



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 06:16 PM JST

PDB ID : 5XRA
Title : Crystal structure of the human CB1 in complex with agonist AM11542
Authors : Hua, T.; Vemuri, K.; Nikas, P.S.; Laprairie, R.B.; Wu, Y.; Qu, L.; Pu, M.; Korde, A.; Shan, J.; Ho, J.H.; Han, G.W.; Ding, K.; Li, X.; Liu, H.; Hanson, M.A.; Zhao, S.; Bohn, L.M.; Makriyannis, A.; Stevens, R.C.; Liu, Z.J.
Deposited on : 2017-06-08
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 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

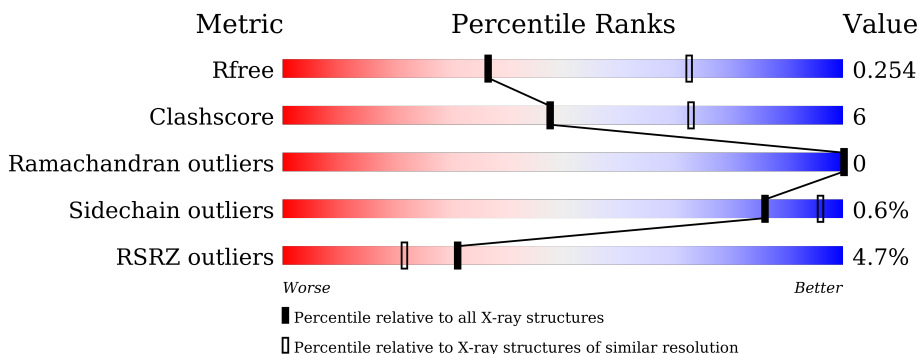
1 Overall quality at a glance

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 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	438	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3461 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.

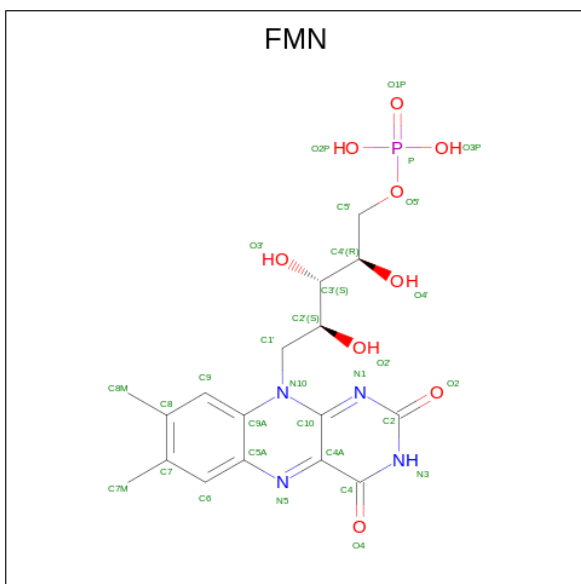
- Molecule 1 is a protein called Cannabinoid receptor 1,Flavodoxin,Cannabinoid receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	428	3311	2162	535	593	21	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

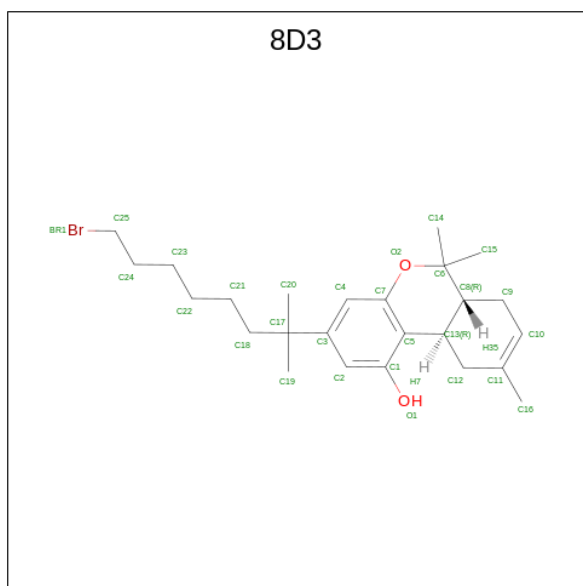
Chain	Residue	Modelled	Actual	Comment	Reference
A	210	ALA	THR	engineered mutation	UNP P21554
A	273	LYS	GLU	engineered mutation	UNP P21554
A	283	VAL	THR	engineered mutation	UNP P21554
A	1002	ALA	-	linker	UNP P21554
A	1098	TRP	TYR	engineered mutation	UNP P00323
A	340	GLU	ARG	engineered mutation	UNP P21554

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



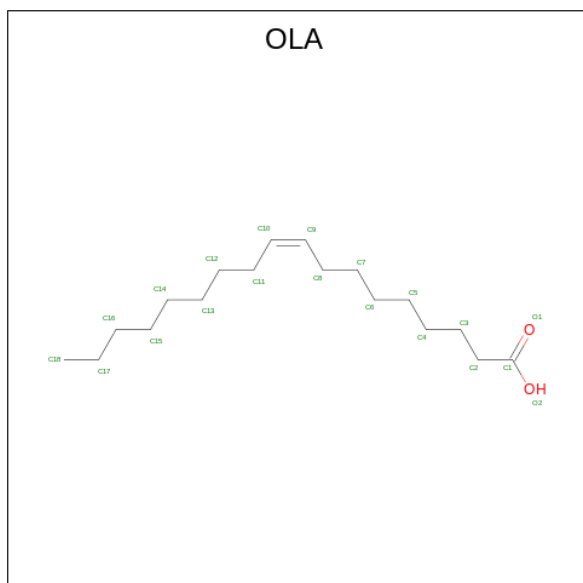
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	17	4	9	1	0	0

- Molecule 3 is (6aR,10aR)-3-(8-bromanyl-2-methyl-octan-2-yl)-6,6,9-trimethyl-6a,7,10,10a-tetrahydrobenzo[c]chromen-1-ol (three-letter code: 8D3) (formula: C₂₅H₃₇BrO₂).



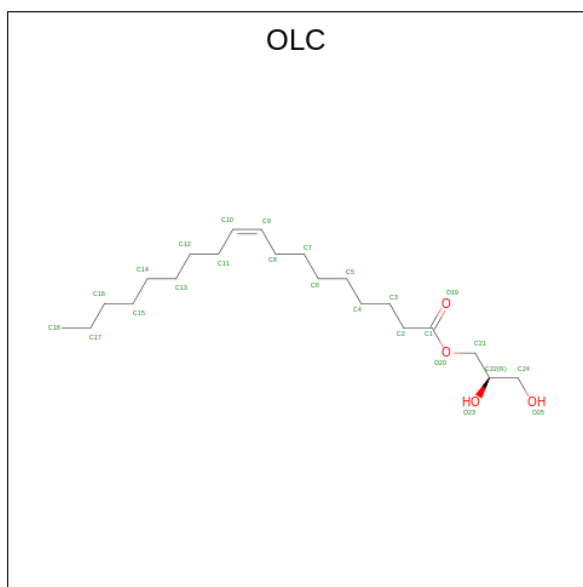
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	O		
3	A	1	28	1	25	2	0	0

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: C₁₈H₃₄O₂).



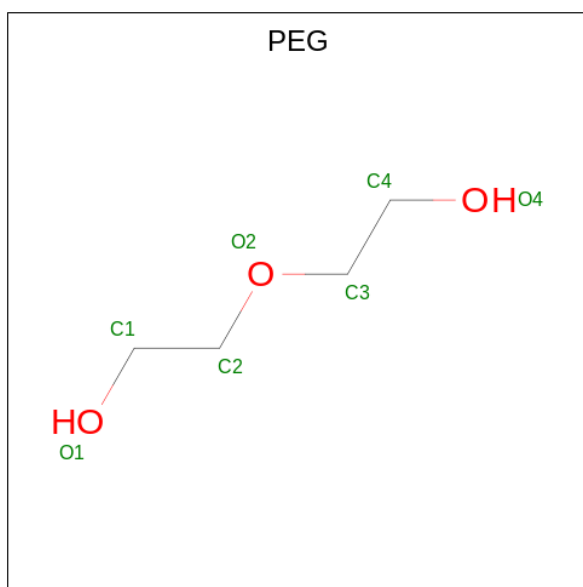
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	11	2		
4	A	1	Total	C	O	0	0
			13	11	2		

- Molecule 5 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



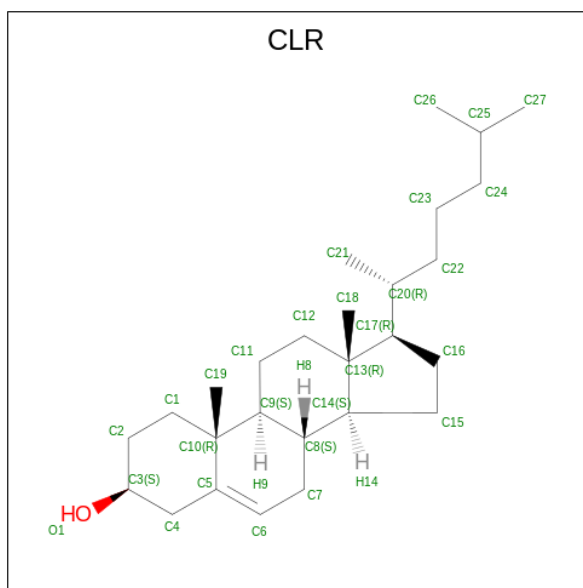
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			17	13	4		
5	A	1	Total	C	O	0	0
			13	9	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).

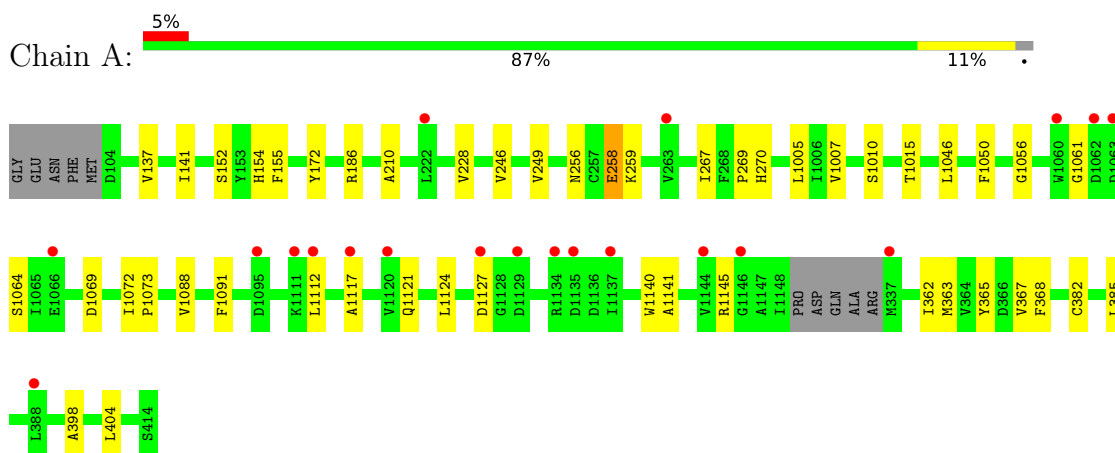


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			28	27	1		

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: Cannabinoid receptor 1,Flavodoxin,Cannabinoid receptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	66.05Å 75.87Å 138.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.91 – 2.80 37.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.6 (37.91-2.80) 92.4 (37.94-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.234 , 0.252 0.235 , 0.254	Depositor DCC
R_{free} test set	805 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	71.2	Xtrriage
Anisotropy	0.228	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3461	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, FMN, OLC, PEG, 8D3, OLA

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	0.27	0/3386	0.41	0/4607

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 [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	3311	0	3311	41	0
2	A	31	0	19	0	0
3	A	28	0	0	0	0
4	A	26	0	32	0	0
5	A	30	0	37	2	0
6	A	7	0	10	0	0
7	A	28	0	46	1	0
All	All	3461	0	3455	42	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 6.

All (42) 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:1112:LEU:HD11	1:A:1117:ALA:CB	1.74	1.18
1:A:1112:LEU:CD1	1:A:1117:ALA:HB3	1.81	1.10
1:A:1088:VAL:HB	1:A:1112:LEU:HD21	1.38	1.03
1:A:1112:LEU:CD1	1:A:1117:ALA:CB	2.42	0.92
1:A:1112:LEU:HD11	1:A:1117:ALA:HB3	1.44	0.92
1:A:1088:VAL:CB	1:A:1112:LEU:HD21	2.14	0.78
1:A:186:ARG:HG3	1:A:270:HIS:ND1	2.02	0.74
1:A:1088:VAL:HB	1:A:1112:LEU:CD2	2.17	0.73
1:A:1069:ASP:O	1:A:1072:ILE:HG12	1.94	0.68
1:A:1112:LEU:CG	1:A:1117:ALA:HB3	2.24	0.67
1:A:1010:SER:HB3	1:A:1015:THR:HB	1.82	0.62
1:A:269:PRO:HB2	1:A:270:HIS:HD2	1.64	0.62
1:A:1112:LEU:HD11	1:A:1117:ALA:HB2	1.78	0.61
1:A:137:VAL:O	1:A:141:ILE:HG12	2.02	0.60
1:A:1112:LEU:HD12	1:A:1117:ALA:HB3	1.85	0.56
1:A:269:PRO:CB	1:A:270:HIS:HD2	2.19	0.56
1:A:1112:LEU:HG	1:A:1117:ALA:HB3	1.88	0.56
1:A:1072:ILE:HG12	1:A:1073:PRO:HD3	1.88	0.55
1:A:256:ASN:OD1	1:A:259:LYS:HB2	2.08	0.52
1:A:1005:LEU:HB2	1:A:1050:PHE:CD1	2.45	0.51
1:A:186:ARG:HH21	1:A:258:GLU:HB2	1.77	0.48
1:A:363:MET:O	1:A:367:VAL:HG23	2.13	0.48
1:A:228:VAL:HG13	5:A:606:OLC:H2	1.96	0.47
1:A:1112:LEU:CD1	1:A:1117:ALA:HB2	2.41	0.47
1:A:1112:LEU:HD11	1:A:1117:ALA:HB1	1.84	0.47
1:A:246:VAL:O	1:A:249:VAL:HG12	2.15	0.46
1:A:1061:GLY:HA3	1:A:1064:SER:O	2.16	0.45
1:A:152:SER:HB3	1:A:154:HIS:CD2	2.52	0.45
1:A:1141:ALA:O	1:A:1145:ARG:HB2	2.17	0.45
1:A:1124:LEU:HD13	1:A:1140:TRP:HB2	2.00	0.44
1:A:1072:ILE:CG1	1:A:1073:PRO:HD3	2.48	0.44
1:A:382:CYS:O	1:A:385:LEU:HB2	2.17	0.43
1:A:1056:GLY:HA3	1:A:1091:PHE:CZ	2.54	0.43
1:A:155:PHE:CD1	1:A:210:ALA:HB2	2.54	0.43
1:A:1127:ASP:OD1	1:A:1127:ASP:N	2.44	0.42
1:A:172:TYR:HD2	5:A:605:OLC:H5A	1.85	0.41
1:A:398:ALA:O	1:A:404:LEU:HD23	2.21	0.41
1:A:267:ILE:HD11	1:A:362:ILE:HG22	2.02	0.41
7:A:608:CLR:H231	7:A:608:CLR:H213	1.80	0.41
1:A:362:ILE:O	1:A:365:TYR:HB2	2.21	0.41
1:A:1007:VAL:HG21	1:A:1046:LEU:HD21	2.03	0.41
1:A:368:PHE:N	1:A:368:PHE:CD2	2.89	0.41

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	424/438 (97%)	415 (98%)	9 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	353/369 (96%)	351 (99%)	2 (1%)	86 96

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

Mol	Chain	Res	Type
1	A	258	GLU
1	A	1121	GLN

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

Mol	Chain	Res	Type
1	A	270	HIS

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
7	CLR	A	608	-	31,31,31	0.67	1 (3%)	48,48,48	1.41	9 (18%)
2	FMN	A	601	-	33,33,33	1.59	8 (24%)	48,50,50	1.42	12 (25%)
5	OLC	A	605	-	16,16,24	0.99	2 (12%)	17,17,25	1.01	1 (5%)
5	OLC	A	606	-	12,12,24	1.09	2 (16%)	13,13,25	1.01	1 (7%)
3	8D3	A	602	-	30,30,30	2.80	6 (20%)	43,45,45	2.27	13 (30%)
4	OLA	A	604	-	12,12,19	0.73	0	12,12,19	1.13	0
6	PEG	A	607	-	6,6,6	0.49	0	5,5,5	0.29	0
4	OLA	A	603	-	12,12,19	0.71	0	12,12,19	1.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLR	A	608	-	-	0/10/68/68	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	A	601	-	-	11/18/18/18	0/3/3/3
5	OLC	A	605	-	-	7/16/16/24	-
5	OLC	A	606	-	-	4/12/12/24	-
3	8D3	A	602	-	-	0/14/42/42	0/3/3/3
4	OLA	A	604	-	-	6/10/10/17	-
6	PEG	A	607	-	-	2/4/4/4	-
4	OLA	A	603	-	-	9/10/10/17	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	8D3	C17-C3	-8.51	1.40	1.53
3	A	602	8D3	C5-C13	-7.73	1.40	1.51
3	A	602	8D3	C6-C8	-5.94	1.44	1.53
3	A	602	8D3	C9-C10	-5.05	1.39	1.50
3	A	602	8D3	C16-C11	-4.32	1.39	1.50
3	A	602	8D3	C12-C11	-3.44	1.41	1.50
2	A	601	FMN	C9A-N10	-3.32	1.35	1.41
2	A	601	FMN	C4-N3	-3.03	1.33	1.38
2	A	601	FMN	O2-C2	-2.83	1.19	1.24
2	A	601	FMN	C4A-C10	-2.70	1.36	1.44
2	A	601	FMN	C5A-N5	-2.64	1.34	1.39
5	A	605	OLC	O20-C1	2.51	1.40	1.33
2	A	601	FMN	C4A-N5	2.49	1.35	1.30
5	A	606	OLC	O20-C1	2.45	1.40	1.33
2	A	601	FMN	O4-C4	-2.42	1.19	1.23
7	A	608	CLR	C10-C9	-2.33	1.52	1.56
2	A	601	FMN	C9A-C5A	-2.25	1.37	1.41
5	A	606	OLC	O20-C21	-2.05	1.40	1.45
5	A	605	OLC	O20-C21	-2.00	1.40	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	8D3	C12-C13-C8	-7.68	92.20	109.74
3	A	602	8D3	O2-C7-C5	-4.94	114.25	122.00
3	A	602	8D3	C12-C13-C5	-4.59	104.73	113.29
3	A	602	8D3	C6-O2-C7	3.66	124.22	117.46
3	A	602	8D3	O2-C7-C4	3.63	122.19	116.42
3	A	602	8D3	C4-C7-C5	-3.59	116.47	121.85
2	A	601	FMN	C1'-N10-C9A	3.47	126.30	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	8D3	C21-C18-C17	-3.16	111.11	117.31
3	A	602	8D3	C7-C5-C13	-3.07	115.94	120.92
2	A	601	FMN	C4-N3-C2	-3.05	120.00	125.64
7	A	608	CLR	C19-C10-C9	-2.96	108.16	111.68
3	A	602	8D3	C5-C13-C8	2.87	118.29	106.47
3	A	602	8D3	C6-C8-C13	-2.76	103.19	109.78
2	A	601	FMN	O4-C4-C4A	-2.66	119.56	126.60
2	A	601	FMN	C7M-C7-C6	-2.65	114.59	119.49
2	A	601	FMN	C4A-C4-N3	2.62	119.85	113.19
5	A	606	OLC	O20-C1-C2	2.61	120.11	111.91
7	A	608	CLR	C13-C14-C8	-2.59	110.54	114.38
7	A	608	CLR	C14-C8-C9	-2.59	105.62	109.09
5	A	605	OLC	O20-C1-C2	2.58	120.00	111.91
7	A	608	CLR	C11-C9-C10	-2.43	109.88	113.08
2	A	601	FMN	C7M-C7-C8	2.38	125.61	120.74
7	A	608	CLR	C21-C20-C22	-2.33	106.71	110.36
2	A	601	FMN	C4A-C10-N10	2.32	119.87	116.48
2	A	601	FMN	C4A-C10-N1	-2.28	119.45	124.73
3	A	602	8D3	O2-C6-C8	-2.27	103.88	109.27
7	A	608	CLR	C3-C4-C5	-2.26	108.19	112.03
2	A	601	FMN	C5A-C9A-N10	2.25	120.28	117.95
3	A	602	8D3	C9-C8-C6	-2.25	107.21	112.49
7	A	608	CLR	C13-C17-C20	-2.21	116.03	119.49
2	A	601	FMN	C9A-C5A-N5	-2.19	120.05	122.43
2	A	601	FMN	C4-C4A-C10	2.14	120.39	116.79
3	A	602	8D3	C16-C11-C12	2.14	119.81	116.16
7	A	608	CLR	C23-C22-C20	-2.12	108.94	115.03
2	A	601	FMN	C10-C4A-N5	-2.08	120.44	124.86
7	A	608	CLR	C18-C13-C14	-2.06	107.87	111.71

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FMN	C1'-C2'-C3'-O3'
2	A	601	FMN	C1'-C2'-C3'-C4'
2	A	601	FMN	O4'-C4'-C5'-O5'
2	A	601	FMN	C5'-O5'-P-O2P
2	A	601	FMN	C5'-O5'-P-O3P
2	A	601	FMN	O2'-C2'-C3'-O3'
2	A	601	FMN	O2'-C2'-C3'-C4'
5	A	605	OLC	O20-C21-C22-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	605	OLC	O20-C21-C22-O23
5	A	606	OLC	C1-C2-C3-C4
6	A	607	PEG	O2-C3-C4-O4
5	A	605	OLC	C2-C1-O20-C21
4	A	603	OLA	C5-C6-C7-C8
5	A	606	OLC	C2-C3-C4-C5
4	A	603	OLA	C1-C2-C3-C4
4	A	603	OLA	C6-C7-C8-C9
5	A	605	OLC	C5-C6-C7-C8
5	A	605	OLC	O19-C1-O20-C21
4	A	603	OLA	C3-C4-C5-C6
4	A	603	OLA	C2-C3-C4-C5
4	A	604	OLA	C3-C4-C5-C6
2	A	601	FMN	C2'-C3'-C4'-O4'
4	A	604	OLA	C6-C7-C8-C9
2	A	601	FMN	O3'-C3'-C4'-O4'
2	A	601	FMN	C2'-C3'-C4'-C5'
4	A	604	OLA	C4-C5-C6-C7
4	A	604	OLA	C1-C2-C3-C4
4	A	603	OLA	C4-C5-C6-C7
5	A	605	OLC	C2-C3-C4-C5
5	A	605	OLC	C7-C8-C9-C10
6	A	607	PEG	O1-C1-C2-O2
4	A	603	OLA	O1-C1-C2-C3
2	A	601	FMN	O3'-C3'-C4'-C5'
4	A	604	OLA	O1-C1-C2-C3
4	A	603	OLA	O2-C1-C2-C3
4	A	604	OLA	O2-C1-C2-C3
4	A	603	OLA	C7-C8-C9-C10
5	A	606	OLC	O20-C1-C2-C3
5	A	606	OLC	O19-C1-C2-C3

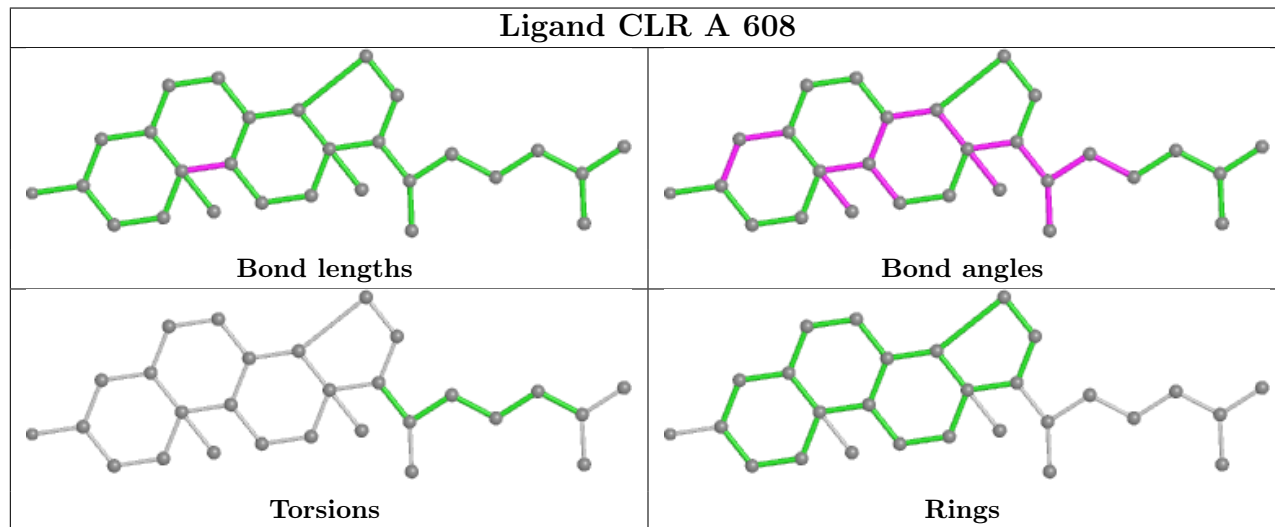
There are no ring outliers.

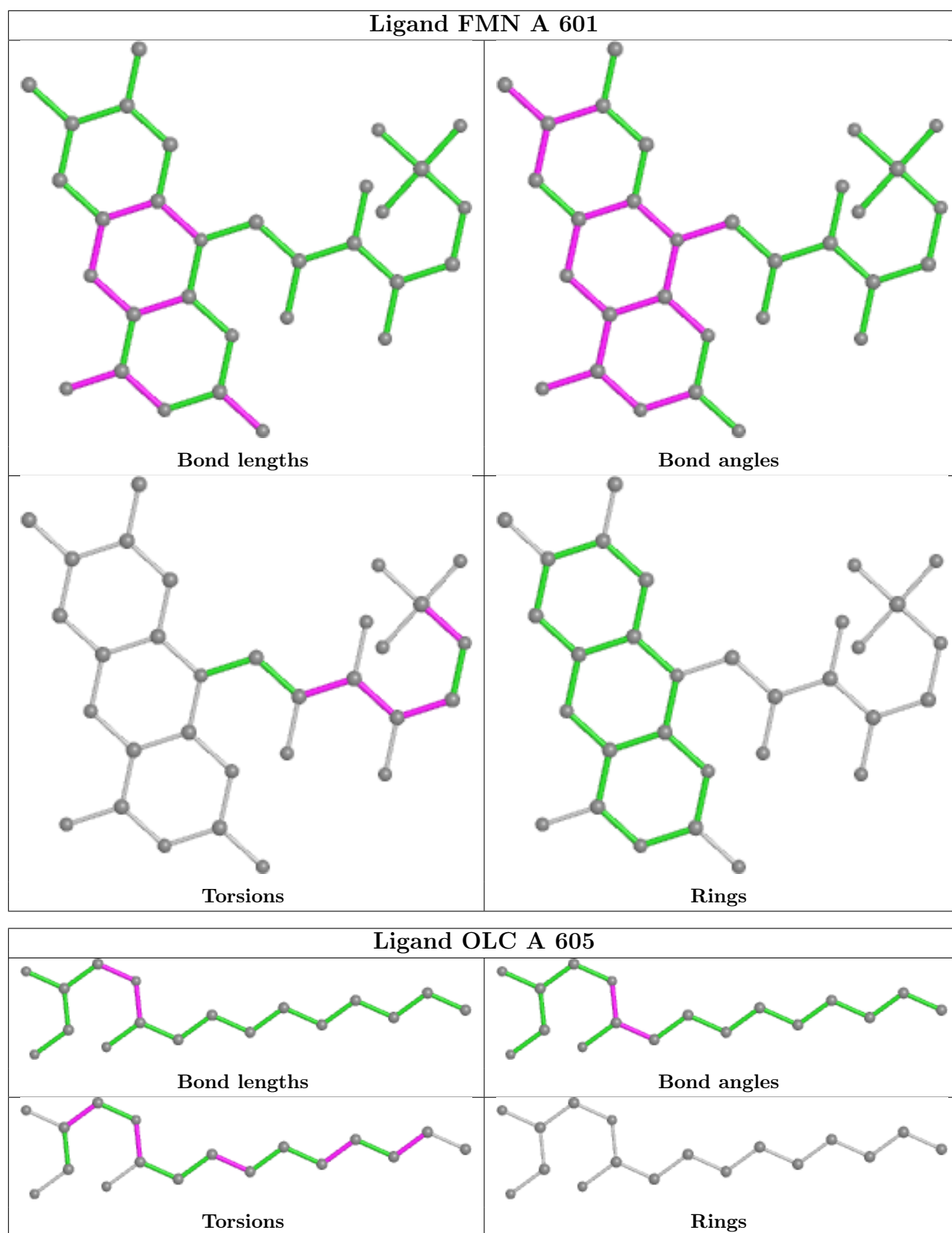
3 monomers are involved in 3 short contacts:

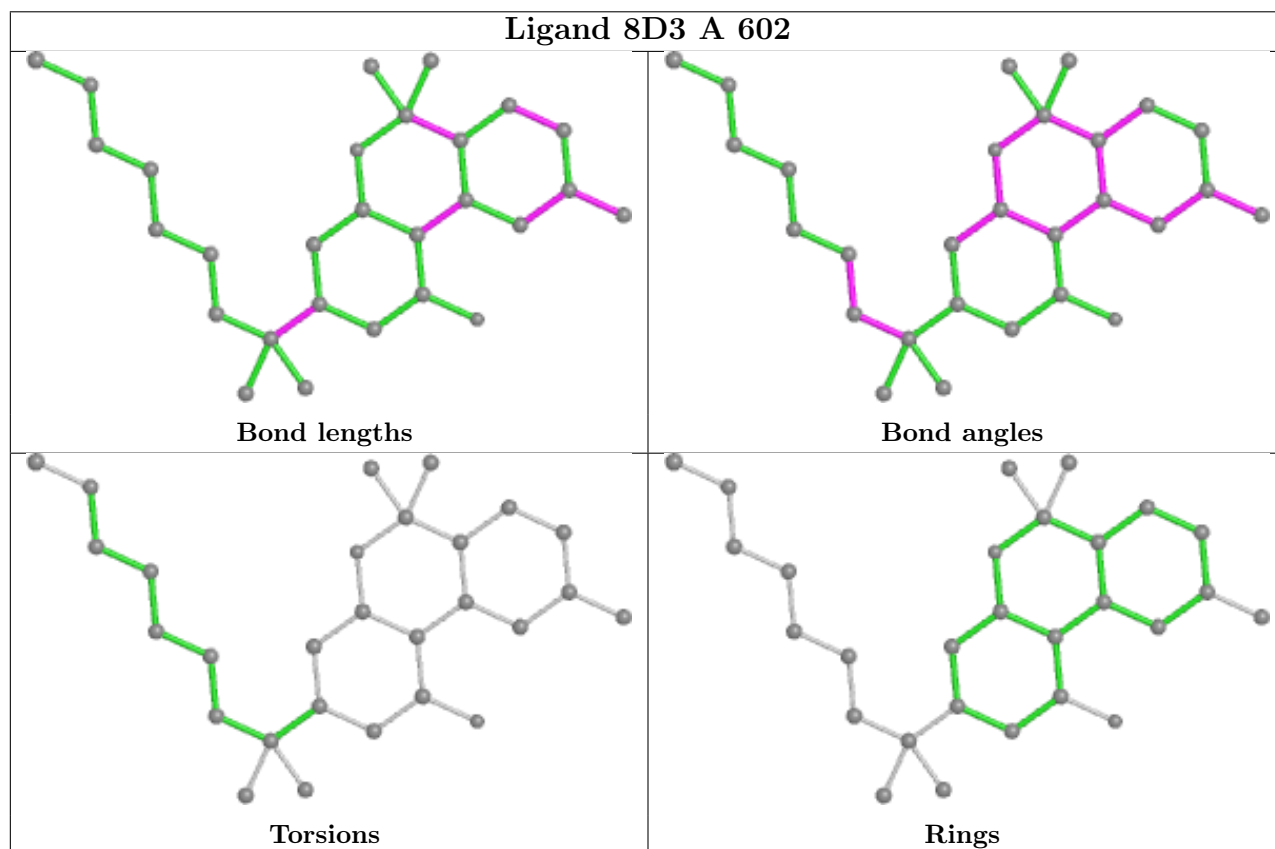
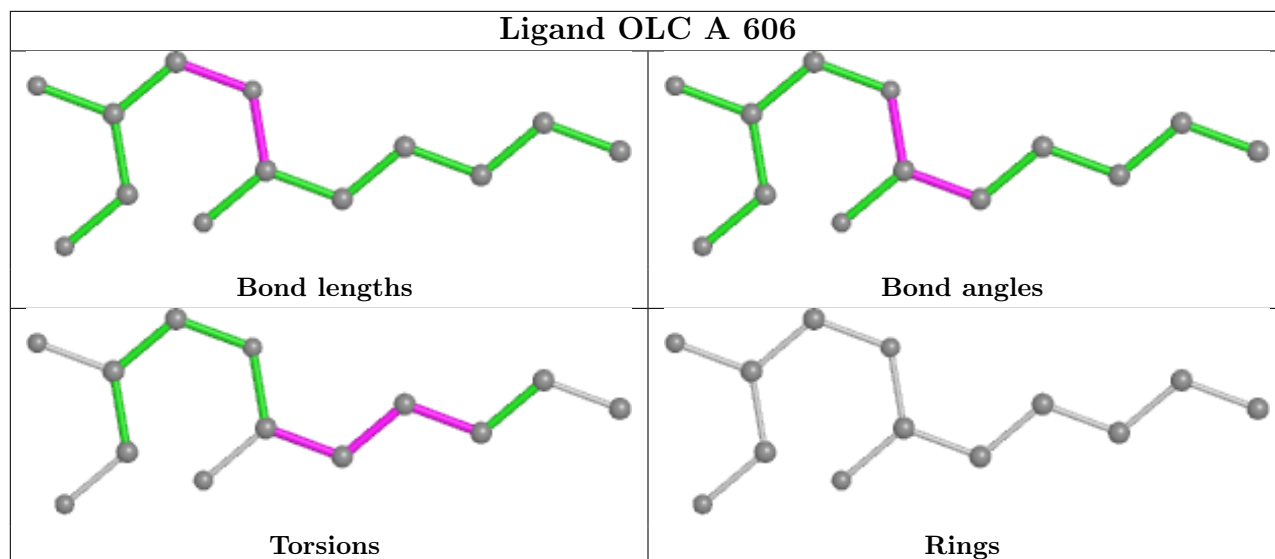
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	608	CLR	1	0
5	A	605	OLC	1	0
5	A	606	OLC	1	0

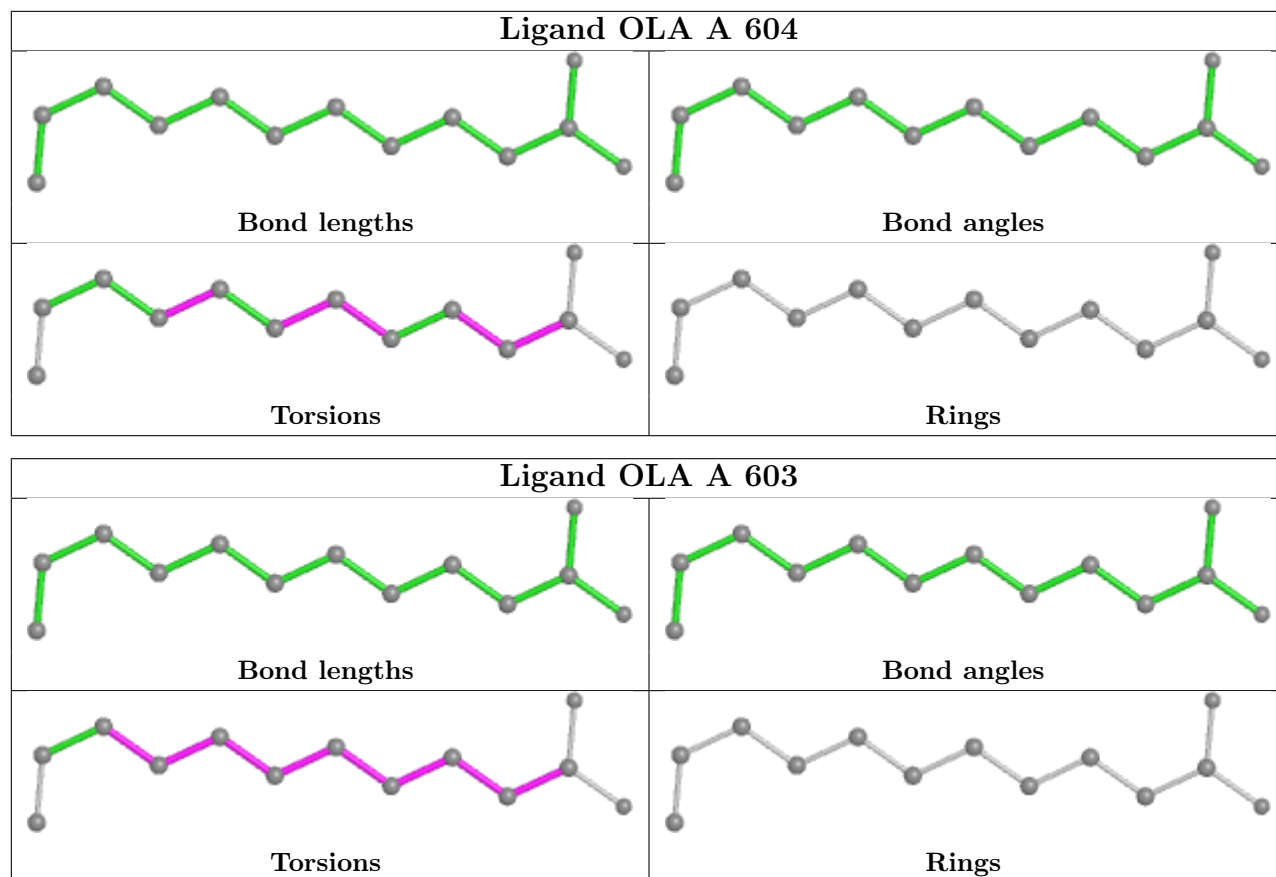
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	428/438 (97%)	-0.07	20 (4%) 31 22	52, 86, 132, 161	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1060	TRP	5.2
1	A	1112	LEU	4.9
1	A	1062	ASP	3.9
1	A	1066	GLU	3.7
1	A	1134	ARG	3.2
1	A	263	VAL	3.1
1	A	1127	ASP	3.1
1	A	1111	LYS	3.0
1	A	1095	ASP	3.0
1	A	1120	VAL	2.9
1	A	1137	ILE	2.9
1	A	1144	VAL	2.6
1	A	1129	ASP	2.5
1	A	1063	ASP	2.5
1	A	1117	ALA	2.5
1	A	1146	GLY	2.5
1	A	337	MET	2.4
1	A	388	LEU	2.2
1	A	222	LEU	2.2
1	A	1135	ASP	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](#)

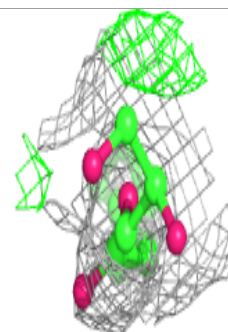
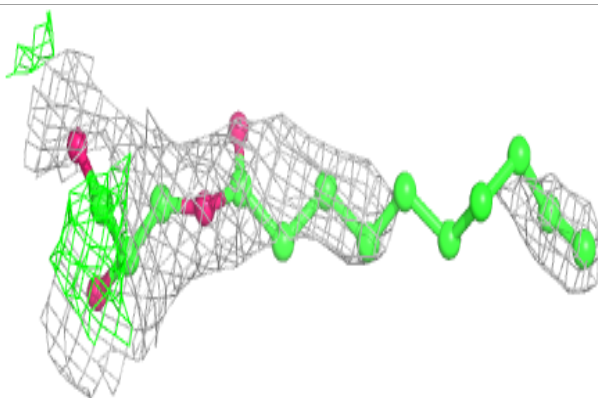
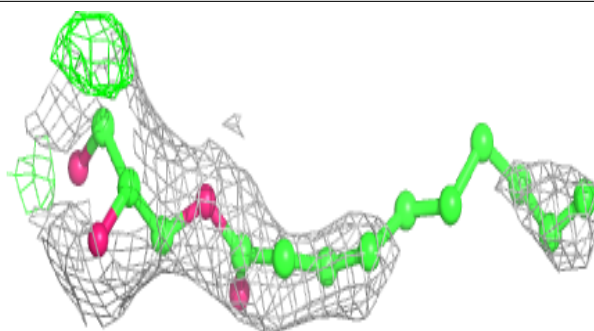
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PEG	A	607	7/7	0.73	0.33	104,106,106,106	0
5	OLC	A	605	17/25	0.77	0.33	85,100,107,108	0
5	OLC	A	606	13/25	0.78	0.29	86,102,105,106	0
4	OLA	A	604	13/20	0.82	0.32	81,84,96,96	0
4	OLA	A	603	13/20	0.88	0.16	80,81,86,89	0
2	FMN	A	601	31/31	0.94	0.25	64,72,79,80	0
3	8D3	A	602	28/28	0.95	0.22	52,59,80,87	0
7	CLR	A	608	28/28	0.96	0.22	58,62,72,73	0

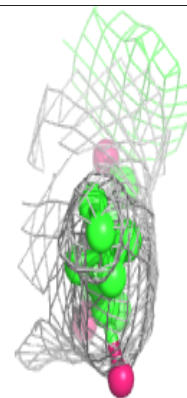
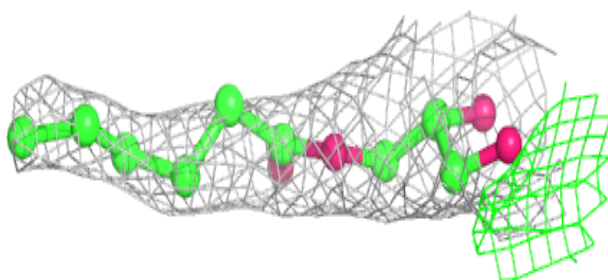
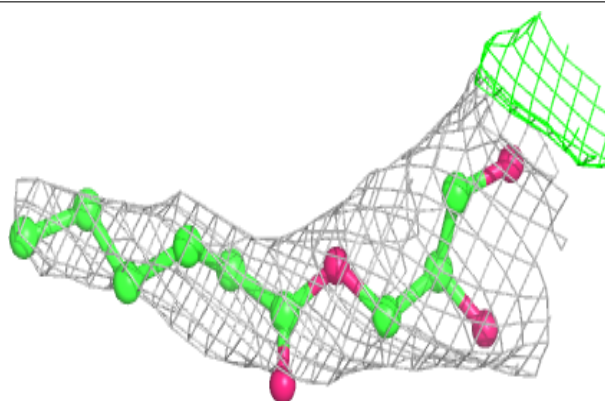
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 605:

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

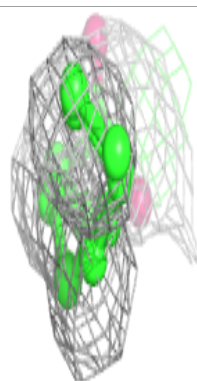
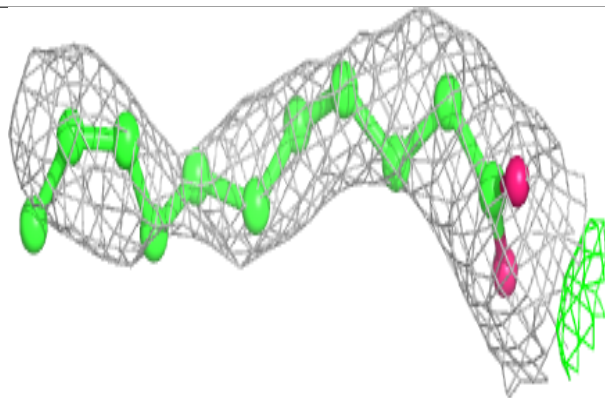
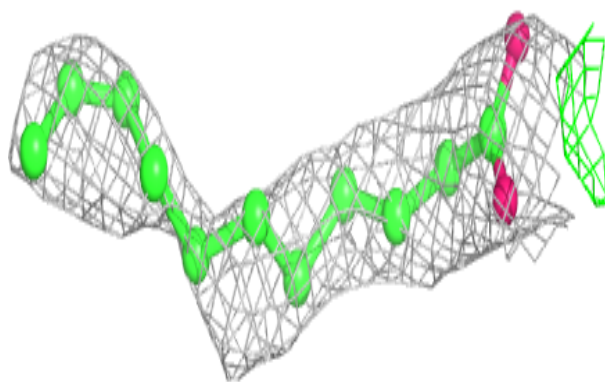
**Electron density around OLC A 606:**

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

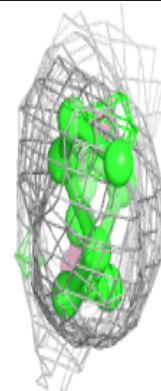
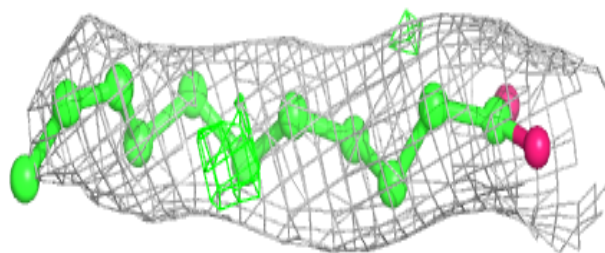
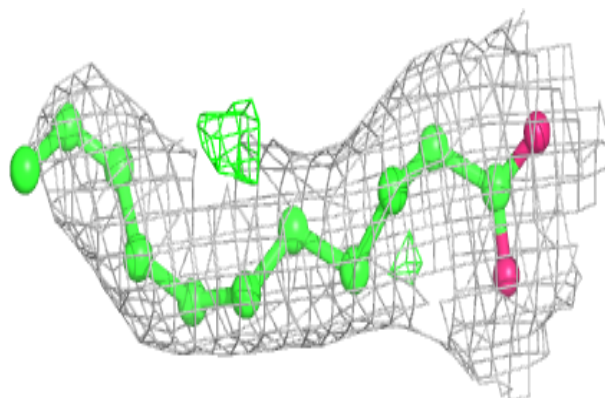


Electron density around OLA A 604:

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

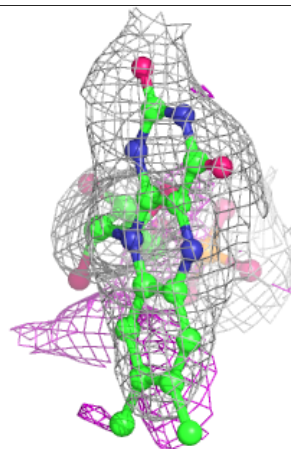
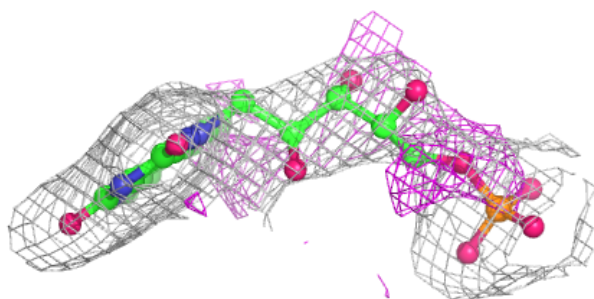
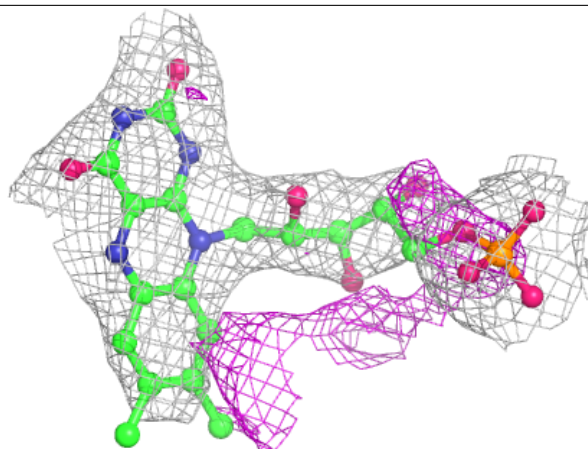
**Electron density around OLA A 603:**

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



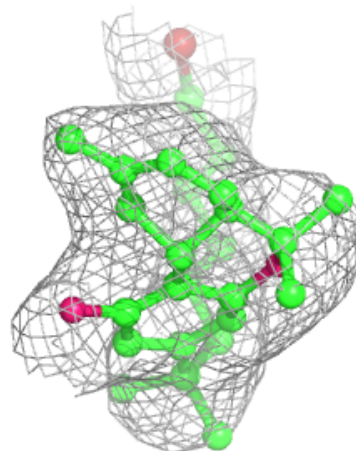
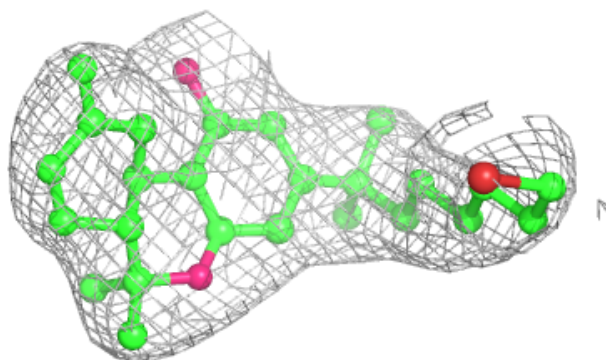
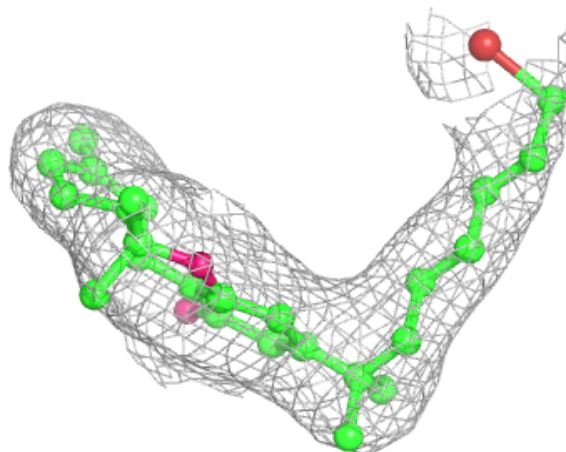
Electron density around FMN A 601:

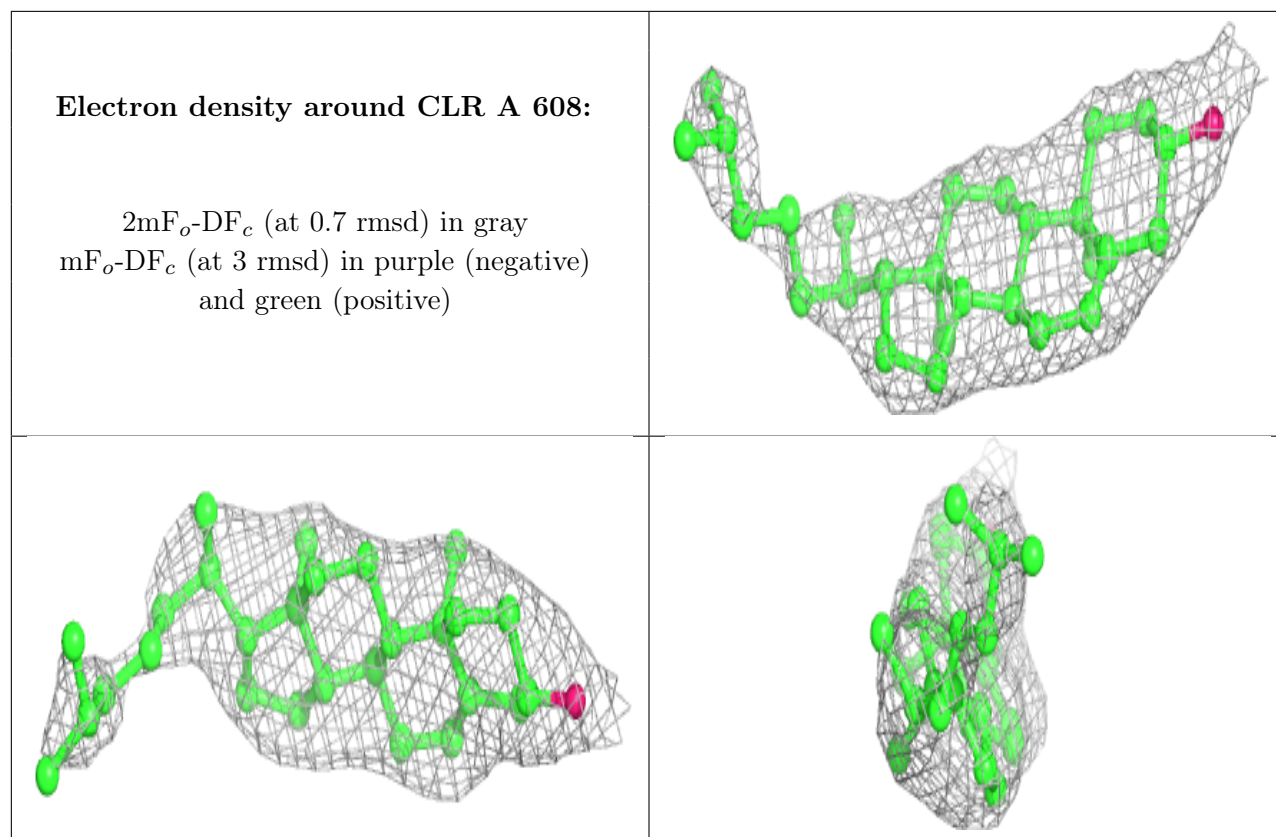
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 8D3 A 602:

$2mF_o-DF_c$ (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.