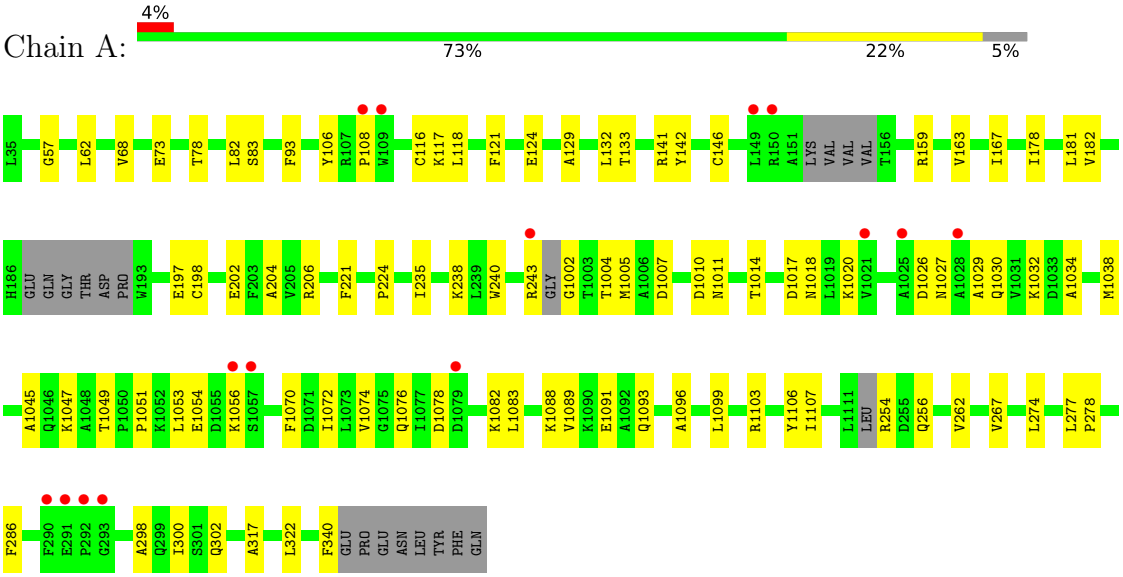
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			37	29	6	1	1		
3	B	1	Total	C	N	O	S	0	0
			37	29	6	1	1		

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.

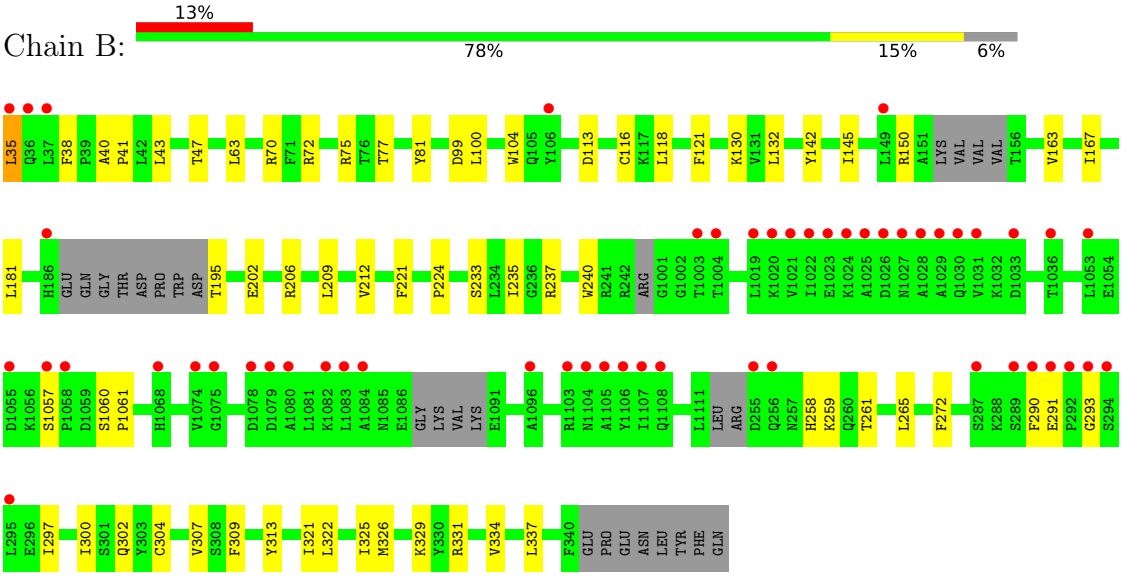
• Molecule 1: Growth hormone secretagogue receptor type 1,Soluble cytochrome b562

Chain A:



• Molecule 1: Growth hormone secretagogue receptor type 1,Soluble cytochrome b562

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.71Å 58.68Å 119.24Å 90.00° 90.60° 90.00°	Depositor
Resolution (Å)	39.78 – 2.94 39.78 – 2.94	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.78-2.94) 100.0 (39.78-2.94)	Depositor EDS
R_{merge}	0.66	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.19.2-4158	Depositor
R, R_{free}	0.227 , 0.265 0.227 , 0.265	Depositor DCC
R_{free} test set	1239 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 79.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6227	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLC, 1KQ

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	0.40	0/3229	0.59	4/4377 (0.1%)
1	B	0.36	0/2930	0.57	3/3998 (0.1%)
All	All	0.38	0/6159	0.58	7/8375 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	150	ARG	NE-CZ-NH1	-8.71	115.95	120.30
1	A	1026	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	B	35	LEU	CA-CB-CG	5.90	128.87	115.30
1	A	73	GLU	CA-CB-CG	-5.78	100.69	113.40
1	A	116	CYS	CA-CB-SG	-5.55	104.01	114.00
1	B	150	ARG	CG-CD-NE	5.46	123.26	111.80
1	A	198	CYS	CA-CB-SG	-5.31	104.44	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	GLU	Peptide

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	3158	0	3245	54	0
1	B	2867	0	2745	38	0
2	A	43	0	63	0	0
2	B	85	0	126	4	0
3	A	37	0	0	0	0
3	B	37	0	0	0	0
All	All	6227	0	6179	94	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 8.

All (94) 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:243:ARG:O	1:A:1002:GLY:N	2.17	0.77
1:A:117:LYS:NZ	1:A:182:VAL:O	2.22	0.73
1:B:145:ILE:HD12	1:B:235:ILE:HD12	1.72	0.71
1:A:181:LEU:HB2	1:A:204:ALA:HB2	1.77	0.66
1:A:146:CYS:HA	1:A:238:LYS:HE3	1.79	0.65
1:A:340:PHE:HB3	2:B:1204:OLC:H24A	1.81	0.62
1:A:1004:THR:HG23	1:A:1007:ASP:H	1.67	0.60
1:A:1053:LEU:HD12	1:A:1056:LYS:HG3	1.84	0.59
1:B:35:LEU:HD23	1:B:195:THR:HG21	1.85	0.59
1:B:132:LEU:HB2	1:B:167:ILE:HG23	1.86	0.58
1:A:254:ARG:O	1:A:256:GLN:NE2	2.37	0.58
1:A:1106:TYR:HB2	1:A:1107:ILE:HD12	1.84	0.58
1:A:1096:ALA:HA	1:A:1099:LEU:HD13	1.86	0.57
1:B:100:LEU:HB3	2:B:1204:OLC:H7A	1.87	0.56
1:A:243:ARG:NH2	1:A:1054:GLU:HG2	2.20	0.56
1:B:202:GLU:CD	1:B:206:ARG:HD3	2.26	0.55
1:A:1078:ASP:O	1:A:1082:LYS:HG3	2.06	0.55
1:B:70:ARG:NH1	1:B:337:LEU:O	2.40	0.55
1:A:1103:ARG:HA	1:A:1107:ILE:HD13	1.90	0.54
1:A:1051:PRO:HA	1:A:1054:GLU:HG3	1.90	0.54
1:A:243:ARG:NH2	1:A:1049:THR:HB	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLU:HG3	1:A:178:ILE:HG13	1.89	0.53
1:A:1027:ASN:HB3	1:A:1030:GLN:HB2	1.91	0.53
1:A:1089:VAL:O	1:A:1093:GLN:HG3	2.08	0.52
1:A:129:ALA:O	1:A:133:THR:HG22	2.09	0.52
1:A:1083:LEU:HD13	1:A:1091:GLU:HB3	1.92	0.52
1:A:106:TYR:O	1:A:108:PRO:HD3	2.10	0.51
1:B:77:THR:HG22	1:B:81:TYR:CE2	2.45	0.51
1:A:202:GLU:HG2	1:A:206:ARG:HD3	1.91	0.51
1:A:221:PHE:O	1:A:224:PRO:HD2	2.10	0.51
1:B:233:SER:O	1:B:237:ARG:HG2	2.11	0.51
1:B:1060:SER:OG	1:B:1061:PRO:HD3	2.10	0.51
1:A:178:ILE:O	1:A:182:VAL:HG22	2.11	0.51
1:A:267:VAL:HG12	1:A:322:LEU:HD13	1.94	0.50
1:B:142:TYR:HA	1:B:235:ILE:HD11	1.93	0.50
1:A:57:GLY:HA3	1:A:93:PHE:CE2	2.46	0.50
1:A:235:ILE:HG21	1:A:262:VAL:HG21	1.94	0.50
1:B:81:TYR:OH	1:B:163:VAL:HG21	2.13	0.48
1:B:261:THR:O	1:B:265:LEU:HG	2.13	0.48
1:B:99:ASP:OD2	1:B:313:TYR:OH	2.22	0.48
1:A:118:LEU:O	1:A:121:PHE:HB3	2.14	0.48
1:B:130:LYS:HD2	1:B:272:PHE:CE1	2.49	0.48
1:B:293:GLY:O	1:B:297:ILE:HG12	2.13	0.48
1:B:72:ARG:HA	1:B:75:ARG:HH11	1.79	0.48
1:B:297:ILE:HA	1:B:300:ILE:HD12	1.96	0.47
1:A:1088:LYS:HB3	1:A:1091:GLU:HB2	1.96	0.47
1:A:277:LEU:HB3	1:A:278:PRO:HD3	1.97	0.47
1:A:286:PHE:HZ	1:A:300:ILE:HG22	1.79	0.47
1:A:1004:THR:HG22	1:A:1007:ASP:OD2	2.14	0.47
1:A:1072:ILE:O	1:A:1076:GLN:HG3	2.16	0.46
1:A:1047:LYS:HE3	1:A:1047:LYS:HB2	1.56	0.46
1:A:1096:ALA:O	1:A:1099:LEU:HB2	2.15	0.46
1:B:99:ASP:HB3	1:B:309:PHE:CE2	2.51	0.45
1:B:113:ASP:O	1:B:116:CYS:HB3	2.17	0.45
1:A:1010:ASP:O	1:A:1014:THR:HG23	2.17	0.45
1:A:1018:ASN:C	1:A:1038:MET:HE2	2.37	0.45
1:A:68:VAL:HG21	1:A:83:SER:HB2	1.99	0.44
1:B:40:ALA:N	1:B:41:PRO:HD2	2.32	0.44
1:B:130:LYS:HD2	1:B:272:PHE:HE1	1.83	0.44
1:B:47:THR:HG23	1:B:100:LEU:HD22	1.99	0.44
1:B:321:ILE:O	1:B:325:ILE:HG12	2.16	0.44
1:B:331:ARG:O	1:B:334:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:HA	1:B:63:LEU:HD23	1.69	0.44
1:A:1029:ALA:HA	1:A:1032:LYS:HE2	1.99	0.44
1:B:329:LYS:N	1:B:329:LYS:HD3	2.33	0.44
2:B:1203:OLC:H2A	2:B:1203:OLC:H21A	1.80	0.44
1:B:118:LEU:O	1:B:121:PHE:HB3	2.19	0.43
1:A:1005:MET:HE2	1:A:1051:PRO:HG3	2.01	0.43
1:A:1017:ASP:HA	1:A:1020:LYS:HE2	2.00	0.42
1:A:298:ALA:O	1:A:302:GLN:HG3	2.19	0.42
1:A:142:TYR:HA	1:A:235:ILE:HD11	2.00	0.42
1:B:1057:SER:HB3	1:B:1061:PRO:HD2	2.00	0.42
1:A:93:PHE:HZ	1:A:317:ALA:HB2	1.83	0.42
1:B:240:TRP:CH2	1:B:259:LYS:HD2	2.54	0.42
1:B:221:PHE:O	1:B:224:PRO:HD2	2.19	0.42
1:A:1034:ALA:O	1:A:1038:MET:HG3	2.20	0.42
1:A:1070:PHE:O	1:A:1074:VAL:HG23	2.20	0.41
1:B:304:CYS:O	1:B:307:VAL:HG22	2.19	0.41
1:B:290:PHE:HD2	1:B:291:GLU:HG3	1.85	0.41
1:A:62:LEU:HD23	1:A:62:LEU:HA	1.77	0.41
1:A:78:THR:CG2	1:A:141:ARG:HH11	2.32	0.41
1:B:181:LEU:HD21	1:B:209:LEU:HB3	2.02	0.41
2:B:1203:OLC:H2A	2:B:1203:OLC:H5	1.72	0.41
1:B:145:ILE:HG12	1:B:258:HIS:ND1	2.36	0.41
1:A:132:LEU:HB2	1:A:167:ILE:HG23	2.03	0.41
1:B:38:PHE:CZ	1:B:302:GLN:HB3	2.56	0.41
1:B:43:LEU:HB3	1:B:104:TRP:CZ2	2.55	0.41
1:B:209:LEU:O	1:B:212:VAL:HG22	2.21	0.41
1:A:1011:ASN:CB	1:A:1045:ALA:HB2	2.51	0.41
1:A:159:ARG:O	1:A:163:VAL:HG23	2.21	0.40
1:A:240:TRP:HA	1:A:1004:THR:OG1	2.21	0.40
1:A:78:THR:O	1:A:82:LEU:HG	2.22	0.40
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.88	0.40
1:B:322:LEU:O	1:B:326:MET:HG3	2.21	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	386/416 (93%)	373 (97%)	13 (3%)	0	100	100
1	B	377/416 (91%)	362 (96%)	15 (4%)	0	100	100
All	All	763/832 (92%)	735 (96%)	28 (4%)	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	341/361 (94%)	341 (100%)	0	100	100
1	B	274/361 (76%)	274 (100%)	0	100	100
All	All	615/722 (85%)	615 (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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	B	1011	ASN
1	B	302	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
2	OLC	B	1201	-	18,18,24	1.00	2 (11%)	18,19,25	0.91	1 (5%)
2	OLC	A	1202	-	24,24,24	0.90	1 (4%)	25,25,25	0.97	1 (4%)
3	1KQ	A	1203	-	36,43,43	6.05	12 (33%)	39,65,65	1.95	9 (23%)
2	OLC	B	1203	-	24,24,24	0.84	2 (8%)	25,25,25	0.93	1 (4%)
3	1KQ	B	1205	-	36,43,43	6.23	10 (27%)	39,65,65	2.12	10 (25%)
2	OLC	A	1201	-	17,17,24	0.95	1 (5%)	18,18,25	1.16	1 (5%)
2	OLC	B	1204	-	24,24,24	0.79	2 (8%)	25,25,25	1.07	1 (4%)
2	OLC	B	1202	-	15,15,24	1.03	1 (6%)	16,16,25	1.10	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	B	1201	-	-	8/18/18/24	-
2	OLC	A	1202	-	-	8/24/24/24	-
3	1KQ	A	1203	-	-	0/10/47/47	0/7/7/7
2	OLC	B	1203	-	-	12/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1KQ	B	1205	-	-	0/10/47/47	0/7/7/7
2	OLC	A	1201	-	-	5/17/17/24	-
2	OLC	B	1204	-	-	13/24/24/24	-
2	OLC	B	1202	-	-	9/15/15/24	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1205	1KQ	C16-N17	-30.73	1.10	1.48
3	A	1203	1KQ	C16-N17	-29.55	1.12	1.48
3	B	1205	1KQ	C20-C19	-13.21	1.42	1.54
3	B	1205	1KQ	C18-C19	-12.42	1.43	1.54
3	A	1203	1KQ	C20-C19	-12.41	1.43	1.54
3	A	1203	1KQ	C18-C19	-12.25	1.43	1.54
3	A	1203	1KQ	C26-N23	6.50	1.48	1.35
3	B	1205	1KQ	C08-C06	-6.03	1.39	1.48
3	B	1205	1KQ	C26-N23	5.46	1.46	1.35
3	A	1203	1KQ	C08-C06	-5.40	1.40	1.48
3	A	1203	1KQ	C28-C26	3.02	1.55	1.52
3	B	1205	1KQ	C14-C12	3.02	1.55	1.51
3	A	1203	1KQ	C28-C29	2.83	1.54	1.51
2	B	1202	OLC	O20-C1	2.81	1.41	1.33
2	A	1202	OLC	O20-C1	2.78	1.41	1.33
3	A	1203	1KQ	C11-C16	2.75	1.54	1.51
2	B	1201	OLC	O20-C1	2.63	1.41	1.33
2	B	1203	OLC	O20-C1	2.56	1.40	1.33
2	A	1201	OLC	O20-C1	2.52	1.40	1.33
3	A	1203	1KQ	C14-C12	2.46	1.54	1.51
2	B	1204	OLC	O20-C1	2.45	1.40	1.33
3	B	1205	1KQ	C11-C16	2.38	1.54	1.51
3	A	1203	1KQ	C33-C29	2.33	1.39	1.36
3	A	1203	1KQ	C22-N23	2.29	1.51	1.47
3	B	1205	1KQ	C28-C26	2.18	1.54	1.52
3	B	1205	1KQ	C28-C29	2.18	1.53	1.51
2	B	1204	OLC	O20-C21	-2.12	1.40	1.45
2	B	1203	OLC	O20-C21	-2.09	1.40	1.45
3	A	1203	1KQ	C24-N23	2.05	1.50	1.47
2	B	1201	OLC	O20-C21	-2.04	1.40	1.45
3	B	1205	1KQ	C22-N23	2.04	1.50	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1205	1KQ	C35-C34-N32	7.06	115.14	107.89
3	A	1203	1KQ	C35-C34-N32	5.85	113.90	107.89
3	A	1203	1KQ	N05-C04-N03	-4.34	121.81	128.60
3	B	1205	1KQ	N05-C04-N03	-4.29	121.89	128.60
3	B	1205	1KQ	C37-C35-S36	4.28	124.60	119.88
2	A	1202	OLC	O20-C1-C2	3.22	122.00	111.91
3	A	1203	1KQ	C04-N05-C06	3.20	120.07	115.74
3	B	1205	1KQ	C09-C08-C06	-3.04	116.48	121.28
2	A	1201	OLC	O20-C1-C2	2.96	121.19	111.91
3	A	1203	1KQ	C15-C14-C12	2.94	106.17	103.31
3	B	1205	1KQ	C15-C14-C12	2.94	106.17	103.31
2	B	1202	OLC	O20-C1-C2	2.93	121.10	111.91
3	A	1203	1KQ	C09-C08-C06	-2.92	116.67	121.28
3	B	1205	1KQ	C04-N03-C02	2.89	121.52	116.97
3	B	1205	1KQ	C07-C02-N03	-2.88	118.87	121.66
2	B	1201	OLC	O20-C1-C2	2.70	120.38	111.91
3	A	1203	1KQ	C04-N03-C02	2.70	121.22	116.97
3	A	1203	1KQ	C07-C02-N03	-2.68	119.07	121.66
2	B	1203	OLC	O20-C1-C2	2.65	120.21	111.91
3	B	1205	1KQ	C34-C35-S36	-2.57	105.70	111.28
3	B	1205	1KQ	C04-N05-C06	2.57	119.22	115.74
2	B	1204	OLC	O20-C1-C2	2.39	119.42	111.91
3	B	1205	1KQ	C07-C06-C08	-2.19	118.94	121.85
3	A	1203	1KQ	C37-C35-C34	2.13	131.34	126.35
3	A	1203	1KQ	C34-C35-S36	-2.04	106.85	111.28

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	OLC	O20-C21-C22-O23
2	B	1201	OLC	O20-C21-C22-C24
2	B	1203	OLC	O19-C1-O20-C21
2	B	1203	OLC	C2-C1-O20-C21
2	A	1202	OLC	O19-C1-O20-C21
2	A	1202	OLC	C2-C1-O20-C21
2	B	1204	OLC	C2-C1-O20-C21
2	B	1204	OLC	O19-C1-O20-C21
2	B	1203	OLC	C13-C14-C15-C16
2	B	1202	OLC	C2-C1-O20-C21
2	B	1201	OLC	O20-C21-C22-O23
2	B	1203	OLC	O20-C21-C22-O23
2	B	1202	OLC	O19-C1-O20-C21

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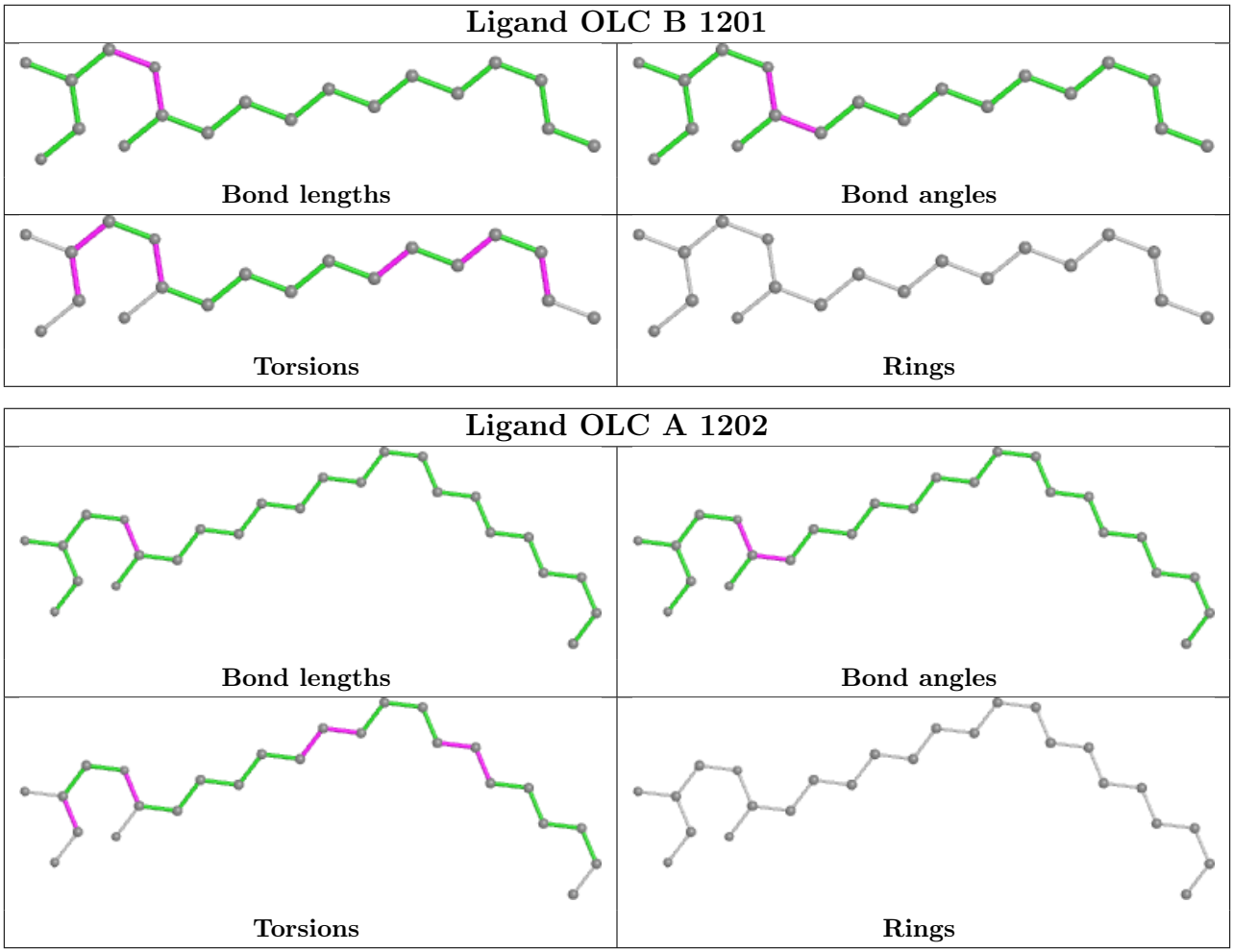
Mol	Chain	Res	Type	Atoms
2	B	1202	OLC	C1-C2-C3-C4
2	B	1204	OLC	C1-C2-C3-C4
2	B	1202	OLC	O20-C21-C22-O23
2	B	1204	OLC	O20-C21-C22-O23
2	B	1202	OLC	O20-C21-C22-C24
2	B	1203	OLC	O20-C21-C22-C24
2	B	1204	OLC	O20-C21-C22-C24
2	B	1204	OLC	C11-C12-C13-C14
2	B	1204	OLC	C3-C4-C5-C6
2	A	1202	OLC	C21-C22-C24-O25
2	B	1204	OLC	C21-C22-C24-O25
2	B	1201	OLC	C5-C6-C7-C8
2	A	1202	OLC	C5-C6-C7-C8
2	B	1204	OLC	C5-C6-C7-C8
2	B	1203	OLC	C6-C7-C8-C9
2	B	1203	OLC	C5-C6-C7-C8
2	B	1202	OLC	C3-C4-C5-C6
2	B	1203	OLC	C11-C12-C13-C14
2	A	1201	OLC	C2-C3-C4-C5
2	B	1204	OLC	C4-C5-C6-C7
2	B	1203	OLC	C14-C15-C16-C17
2	B	1204	OLC	O23-C22-C24-O25
2	A	1202	OLC	C6-C7-C8-C9
2	B	1201	OLC	C7-C8-C9-C10
2	B	1203	OLC	C2-C3-C4-C5
2	B	1202	OLC	C4-C5-C6-C7
2	B	1202	OLC	C5-C6-C7-C8
2	A	1201	OLC	O20-C21-C22-C24
2	B	1201	OLC	C9-C10-C11-C12
2	A	1202	OLC	O23-C22-C24-O25
2	B	1202	OLC	O23-C22-C24-O25
2	A	1201	OLC	C5-C6-C7-C8
2	B	1204	OLC	C2-C3-C4-C5
2	A	1202	OLC	C10-C11-C12-C13
2	B	1203	OLC	C9-C10-C11-C12
2	B	1204	OLC	C7-C8-C9-C10
2	A	1201	OLC	C7-C8-C9-C10
2	B	1201	OLC	O23-C22-C24-O25
2	B	1201	OLC	C2-C1-O20-C21
2	B	1203	OLC	C3-C4-C5-C6
2	B	1201	OLC	O19-C1-O20-C21
2	A	1202	OLC	C11-C12-C13-C14

There are no ring outliers.

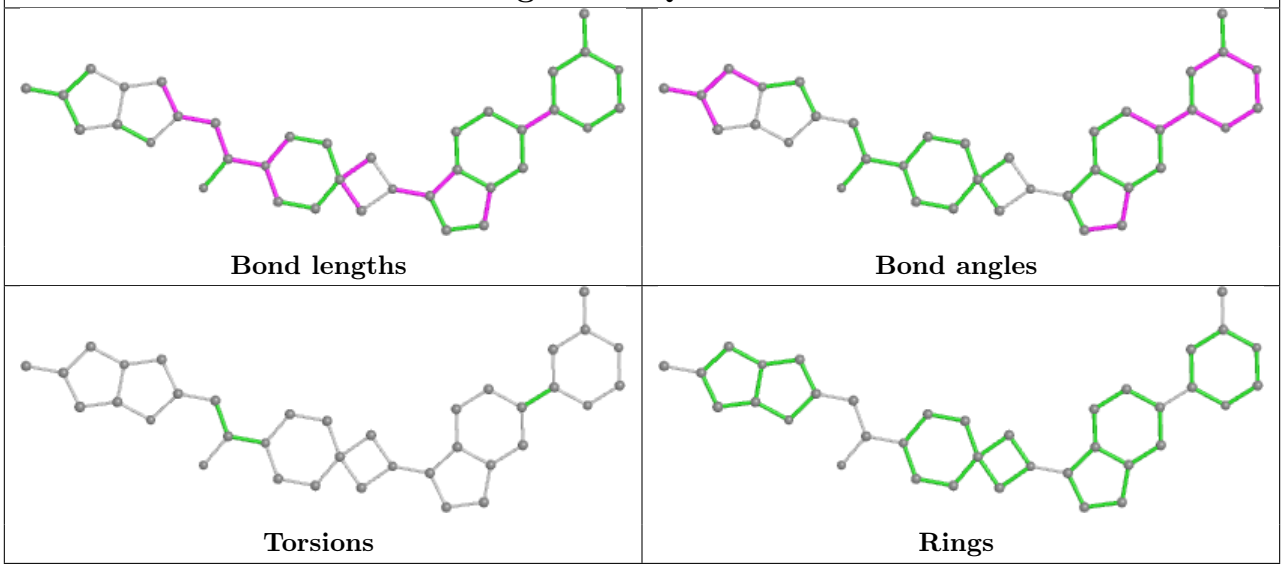
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1203	OLC	2	0
2	B	1204	OLC	2	0

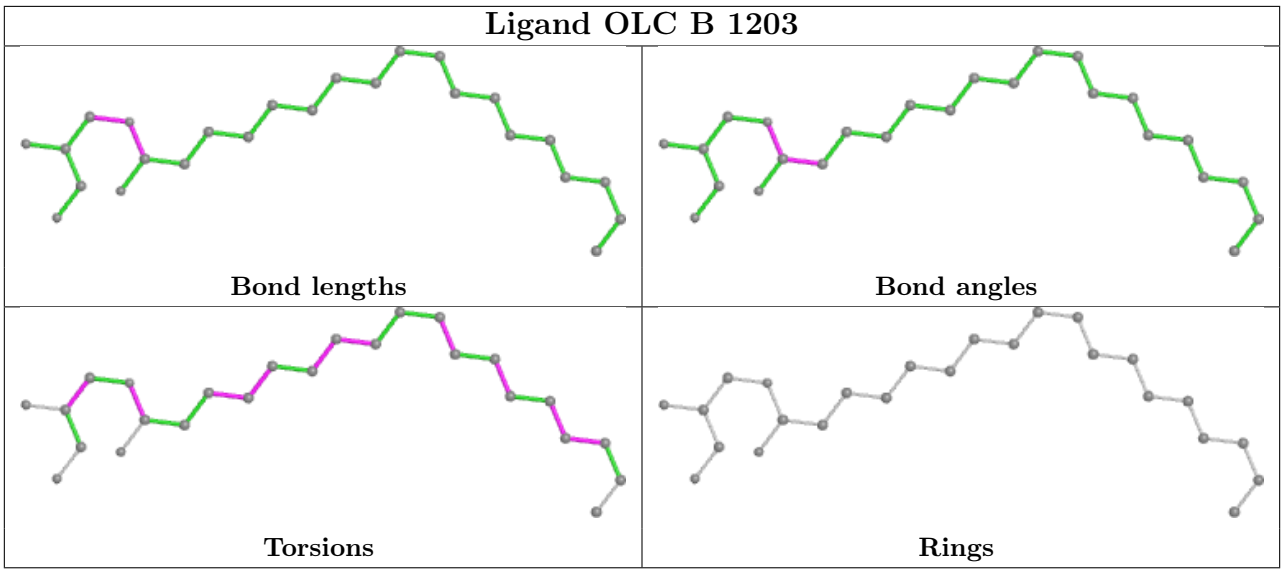
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



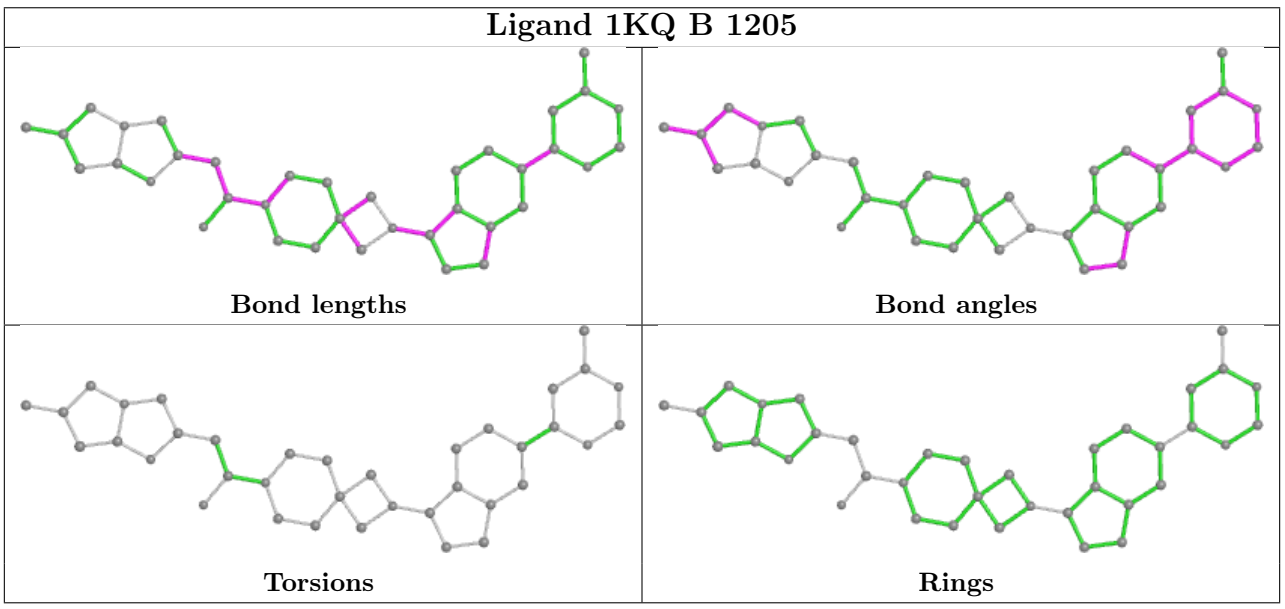
Ligand 1KQ A 1203

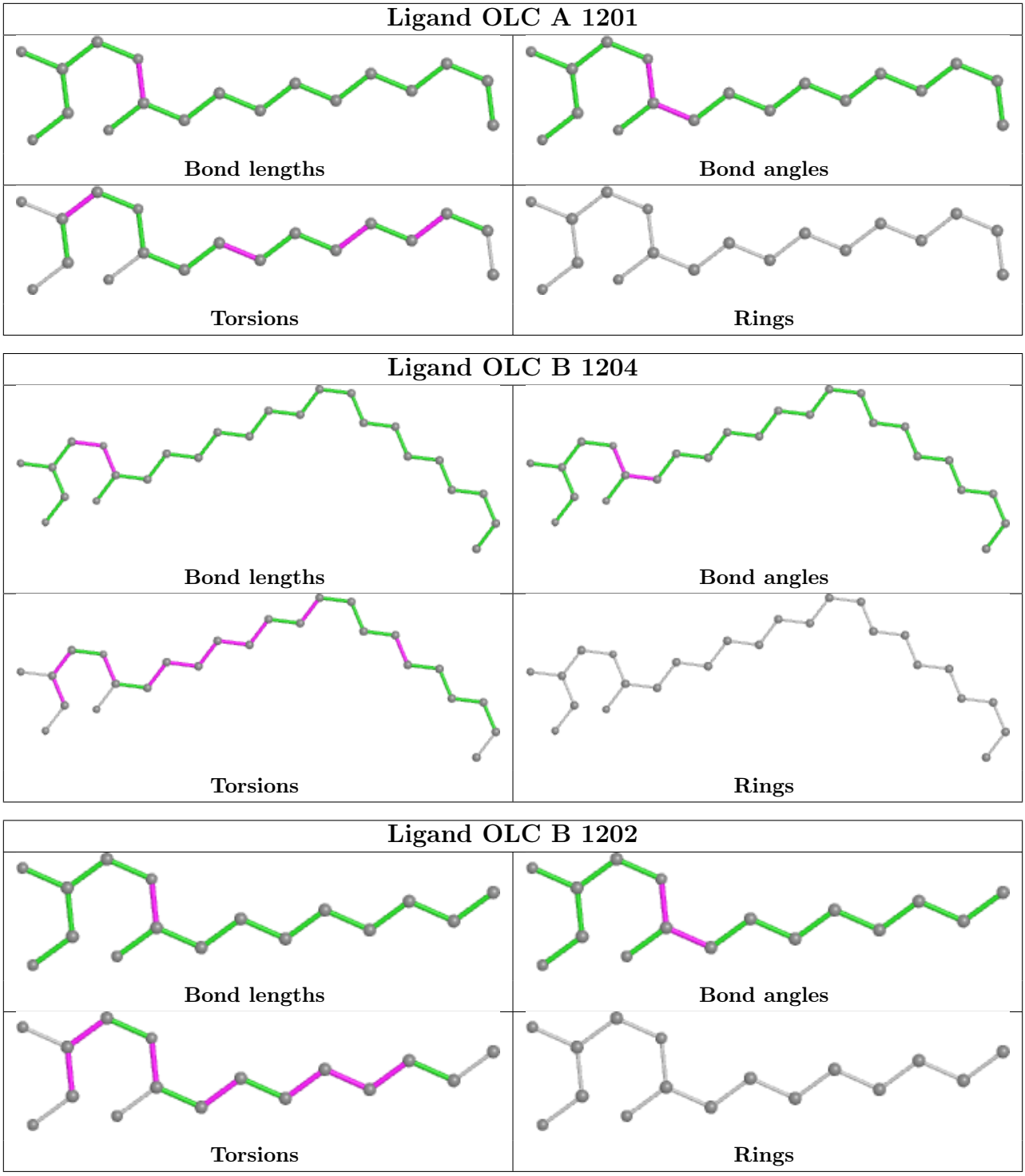


Ligand OLC B 1203



Ligand 1KQ B 1205





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	396/416 (95%)	0.05	15 (3%) 40 39	28, 52, 106, 131	0
1	B	389/416 (93%)	0.54	53 (13%) 3 2	38, 69, 214, 235	0
All	All	785/832 (94%)	0.29	68 (8%) 10 8	28, 62, 198, 235	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1028	ALA	7.7
1	B	1027	ASN	7.1
1	B	1020	LYS	6.5
1	A	290	PHE	5.8
1	B	1030	GLN	5.5
1	A	293	GLY	5.3
1	B	1104	ASN	5.2
1	B	1026	ASP	4.9
1	B	1074	VAL	4.8
1	B	291	GLU	4.8
1	B	290	PHE	4.4
1	A	109	TRP	4.4
1	B	1025	ALA	4.3
1	B	1029	ALA	4.2
1	B	294	SER	4.1
1	B	1084	ALA	4.1
1	B	287	SER	4.0
1	B	292	PRO	4.0
1	B	35	LEU	3.9
1	B	1019	LEU	3.8
1	A	1028	ALA	3.8
1	B	1075	GLY	3.7
1	A	292	PRO	3.7
1	B	293	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	1021	VAL	3.6
1	B	36	GLN	3.6
1	B	1058	PRO	3.6
1	B	37	LEU	3.6
1	B	1106	TYR	3.5
1	A	1021	VAL	3.4
1	A	108	PRO	3.4
1	A	150	ARG	3.3
1	B	1057	SER	3.3
1	B	1024	LYS	3.3
1	B	1004	THR	3.1
1	B	1055	ASP	3.1
1	B	1036	THR	3.1
1	B	1107	ILE	3.0
1	B	1003	THR	3.0
1	B	1022	ILE	2.9
1	B	1080	ALA	2.8
1	B	186	HIS	2.8
1	A	243	ARG	2.6
1	A	1025	ALA	2.6
1	A	291	GLU	2.6
1	B	1078	ASP	2.6
1	B	1108	GLN	2.5
1	B	106	TYR	2.5
1	A	1057	SER	2.5
1	B	1023	GLU	2.5
1	B	1079	ASP	2.5
1	B	289	SER	2.5
1	B	1033	ASP	2.4
1	B	295	LEU	2.4
1	B	1031	VAL	2.3
1	B	149	LEU	2.3
1	A	149	LEU	2.3
1	B	1068	HIS	2.3
1	B	256	GLN	2.3
1	B	1082	LYS	2.2
1	B	1096	ALA	2.1
1	A	1056	LYS	2.1
1	A	1079	ASP	2.1
1	B	1083	LEU	2.0
1	B	1105	ALA	2.0
1	B	255	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	1053	LEU	2.0
1	B	1103	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

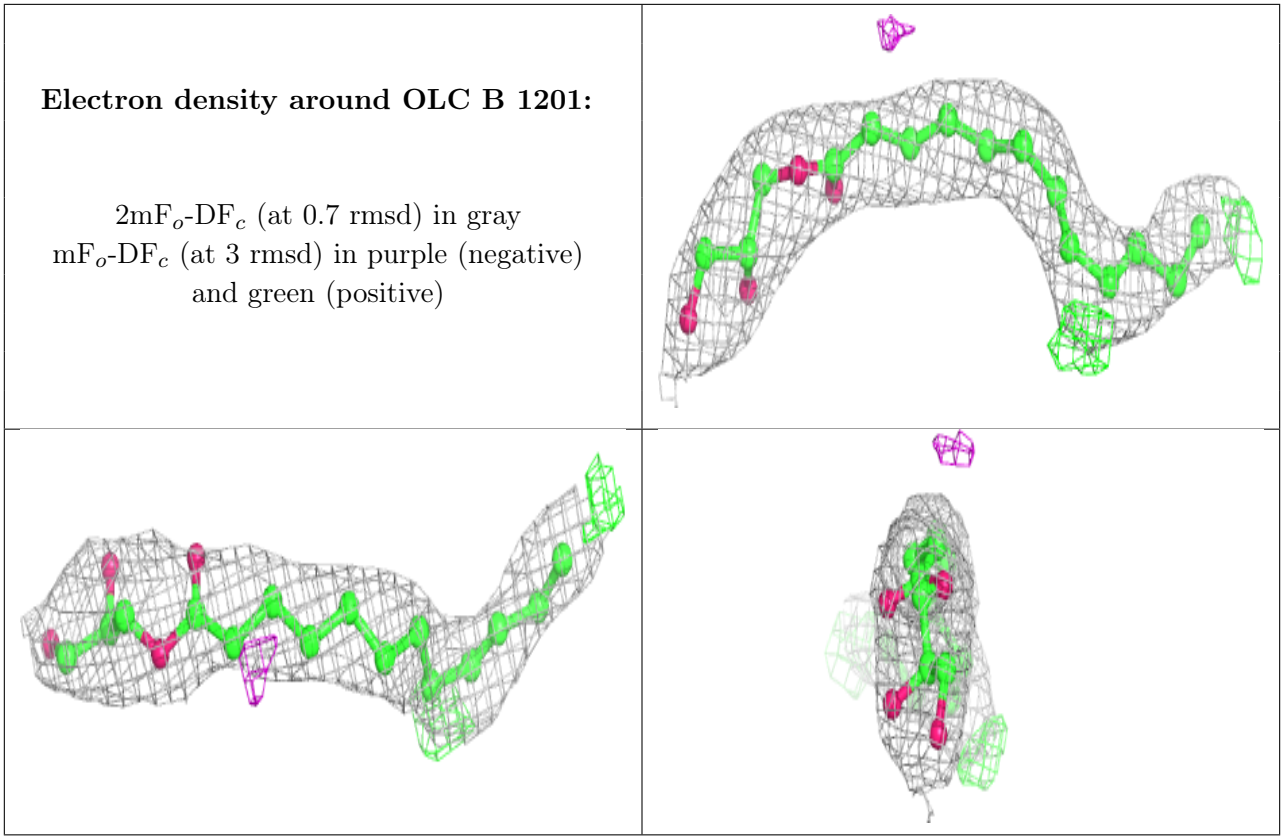
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OLC	B	1201	19/25	0.81	0.28	35,56,79,82	0
2	OLC	B	1203	25/25	0.83	0.27	51,70,95,102	0
2	OLC	B	1202	16/25	0.85	0.22	46,69,84,87	0
2	OLC	A	1201	18/25	0.86	0.23	38,61,78,86	0
2	OLC	A	1202	25/25	0.88	0.28	34,59,72,76	0
2	OLC	B	1204	25/25	0.89	0.27	45,59,78,85	0
3	1KQ	A	1203	37/37	0.93	0.22	22,41,52,58	0
3	1KQ	B	1205	37/37	0.95	0.18	37,52,63,67	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.

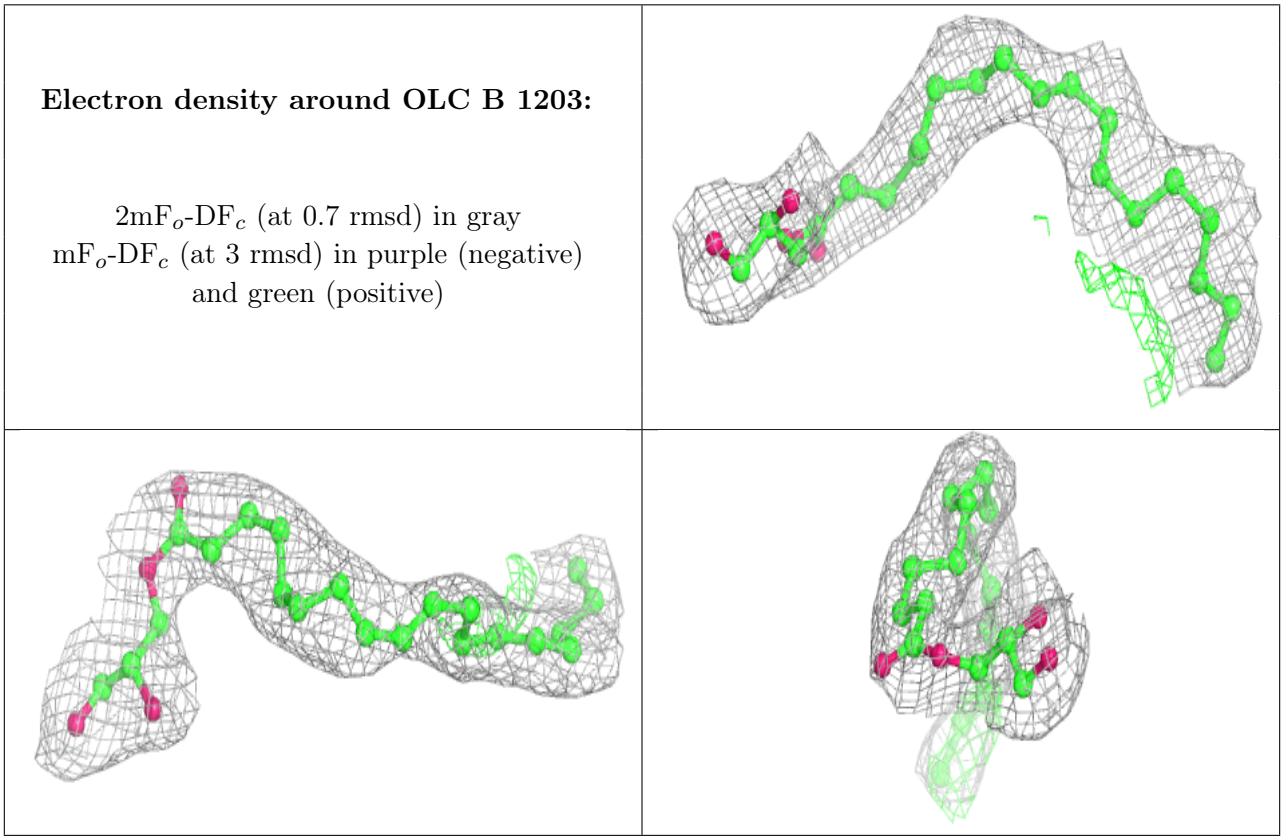
Electron density around OLC B 1201:

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



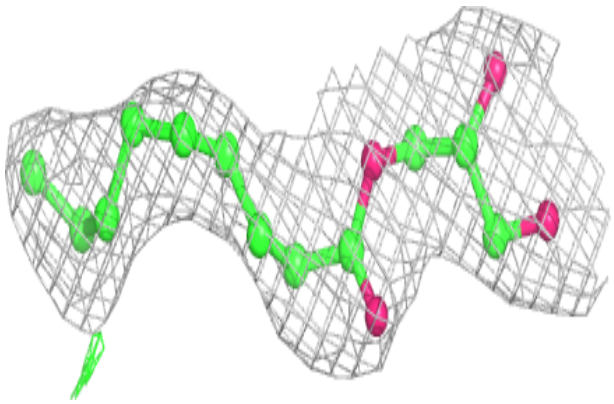
Electron density around OLC B 1203:

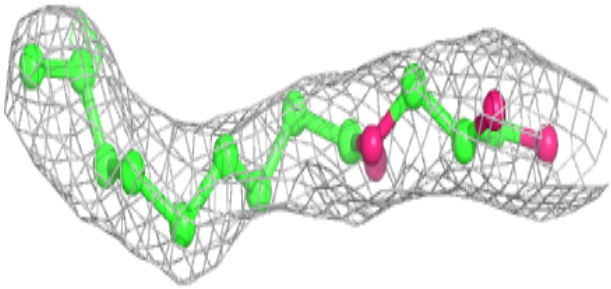
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

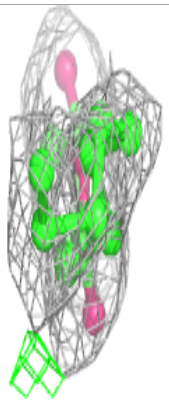


Electron density around OLC B 1202:

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

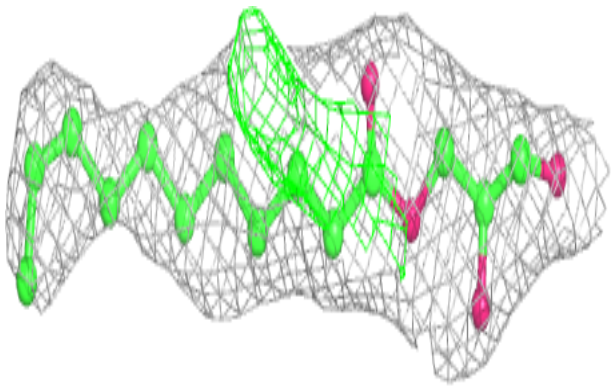


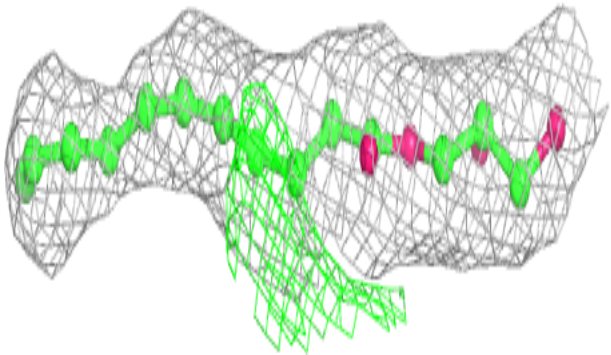


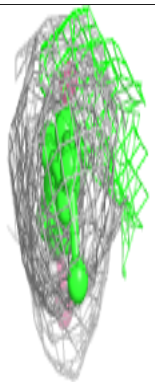


Electron density around OLC A 1201:

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

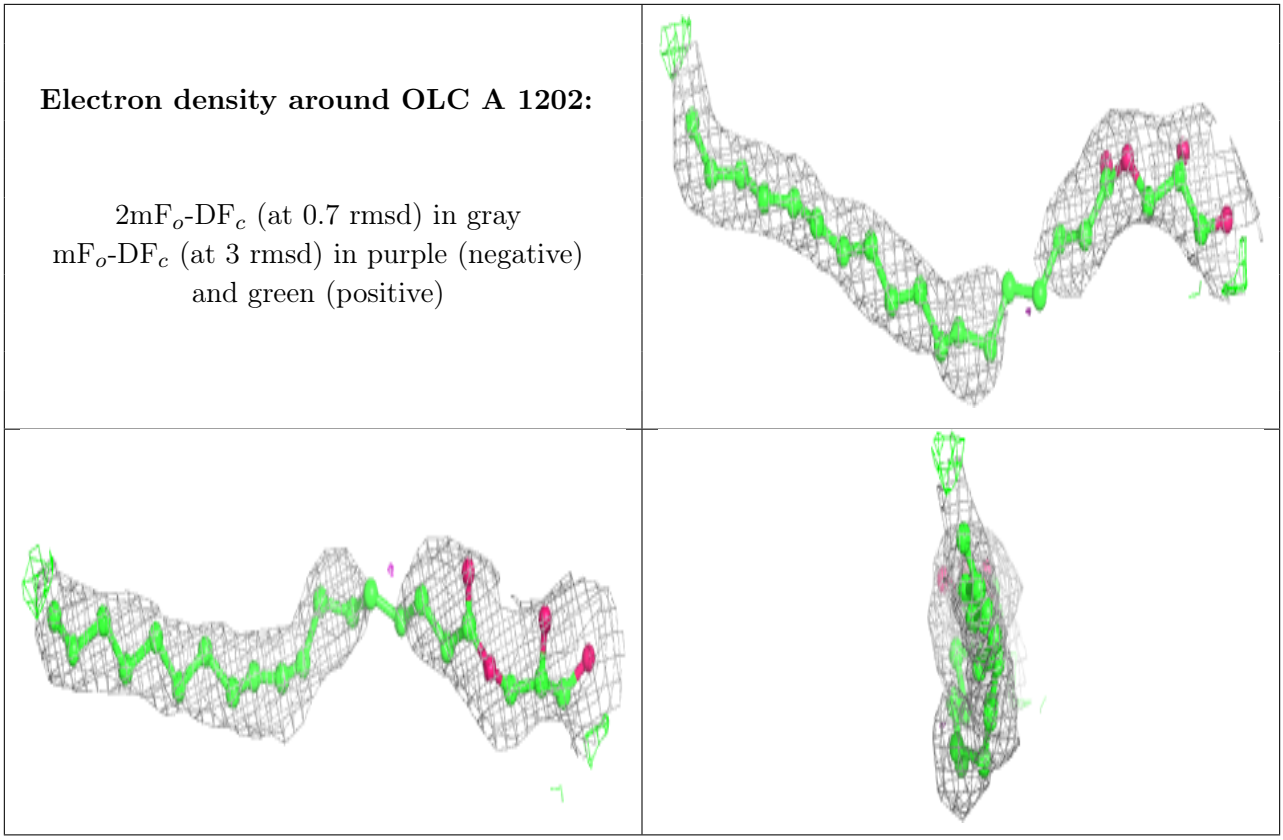






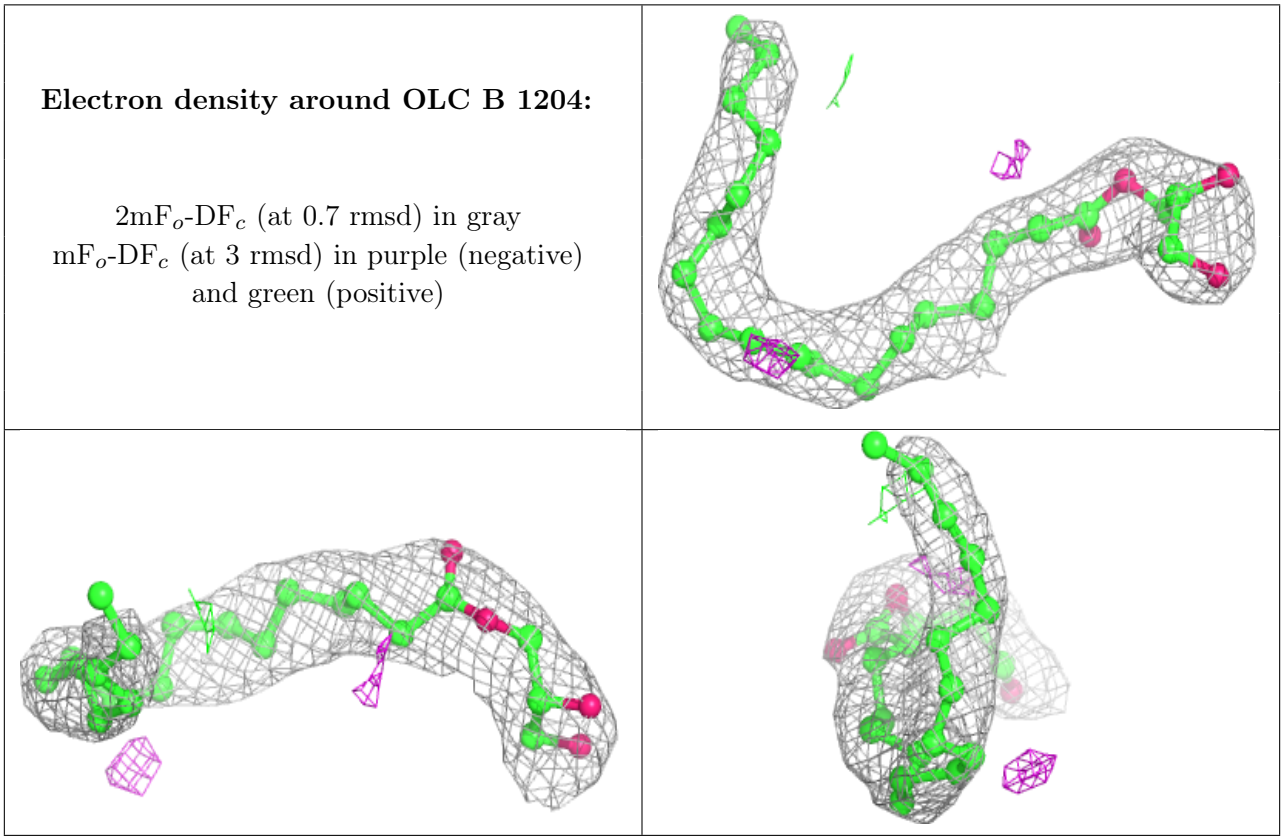
Electron density around OLC A 1202:

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



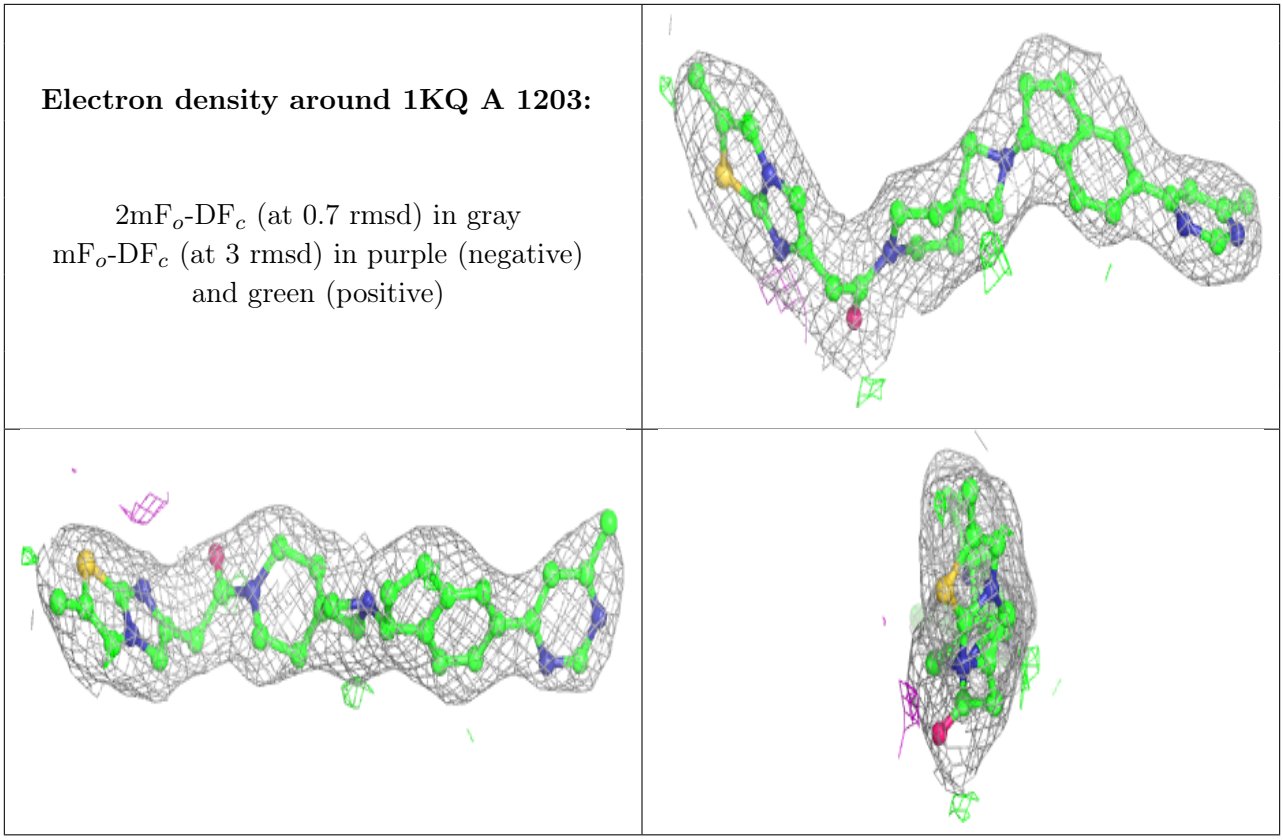
Electron density around OLC B 1204:

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



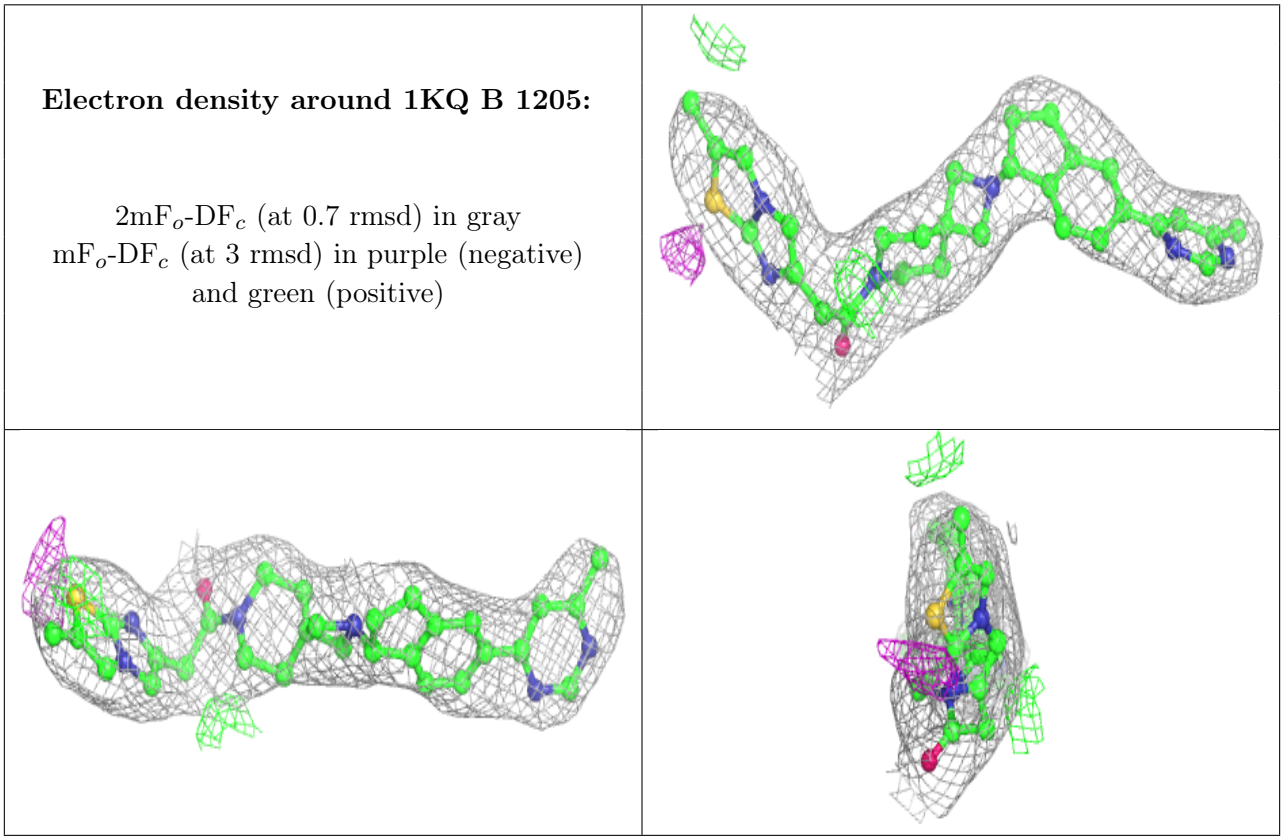
Electron density around 1KQ A 1203:

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



Electron density around 1KQ B 1205:

$2mF_o$-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.