



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:56 PM UTC

PDB ID : 5DSG / pdb_00005dsg
Title : Structure of the M4 muscarinic acetylcholine receptor (M4-mT4L) bound to tiotropium
Authors : Thal, D.M.; Kobilka, B.K.; Sexton, P.M.; Christopoulos, A.
Deposited on : 2015-09-17
Resolution : 2.60 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

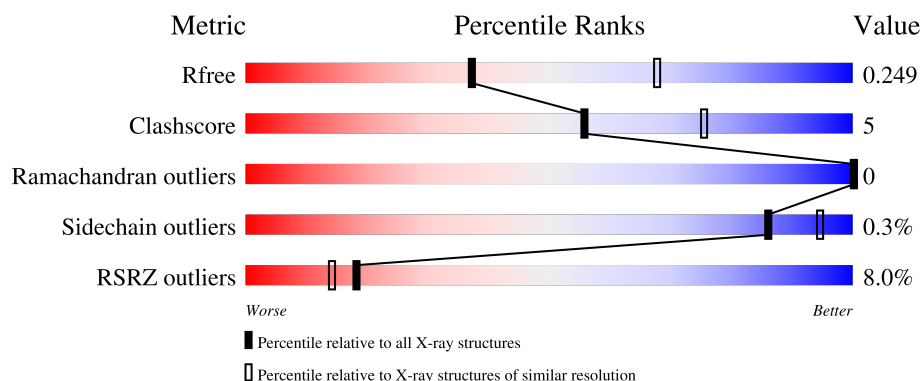
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	422	
1	B	422	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6516 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 Muscarinic acetylcholine receptor M4,Endolysin,Endolysin,Muscarinic acetylcholine receptor M4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3058	2004	499	533	22			
1	B	399	Total	C	N	O	S	0	0	0
			3115	2041	512	541	21			

There are 38 discrepancies between the modelled and reference sequences:

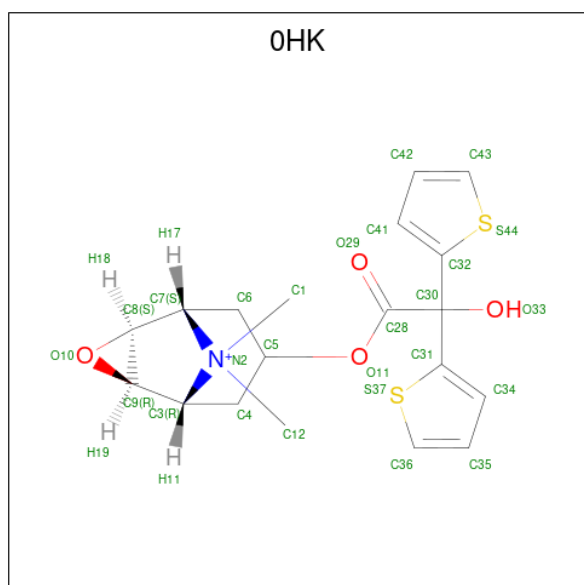
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	expression tag	UNP P08173
A	21	PRO	-	expression tag	UNP P08173
A	1012	GLY	-	linker	UNP P00720
A	1013	GLY	-	linker	UNP P00720
A	1014	GLY	-	linker	UNP P00720
A	1015	SER	-	linker	UNP P00720
A	1016	GLY	-	linker	UNP P00720
A	1017	GLY	-	linker	UNP P00720
A	1054	ALA	CYS	engineered mutation	UNP P00720
A	1094	ARG	ILE	engineered mutation	UNP P00720
A	479	ARG	-	expression tag	UNP P08173
A	480	HIS	-	expression tag	UNP P08173
A	481	HIS	-	expression tag	UNP P08173
A	482	HIS	-	expression tag	UNP P08173
A	483	HIS	-	expression tag	UNP P08173
A	484	HIS	-	expression tag	UNP P08173
A	485	HIS	-	expression tag	UNP P08173
A	486	HIS	-	expression tag	UNP P08173
A	487	HIS	-	expression tag	UNP P08173
B	20	GLY	-	expression tag	UNP P08173
B	21	PRO	-	expression tag	UNP P08173
B	1012	GLY	-	linker	UNP P00720
B	1013	GLY	-	linker	UNP P00720
B	1014	GLY	-	linker	UNP P00720

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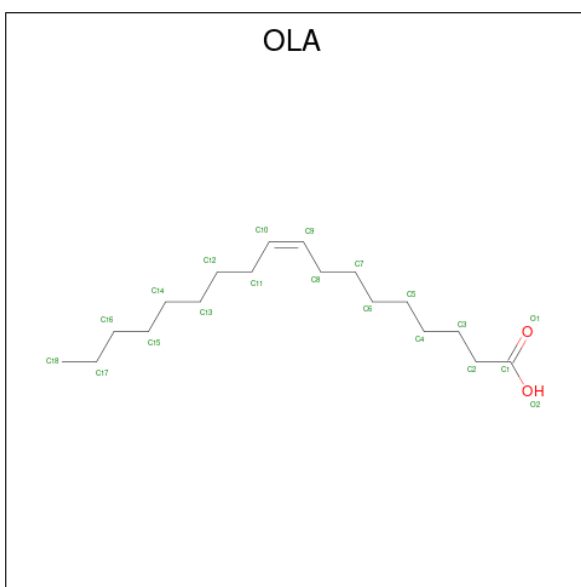
Chain	Residue	Modelled	Actual	Comment	Reference
B	1015	SER	-	linker	UNP P00720
B	1016	GLY	-	linker	UNP P00720
B	1017	GLY	-	linker	UNP P00720
B	1054	ALA	CYS	conflict	UNP P00720
B	1094	ARG	ILE	conflict	UNP P00720
B	479	ARG	-	expression tag	UNP P08173
B	480	HIS	-	expression tag	UNP P08173
B	481	HIS	-	expression tag	UNP P08173
B	482	HIS	-	expression tag	UNP P08173
B	483	HIS	-	expression tag	UNP P08173
B	484	HIS	-	expression tag	UNP P08173
B	485	HIS	-	expression tag	UNP P08173
B	486	HIS	-	expression tag	UNP P08173
B	487	HIS	-	expression tag	UNP P08173

- Molecule 2 is (1R,2R,4S,5S,7S)-7-{[hydroxy(dithiophen-2-yl)acetyl]oxy}-9,9-dimethyl-3-oxa-9-azoniatricyclo[3.3.1.0 2,4]nonane (CCD ID: 0HK) (formula: C₁₉H₂₂NO₄S₂).



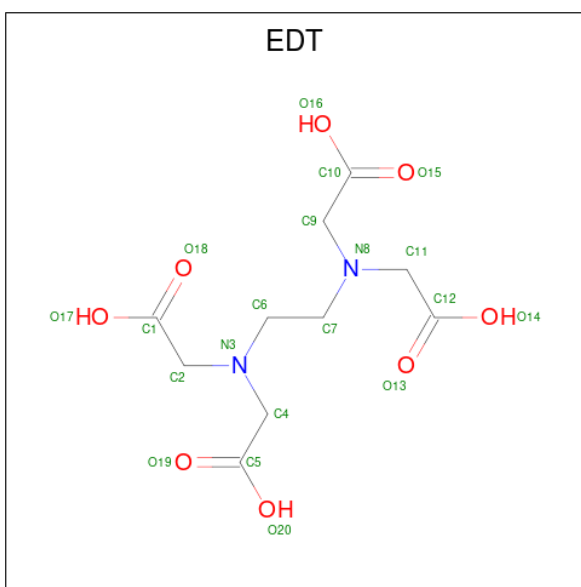
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	19	1	4	2		
2	B	1	Total	C	N	O	S	0	0
			26	19	1	4	2		

- Molecule 3 is OLEIC ACID (CCD ID: OLA) (formula: C₁₈H₃₄O₂).



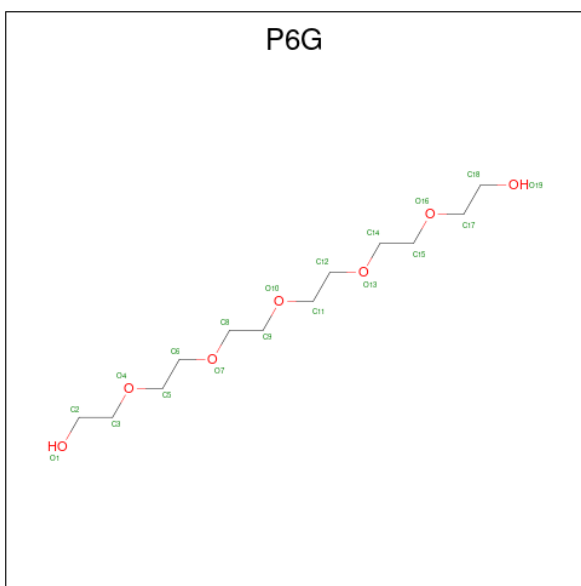
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	10	2		
3	A	1	Total	C	O	0	0
			14	12	2		
3	A	1	Total	C	O	0	0
			20	18	2		
3	B	1	Total	C	O	0	0
			20	18	2		
3	B	1	Total	C	O	0	0
			20	18	2		

- Molecule 4 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (CCD ID: EDT) (formula: C₁₀H₁₆N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			20	10	2	8		

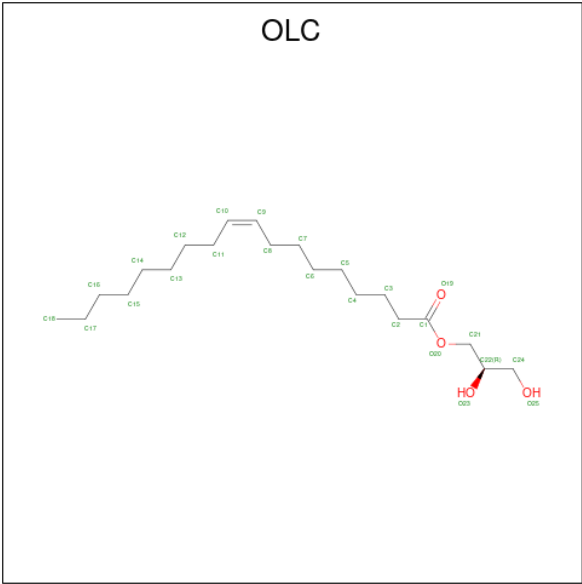
- Molecule 5 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		
5	B	1	Total	C	O	0	0
			19	12	7		

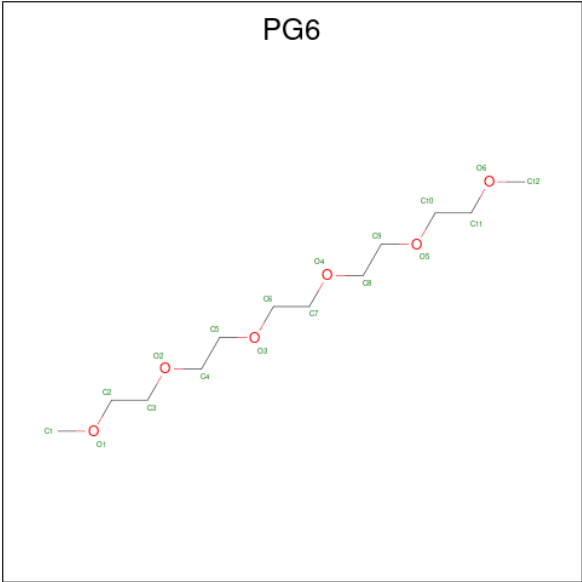
- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula:

C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			25	21	4		
6	A	1	Total	C	O	0	0
			18	14	4		
6	A	1	Total	C	O	0	0
			25	21	4		
6	B	1	Total	C	O	0	0
			17	13	4		
6	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 7 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (CCD ID: PG6) (formula: C₁₂H₂₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	17	Total	O	0	0
			17	17		
8	B	10	Total	O	0	0
			10	10		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.49Å 172.04Å 60.66Å 90.00° 94.37° 90.00°	Depositor
Resolution (Å)	28.53 – 2.60 28.53 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.53-2.60) 94.8 (28.53-2.60)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.227 , 0.240 0.236 , 0.249	Depositor DCC
R_{free} test set	2264 reflections (7.28%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.9	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6516	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: PG6, OLA, EDT, OLC, 0HK, P6G

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	0.28	0/3132	0.72	0/4283
1	B	0.28	0/3190	0.73	1/4362 (0.0%)
All	All	0.28	0/6322	0.72	1/8645 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1021	GLU	N-CA-C	-5.94	104.93	111.82

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	3058	0	3044	30	0
1	B	3115	0	3104	25	0
2	A	26	0	22	3	0
2	B	26	0	22	3	0
3	A	46	0	66	0	0
3	B	40	0	66	2	0
4	A	20	0	12	3	0
5	A	19	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	19	0	26	1	0
6	A	68	0	103	6	0
6	B	42	0	62	6	0
7	B	10	0	12	1	0
8	A	17	0	0	0	0
8	B	10	0	0	0	0
All	All	6516	0	6565	61	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 (61) 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:136:LYS:HD2	6:A:1207:OLC:H24A	1.79	0.64
1:A:106:ASP:OD1	1:A:178:ARG:NH2	2.32	0.63
1:A:435:TRP:HB3	5:A:1205:P6G:H141	1.81	0.63
1:A:1044:VAL:HG21	1:A:1075:LEU:HB3	1.82	0.61
1:A:186:PHE:HA	5:A:1205:P6G:H61	1.84	0.60
1:B:462:LYS:O	1:B:466:HIS:ND1	2.35	0.60
1:A:416:TYR:HE2	2:A:1201:0HK:H1	1.69	0.58
1:A:20:GLY:N	4:A:1204:EDT:O15	2.38	0.57
3:B:1203:OLA:H71	3:B:1204:OLA:H31	1.84	0.57
1:B:416:TYR:HE2	2:B:1201:0HK:H1	1.70	0.56
1:A:450:PRO:HA	1:A:453:TYR:HD2	1.71	0.56
1:B:391:MET:HE3	1:B:396:ARG:HG2	1.89	0.55
1:A:72:PHE:HD2	6:A:1206:OLC:H4A	1.73	0.52
1:B:203:ALA:HA	6:B:1206:OLC:H18A	1.92	0.52
1:B:422:VAL:HB	1:B:430:ILE:HD11	1.92	0.52
1:A:192:ASN:HD22	1:A:195:VAL:HG23	1.75	0.51
1:B:130:ARG:HH12	1:B:395:GLU:HB3	1.75	0.51
6:A:1206:OLC:H7	6:B:1202:OLC:H3	1.93	0.50
1:B:1071:PHE:HA	7:B:1207:PG6:H62	1.94	0.49
1:B:187:ILE:H	5:B:1205:P6G:H21	1.77	0.49
1:A:138:LEU:HD12	1:A:1021:GLU:HG2	1.95	0.48
1:B:192:ASN:HD22	1:B:195:VAL:HG23	1.77	0.48
1:A:69:TYR:CE1	6:A:1206:OLC:H21	2.49	0.47
1:B:1074:SER:OG	1:B:1089:ASN:ND2	2.37	0.47
1:B:1022:LYS:O	1:B:1025:ASN:HB2	2.14	0.47
1:A:113:TYR:CZ	2:A:1201:0HK:H19	2.50	0.47
1:A:154:ALA:HA	6:B:1202:OLC:H4A	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PHE:HE1	6:A:1208:OLC:H5A	1.81	0.46
4:A:1204:EDT:H111	4:A:1204:EDT:H061	1.74	0.46
1:B:154:ALA:HA	3:B:1203:OLA:H61	1.96	0.46
1:A:410:ILE:O	1:A:414:THR:OG1	2.31	0.46
1:A:1050:ALA:HA	1:A:1053:ARG:HG2	1.97	0.46
1:A:157:TRP:HB3	6:B:1202:OLC:H8	1.98	0.45
1:A:1074:SER:OG	1:A:1089:ASN:ND2	2.39	0.45
1:B:163:LEU:HD13	6:B:1206:OLC:H14	1.97	0.45
1:A:163:LEU:HD13	6:A:1208:OLC:H15A	1.99	0.45
1:A:130:ARG:O	1:A:134:VAL:HG23	2.17	0.45
1:B:1022:LYS:HA	1:B:1025:ASN:HD22	1.80	0.45
1:A:86:MET:O	1:A:90:THR:HG23	2.17	0.45
1:A:125:ILE:HD13	1:A:152:MET:HB3	2.00	0.44
1:B:86:MET:O	1:B:90:THR:HG23	2.17	0.44
1:A:116:SER:HB3	1:A:413:TRP:HH2	1.83	0.44
1:A:112:ASP:OD2	1:A:443:TYR:OH	2.35	0.43
1:B:116:SER:HB3	1:B:413:TRP:HH2	1.82	0.43
1:B:206:LEU:HB3	1:B:207:PRO:HD3	2.01	0.43
1:B:83:ALA:O	1:B:87:ASN:ND2	2.51	0.43
1:B:415:PRO:O	1:B:419:MET:HG3	2.19	0.43
1:B:1089:ASN:HA	1:B:1092:LYS:HE2	2.00	0.43
1:A:66:VAL:HG13	1:A:149:ALA:HB2	2.01	0.43
4:A:1204:EDT:H022	4:A:1204:EDT:H072	1.58	0.43
1:B:223:ARG:HG3	1:B:1005:GLU:CD	2.43	0.42
1:A:1035:ILE:HG12	1:A:1060:VAL:HG21	2.01	0.42
1:B:1044:VAL:HG21	1:B:1075:LEU:HD22	2.02	0.42
2:B:1201:0HK:O10	2:B:1201:0HK:H20	2.20	0.41
1:B:113:TYR:CZ	2:B:1201:0HK:H19	2.56	0.41
1:B:1042:LYS:HB3	1:B:1043:PRO:HD3	2.03	0.41
1:A:1006:MET:HG3	1:A:1118:TYR:CZ	2.56	0.41
2:A:1201:0HK:H20	2:A:1201:0HK:O10	2.21	0.41
1:A:1048:LEU:HD23	1:A:1053:ARG:HA	2.03	0.41
1:A:401:THR:O	1:A:405:ILE:HG12	2.22	0.40
1:B:197:PHE:CE2	6:B:1202:OLC:H5A	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/422 (92%)	383 (99%)	3 (1%)	0	100	100
1	B	395/422 (94%)	391 (99%)	4 (1%)	0	100	100
All	All	781/844 (92%)	774 (99%)	7 (1%)	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	324/361 (90%)	323 (100%)	1 (0%)	86	94
1	B	327/361 (91%)	326 (100%)	1 (0%)	86	94
All	All	651/722 (90%)	649 (100%)	2 (0%)	86	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	B	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN

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Mol	Chain	Res	Type
1	B	192	ASN
1	B	1025	ASN
1	B	417	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	$\# Z > 2$
4	EDT	A	1204	-	19,19,19	0.89	0	24,24,24	0.95	0
6	OLC	A	1208	-	24,24,24	0.94	1 (4%)	25,25,25	0.86	1 (4%)
3	OLA	B	1203	-	19,19,19	0.80	1 (5%)	19,19,19	0.91	1 (5%)
5	P6G	A	1205	-	18,18,18	0.46	0	17,17,17	0.31	0
6	OLC	B	1206	-	24,24,24	0.94	1 (4%)	25,25,25	0.80	1 (4%)
2	0HK	A	1201	-	28,30,30	1.80	10 (35%)	40,48,48	4.35	20 (50%)
6	OLC	A	1207	-	17,17,24	1.09	1 (5%)	18,18,25	1.09	1 (5%)
7	PG6	B	1207	-	9,9,17	0.45	0	8,8,16	0.33	0
6	OLC	B	1202	-	16,16,24	1.14	1 (6%)	17,17,25	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OLA	A	1203	-	13,13,19	0.97	1 (7%)	13,13,19	1.08	1 (7%)
3	OLA	A	1209	-	19,19,19	0.80	1 (5%)	19,19,19	0.91	1 (5%)
5	P6G	B	1205	-	18,18,18	0.46	0	17,17,17	0.31	0
3	OLA	A	1202	-	11,11,19	1.06	1 (9%)	11,11,19	1.16	1 (9%)
2	0HK	B	1201	-	28,30,30	1.80	10 (35%)	40,48,48	4.32	20 (50%)
3	OLA	B	1204	-	19,19,19	0.81	1 (5%)	19,19,19	0.92	1 (5%)
6	OLC	A	1206	-	24,24,24	0.93	1 (4%)	25,25,25	0.89	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDT	A	1204	-	-	9/21/21/21	-
6	OLC	A	1208	-	-	1/24/24/24	-
3	OLA	B	1203	-	-	10/17/17/17	-
5	P6G	A	1205	-	-	2/16/16/16	-
6	OLC	B	1206	-	-	2/24/24/24	-
2	0HK	A	1201	-	-	4/22/55/55	0/6/5/5
6	OLC	A	1207	-	-	4/17/17/24	-
7	PG6	B	1207	-	-	0/7/7/15	-
6	OLC	B	1202	-	-	0/16/16/24	-
3	OLA	A	1203	-	-	7/11/11/17	-
3	OLA	A	1209	-	-	10/17/17/17	-
5	P6G	B	1205	-	-	2/16/16/16	-
3	OLA	A	1202	-	-	6/9/9/17	-
2	0HK	B	1201	-	-	4/22/55/55	0/6/5/5
3	OLA	B	1204	-	-	8/17/17/17	-
6	OLC	A	1206	-	-	4/24/24/24	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1206	OLC	O20-C1	4.36	1.46	1.33
6	A	1206	OLC	O20-C1	4.34	1.46	1.33
6	A	1208	OLC	O20-C1	4.33	1.46	1.33
6	B	1202	OLC	O20-C1	4.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1207	OLC	O20-C1	4.27	1.45	1.33
2	B	1201	0HK	C1-N2	-4.16	1.43	1.51
2	A	1201	0HK	C1-N2	-4.14	1.43	1.51
2	A	1201	0HK	O11-C28	3.66	1.41	1.34
2	B	1201	0HK	O11-C28	3.64	1.41	1.34
3	A	1202	OLA	C10-C9	2.86	1.47	1.29
3	A	1203	OLA	C10-C9	2.79	1.47	1.31
3	A	1209	OLA	C10-C9	2.78	1.47	1.31
3	B	1204	OLA	C10-C9	2.78	1.47	1.31
3	B	1203	OLA	C10-C9	2.78	1.47	1.31
2	A	1201	0HK	C32-S44	2.66	1.78	1.70
2	B	1201	0HK	C30-C28	-2.66	1.50	1.54
2	B	1201	0HK	C32-S44	2.64	1.78	1.70
2	A	1201	0HK	C30-C28	-2.60	1.51	1.54
2	A	1201	0HK	C12-N2	-2.58	1.46	1.51
2	B	1201	0HK	C12-N2	-2.55	1.46	1.51
2	B	1201	0HK	O33-C30	-2.51	1.37	1.42
2	B	1201	0HK	C31-S37	2.45	1.78	1.70
2	A	1201	0HK	C31-S37	2.44	1.78	1.70
2	A	1201	0HK	O33-C30	-2.38	1.38	1.42
2	B	1201	0HK	C43-S44	2.24	1.80	1.70
2	A	1201	0HK	C43-S44	2.23	1.80	1.70
2	A	1201	0HK	O11-C5	-2.12	1.41	1.46
2	B	1201	0HK	O11-C5	-2.11	1.41	1.46
2	A	1201	0HK	C36-S37	2.08	1.79	1.70
2	B	1201	0HK	C36-S37	2.07	1.79	1.70

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	0HK	C6-C7-N2	12.08	116.42	108.82
2	B	1201	0HK	C6-C7-N2	11.91	116.31	108.82
2	A	1201	0HK	C4-C3-N2	9.62	114.87	108.82
2	B	1201	0HK	C4-C3-N2	9.56	114.83	108.82
2	A	1201	0HK	C7-C8-C9	-9.38	101.71	107.46
2	B	1201	0HK	C7-C8-C9	-9.19	101.83	107.46
2	A	1201	0HK	C8-C7-N2	7.89	108.44	103.54
2	B	1201	0HK	C8-C7-N2	7.71	108.33	103.54
2	B	1201	0HK	C3-C9-C8	-7.40	102.92	107.46
2	A	1201	0HK	C3-C9-C8	-7.18	103.06	107.46
2	A	1201	0HK	C9-C3-N2	7.15	107.98	103.54
2	B	1201	0HK	C9-C3-N2	7.10	107.95	103.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	0HK	O10-C9-C3	6.27	122.97	117.11
2	A	1201	0HK	O10-C9-C3	6.20	122.91	117.11
2	A	1201	0HK	C6-C7-C8	-6.04	102.05	107.04
2	B	1201	0HK	C6-C7-C8	-5.67	102.36	107.04
2	B	1201	0HK	O10-C8-C7	5.41	122.17	117.11
2	A	1201	0HK	O10-C8-C7	5.36	122.12	117.11
2	B	1201	0HK	C42-C43-S44	-4.67	101.60	113.02
2	A	1201	0HK	C42-C43-S44	-4.66	101.63	113.02
2	A	1201	0HK	C35-C36-S37	-4.46	102.11	113.02
2	B	1201	0HK	C35-C36-S37	-4.46	102.12	113.02
2	B	1201	0HK	O11-C28-C30	3.97	116.97	110.92
2	B	1201	0HK	C41-C32-S44	-3.92	101.72	110.95
2	A	1201	0HK	C41-C32-S44	-3.90	101.76	110.95
2	A	1201	0HK	O11-C28-C30	3.86	116.82	110.92
2	A	1201	0HK	C34-C31-S37	-3.79	102.01	110.95
2	B	1201	0HK	C34-C31-S37	-3.77	102.07	110.95
2	A	1201	0HK	C4-C3-C9	-3.56	104.10	107.04
2	B	1201	0HK	C4-C3-C9	-3.53	104.12	107.04
2	B	1201	0HK	C5-O11-C28	3.32	122.82	117.64
2	A	1201	0HK	C5-O11-C28	3.31	122.80	117.64
6	B	1202	OLC	O20-C1-C2	2.98	120.93	111.83
6	A	1207	OLC	O20-C1-C2	2.91	120.72	111.83
6	A	1206	OLC	O20-C1-C2	2.80	120.38	111.83
6	A	1208	OLC	O20-C1-C2	2.67	119.98	111.83
2	A	1201	0HK	C36-S37-C31	2.60	97.98	92.97
2	B	1201	0HK	C36-S37-C31	2.58	97.94	92.97
2	B	1201	0HK	C43-S44-C32	2.54	97.88	92.97
2	A	1201	0HK	C43-S44-C32	2.53	97.86	92.97
2	A	1201	0HK	C1-N2-C7	2.49	116.56	113.03
6	B	1206	OLC	O20-C1-C2	2.48	119.39	111.83
2	B	1201	0HK	C1-N2-C7	2.44	116.49	113.03
3	A	1202	OLA	O2-C1-C2	2.09	120.59	114.00
2	B	1201	0HK	C42-C41-C32	2.09	119.75	109.83
3	B	1203	OLA	O2-C1-C2	2.08	120.56	114.00
2	A	1201	0HK	C42-C41-C32	2.08	119.70	109.83
3	A	1209	OLA	O2-C1-C2	2.04	120.44	114.00
3	B	1204	OLA	O2-C1-C2	2.03	120.41	114.00
3	A	1203	OLA	O2-C1-C2	2.03	120.41	114.00

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1204	EDT	N3-C4-C5-O20
4	A	1204	EDT	N3-C4-C5-O19
4	A	1204	EDT	O18-C1-C2-N3
4	A	1204	EDT	O17-C1-C2-N3
4	A	1204	EDT	O16-C10-C9-N8
6	A	1206	OLC	O20-C21-C22-C24
4	A	1204	EDT	C7-C6-N3-C2
6	A	1206	OLC	O20-C21-C22-O23
4	A	1204	EDT	O15-C10-C9-N8
4	A	1204	EDT	N8-C11-C12-O13
4	A	1204	EDT	N8-C11-C12-O14
3	A	1202	OLA	C1-C2-C3-C4
3	B	1203	OLA	C1-C2-C3-C4
3	A	1209	OLA	C1-C2-C3-C4
3	B	1204	OLA	C1-C2-C3-C4
3	A	1203	OLA	C1-C2-C3-C4
3	B	1203	OLA	C5-C6-C7-C8
3	B	1203	OLA	C12-C13-C14-C15
3	B	1204	OLA	C4-C5-C6-C7
3	A	1202	OLA	C3-C4-C5-C6
3	A	1209	OLA	C5-C6-C7-C8
3	B	1203	OLA	C4-C5-C6-C7
3	A	1203	OLA	C11-C10-C9-C8
3	B	1204	OLA	C11-C10-C9-C8
6	A	1207	OLC	O20-C21-C22-O23
3	A	1209	OLA	C11-C10-C9-C8
3	B	1204	OLA	C3-C4-C5-C6
3	A	1209	OLA	C4-C5-C6-C7
3	A	1203	OLA	C3-C4-C5-C6
3	B	1203	OLA	C11-C10-C9-C8
3	A	1203	OLA	C4-C5-C6-C7
6	A	1206	OLC	C5-C6-C7-C8
6	B	1206	OLC	C1-C2-C3-C4
3	A	1202	OLA	C4-C5-C6-C7
6	B	1206	OLC	C6-C7-C8-C9
2	A	1201	0HK	C32-C30-C31-S37
2	B	1201	0HK	C32-C30-C31-S37
3	A	1209	OLA	C11-C12-C13-C14
3	A	1203	OLA	C2-C3-C4-C5
2	A	1201	0HK	O33-C30-C31-C34
2	A	1201	0HK	O33-C30-C31-S37
2	B	1201	0HK	O33-C30-C31-C34
3	A	1209	OLA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	B	1205	P6G	C5-C6-O7-C8
5	A	1205	P6G	O7-C8-C9-O10
3	A	1203	OLA	C9-C10-C11-C12
3	B	1204	OLA	C9-C10-C11-C12
3	A	1202	OLA	C7-C8-C9-C10
3	B	1204	OLA	C6-C7-C8-C9
3	B	1203	OLA	C3-C4-C5-C6
6	A	1208	OLC	C3-C4-C5-C6
6	A	1207	OLC	O20-C21-C22-C24
5	B	1205	P6G	O7-C8-C9-O10
3	A	1209	OLA	C12-C13-C14-C15
3	A	1209	OLA	C14-C15-C16-C17
3	A	1209	OLA	C9-C10-C11-C12
3	B	1204	OLA	O2-C1-C2-C3
3	A	1203	OLA	C7-C8-C9-C10
3	A	1202	OLA	C5-C6-C7-C8
6	A	1207	OLC	C2-C1-O20-C21
3	B	1204	OLA	O1-C1-C2-C3
2	A	1201	0HK	C32-C30-C31-C34
2	B	1201	0HK	C32-C30-C31-C34
5	A	1205	P6G	O13-C14-C15-O16
3	A	1209	OLA	C7-C8-C9-C10
3	B	1203	OLA	C7-C8-C9-C10
6	A	1207	OLC	O19-C1-O20-C21
3	B	1203	OLA	C9-C10-C11-C12
6	A	1206	OLC	O20-C1-C2-C3
3	B	1203	OLA	C13-C14-C15-C16
3	B	1203	OLA	C11-C12-C13-C14
2	B	1201	0HK	O33-C30-C31-S37
3	A	1202	OLA	O2-C1-C2-C3

There are no ring outliers.

13 monomers are involved in 26 short contacts:

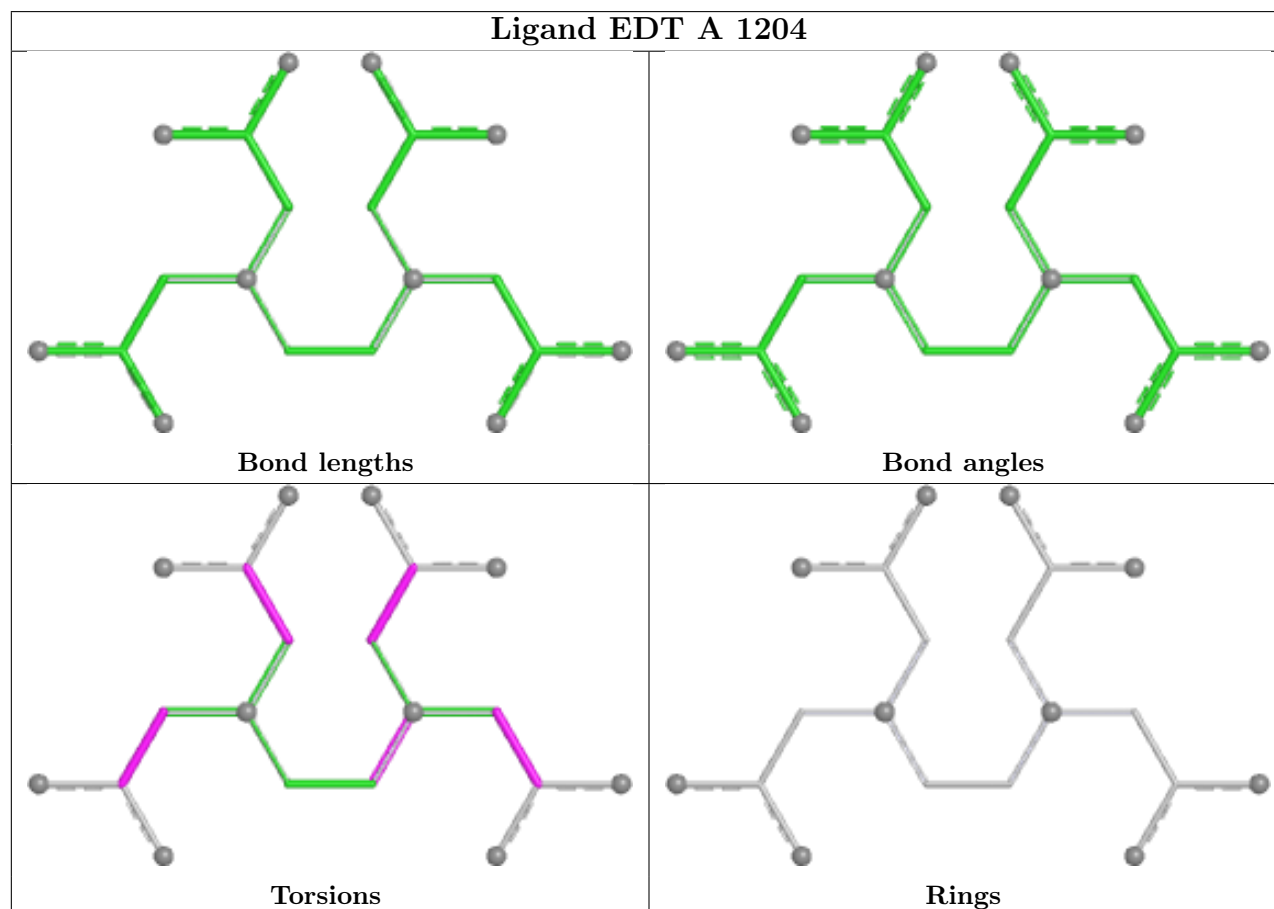
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1204	EDT	3	0
6	A	1208	OLC	2	0
3	B	1203	OLA	2	0
5	A	1205	P6G	2	0
6	B	1206	OLC	2	0
2	A	1201	0HK	3	0
6	A	1207	OLC	1	0

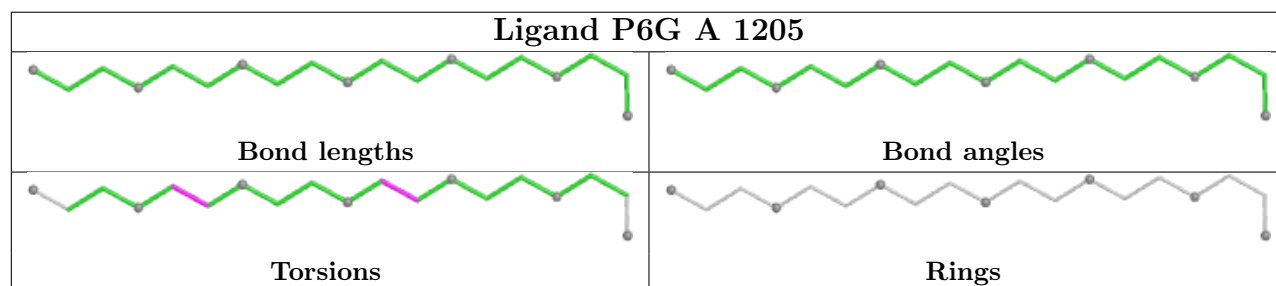
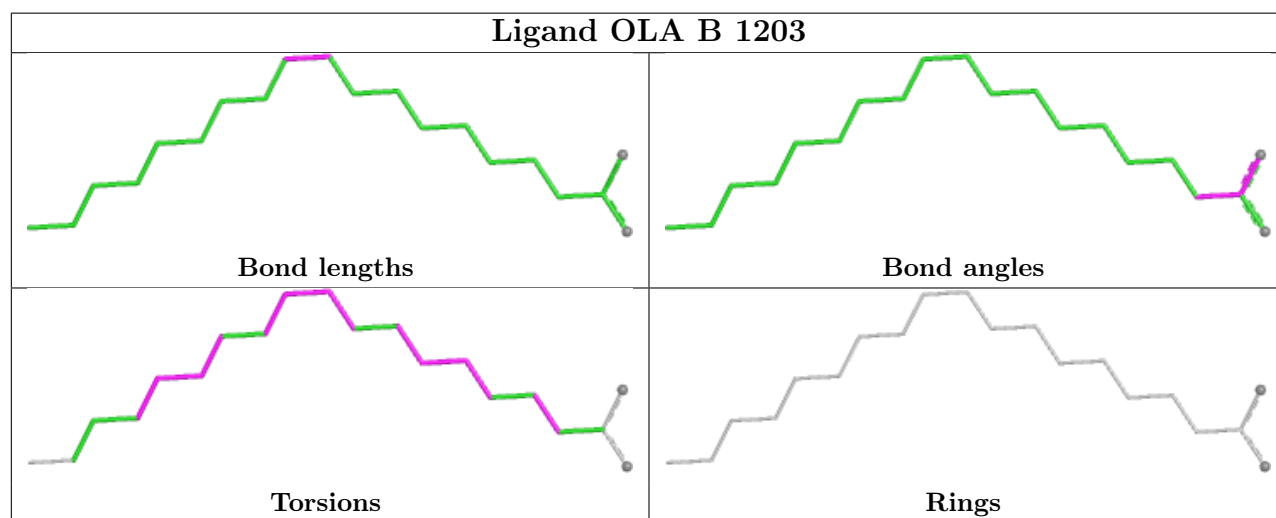
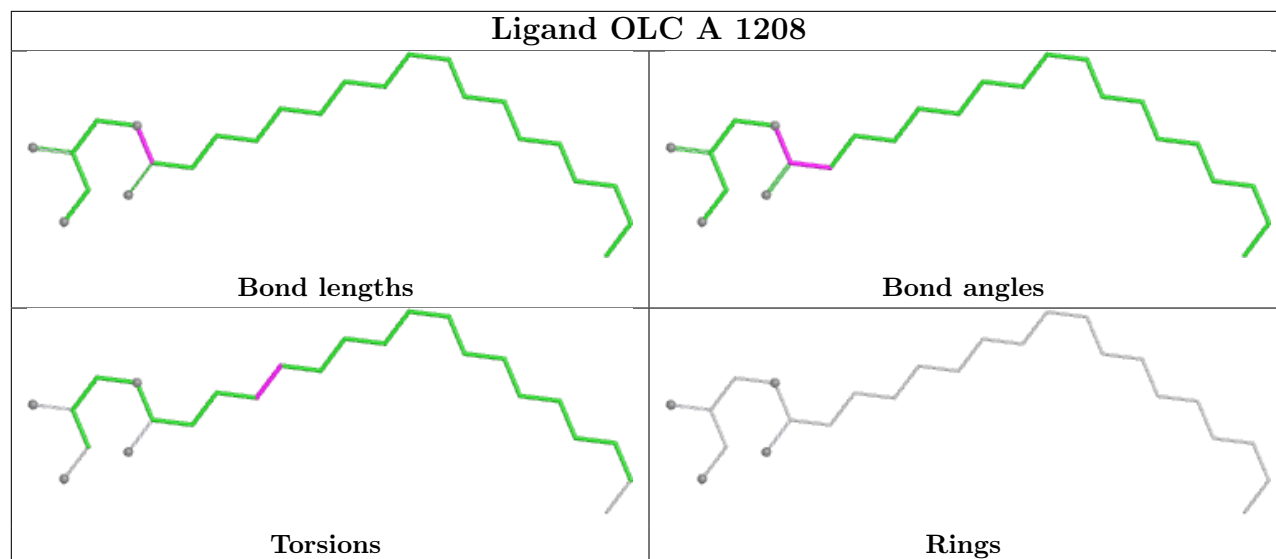
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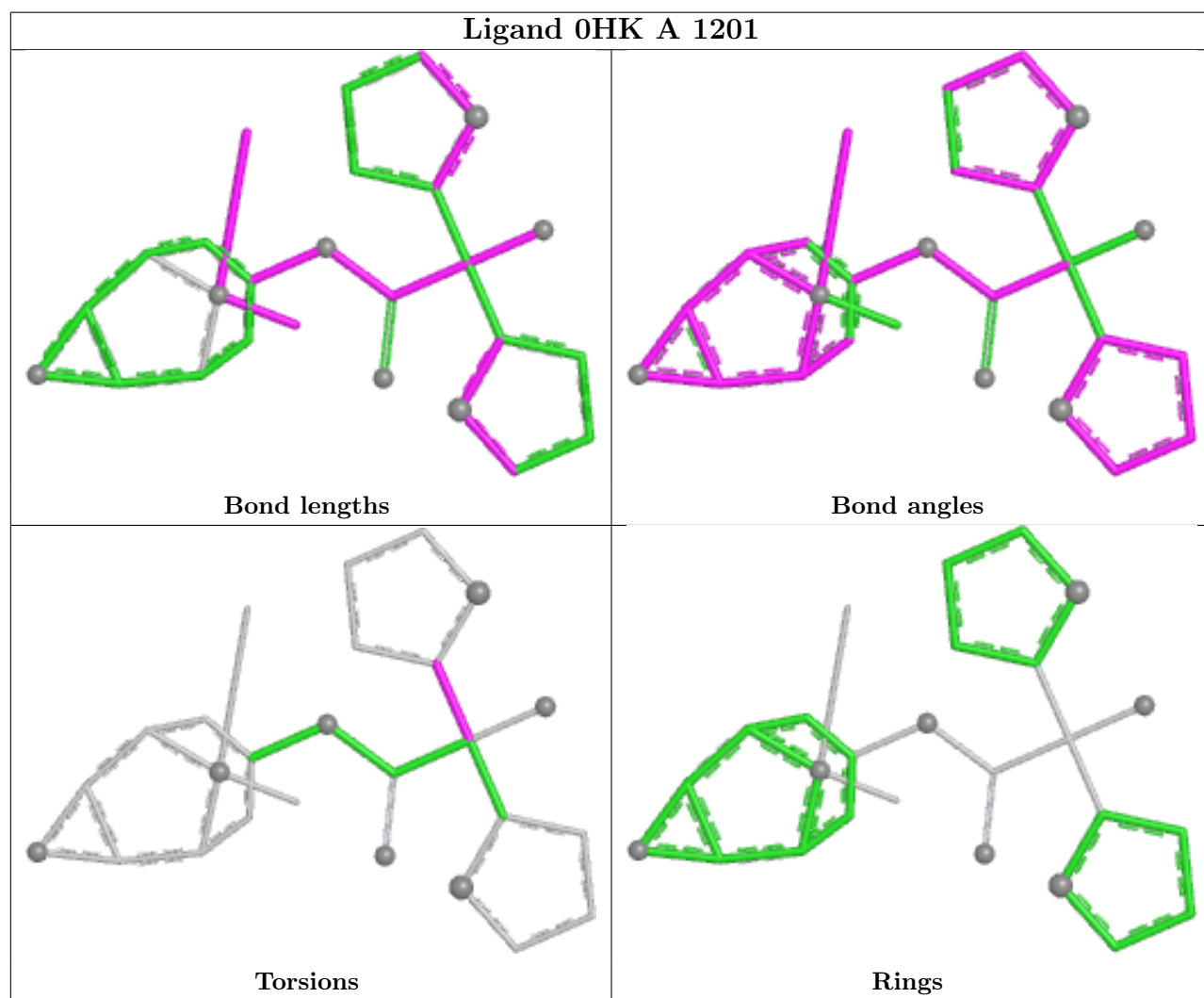
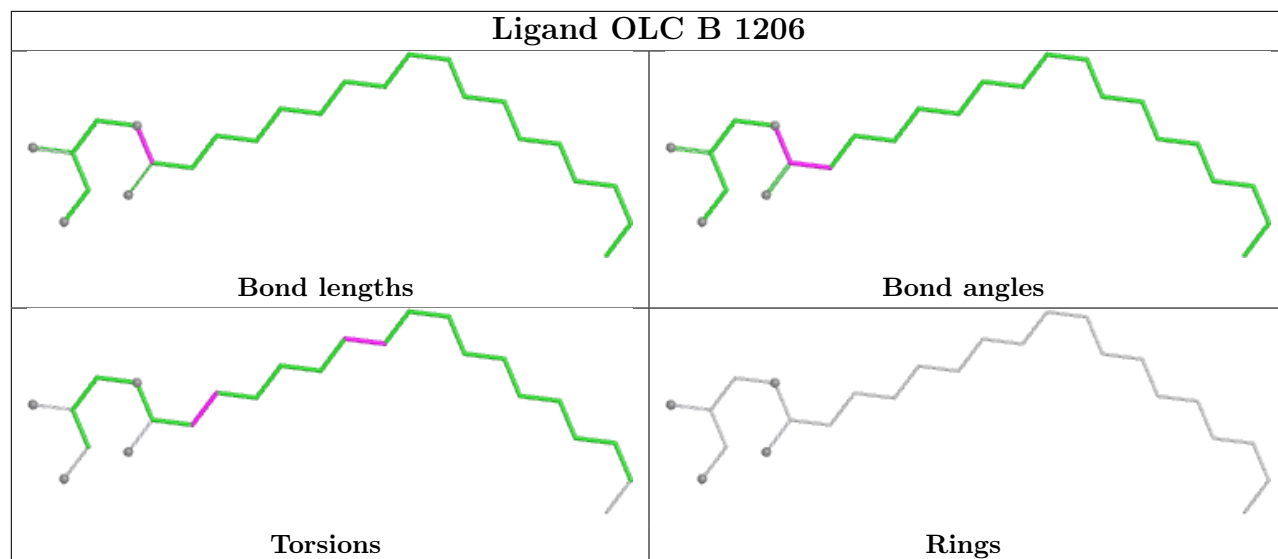
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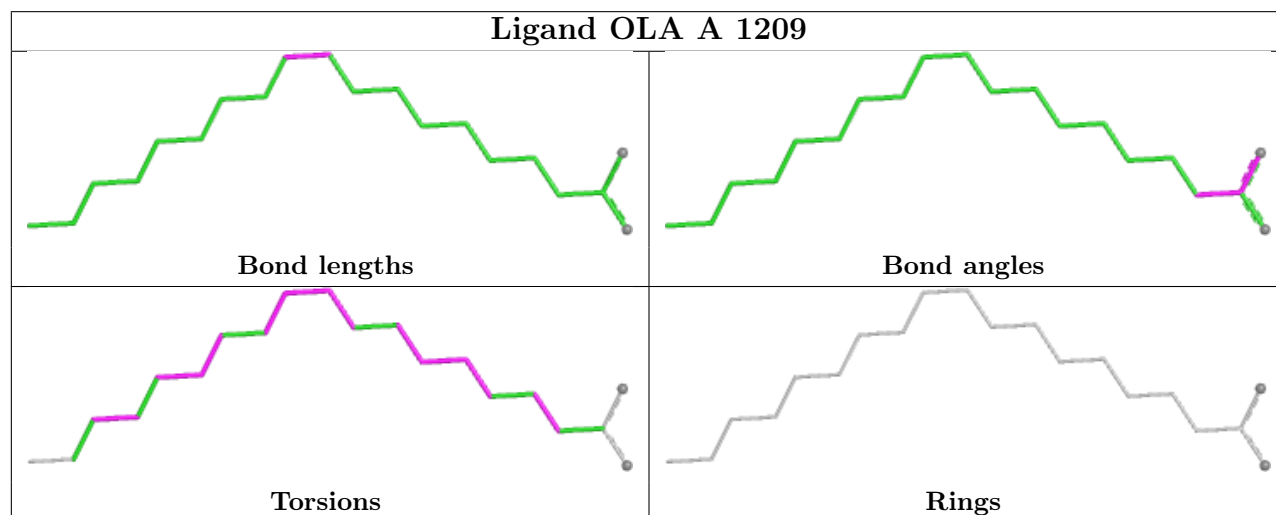
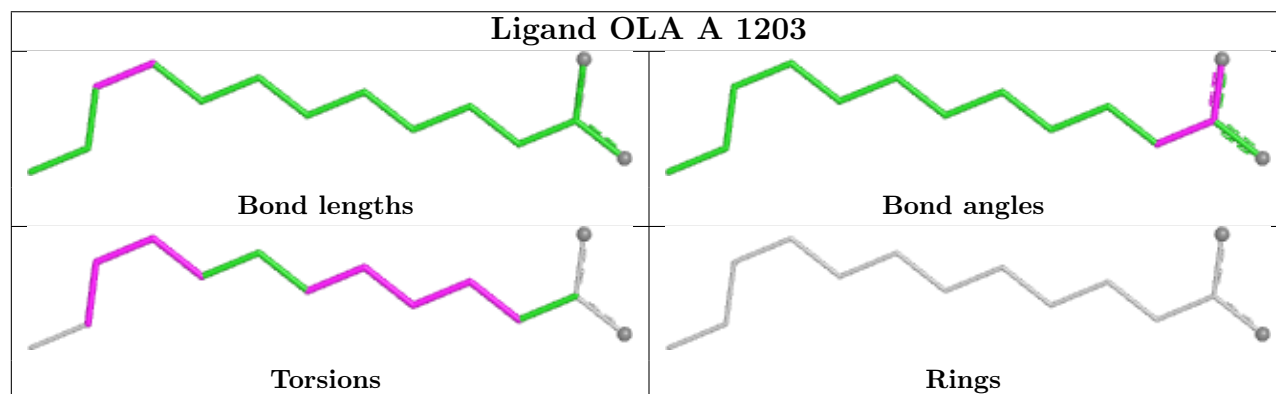
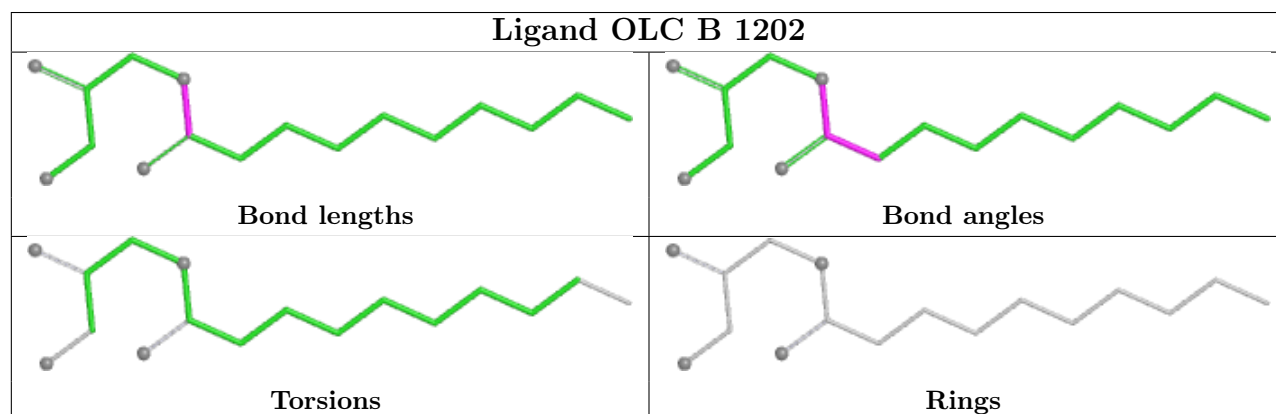
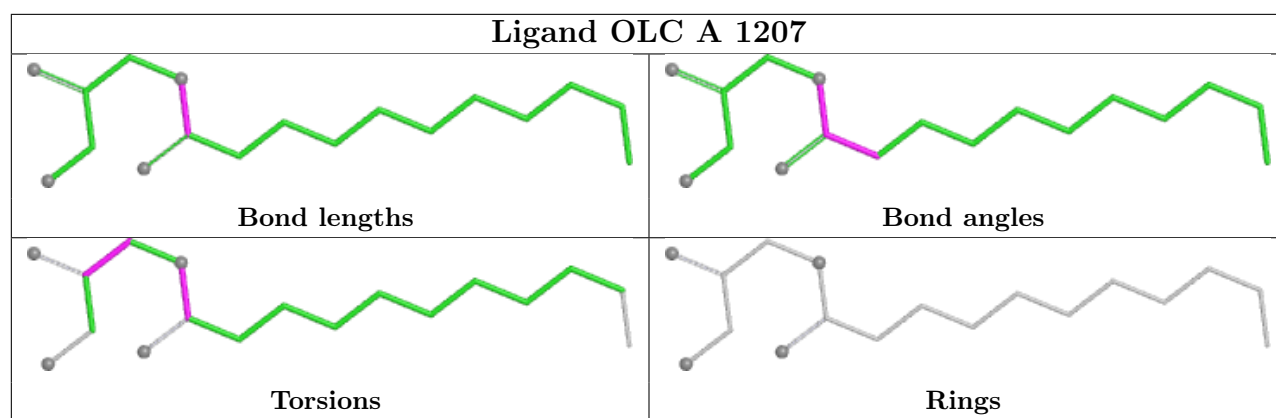
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1207	PG6	1	0
6	B	1202	OLC	4	0
5	B	1205	P6G	1	0
2	B	1201	0HK	3	0
3	B	1204	OLA	1	0
6	A	1206	OLC	3	0

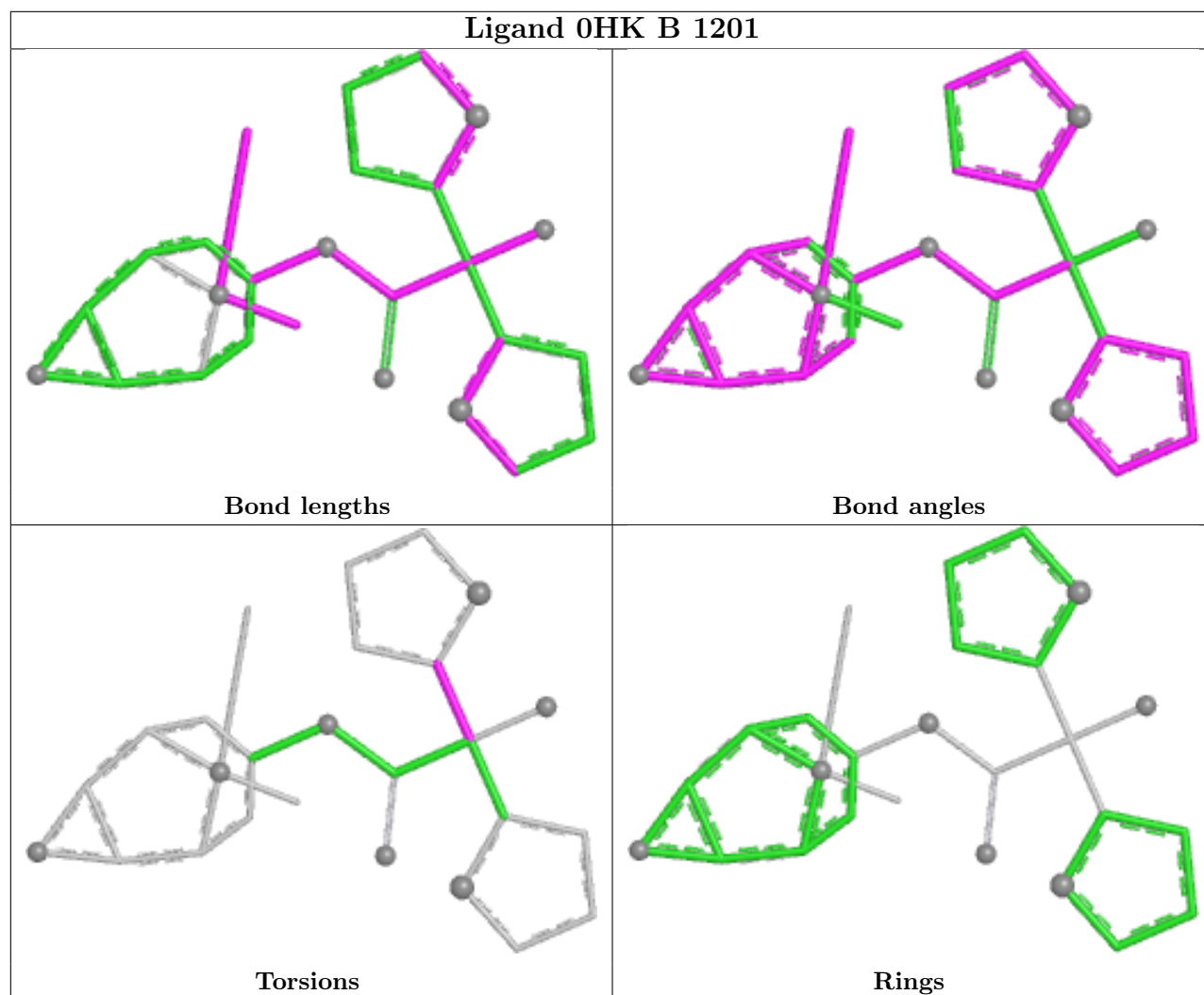
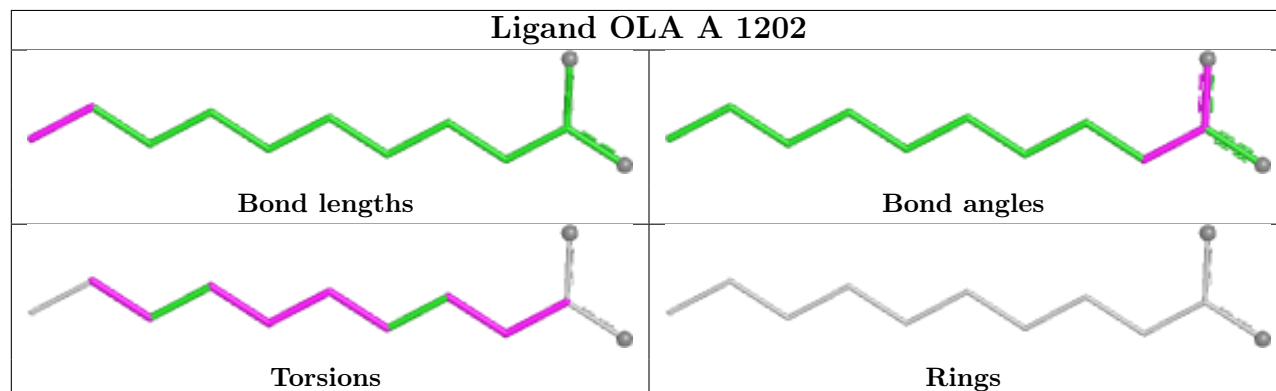
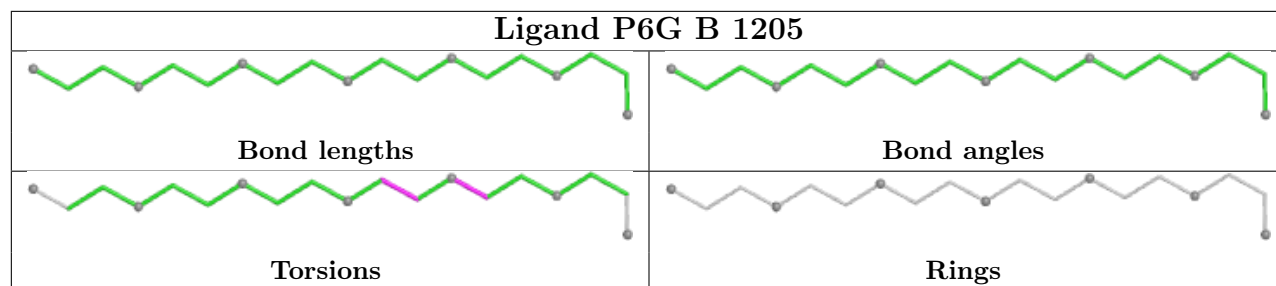
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

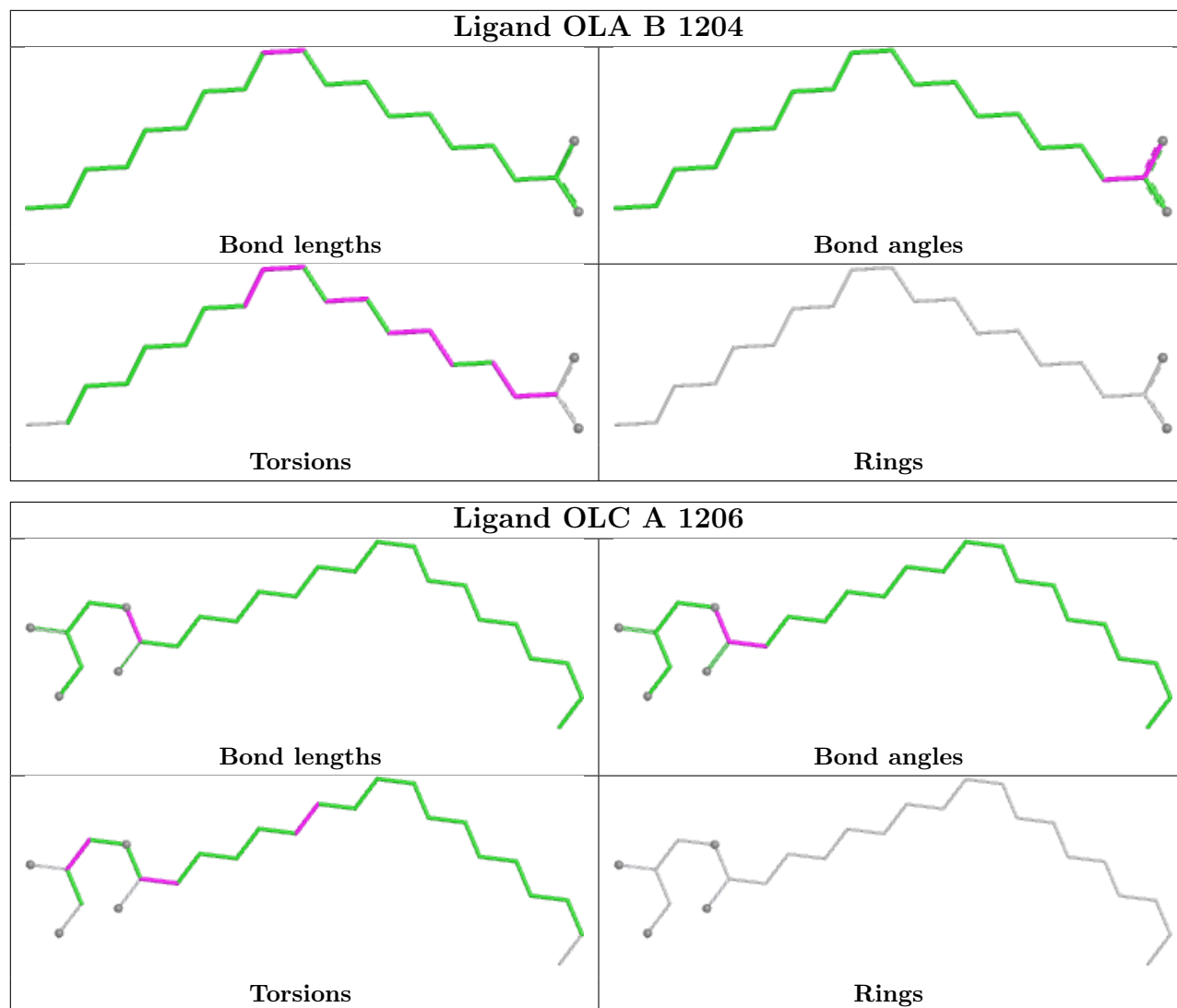












5.7 Other polymers [i](#)

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	392/422 (92%)	0.65	34 (8%) 16 12	40, 64, 127, 167	0
1	B	399/422 (94%)	0.60	29 (7%) 21 17	42, 66, 114, 162	0
All	All	791/844 (93%)	0.62	63 (7%) 18 14	40, 65, 122, 167	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	396	ARG	4.9
1	B	1017	GLY	4.7
1	B	1018	ASP	4.5
1	A	66	VAL	4.1
1	B	453	TYR	4.0
1	A	67	ASN	3.9
1	B	454	ALA	3.5
1	B	1091	ALA	3.5
1	A	1108	THR	3.4
1	B	392	ALA	3.4
1	A	222	SER	3.3
1	A	224	SER	3.2
1	A	1088	VAL	3.2
1	A	1051	VAL	3.1
1	B	1020	ALA	3.1
1	B	1024	PHE	3.0
1	A	453	TYR	2.8
1	A	458	ALA	2.8
1	A	398	VAL	2.8
1	B	66	VAL	2.8
1	B	468	LEU	2.7
1	B	394	ARG	2.7
1	A	1020	ALA	2.7
1	A	468	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1037	ARG	2.6
1	A	1087	ALA	2.6
1	B	1090	LEU	2.6
1	B	469	LEU	2.6
1	B	1026	GLN	2.6
1	A	1115	TRP	2.5
1	A	403	PHE	2.5
1	A	1117	ALA	2.5
1	B	402	ILE	2.5
1	A	223	ARG	2.4
1	A	397	LYS	2.4
1	A	1050	ALA	2.4
1	A	1049	ASP	2.4
1	B	471	GLN	2.4
1	A	226	VAL	2.4
1	B	403	PHE	2.4
1	B	473	ARG	2.4
1	B	1061	PHE	2.3
1	B	455	LEU	2.3
1	A	122	ASN	2.3
1	A	1111	ARG	2.3
1	A	470	CYS	2.3
1	B	67	ASN	2.3
1	A	469	LEU	2.3
1	A	454	ALA	2.3
1	A	221	ALA	2.2
1	B	24	HIS	2.2
1	A	1079	GLN	2.2
1	A	1085	GLU	2.1
1	B	452	CYS	2.1
1	A	1048	LEU	2.1
1	B	215	TYR	2.1
1	A	1019	GLU	2.1
1	B	1011	GLU	2.1
1	A	467	LEU	2.1
1	A	1003	ILE	2.1
1	B	397	LYS	2.1
1	B	138	LEU	2.1
1	B	28	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

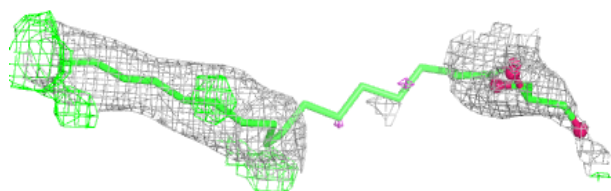
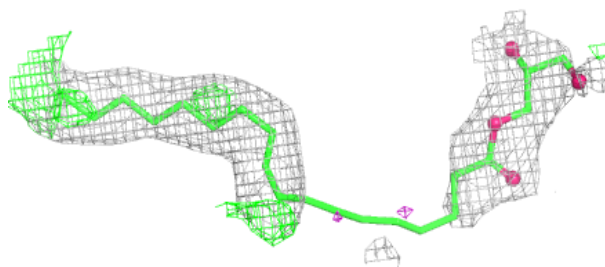
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PG6	B	1207	10/18	0.62	0.19	90,91,91,91	0
6	OLC	A	1208	25/25	0.73	0.22	57,86,91,91	0
3	OLA	A	1202	12/20	0.78	0.17	79,82,91,92	0
6	OLC	A	1207	18/25	0.79	0.18	73,79,94,95	0
3	OLA	A	1209	20/20	0.80	0.18	73,79,83,83	0
6	OLC	B	1206	25/25	0.81	0.17	53,76,86,87	0
5	P6G	B	1205	19/19	0.81	0.23	75,81,85,86	0
3	OLA	A	1203	14/20	0.82	0.19	83,84,89,91	0
6	OLC	A	1206	25/25	0.83	0.19	70,74,90,91	0
3	OLA	B	1204	20/20	0.84	0.20	59,70,73,73	0
6	OLC	B	1202	17/25	0.85	0.19	79,82,91,91	0
4	EDT	A	1204	20/20	0.86	0.13	70,74,80,80	0
3	OLA	B	1203	20/20	0.86	0.19	76,79,87,88	0
5	P6G	A	1205	19/19	0.87	0.18	65,69,86,86	0
2	0HK	B	1201	26/26	0.95	0.09	40,47,54,67	0
2	0HK	A	1201	26/26	0.96	0.08	42,47,48,64	0

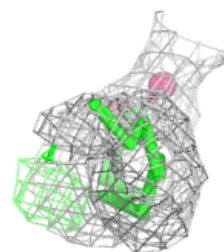
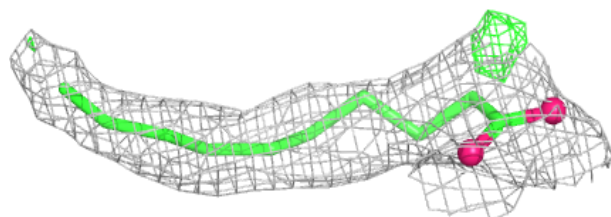
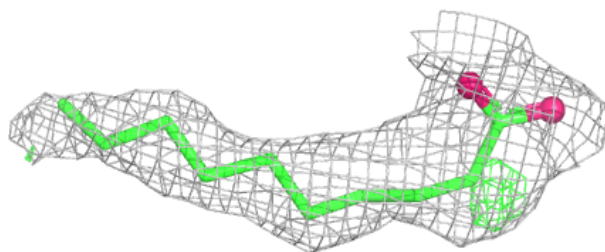
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around OLC A 1208:

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

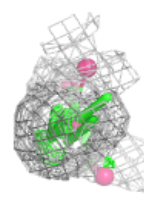
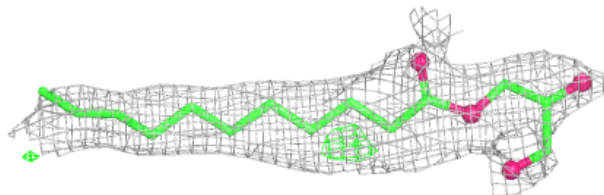
**Electron density around OLA A 1202:**

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

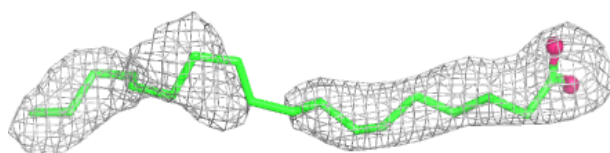
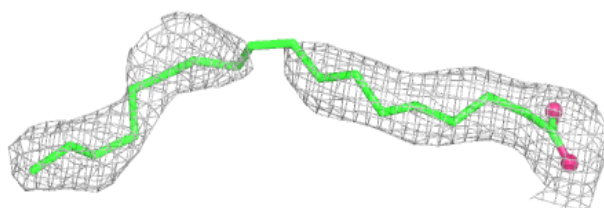


Electron density around OLC A 1207:

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

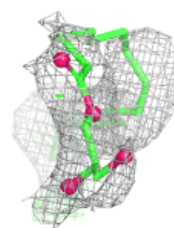
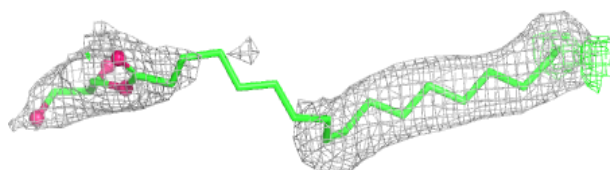
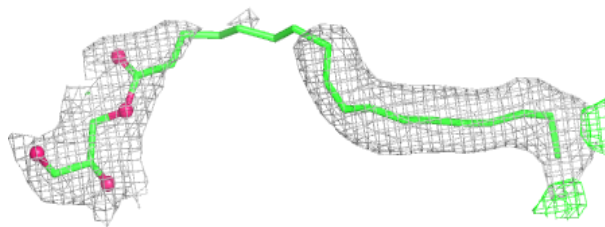
**Electron density around OLA A 1209:**

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



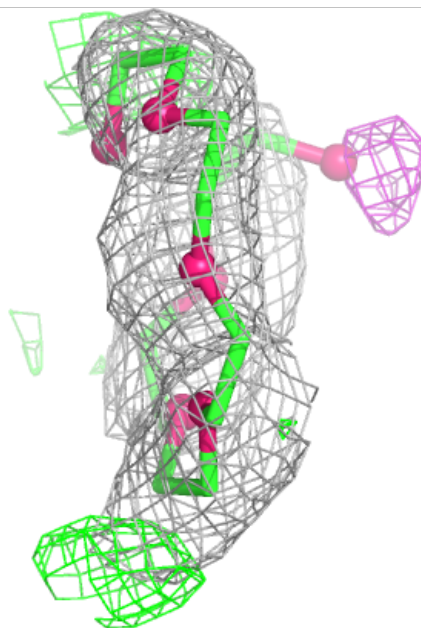
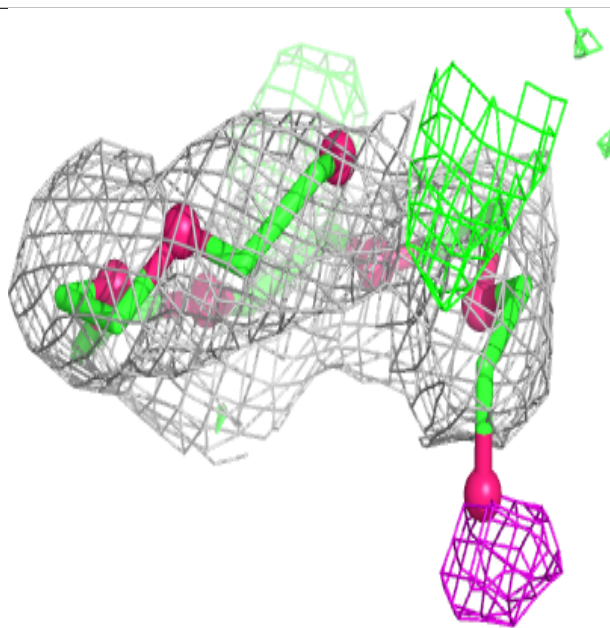
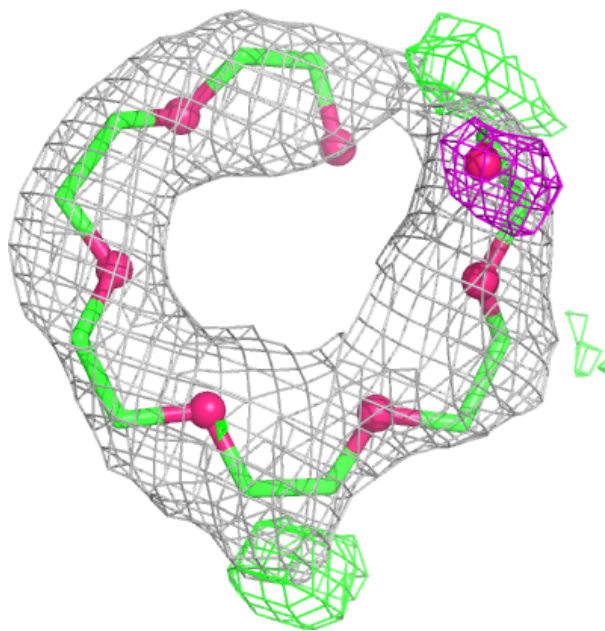
Electron density around OLC B 1206:

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



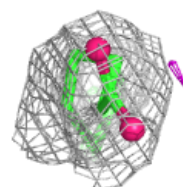
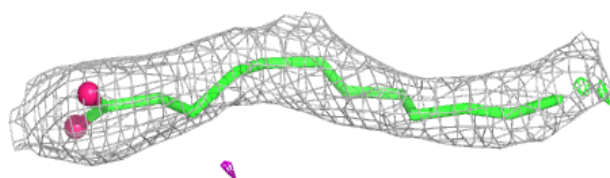
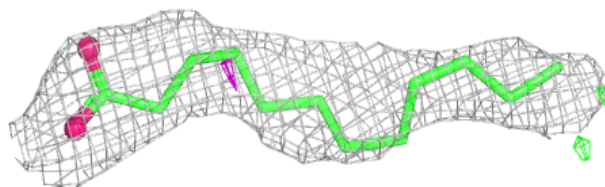
Electron density around P6G B 1205:

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

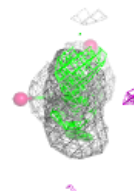
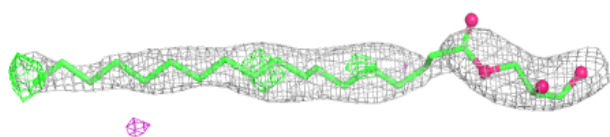
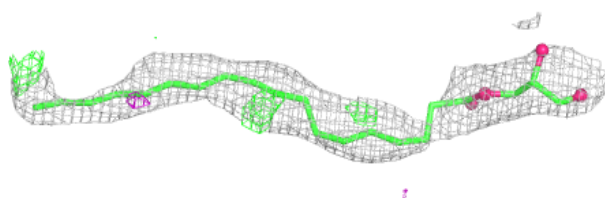


Electron density around OLA A 1203:

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

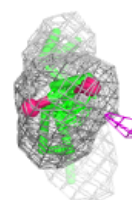
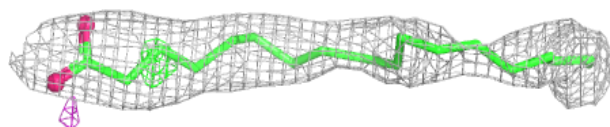
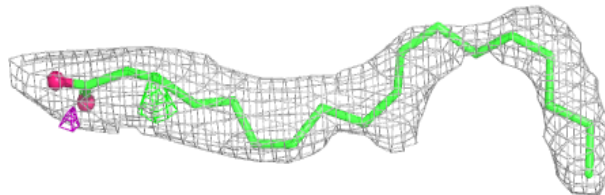
**Electron density around OLC A 1206:**

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

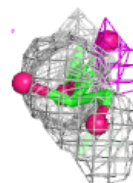
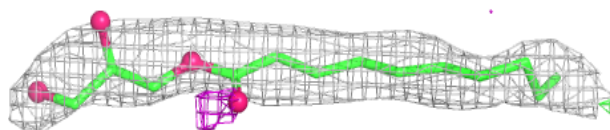
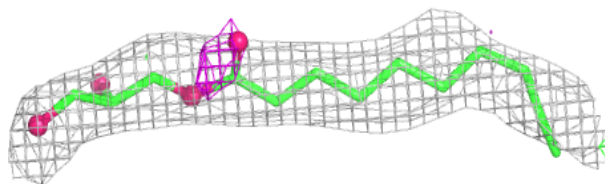


Electron density around OLA B 1204:

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

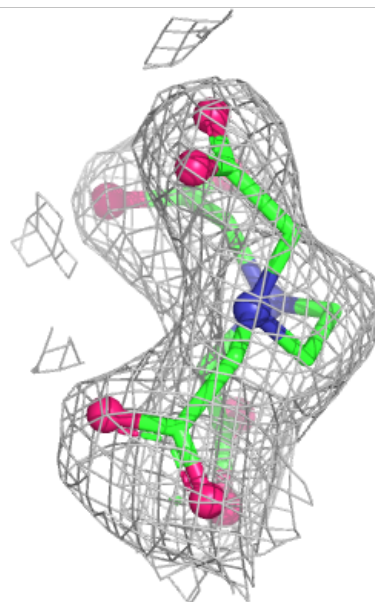
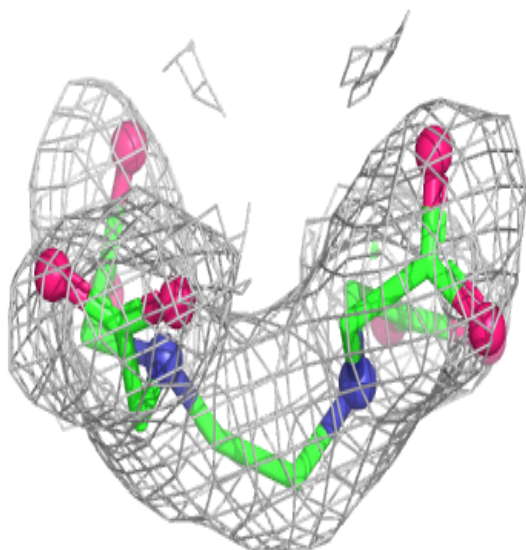
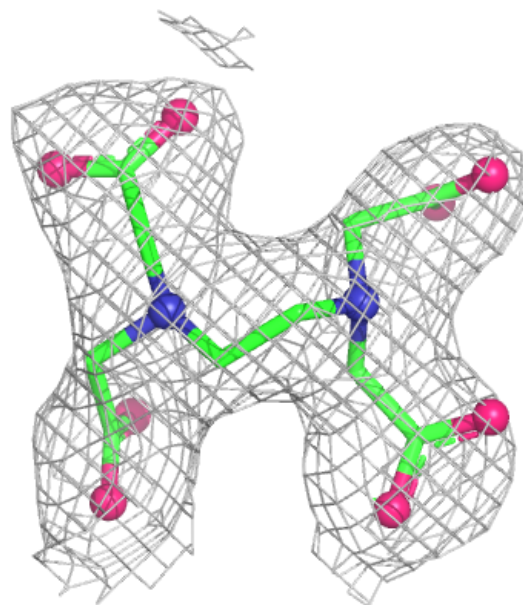
**Electron density around OLC B 1202:**

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



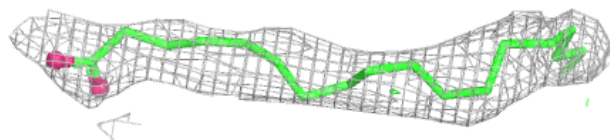
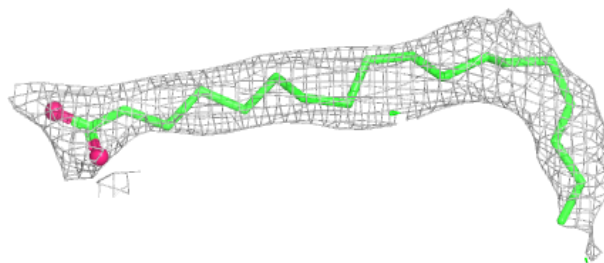
Electron density around EDT A 1204:

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



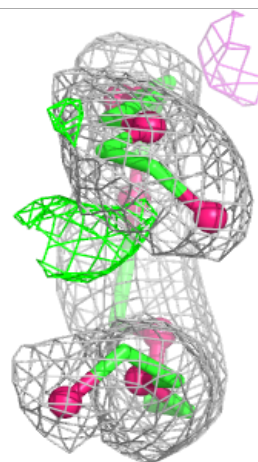
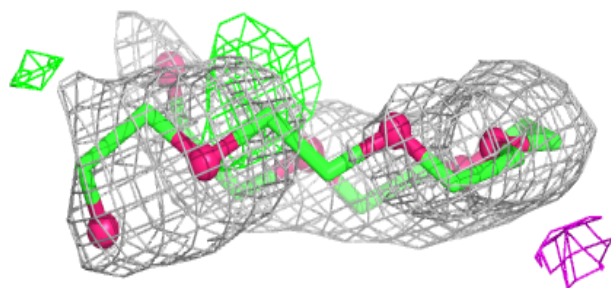
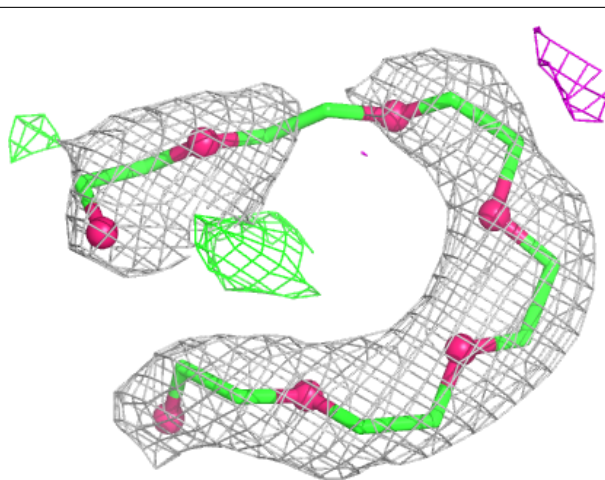
Electron density around OLA B 1203:

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



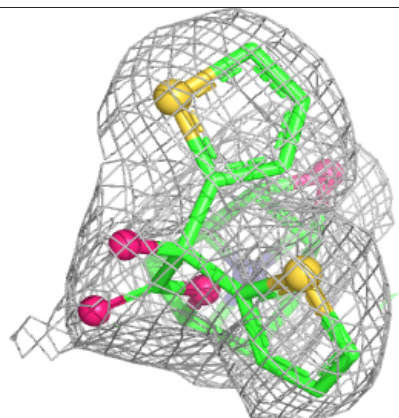
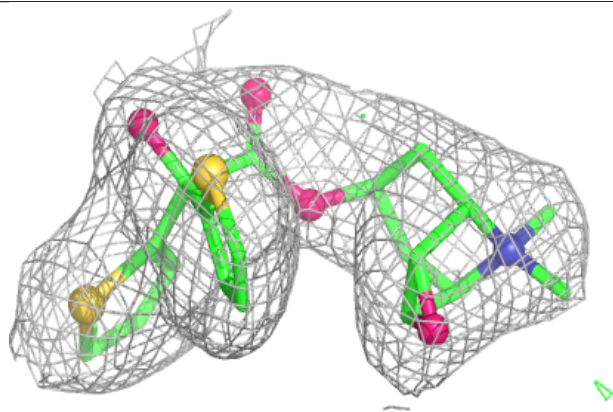
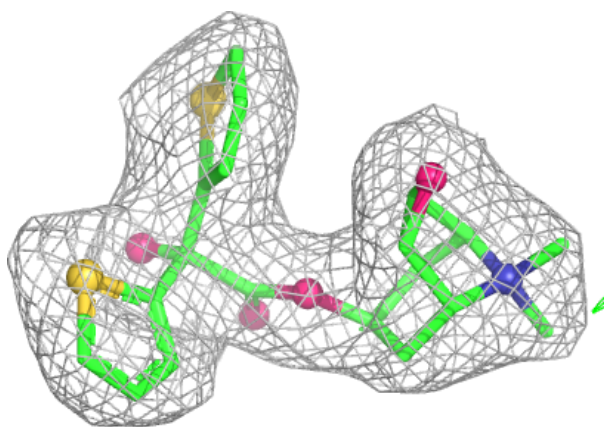
Electron density around P6G A 1205:

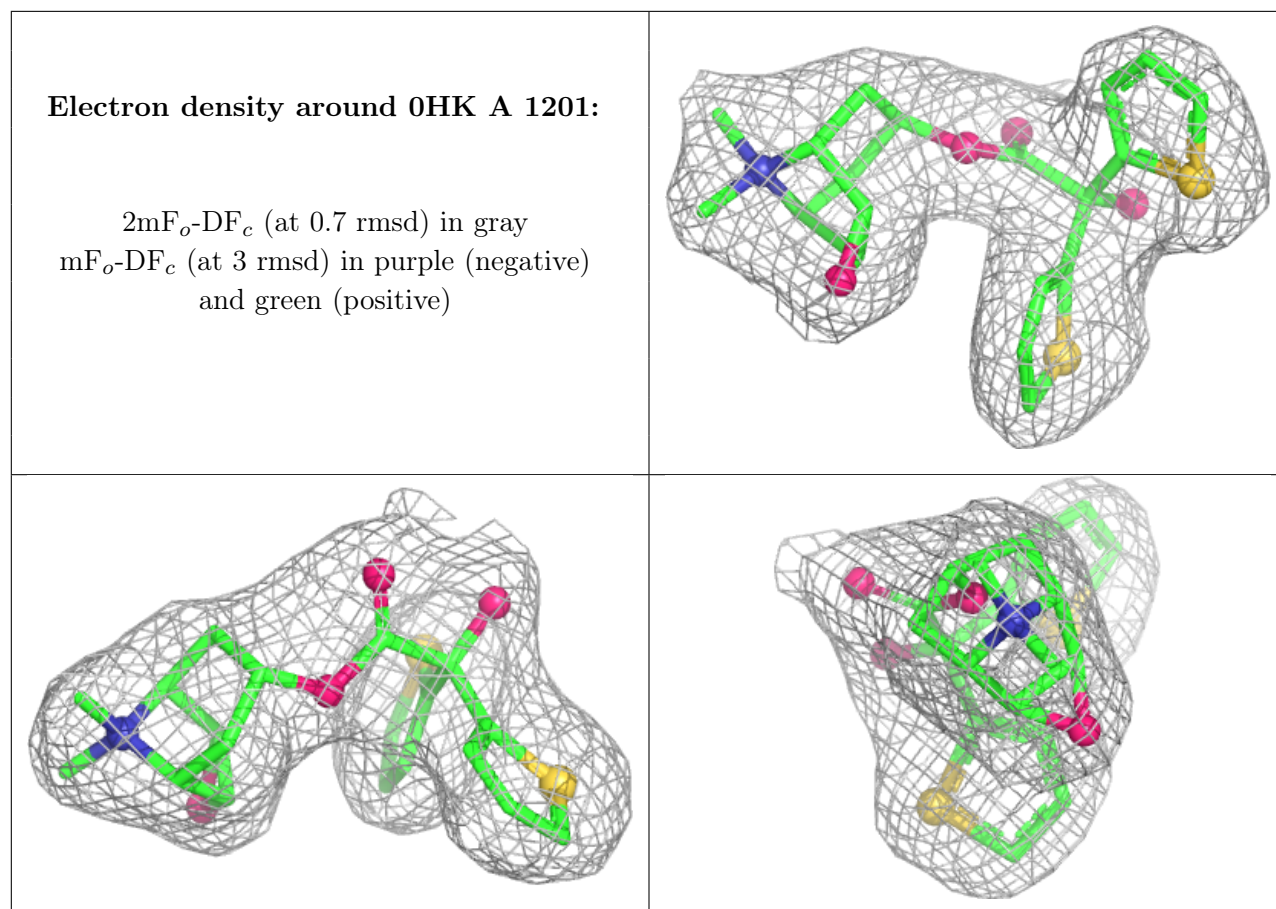
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around OHK 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.