



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:12 PM BST

PDB ID : 4JKV
Title : Structure of the human smoothened 7TM receptor in complex with an antitumor agent
Authors : Wang, C.; Wu, H.; Katritch, V.; Han, G.W.; Huang, X.; Liu, W.; Siu, F.Y.; Roth, B.L.; Cherezov, V.; Stevens, R.C.; GPCR Network (GPCR)
Deposited on : 2013-03-11
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

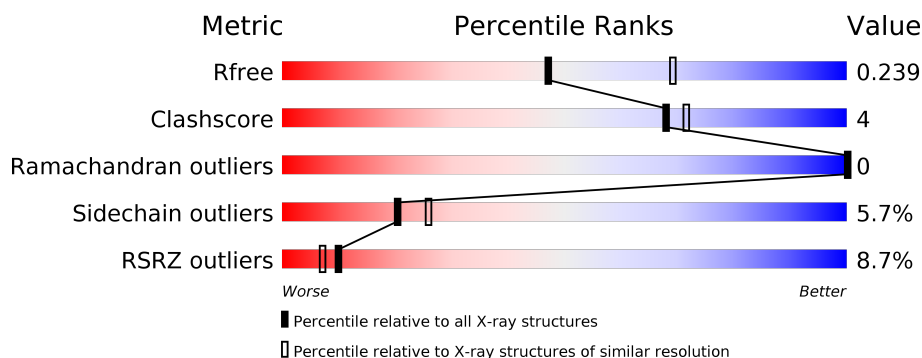
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	<div> <div>9%</div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
1	B	475	<div> <div>7%</div> <div>81%</div> <div>12%</div> <div>• 5%</div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7390 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

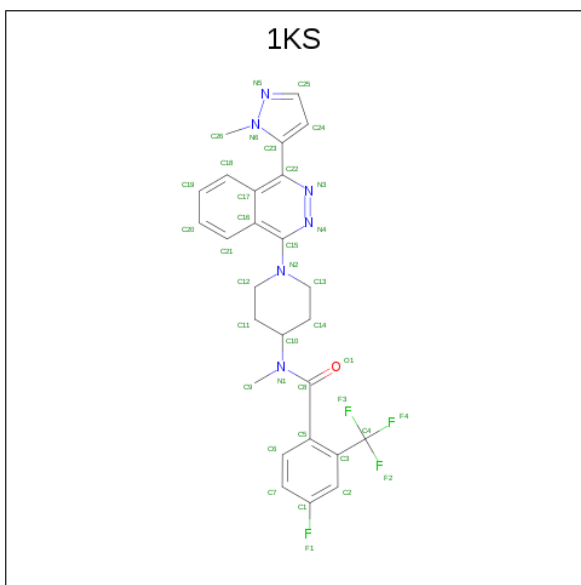
- Molecule 1 is a protein called Soluble cytochrome b562, Smoothened homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3532	2297	578	635	22			
1	B	450	Total	C	N	O	S	0	1	0
			3511	2278	578	635	20			

There are 12 discrepancies between the modelled and reference sequences:

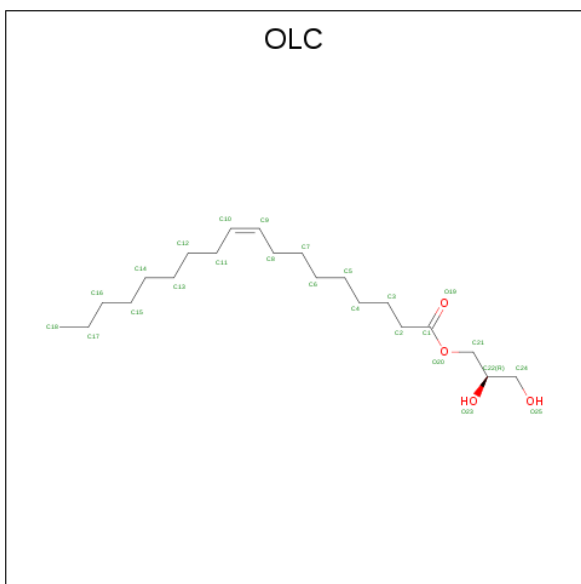
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P0ABE7
A	-1	GLY	-	EXPRESSION TAG	UNP P0ABE7
A	0	THR	-	EXPRESSION TAG	UNP P0ABE7
A	7	TRP	MET	ENGINEERED MUTATION	UNP P0ABE7
A	102	ILE	HIS	ENGINEERED MUTATION	UNP P0ABE7
A	106	LEU	-	LINKER	UNP P0ABE7
B	-2	GLY	-	EXPRESSION TAG	UNP P0ABE7
B	-1	GLY	-	EXPRESSION TAG	UNP P0ABE7
B	0	THR	-	EXPRESSION TAG	UNP P0ABE7
B	7	TRP	MET	ENGINEERED MUTATION	UNP P0ABE7
B	102	ILE	HIS	ENGINEERED MUTATION	UNP P0ABE7
B	106	LEU	-	LINKER	UNP P0ABE7

- Molecule 2 is 4-fluoro-N-methyl-N-{1-[4-(1-methyl-1H-pyrazol-5-yl)phthalazin-1-yl]piperidin-4-yl}-2-(trifluoromethyl)benzamide (three-letter code: 1KS) (formula: C₂₆H₂₄F₄N₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 37	C 26	F 4	N 6	O 1	0	0
2	B	1	Total 37	C 26	F 4	N 6	O 1	0	0

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



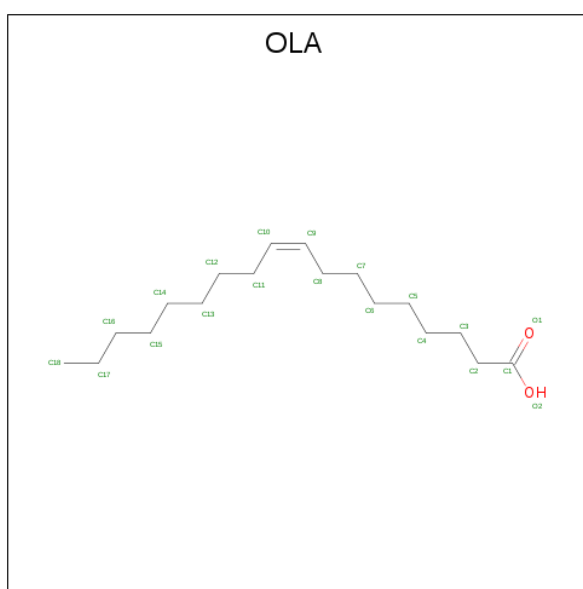
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	11	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	11	4		
3	A	1	Total	C	O	0	0
			14	10	4		
3	B	1	Total	C	O	0	0
			13	9	4		
3	B	1	Total	C	O	0	0
			14	10	4		

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



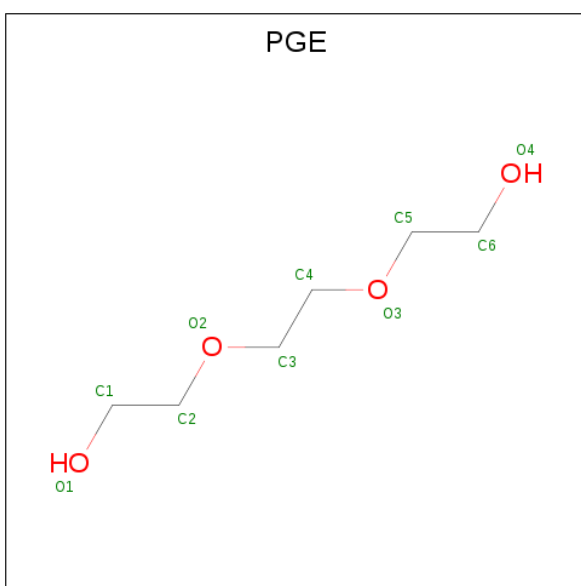
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	18	2		
4	A	1	Total	C	O	0	0
			15	13	2		
4	B	1	Total	C	O	0	0
			20	18	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



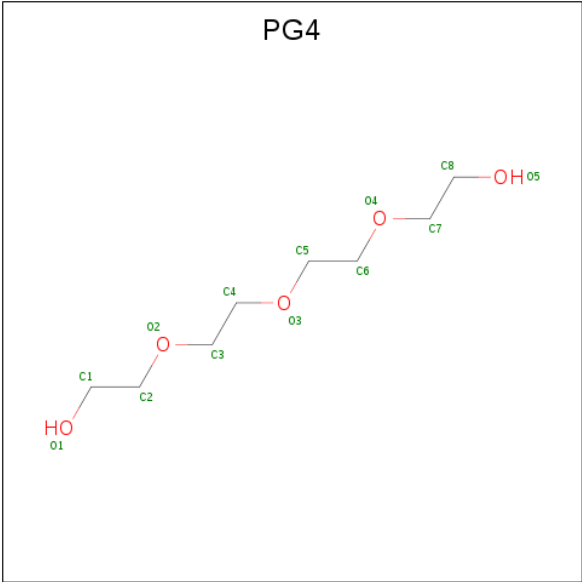
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		

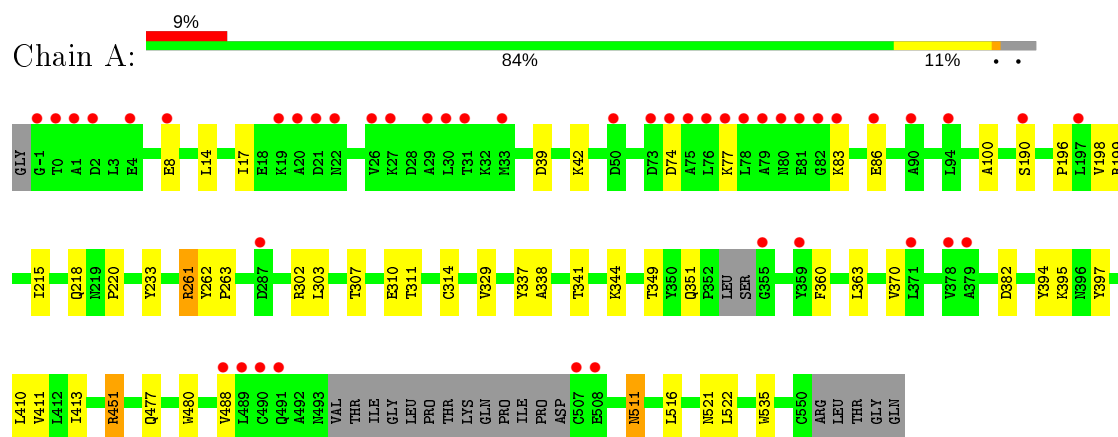
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	49	Total	O	0	0
			49	49		
8	B	61	Total	O	0	0
			61	61		

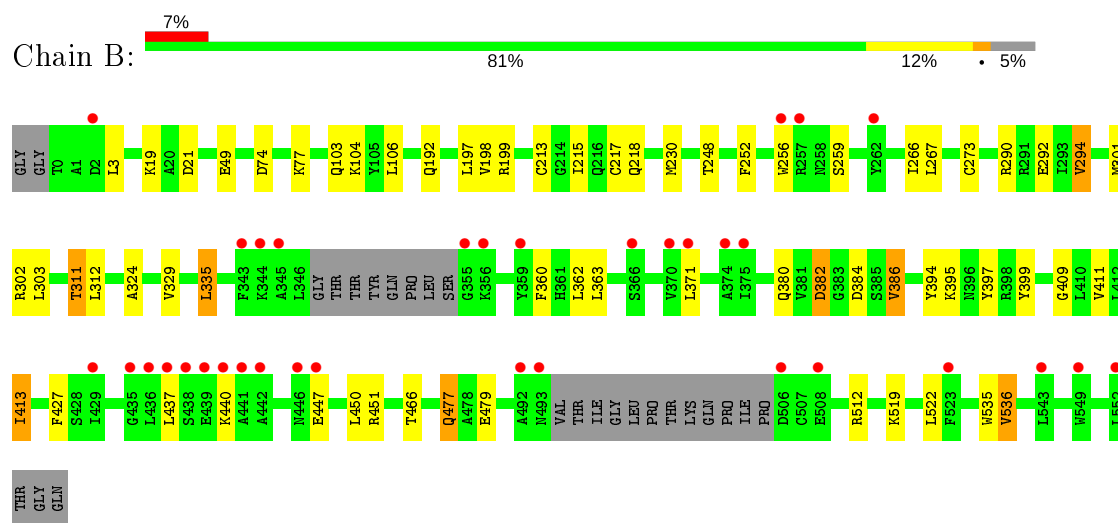
3 Residue-property plots [i](#)

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: Soluble cytochrome b562, Smoothened homolog



- Molecule 1: Soluble cytochrome b562, Smoothened homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.44Å 98.18Å 84.29Å 90.00° 103.27° 90.00°	Depositor
Resolution (Å)	42.12 – 2.45 41.02 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.12-2.45) 99.5 (41.02-2.45)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.200 , 0.231 0.205 , 0.239	Depositor DCC
R_{free} test set	2202 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7390	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 6.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLA, OLC, PG4, PGE, 1KS, PEG

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	0.47	0/3621	0.60	0/4926
1	B	0.46	0/3598	0.60	0/4894
All	All	0.46	0/7219	0.60	0/9820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3532	0	3446	26	0
1	B	3511	0	3400	31	0
2	A	37	0	24	1	0
2	B	37	0	24	2	0
3	A	44	0	55	0	0
3	B	27	0	32	2	0
4	A	35	0	53	0	0
4	B	20	0	33	0	0
5	A	7	0	10	0	0
5	B	7	0	10	1	0
6	A	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	13	0	18	2	0
8	A	49	0	0	1	0
8	B	61	0	0	0	0
All	All	7390	0	7119	55	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 4.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LEU:H	5:B:605:PEG:H21	1.61	0.66
1:B:329:VAL:HB	1:B:411:VAL:HG21	1.79	0.64
1:A:382:ASP:HB2	1:A:394:TYR:HB2	1.83	0.60
1:B:302:ARG:HH12	1:B:311:THR:HG22	1.66	0.60
1:A:480:TRP:HD1	1:A:511:ASN:HD22	1.52	0.57
1:A:261:ARG:HH11	1:A:262:TYR:H	1.52	0.57
1:A:329:VAL:HB	1:A:411:VAL:HG21	1.89	0.54
1:B:104:LYS:HA	1:B:199:ARG:HB3	1.91	0.52
1:A:363:LEU:HD22	1:B:363:LEU:HA	1.90	0.52
1:A:196:PRO:HG2	1:A:488:VAL:HG22	1.90	0.52
1:A:302:ARG:HH12	1:A:311:THR:HG22	1.74	0.52
1:B:522:LEU:HD11	2:B:601:IKS:H11	1.91	0.51
1:A:14:LEU:HA	1:A:17:ILE:HD12	1.92	0.50
1:B:519:LYS:HD2	3:B:603:OLC:H21	1.94	0.50
1:A:74:ASP:HA	1:A:77:LYS:HE2	1.94	0.50
1:B:397:TYR:HB3	1:B:477:GLN:HB3	1.94	0.48
1:B:301:MET:HE2	2:B:601:IKS:H21	1.94	0.48
1:B:294:VAL:HG22	1:B:384:ASP:H	1.79	0.48
1:A:302:ARG:HH21	1:A:310:GLU:HB3	1.78	0.48
1:B:230:MET:HG2	1:B:386:VAL:HG23	1.94	0.48
1:B:267:LEU:HG	1:B:535:TRP:CD2	2.49	0.47
1:A:302:ARG:NH2	1:A:310:GLU:HB3	2.30	0.47
1:A:516:LEU:HD13	7:A:609:PG4:H72	1.96	0.47
1:B:292:GLU:HG2	3:B:602:OLC:H22	1.96	0.47
1:B:248:THR:HG23	1:B:536:VAL:HB	1.97	0.47
1:B:382:ASP:HB2	1:B:394:TYR:HB2	1.98	0.46
1:B:409:GLY:O	1:B:413:ILE:HG23	2.15	0.46
1:B:74:ASP:HA	1:B:77:LYS:HE2	1.97	0.46
1:A:337:TYR:CZ	1:A:341:THR:HG21	2.51	0.46
1:A:303:LEU:HD22	1:A:395:LYS:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ARG:NH1	1:A:535:TRP:O	2.49	0.45
1:A:83:LYS:HB3	1:A:86:GLU:HB2	1.99	0.45
1:A:370:VAL:HG12	1:B:371:LEU:HD21	1.99	0.45
1:A:522:LEU:HD11	2:A:601:1KS:H11	1.98	0.45
1:B:290:ARG:O	1:B:294:VAL:HB	2.17	0.45
1:B:273:CYS:O	1:B:324:ALA:HB1	2.18	0.44
1:B:215:ILE:HG23	1:B:301:MET:HG2	2.00	0.44
1:B:303:LEU:HD22	1:B:395:LYS:HG3	1.98	0.43
1:B:197:LEU:HB3	1:B:213:CYS:HB3	1.99	0.43
1:B:292:GLU:OE1	1:B:311:THR:HG21	2.17	0.43
1:A:215:ILE:HD11	1:A:220:PRO:HG3	2.00	0.43
1:A:263:PRO:HB3	1:A:338:ALA:HB1	2.00	0.43
1:A:233:TYR:HD1	7:A:609:PG4:H31	1.84	0.43
1:A:314:CYS:HB3	8:A:709:HOH:O	2.19	0.43
1:A:397:TYR:HB3	1:A:477:GLN:HB3	2.01	0.42
1:B:302:ARG:HH22	1:B:311:THR:HG22	1.83	0.42
1:B:3:LEU:HG	1:B:106:LEU:HD21	2.02	0.42
1:A:100:ALA:HA	1:A:198:VAL:HG13	2.02	0.41
1:B:266:ILE:HG22	1:B:335:LEU:HD12	2.02	0.41
1:A:341:THR:HA	1:A:344:LYS:HB2	2.02	0.41
1:B:217:CYS:SG	1:B:294:VAL:HG12	2.60	0.41
1:A:39:ASP:HA	1:A:42:LYS:HE2	2.03	0.41
1:B:252:PHE:CD2	1:B:259:SER:HB3	2.55	0.41
1:B:397:TYR:CB	1:B:477:GLN:HB3	2.51	0.41
1:B:380:GLN:HG3	1:B:399:TYR:CE2	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	448/475 (94%)	435 (97%)	13 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	445/475 (94%)	435 (98%)	10 (2%)	0	100	100
All	All	893/950 (94%)	870 (97%)	23 (3%)	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	365/396 (92%)	351 (96%)	14 (4%)	33	43
1	B	360/396 (91%)	333 (92%)	27 (8%)	13	16
All	All	725/792 (92%)	684 (94%)	41 (6%)	20	26

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	190	SER
1	A	199	ARG
1	A	218	GLN
1	A	261	ARG
1	A	307	THR
1	A	349	THR
1	A	351	GLN
1	A	360	PHE
1	A	410	LEU
1	A	413	ILE
1	A	451	ARG
1	A	511	ASN
1	A	521	ASN
1	B	19	LYS
1	B	21	ASP
1	B	49	GLU
1	B	103	GLN

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Mol	Chain	Res	Type
1	B	192	GLN
1	B	198	VAL
1	B	218	GLN
1	B	256	TRP
1	B	294	VAL
1	B	311	THR
1	B	335	LEU
1	B	360	PHE
1	B	362	LEU
1	B	382	ASP
1	B	386	VAL
1	B	413	ILE
1	B	427	PHE
1	B	437	LEU
1	B	440	LYS
1	B	447	GLU
1	B	450	LEU
1	B	451	ARG
1	B	466	THR
1	B	477	GLN
1	B	479	GLU
1	B	512	ARG
1	B	536	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	511	ASN
1	A	521	ASN
1	B	22	ASN
1	B	71	GLN
1	B	396	ASN

5.3.3 RNA ⓘ

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](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	OLC	B	602	-	12,12,24	1.35	1 (8%)	13,13,25	1.08	2 (15%)
3	OLC	A	604	-	13,13,24	1.32	1 (7%)	14,14,25	0.97	1 (7%)
4	OLA	B	604	-	16,19,19	0.28	0	15,19,19	0.53	0
3	OLC	A	603	-	14,14,24	1.31	1 (7%)	15,15,25	1.11	1 (6%)
3	OLC	B	603	-	13,13,24	1.32	1 (7%)	14,14,25	0.92	1 (7%)
5	PEG	B	605	-	6,6,6	0.12	0	5,5,5	0.07	0
4	OLA	A	605	-	16,19,19	0.27	0	15,19,19	0.56	0
4	OLA	A	606	-	11,14,19	0.29	0	10,14,19	0.52	0
5	PEG	A	607	-	6,6,6	0.11	0	5,5,5	0.06	0
7	PG4	A	609	-	12,12,12	0.19	0	11,11,11	0.14	0
3	OLC	A	602	-	14,14,24	1.29	1 (7%)	15,15,25	0.99	1 (6%)
2	1KS	A	601	-	40,41,41	2.55	9 (22%)	55,61,61	1.46	8 (14%)
6	PGE	A	608	-	9,9,9	0.16	0	8,8,8	0.16	0
2	1KS	B	601	-	40,41,41	2.45	10 (25%)	55,61,61	1.35	8 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	B	602	-	-	4/12/12/24	-
3	OLC	A	604	-	-	6/13/13/24	-
4	OLA	B	604	-	-	5/15/17/17	-
3	OLC	A	603	-	-	8/14/14/24	-
3	OLC	B	603	-	-	10/13/13/24	-
5	PEG	B	605	-	-	2/4/4/4	-
4	OLA	A	605	-	-	9/15/17/17	-
4	OLA	A	606	-	-	3/10/12/17	-
5	PEG	A	607	-	-	1/4/4/4	-
7	PG4	A	609	-	-	4/10/10/10	-
3	OLC	A	602	-	-	4/14/14/24	-
2	1KS	A	601	-	-	2/24/36/36	0/5/5/5
6	PGE	A	608	-	-	3/7/7/7	-
2	1KS	B	601	-	-	2/24/36/36	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	1KS	C2-C1	7.92	1.50	1.37
2	B	601	1KS	C2-C1	7.39	1.50	1.37
2	A	601	1KS	C5-C3	6.94	1.52	1.40
2	A	601	1KS	C7-C6	6.71	1.51	1.38
2	B	601	1KS	C7-C6	6.45	1.50	1.38
2	B	601	1KS	C5-C3	6.38	1.51	1.40
2	B	601	1KS	C8-N1	5.99	1.46	1.34
2	A	601	1KS	C8-N1	5.93	1.46	1.34
3	A	603	OLC	O20-C1	4.72	1.47	1.33
3	A	602	OLC	O20-C1	4.64	1.46	1.33
3	A	604	OLC	O20-C1	4.58	1.46	1.33
3	B	603	OLC	O20-C1	4.53	1.46	1.33
3	B	602	OLC	O20-C1	4.50	1.46	1.33
2	A	601	1KS	C15-N2	3.96	1.48	1.37
2	B	601	1KS	C15-N2	3.68	1.48	1.37
2	A	601	1KS	C23-C22	3.43	1.55	1.49
2	B	601	1KS	C23-C22	3.37	1.55	1.49
2	B	601	1KS	C24-C25	2.67	1.41	1.38
2	A	601	1KS	C26-N6	-2.54	1.42	1.47
2	B	601	1KS	C23-N6	2.48	1.41	1.36
2	B	601	1KS	C26-N6	-2.45	1.42	1.47
2	A	601	1KS	C23-N6	2.41	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	1KS	C24-C25	2.38	1.41	1.38
2	B	601	1KS	C25-N5	2.27	1.38	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	1KS	C16-C15-N4	-4.82	119.36	126.80
2	B	601	1KS	C16-C15-N4	-4.44	119.95	126.80
2	A	601	1KS	C23-C22-C17	-3.41	117.89	123.19
2	A	601	1KS	C14-C10-N1	3.00	117.72	111.78
2	A	601	1KS	C23-C22-N3	2.98	118.42	113.80
3	A	603	OLC	O20-C1-C2	2.84	120.82	111.91
3	B	602	OLC	O20-C1-C2	2.72	120.45	111.91
3	A	602	OLC	O20-C1-C2	2.56	119.95	111.91
3	A	604	OLC	O20-C1-C2	2.34	119.26	111.91
2	B	601	1KS	C14-C13-N2	2.34	115.93	111.10
2	B	601	1KS	C23-C22-C17	-2.32	119.58	123.19
2	B	601	1KS	C14-C10-N1	2.28	116.30	111.78
3	B	603	OLC	O20-C1-C2	2.23	118.92	111.91
2	B	601	1KS	C11-C12-N2	2.19	115.62	111.10
2	A	601	1KS	C7-C1-C2	-2.18	120.45	123.29
2	A	601	1KS	C11-C12-N2	2.16	115.55	111.10
2	A	601	1KS	C3-C2-C1	2.13	120.50	117.56
2	A	601	1KS	C15-N4-N3	2.09	122.67	118.65
2	B	601	1KS	C3-C2-C1	2.09	120.44	117.56
3	B	602	OLC	O20-C1-O19	-2.08	118.35	123.59
2	B	601	1KS	C23-N6-N5	2.03	113.51	111.96
2	B	601	1KS	C15-N4-N3	2.00	122.50	118.65

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	OLA	C1-C2-C3-C4
2	A	601	1KS	C16-C15-N2-C13
2	A	601	1KS	N3-C22-C23-C24
2	B	601	1KS	C16-C15-N2-C13
2	B	601	1KS	N3-C22-C23-C24
3	A	603	OLC	O19-C1-O20-C21
3	A	603	OLC	C2-C1-O20-C21
3	B	603	OLC	C2-C1-O20-C21
3	B	603	OLC	O19-C1-O20-C21

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Mol	Chain	Res	Type	Atoms
3	B	602	OLC	C2-C1-O20-C21
3	B	602	OLC	O19-C1-O20-C21
3	B	602	OLC	C1-C2-C3-C4
3	A	602	OLC	C1-C2-C3-C4
4	B	604	OLA	C4-C5-C6-C7
3	A	603	OLC	C2-C3-C4-C5
4	A	605	OLA	C5-C6-C7-C8
3	A	604	OLC	C2-C1-O20-C21
3	A	603	OLC	C3-C4-C5-C6
3	A	602	OLC	C4-C5-C6-C7
3	A	604	OLC	C1-C2-C3-C4
3	A	603	OLC	C1-C2-C3-C4
3	A	604	OLC	C2-C3-C4-C5
3	B	603	OLC	C21-C22-C24-O25
4	A	605	OLA	C12-C13-C14-C15
3	A	602	OLC	C2-C3-C4-C5
4	A	606	OLA	C5-C6-C7-C8
4	A	605	OLA	C2-C3-C4-C5
3	B	603	OLC	C2-C3-C4-C5
3	A	604	OLC	O19-C1-O20-C21
3	B	603	OLC	C3-C4-C5-C6
4	B	604	OLA	C13-C14-C15-C16
3	A	603	OLC	C4-C5-C6-C7
3	B	603	OLC	O23-C22-C24-O25
4	A	605	OLA	C10-C11-C12-C13
4	B	604	OLA	C15-C16-C17-C18
3	B	603	OLC	C4-C5-C6-C7
3	B	602	OLC	C3-C4-C5-C6
4	A	606	OLA	C2-C3-C4-C5
4	B	604	OLA	C2-C3-C4-C5
3	B	603	OLC	C1-C2-C3-C4
7	A	609	PG4	C1-C2-O2-C3
4	A	605	OLA	C3-C4-C5-C6
7	A	609	PG4	C4-C3-O2-C2
5	B	605	PEG	C1-C2-O2-C3
4	B	604	OLA	C14-C15-C16-C17
4	A	605	OLA	C4-C5-C6-C7
6	A	608	PGE	O3-C5-C6-O4
5	A	607	PEG	C4-C3-O2-C2
6	A	608	PGE	C1-C2-O2-C3
7	A	609	PG4	C5-C6-O4-C7
4	A	606	OLA	C10-C11-C12-C13

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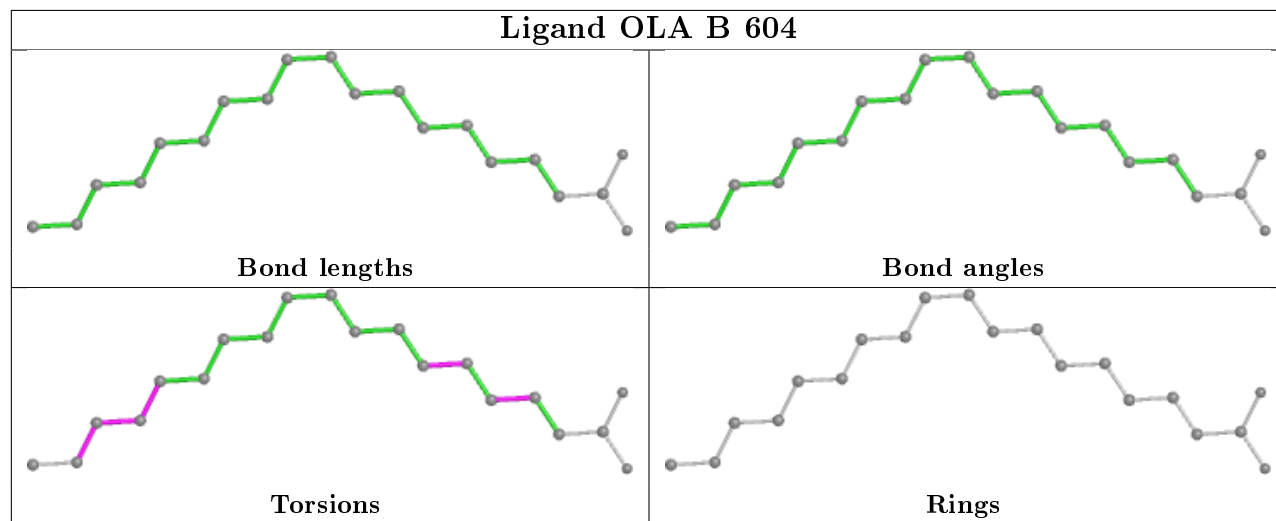
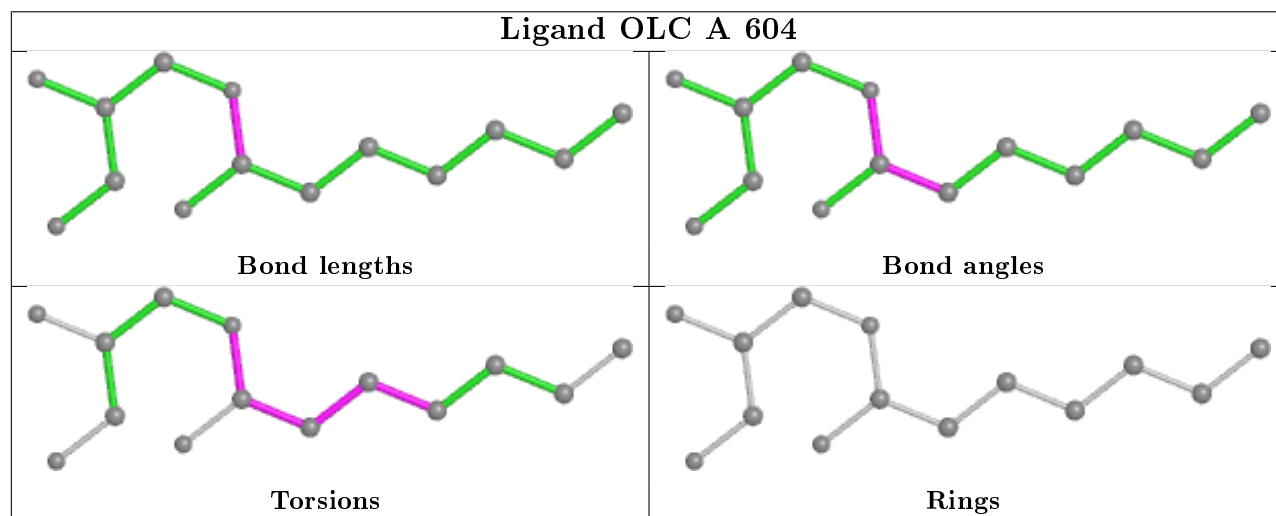
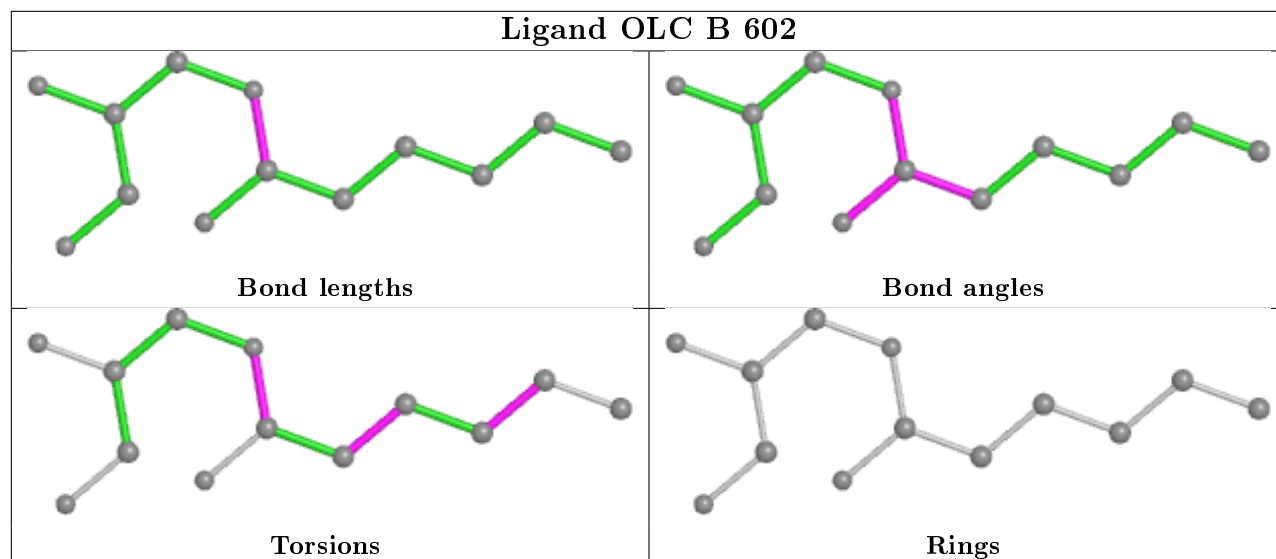
Mol	Chain	Res	Type	Atoms
5	B	605	PEG	C4-C3-O2-C2
6	A	608	PGE	C3-C4-O3-C5
3	A	603	OLC	O23-C22-C24-O25
4	A	605	OLA	C7-C8-C9-C10
4	A	605	OLA	C11-C12-C13-C14
3	A	603	OLC	C5-C6-C7-C8
3	B	603	OLC	O20-C1-C2-C3
3	A	604	OLC	O20-C1-C2-C3
3	B	603	OLC	O19-C1-C2-C3
3	A	604	OLC	O19-C1-C2-C3
7	A	609	PG4	O2-C3-C4-O3
3	A	602	OLC	O20-C1-C2-C3

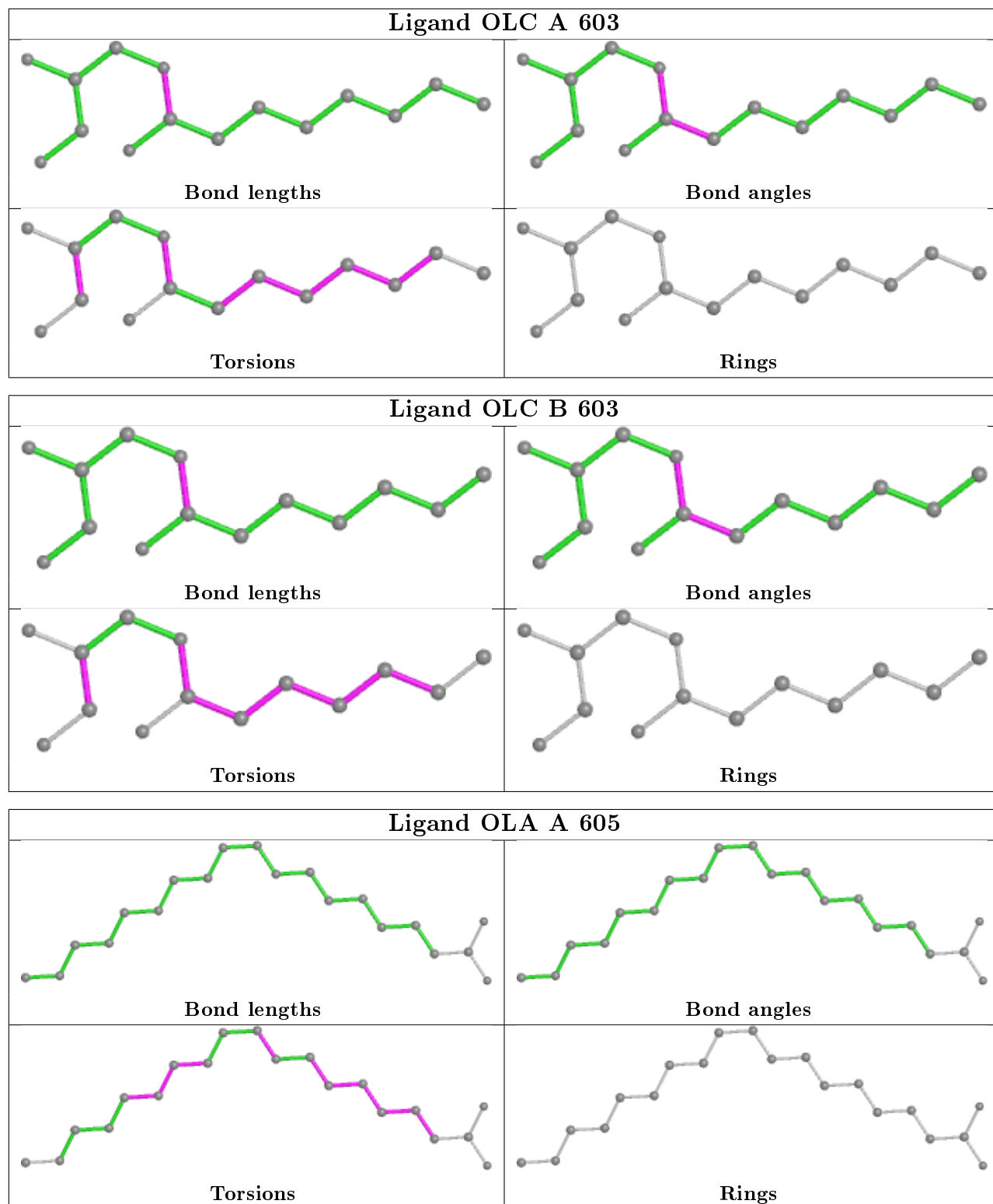
There are no ring outliers.

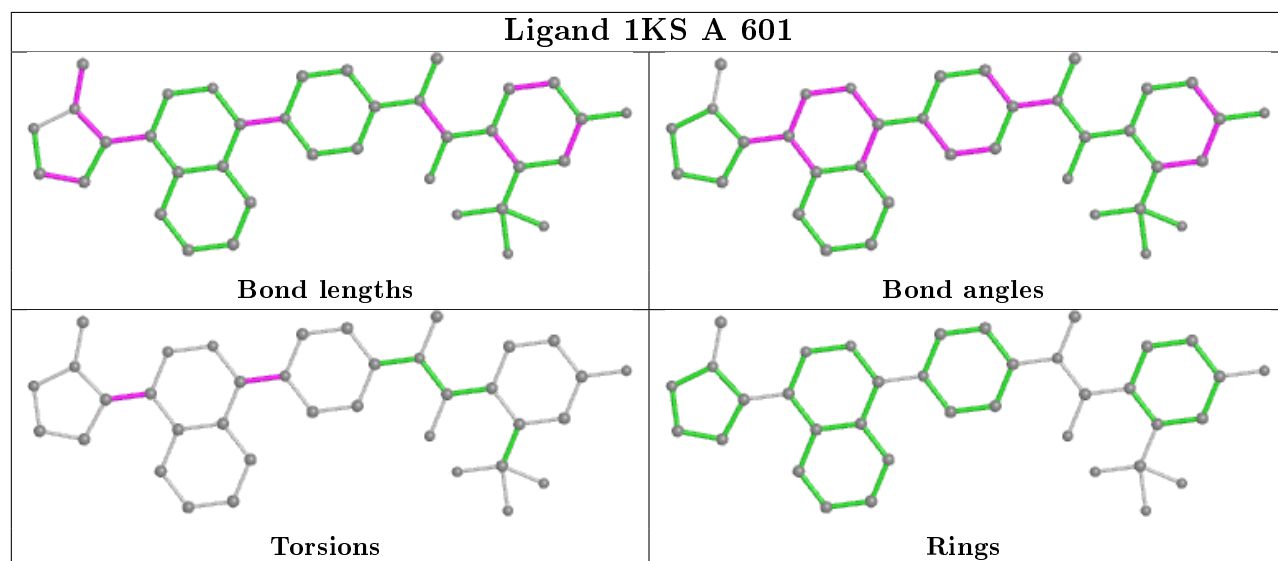
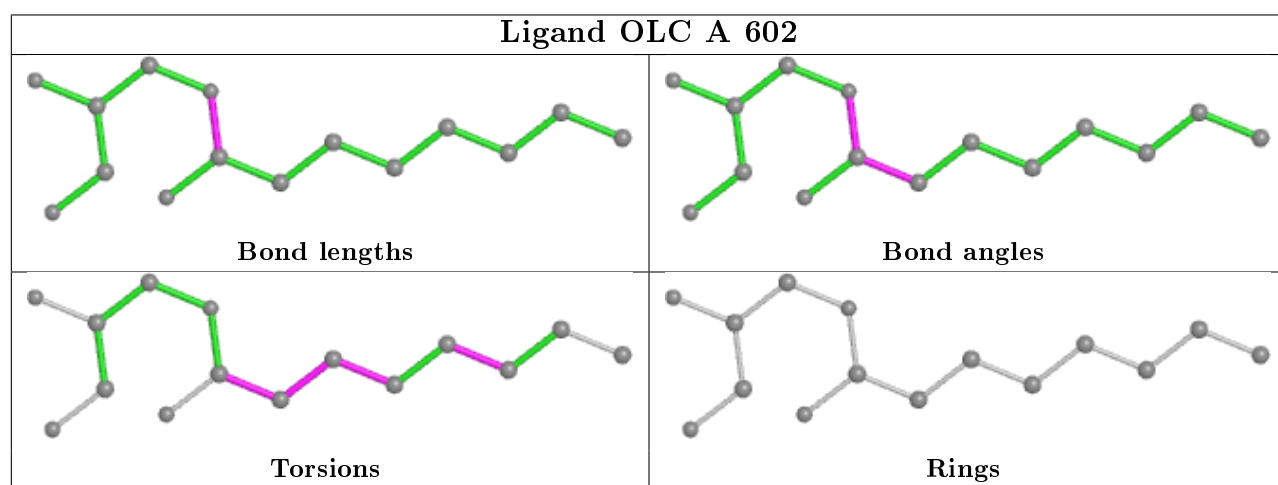
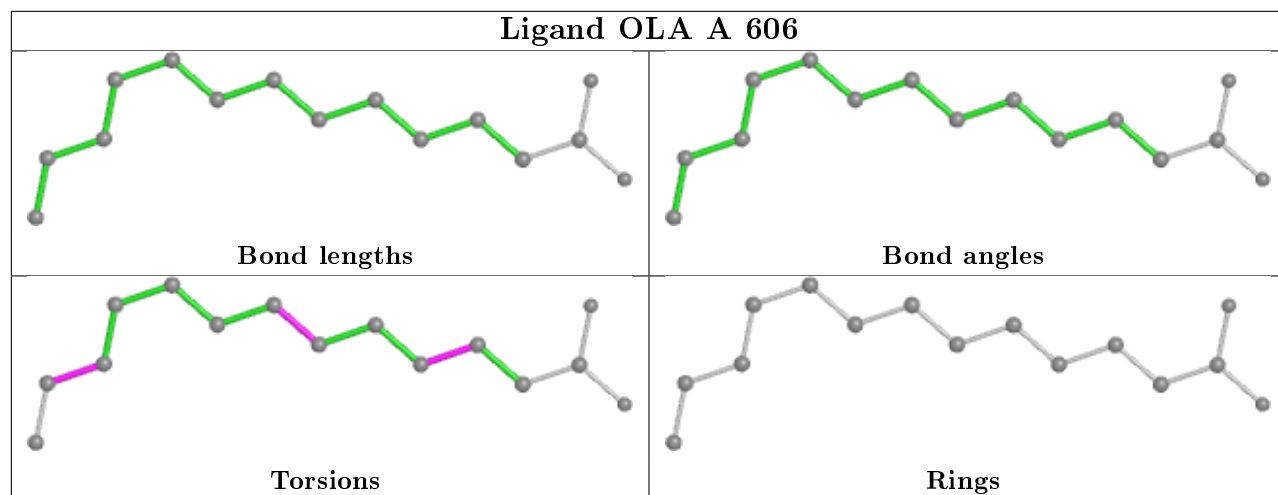
6 monomers are involved in 8 short contacts:

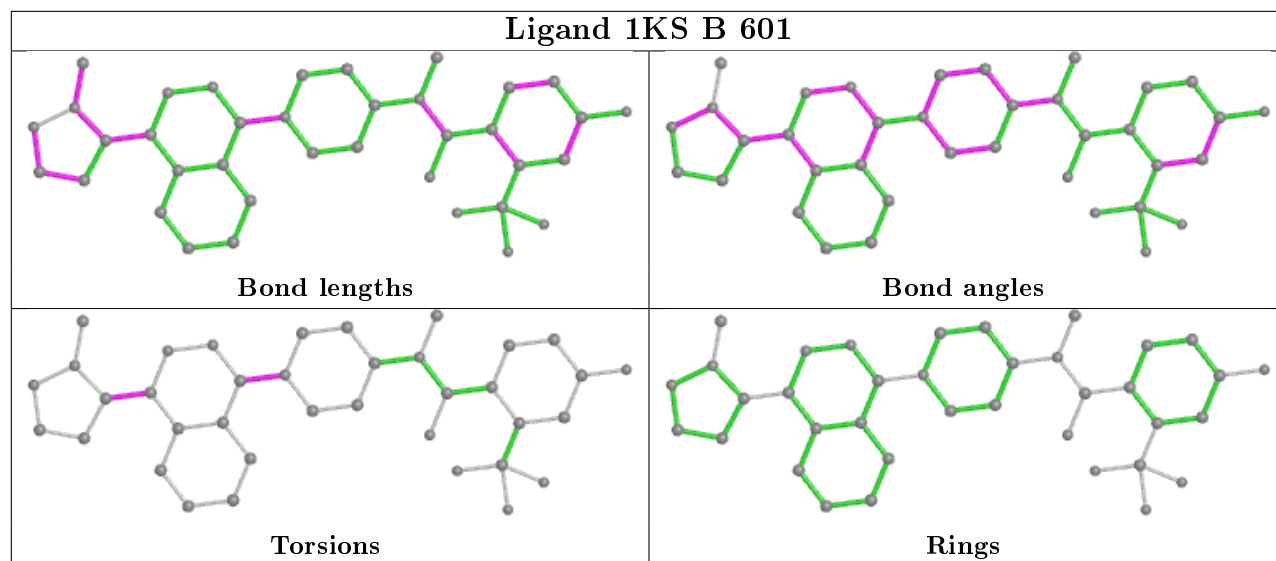
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	OLC	1	0
3	B	603	OLC	1	0
5	B	605	PEG	1	0
7	A	609	PG4	2	0
2	A	601	1KS	1	0
2	B	601	1KS	2	0

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 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	454/475 (95%)	0.62	45 (9%) 7 5	42, 66, 134, 165	0
1	B	450/475 (94%)	0.41	34 (7%) 13 10	42, 66, 127, 220	0
All	All	904/950 (95%)	0.51	79 (8%) 10 7	42, 66, 131, 220	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	435	GLY	12.4
1	A	21	ASP	9.2
1	A	82	GLY	9.1
1	A	80	ASN	8.7
1	A	78	LEU	8.2
1	B	345	ALA	7.6
1	B	438	SER	7.3
1	B	436	LEU	6.0
1	B	493	ASN	5.8
1	A	83	LYS	5.7
1	A	75	ALA	5.2
1	A	79	ALA	5.0
1	B	437	LEU	4.9
1	A	507	CYS	4.9
1	A	76	LEU	4.8
1	A	2	ASP	4.8
1	B	441	ALA	4.6
1	A	0	THR	4.6
1	B	446	ASN	4.6
1	A	1	ALA	4.5
1	B	262	TYR	4.3
1	A	4	GLU	4.2
1	A	190	SER	4.2
1	A	77	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	81	GLU	4.1
1	B	343	PHE	3.9
1	B	442	ALA	3.9
1	B	552	LEU	3.9
1	A	20	ALA	3.8
1	A	-1	GLY	3.8
1	B	440	LYS	3.7
1	B	543	LEU	3.6
1	B	355	GLY	3.5
1	A	26	VAL	3.4
1	B	549	TRP	3.2
1	A	19	LYS	3.2
1	B	2	ASP	3.1
1	B	429	ILE	3.1
1	A	8	GLU	3.0
1	A	22	ASN	3.0
1	B	257	ARG	3.0
1	B	439	GLU	2.9
1	A	31	THR	2.9
1	A	90	ALA	2.9
1	B	359	TYR	2.8
1	A	73	ASP	2.8
1	A	359	TYR	2.8
1	A	50	ASP	2.7
1	A	488	VAL	2.7
1	A	489	LEU	2.7
1	A	94	LEU	2.6
1	A	29	ALA	2.6
1	A	33	MET	2.6
1	A	197	LEU	2.4
1	A	379	ALA	2.4
1	B	508	GLU	2.4
1	A	490	CYS	2.4
1	A	355	GLY	2.4
1	A	287	ASP	2.3
1	A	491	GLN	2.3
1	A	86	GLU	2.3
1	A	74	ASP	2.3
1	A	27	LYS	2.3
1	A	378	VAL	2.3
1	B	356	LYS	2.2
1	B	344	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	256	TRP	2.2
1	B	374	ALA	2.2
1	A	30	LEU	2.2
1	B	371	LEU	2.2
1	B	506	ASP	2.1
1	B	492	ALA	2.1
1	B	375	ILE	2.0
1	B	523	PHE	2.0
1	B	370	VAL	2.0
1	B	447	GLU	2.0
1	A	371	LEU	2.0
1	B	366	SER	2.0
1	A	508	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 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.

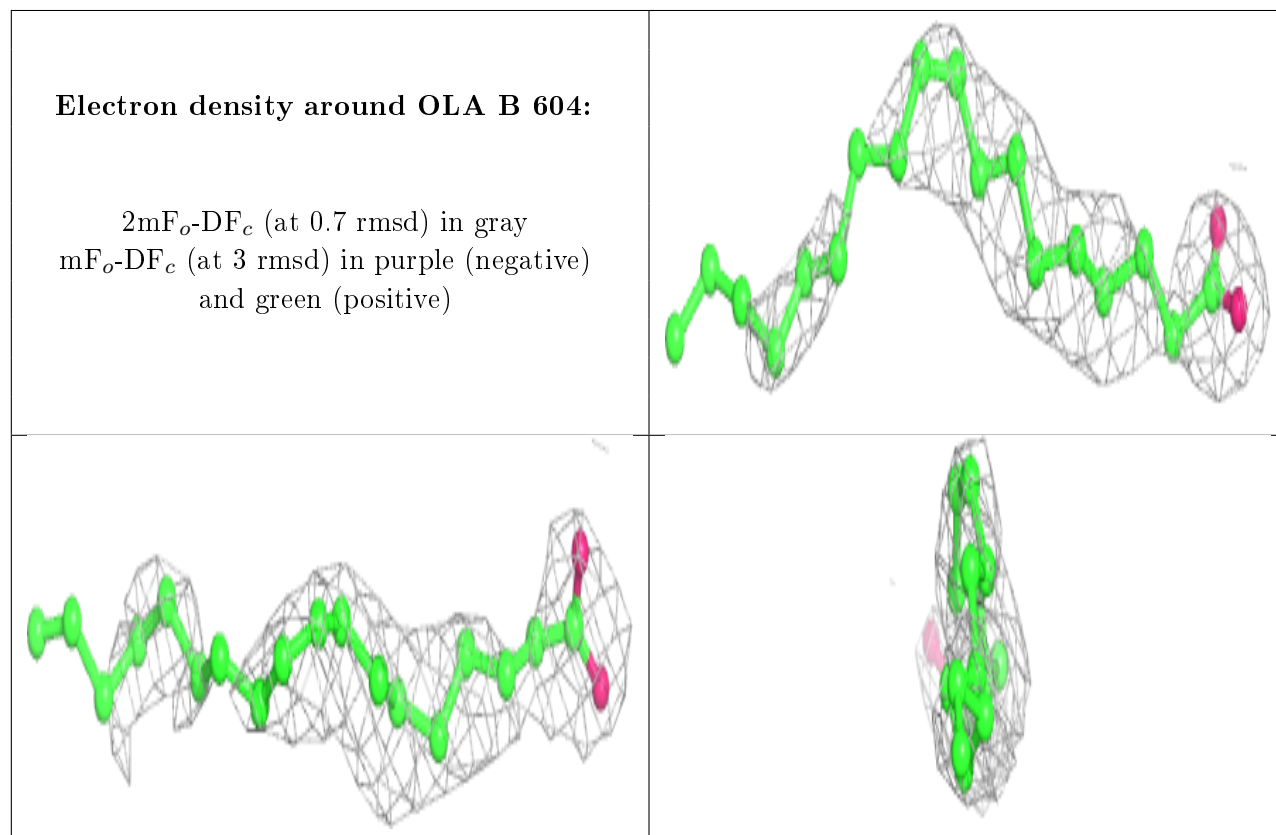
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	OLA	B	604	20/20	0.62	0.39	98,101,110,110	0
5	PEG	B	605	7/7	0.62	0.31	100,101,103,103	0
3	OLC	A	603	15/25	0.71	0.34	82,92,99,99	0
7	PG4	A	609	13/13	0.72	0.22	90,99,102,103	0
3	OLC	B	603	14/25	0.75	0.22	75,83,88,88	0
3	OLC	B	602	13/25	0.77	0.32	89,94,98,99	0
5	PEG	A	607	7/7	0.78	0.23	88,89,90,90	0
3	OLC	A	604	14/25	0.80	0.32	87,92,93,94	0
3	OLC	A	602	15/25	0.85	0.29	86,98,105,106	0
4	OLA	A	606	15/20	0.86	0.20	86,93,105,105	0

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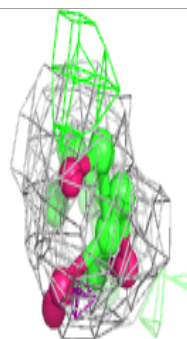
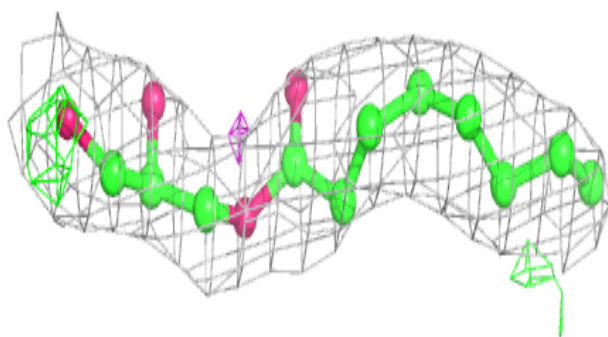
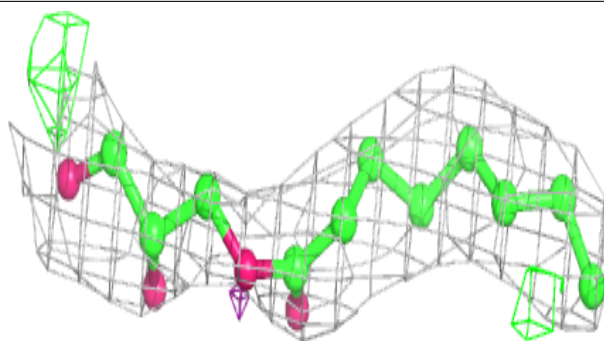
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PGE	A	608	10/10	0.90	0.27	58,62,70,71	0
4	OLA	A	605	20/20	0.92	0.43	79,81,94,96	0
2	1KS	A	601	37/37	0.94	0.18	57,60,71,72	0
2	1KS	B	601	37/37	0.96	0.19	53,56,61,67	0

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.

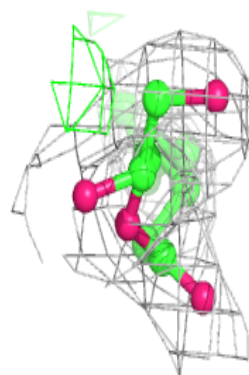
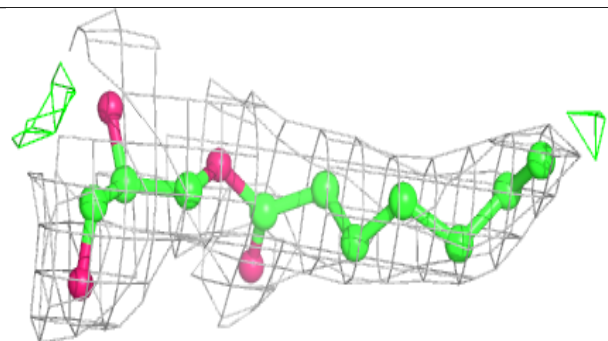
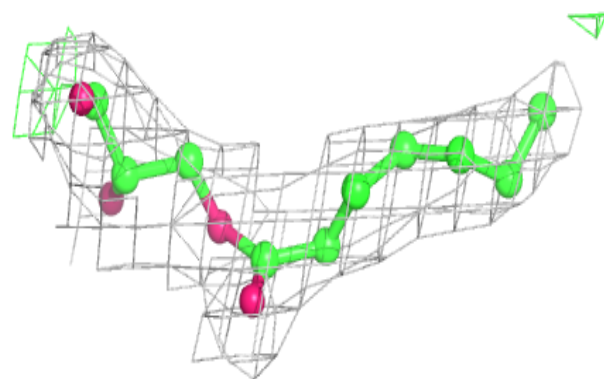


Electron density around OLC A 603:

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

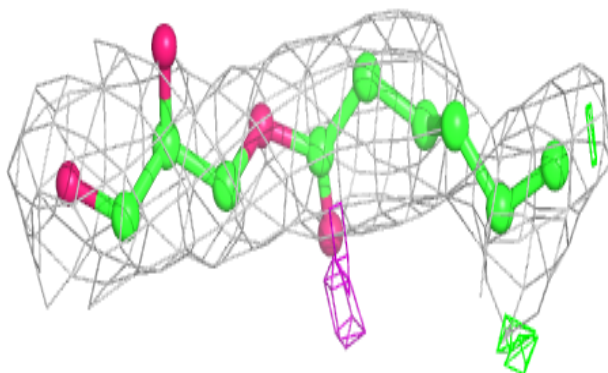
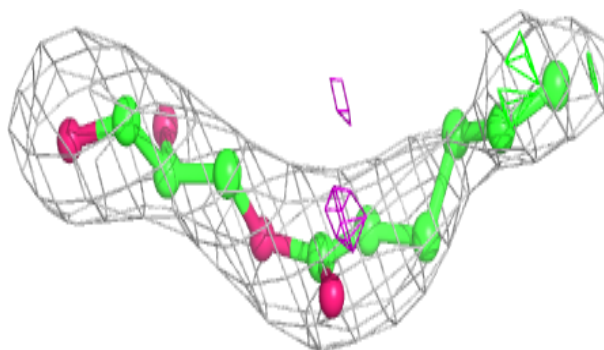
**Electron density around OLC B 603:**

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

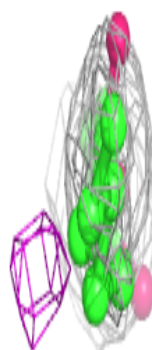
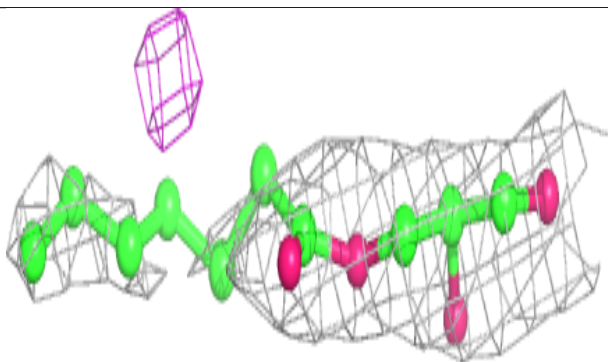
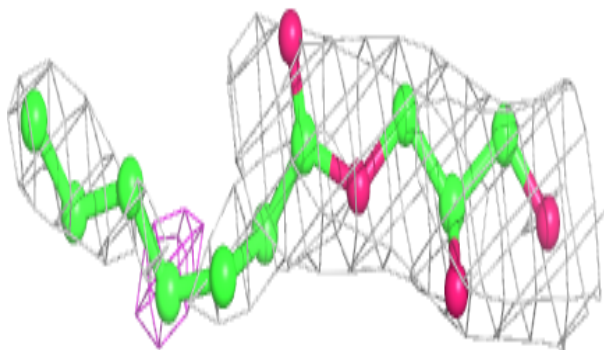


Electron density around OLC B 602:

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

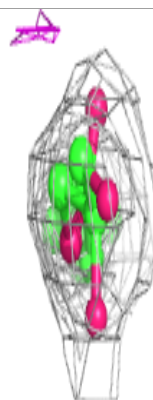
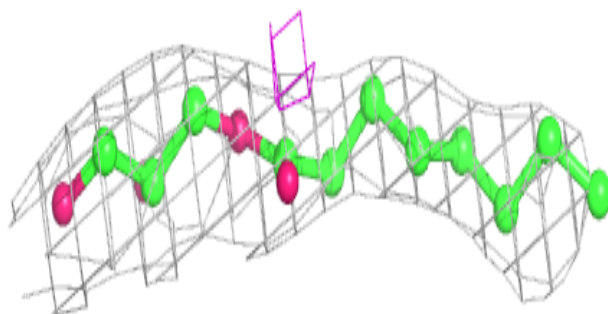
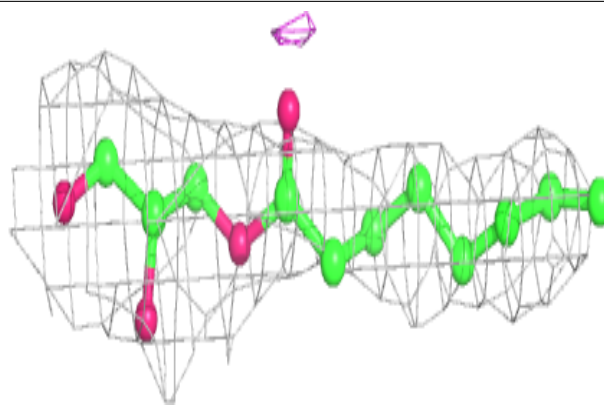
**Electron density around OLC A 604:**

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

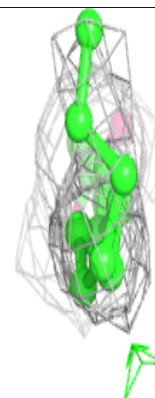
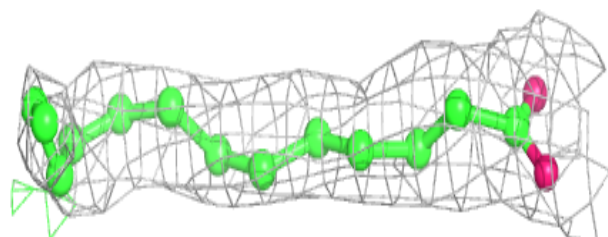
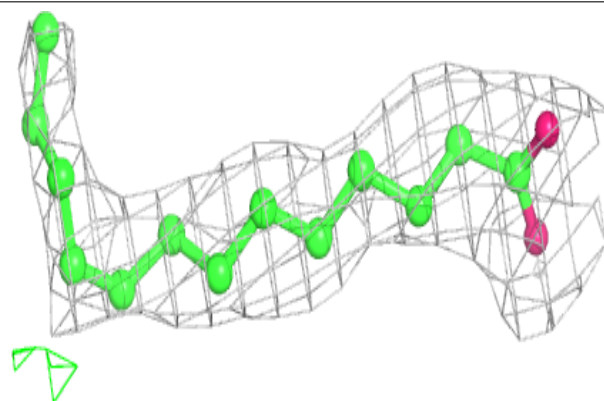


Electron density around OLC A 602:

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

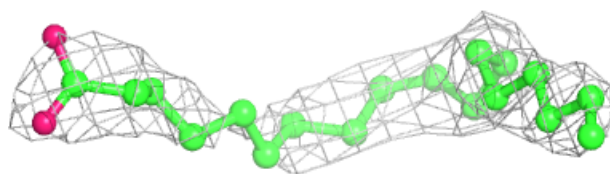
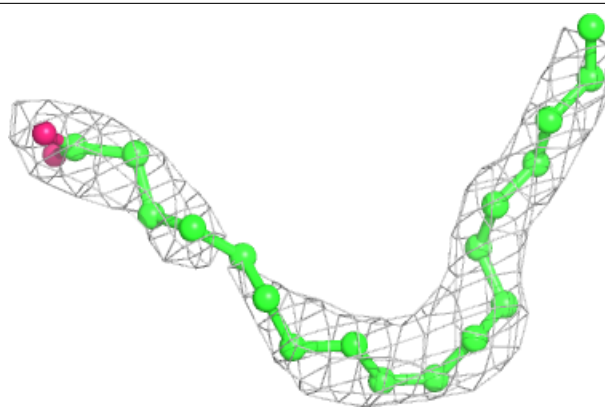
**Electron density around OLA A 606:**

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

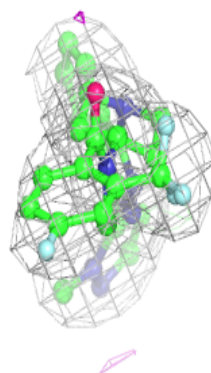
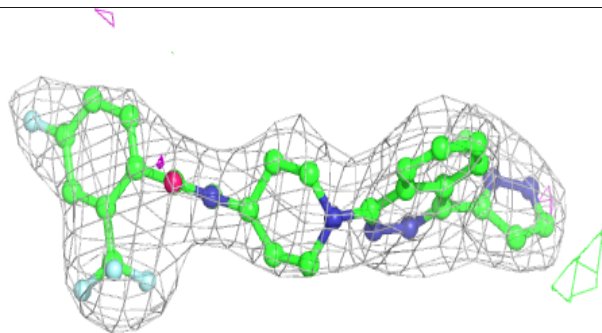
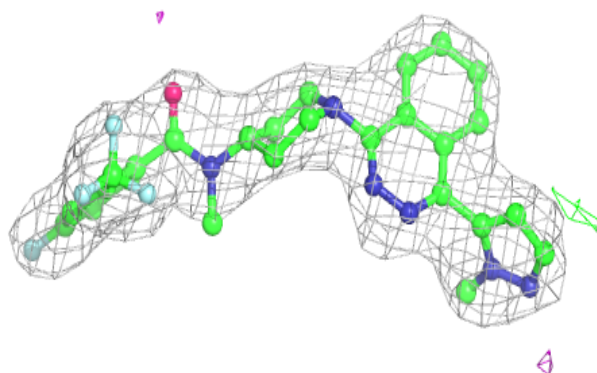


Electron density around OLA A 605:

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

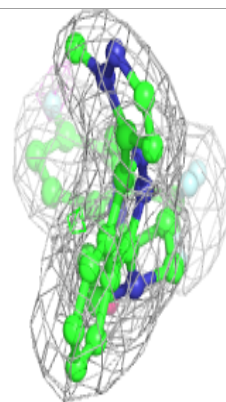
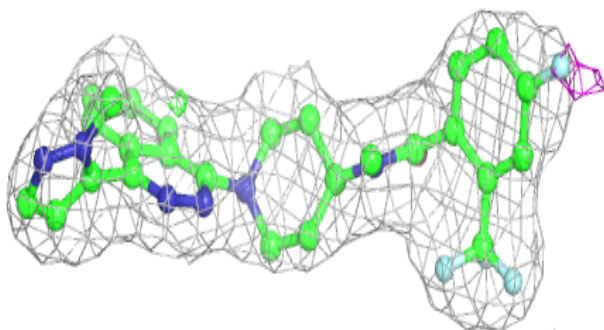
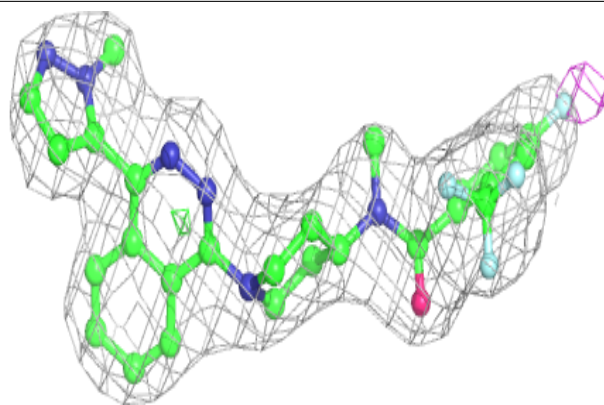
**Electron density around 1KS A 601:**

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



Electron density around 1KS B 601:

$2mF_o-DF_c$ (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.