



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:24 PM UTC

PDB ID : 8AGM / pdb_00008agm
Title : Limonene epoxide low pH soak of epoxide hydrolase from metagenomic source ch65
Authors : Isupov, M.N.; De Rose, S.A.; Mitchell, D.; Littlechild, J.A.
Deposited on : 2022-07-20
Resolution : 1.97 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

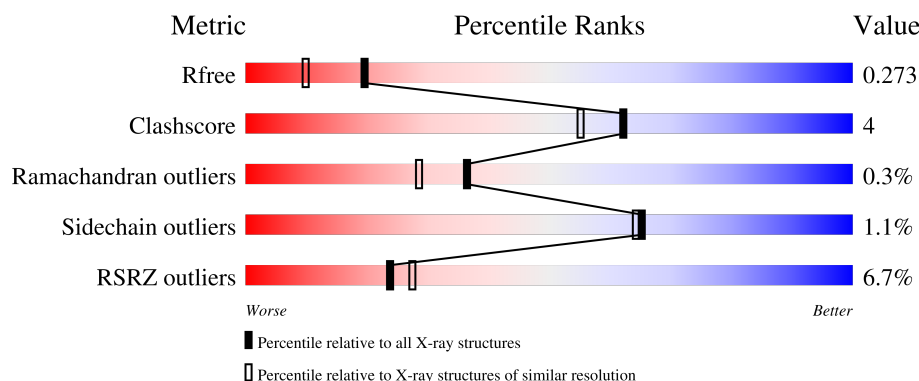
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	AAA	299	8% 86% 9% ..
1	BBB	299	% 89% 7% .
1	CCC	299	7% 85% 11% ..
1	DDD	299	9% 88% 9% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LEO	CCC	301[B]	-	-	X	-
2	LEO	DDD	301[B]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10237 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 Alpha/beta epoxide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	287	Total	C	N	O	S	0	12	0
			2442	1611	405	419	7			
1	BBB	289	Total	C	N	O	S	0	12	0
			2454	1622	404	421	7			
1	CCC	290	Total	C	N	O	S	0	16	0
			2495	1648	412	428	7			
1	DDD	293	Total	C	N	O	S	0	15	0
			2515	1656	420	431	8			

There are 24 discrepancies between the modelled and reference sequences:

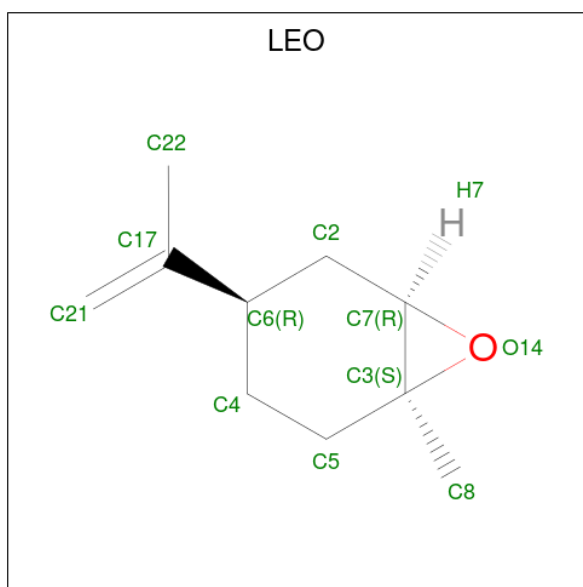
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	294	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	295	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	296	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	297	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	298	HIS	-	expression tag	UNP A0A1U9WZ52
AAA	299	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	294	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	295	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	296	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	297	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	298	HIS	-	expression tag	UNP A0A1U9WZ52
BBB	299	HIS	-	expression tag	UNP A0A1U9WZ52
CCC	294	HIS	-	expression tag	UNP A0A1U9WZ52
CCC	295	HIS	-	expression tag	UNP A0A1U9WZ52
CCC	296	HIS	-	expression tag	UNP A0A1U9WZ52
CCC	297	HIS	-	expression tag	UNP A0A1U9WZ52
CCC	298	HIS	-	expression tag	UNP A0A1U9WZ52
CCC	299	HIS	-	expression tag	UNP A0A1U9WZ52
DDD	294	HIS	-	expression tag	UNP A0A1U9WZ52
DDD	295	HIS	-	expression tag	UNP A0A1U9WZ52
DDD	296	HIS	-	expression tag	UNP A0A1U9WZ52

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	297	HIS	-	expression tag	UNP A0A1U9WZ52
DDD	298	HIS	-	expression tag	UNP A0A1U9WZ52
DDD	299	HIS	-	expression tag	UNP A0A1U9WZ52

- Molecule 2 is D-LIMONENE 1,2-EPOXIDE (CCD ID: LEO) (formula: $C_{10}H_{16}O$) (labeled as "Ligand of Interest" by depositor).

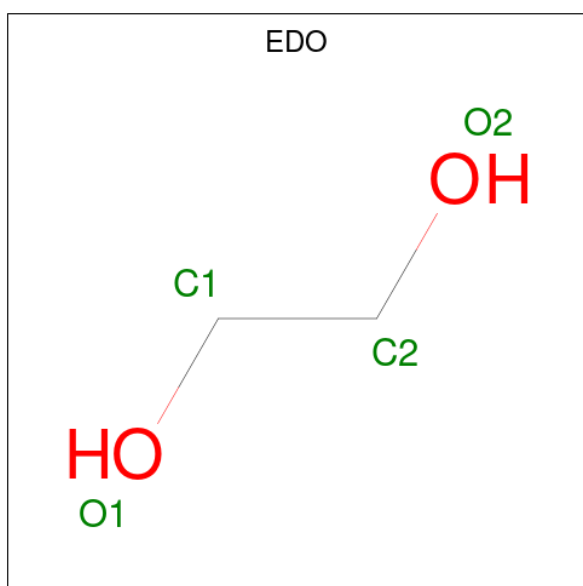


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	1
			11	10	1		
2	AAA	1	Total	C	O	0	0
			11	10	1		
2	BBB	1	Total	C	O	0	1
			11	10	1		
2	BBB	1	Total	C	O	0	0
			11	10	1		
2	CCC	1	Total	C	O	0	1
			11	10	1		
2	CCC	1	Total	C	O	0	0
			11	10	1		
2	DDD	1	Total	C	O	0	1
			11	10	1		
2	DDD	1	Total	C	O	0	0
			11	10	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	2	Total Cl 2 2	0	0
3	BBB	2	Total Cl 2 2	0	0
3	CCC	2	Total Cl 2 2	0	0
3	DDD	2	Total Cl 2 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total C O 4 2 2	0	0

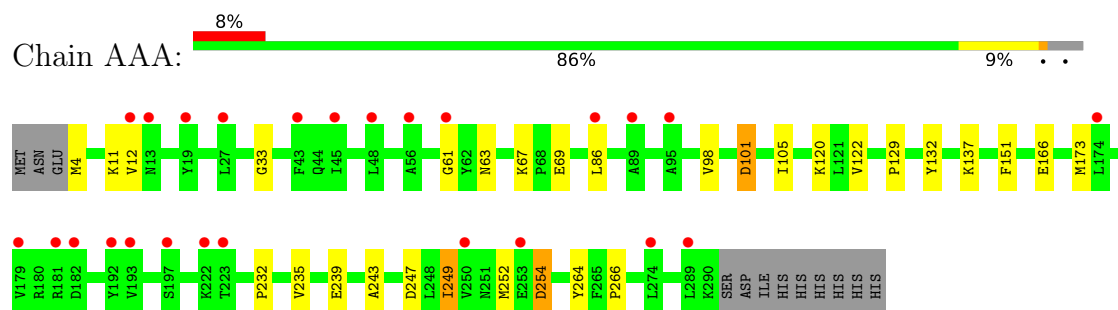
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	40	Total O 40 40	0	0
5	BBB	80	Total O 80 80	0	0
5	CCC	52	Total O 52 52	0	0
5	DDD	59	Total O 59 59	0	0

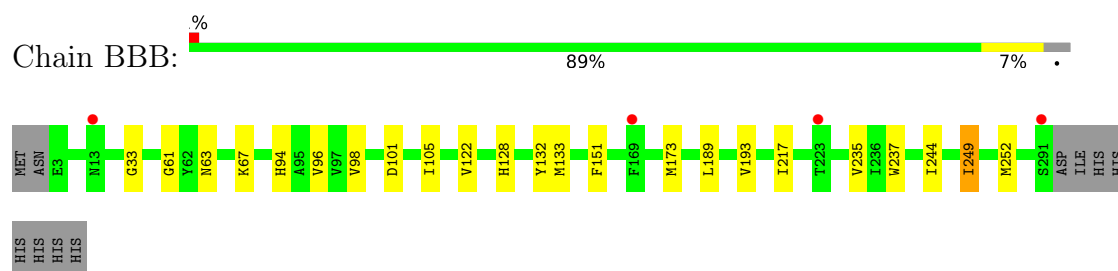
3 Residue-property plots [i](#)

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.

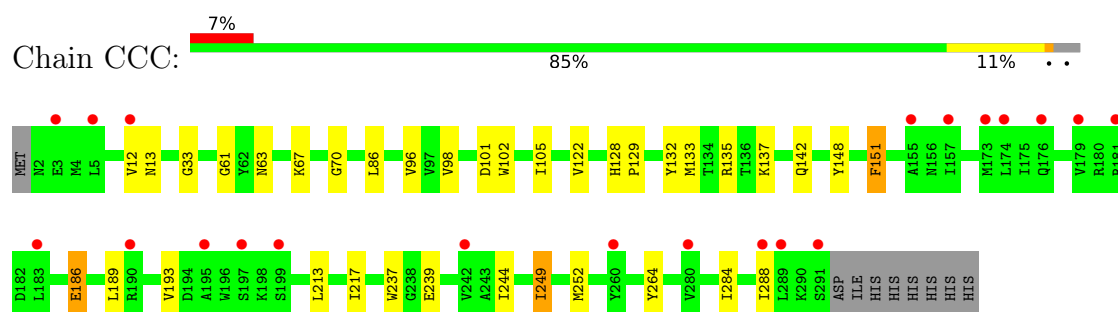
- Molecule 1: Alpha/beta epoxide hydrolase



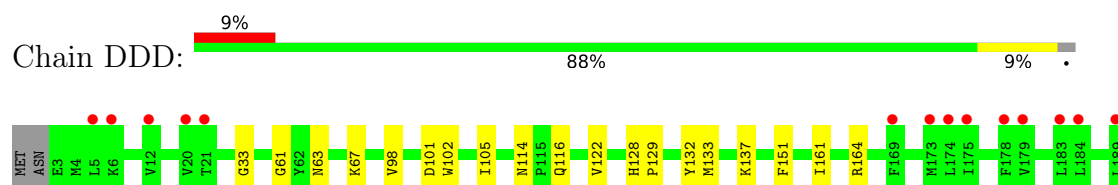
- Molecule 1: Alpha/beta epoxide hydrolase

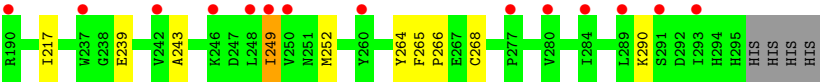


- Molecule 1: Alpha/beta epoxide hydrolase



- Molecule 1: Alpha/beta epoxide hydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.98Å 47.42Å 142.81Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	96.13 – 1.97 96.13 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.6 (96.13-1.97) 99.6 (96.13-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0267, BUSTER	Depositor
R, R_{free}	0.232 , 0.270 0.235 , 0.273	Depositor DCC
R_{free} test set	4467 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.808	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10237	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: EDO, CL, LEO

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	AAA	0.77	0/2539	1.20	4/3439 (0.1%)
1	BBB	0.80	0/2553	1.16	2/3462 (0.1%)
1	CCC	0.76	0/2612	1.18	5/3537 (0.1%)
1	DDD	0.79	0/2630	1.18	1/3560 (0.0%)
All	All	0.78	0/10334	1.18	12/13998 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	151	PHE	CA-CB-CG	5.73	119.53	113.80
1	BBB	151	PHE	CA-CB-CG	5.56	119.36	113.80
1	AAA	151	PHE	CA-CB-CG	5.52	119.32	113.80
1	DDD	151	PHE	CA-CB-CG	5.48	119.28	113.80
1	AAA	247	ASP	CA-CB-CG	5.40	118.00	112.60
1	BBB	96	VAL	N-CA-C	-5.40	101.77	108.89
1	CCC	13	ASN	CA-CB-CG	5.33	117.93	112.60
1	CCC	70	GLY	CA-C-N	5.22	127.62	120.46
1	CCC	70	GLY	C-N-CA	5.22	127.62	120.46
1	AAA	254	ASP	CA-CB-CG	5.14	117.74	112.60
1	AAA	101	ASP	CA-CB-CG	5.05	117.65	112.60
1	CCC	135	ARG	N-CA-C	5.02	117.86	111.69

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	AAA	2442	0	2504	17	0
1	BBB	2454	0	2512	13	0
1	CCC	2495	0	2567	28	0
1	DDD	2515	0	2577	23	0
2	AAA	22	0	30	6	0
2	BBB	22	0	30	4	0
2	CCC	22	0	30	10	0
2	DDD	22	0	30	10	0
3	AAA	2	0	0	0	0
3	BBB	2	0	0	0	0
3	CCC	2	0	0	0	0
3	DDD	2	0	0	0	0
4	BBB	4	0	6	0	0
5	AAA	40	0	0	1	0
5	BBB	80	0	0	0	0
5	CCC	52	0	0	1	0
5	DDD	59	0	0	3	0
All	All	10237	0	10286	83	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 (83) 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:DDD:105:ILE:CD1	2:DDD:301[B]:LEO:H51	1.90	1.00
1:DDD:137:LYS:HE3	5:DDD:422:HOH:O	1.76	0.85
1:CCC:105:ILE:HD11	2:CCC:301[B]:LEO:H51	1.60	0.83
1:CCC:105:ILE:CD1	2:CCC:301[B]:LEO:H51	2.09	0.82
1:DDD:105:ILE:HD11	2:DDD:301[B]:LEO:H51	1.61	0.82
2:DDD:301[B]:LEO:H222	5:DDD:418:HOH:O	1.80	0.81
1:CCC:133[B]:MET:SD	1:CCC:217:ILE:HG22	2.28	0.73
1:BBB:133[B]:MET:SD	1:BBB:217:ILE:HG22	2.32	0.69
1:DDD:133[B]:MET:SD	1:DDD:217:ILE:HG22	2.33	0.69
1:CCC:102:TRP:CE2	2:CCC:301[B]:LEO:H82	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:128:HIS:HB2	1:CCC:252:MET:HE1	1.77	0.66
1:BBB:128:HIS:HB2	1:BBB:252:MET:HE1	1.77	0.66
1:AAA:101:ASP:CG	2:AAA:301[A]:LEO:H81	2.24	0.63
1:CCC:137:LYS:HE3	5:CCC:431:HOH:O	2.00	0.61
1:BBB:244:ILE:HG12	2:BBB:302[A]:LEO:H211	1.82	0.60
1:DDD:114:ASN:HD22	1:DDD:116:GLN:HE22	1.49	0.60
1:BBB:61:GLY:HA2	1:BBB:67:LYS:HG2	1.84	0.59
1:DDD:105:ILE:HD12	2:DDD:301[B]:LEO:H51	1.78	0.59
1:CCC:129:PRO:HA	1:CCC:132[B]:TYR:CE2	2.38	0.59
1:DDD:101:ASP:CG	2:DDD:301[B]:LEO:H81	2.28	0.59
1:AAA:61:GLY:HA2	1:AAA:67:LYS:HG2	1.85	0.58
1:AAA:249:ILE:HD11	1:AAA:264:TYR:CE1	2.40	0.57
1:DDD:249:ILE:HD11	1:DDD:264:TYR:CE1	2.40	0.57
1:CCC:61:GLY:HA2	1:CCC:67:LYS:HG2	1.87	0.56
1:DDD:61:GLY:HA2	1:DDD:67:LYS:HG2	1.86	0.56
1:DDD:105:ILE:HD11	2:DDD:301[B]:LEO:C5	2.35	0.56
1:CCC:249[A]:ILE:HD11	1:CCC:264:TYR:CE1	2.41	0.56
1:DDD:249:ILE:HD11	1:DDD:264:TYR:HE1	1.72	0.55
1:AAA:249:ILE:HD11	1:AAA:264:TYR:HE1	1.70	0.55
1:BBB:132[B]:TYR:HD1	1:BBB:133[B]:MET:HE2	1.73	0.53
1:AAA:105:ILE:CD1	2:AAA:301[A]:LEO:H51	2.39	0.53
1:AAA:129:PRO:HA	1:AAA:132[A]:TYR:CE2	2.44	0.53
1:BBB:189:LEU:O	1:BBB:193:VAL:HG23	2.09	0.52
1:CCC:213:LEU:HD11	2:CCC:301[B]:LEO:H52	1.92	0.52
1:AAA:101:ASP:OD1	2:AAA:301[A]:LEO:H81	2.10	0.51
1:CCC:142:GLN:HE22	2:CCC:301[B]:LEO:H212	1.77	0.50
1:CCC:102:TRP:CE2	2:CCC:301[B]:LEO:C8	2.92	0.50
1:AAA:33:GLY:HA3	1:AAA:101:ASP:HB3	1.94	0.49
1:DDD:129:PRO:HA	1:DDD:132[B]:TYR:CE2	2.48	0.49
1:CCC:33:GLY:HA3	1:CCC:101:ASP:HB3	1.96	0.48
1:DDD:128:HIS:HB2	1:DDD:252[A]:MET:HE1	1.94	0.48
1:AAA:137:LYS:HE3	5:AAA:413:HOH:O	2.14	0.47
1:BBB:173:MET:HB3	2:BBB:303:LEO:H41	1.95	0.47
1:DDD:33:GLY:HA3	1:DDD:101:ASP:HB3	1.95	0.47
1:CCC:237[B]:TRP:CZ3	1:CCC:239:GLU:HA	2.50	0.47
1:BBB:101:ASP:CG	2:BBB:302[A]:LEO:H81	2.39	0.47
1:BBB:33:GLY:HA3	1:BBB:101:ASP:HB3	1.96	0.47
1:DDD:102:TRP:CD1	2:DDD:301[B]:LEO:H82	2.50	0.46
1:AAA:12:VAL:HG11	1:AAA:86:LEU:HA	1.98	0.46
1:CCC:12:VAL:HG11	1:CCC:86:LEU:HA	1.96	0.46
1:CCC:122:VAL:HG11	1:CCC:284:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:96:VAL:HG11	1:CCC:288:ILE:HG12	1.98	0.46
1:CCC:102:TRP:NE1	2:CCC:301[B]:LEO:H82	2.29	0.45
2:DDD:302:LEO:H82	5:DDD:423:HOH:O	2.17	0.45
1:CCC:186[A]:GLU:CD	1:CCC:186[A]:GLU:H	2.24	0.45
1:CCC:244:ILE:HG12	2:CCC:301[B]:LEO:C21	2.47	0.45
1:CCC:105:ILE:HD11	2:CCC:301[B]:LEO:C5	2.42	0.45
1:CCC:133[B]:MET:SD	1:CCC:217:ILE:CG2	3.03	0.44
1:BBB:105:ILE:CD1	2:BBB:302[A]:LEO:H51	2.47	0.44
1:DDD:101:ASP:OD1	2:DDD:301[B]:LEO:H81	2.18	0.43
1:BBB:235:VAL:HG11	1:BBB:249[B]:ILE:HD11	1.99	0.43
1:DDD:265:PHE:HB3	1:DDD:268:CYS:HB2	1.99	0.43
1:CCC:142:GLN:NE2	2:CCC:301[B]:LEO:H212	2.33	0.43
1:AAA:243:ALA:HB2	2:AAA:302:LEO:H82	2.01	0.43
1:BBB:98:VAL:HG22	1:BBB:122:VAL:HB	2.01	0.43
1:DDD:161:ILE:HA	1:DDD:164[B]:ARG:HD2	2.00	0.42
1:CCC:148:TYR:HA	1:CCC:151:PHE:HB3	2.01	0.42
1:AAA:235:VAL:HG11	1:AAA:252[A]:MET:HE1	2.00	0.42
1:AAA:120:LYS:HG2	1:AAA:232:PRO:HB2	2.00	0.42
1:DDD:98:VAL:HG22	1:DDD:122:VAL:HB	2.01	0.42
1:CCC:98:VAL:HG22	1:CCC:122:VAL:HB	2.03	0.41
1:DDD:105:ILE:HG23	1:DDD:129:PRO:HG3	2.03	0.41
1:AAA:173:MET:HB3	2:AAA:302:LEO:H41	2.03	0.41
1:AAA:98:VAL:HG22	1:AAA:122:VAL:HB	2.03	0.41
1:BBB:237[B]:TRP:HZ2	1:BBB:244:ILE:HG21	1.86	0.41
1:CCC:189:LEU:O	1:CCC:193:VAL:HG23	2.20	0.41
1:CCC:249[A]:ILE:HD11	1:CCC:264:TYR:HE1	1.85	0.41
1:AAA:243:ALA:HB2	2:AAA:302:LEO:C8	2.51	0.40
1:CCC:132[B]:TYR:HD1	1:CCC:133[B]:MET:HE2	1.86	0.40
1:DDD:239:GLU:HB2	1:DDD:266:PRO:HA	2.04	0.40
1:AAA:239:GLU:HB2	1:AAA:266:PRO:HA	2.04	0.40
1:DDD:243:ALA:HB2	2:DDD:302:LEO:H83	2.02	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	AAA	297/299 (99%)	284 (96%)	12 (4%)	1 (0%)	36	28
1	BBB	299/299 (100%)	291 (97%)	7 (2%)	1 (0%)	36	28
1	CCC	304/299 (102%)	292 (96%)	11 (4%)	1 (0%)	36	28
1	DDD	306/299 (102%)	296 (97%)	9 (3%)	1 (0%)	36	28
All	All	1206/1196 (101%)	1163 (96%)	39 (3%)	4 (0%)	36	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	63	ASN
1	BBB	63	ASN
1	CCC	63	ASN
1	DDD	63	ASN

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	AAA	266/267 (100%)	260 (98%)	6 (2%)	44	38
1	BBB	268/267 (100%)	265 (99%)	3 (1%)	65	64
1	CCC	274/267 (103%)	270 (98%)	4 (2%)	57	54
1	DDD	276/267 (103%)	275 (100%)	1 (0%)	84	85
All	All	1084/1068 (102%)	1070 (99%)	14 (1%)	65	58

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	4	MET
1	AAA	11	LYS
1	AAA	69	GLU
1	AAA	166	GLU

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Mol	Chain	Res	Type
1	AAA	249	ILE
1	AAA	254	ASP
1	BBB	94	HIS
1	BBB	249[A]	ILE
1	BBB	249[B]	ILE
1	CCC	186[A]	GLU
1	CCC	186[B]	GLU
1	CCC	249[A]	ILE
1	CCC	249[B]	ILE
1	DDD	249	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	LEO	AAA	301[A]	-	12,12,12	0.74	0	19,19,19	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	BBB	301	-	3,3,3	0.56	0	2,2,2	0.25	0
2	LEO	AAA	302	-	12,12,12	0.66	0	19,19,19	0.46	0
2	LEO	CCC	302	-	12,12,12	0.66	0	19,19,19	0.62	0
2	LEO	DDD	302	-	12,12,12	0.63	0	19,19,19	0.67	0
2	LEO	CCC	301[B]	-	12,12,12	0.82	0	19,19,19	0.89	0
2	LEO	DDD	301[B]	-	12,12,12	0.76	0	19,19,19	0.85	0
2	LEO	BBB	302[A]	-	12,12,12	0.66	0	19,19,19	0.58	0
2	LEO	BBB	303	-	12,12,12	0.65	0	19,19,19	0.47	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
2	LEO	AAA	301[A]	-	-	4/4/22/22	0/2/2/2
4	EDO	BBB	301	-	-	0/1/1/1	-
2	LEO	AAA	302	-	-	0/4/22/22	0/2/2/2
2	LEO	CCC	302	-	-	4/4/22/22	0/2/2/2
2	LEO	DDD	302	-	-	0/4/22/22	0/2/2/2
2	LEO	CCC	301[B]	-	-	0/4/22/22	0/2/2/2
2	LEO	DDD	301[B]	-	-	4/4/22/22	0/2/2/2
2	LEO	BBB	302[A]	-	-	0/4/22/22	0/2/2/2
2	LEO	BBB	303	-	-	0/4/22/22	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	301[A]	LEO	C6-C2-C7	2.20	116.06	110.96

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	CCC	302	LEO	C21-C17-C6-C2
2	DDD	301[B]	LEO	C21-C17-C6-C2
2	DDD	301[B]	LEO	C22-C17-C6-C2
2	CCC	302	LEO	C22-C17-C6-C2
2	AAA	301[A]	LEO	C21-C17-C6-C2

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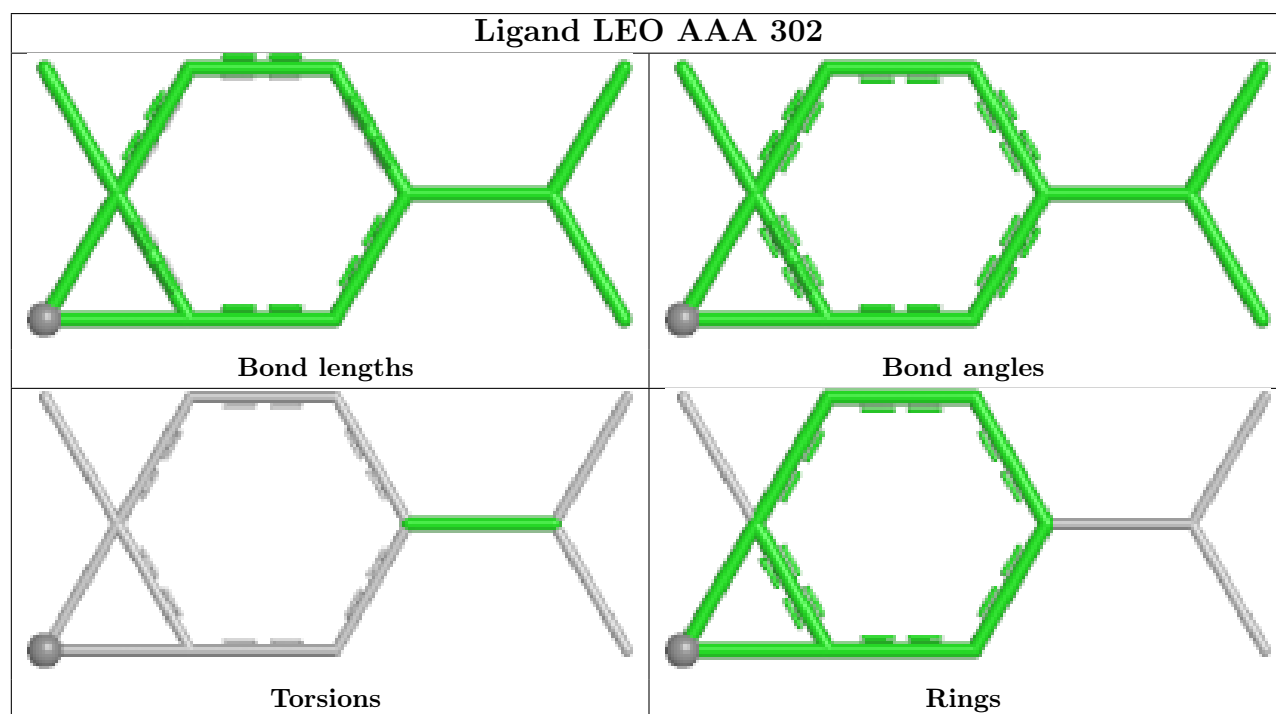
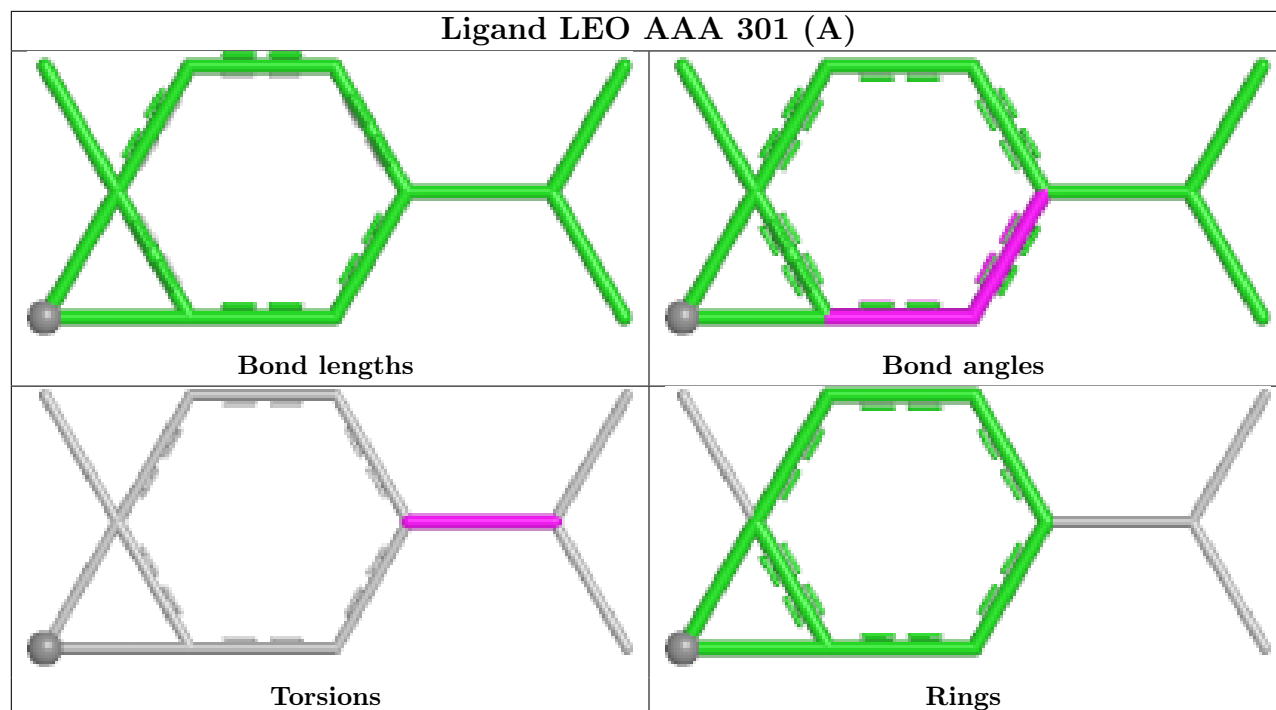
Mol	Chain	Res	Type	Atoms
2	AAA	301[A]	LEO	C22-C17-C6-C2
2	DDD	301[B]	LEO	C22-C17-C6-C4
2	AAA	301[A]	LEO	C22-C17-C6-C4
2	AAA	301[A]	LEO	C21-C17-C6-C4
2	CCC	302	LEO	C22-C17-C6-C4
2	CCC	302	LEO	C21-C17-C6-C4
2	DDD	301[B]	LEO	C21-C17-C6-C4

There are no ring outliers.

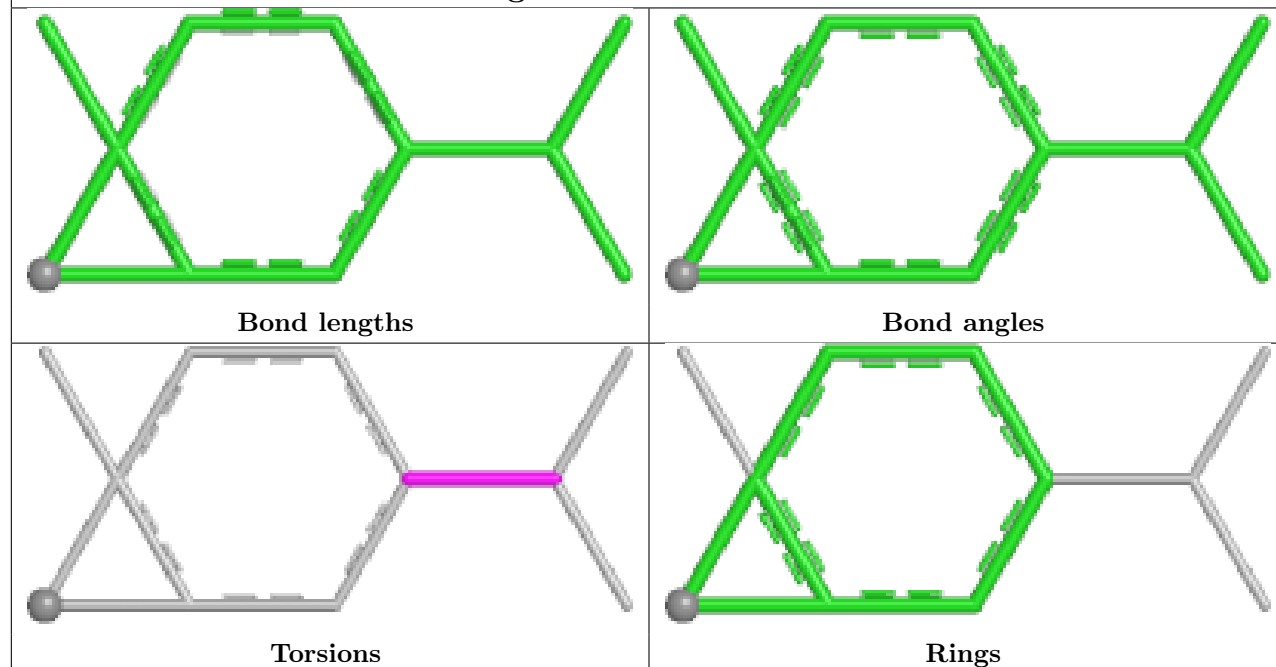
7 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	301[A]	LEO	3	0
2	AAA	302	LEO	3	0
2	DDD	302	LEO	2	0
2	CCC	301[B]	LEO	10	0
2	DDD	301[B]	LEO	8	0
2	BBB	302[A]	LEO	3	0
2	BBB	303	LEO	1	0

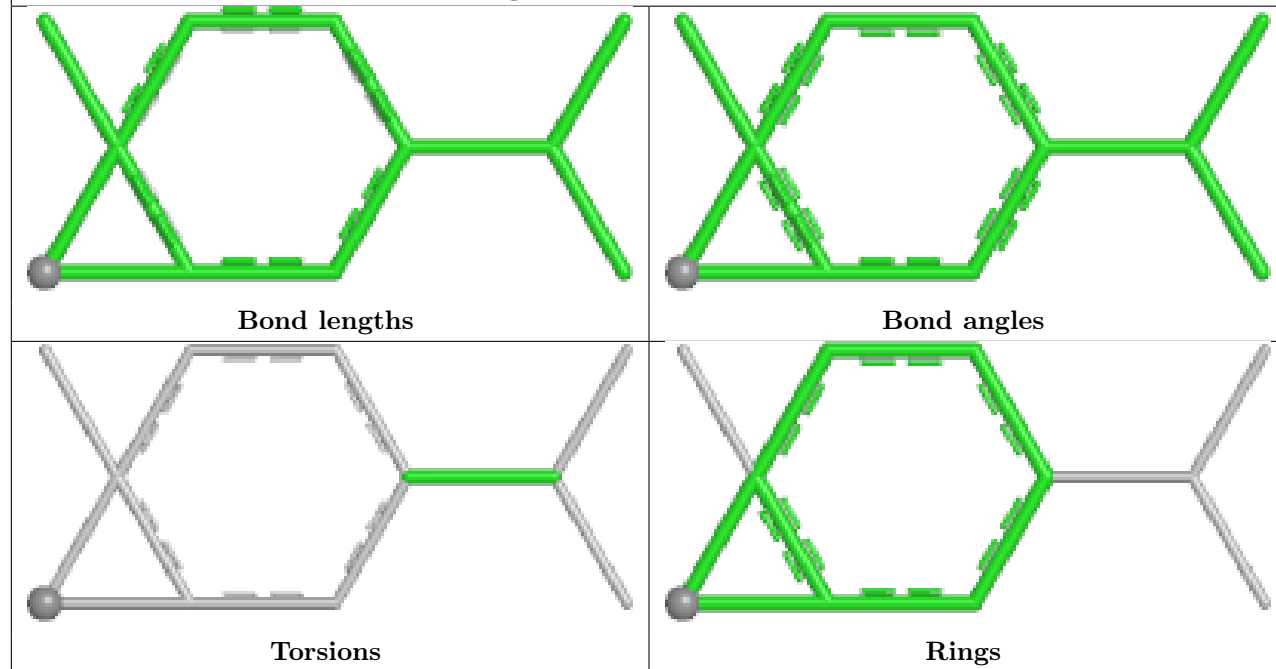
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

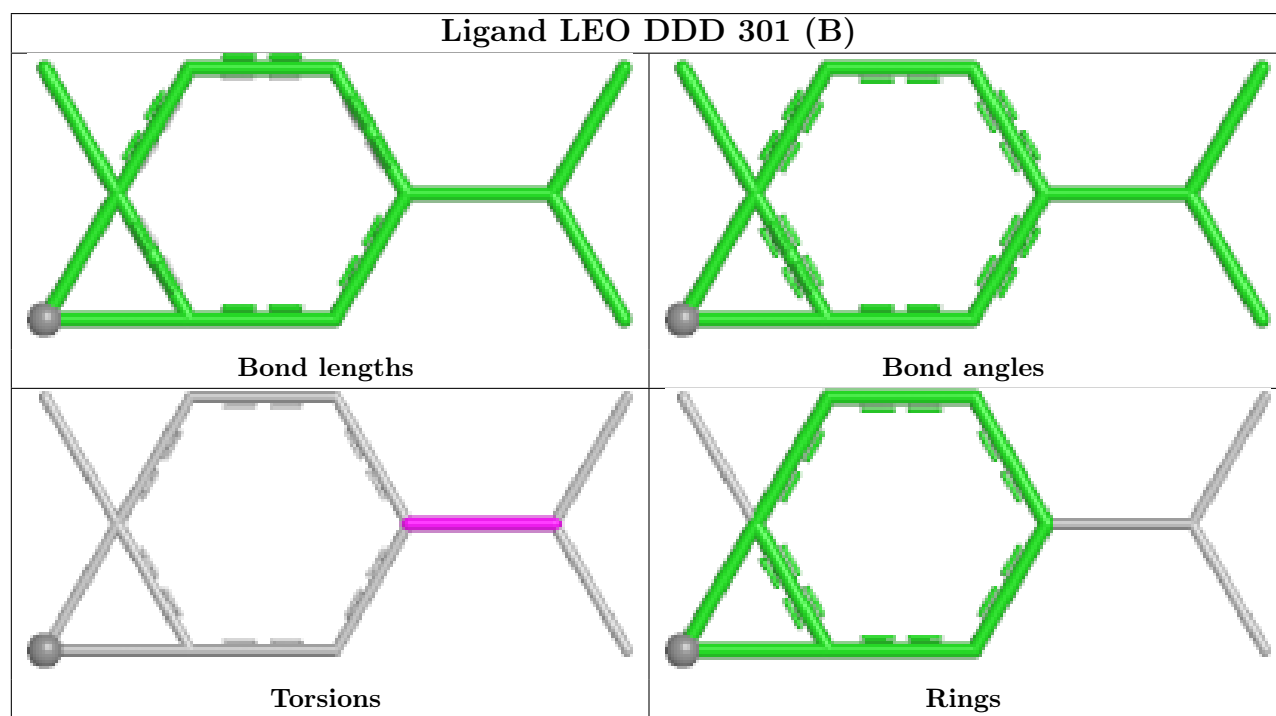
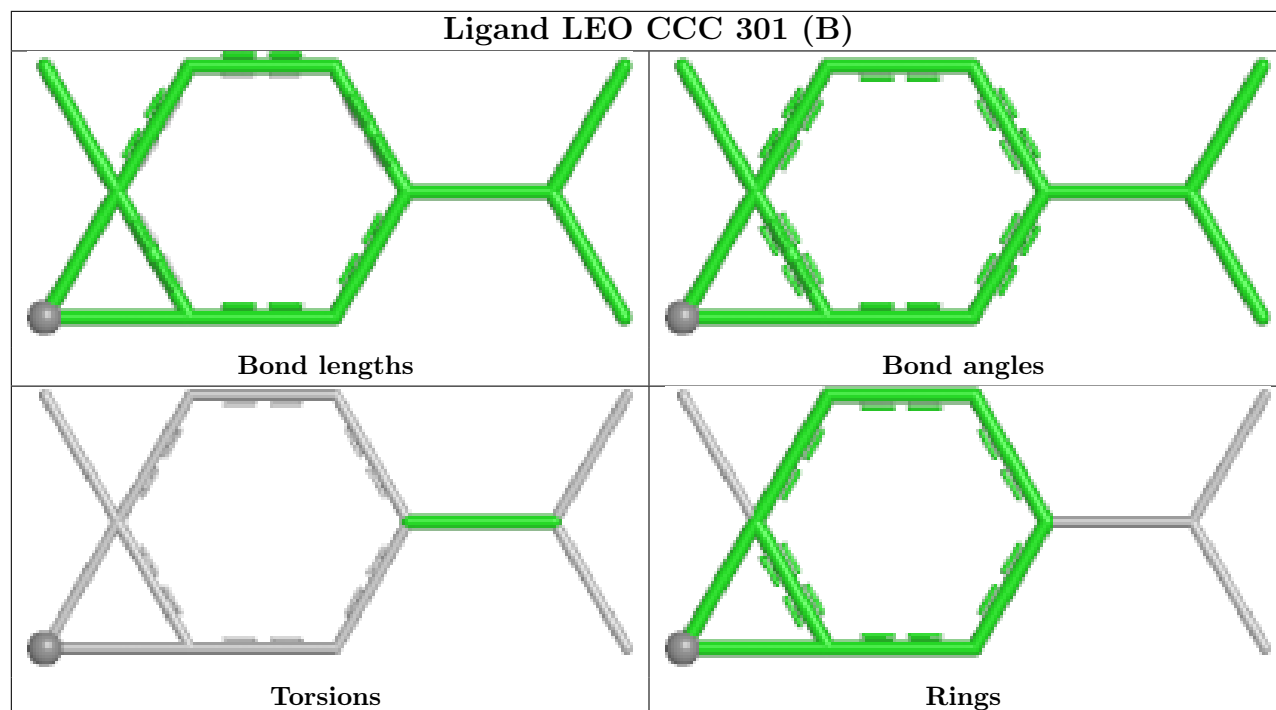


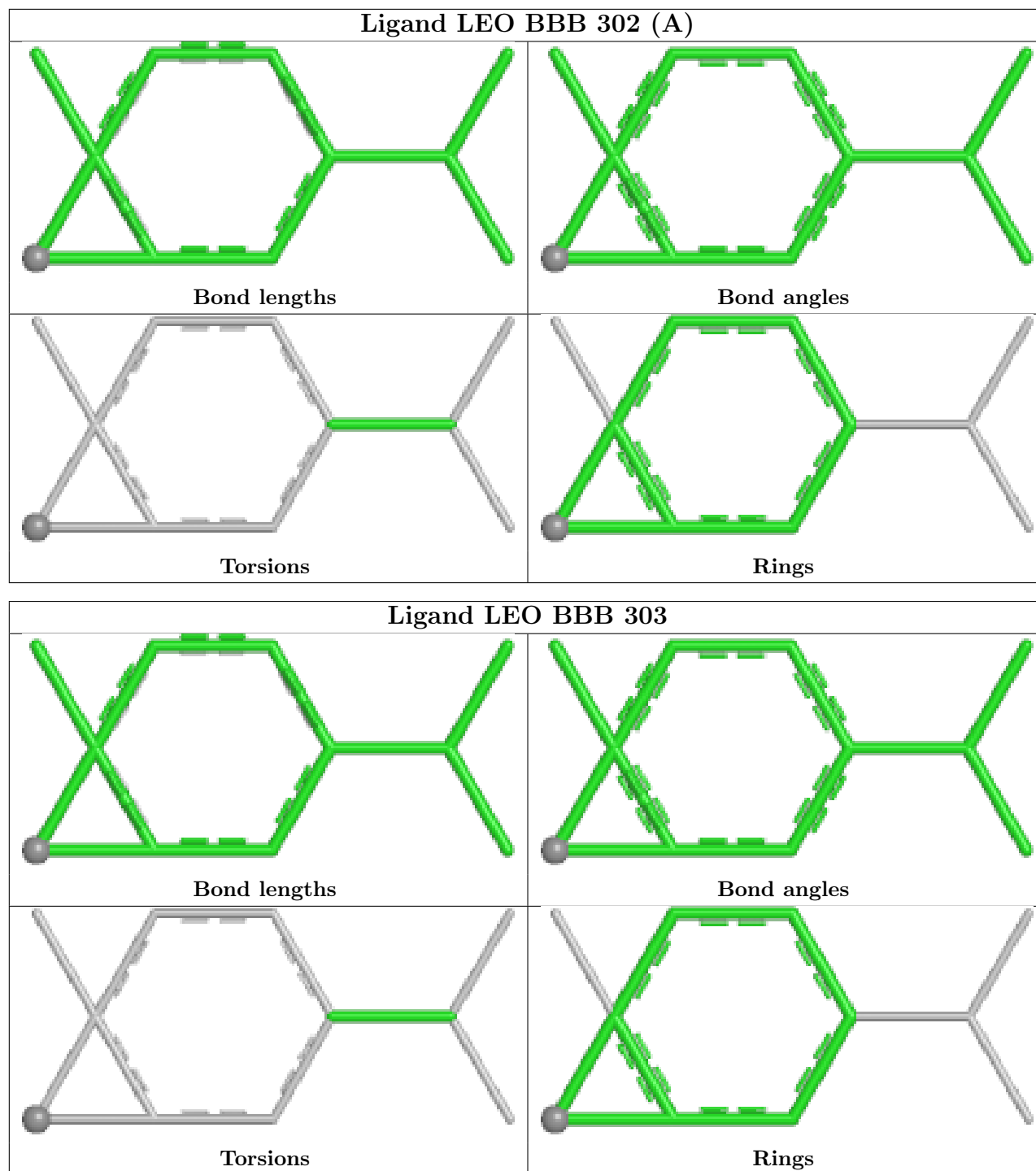
Ligand LEO CCC 302



Ligand LEO DDD 302







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	AAA	287/299 (95%)	0.83	25 (8%) 16 18	31, 64, 91, 143	12 (4%)
1	BBB	289/299 (96%)	0.29	4 (1%) 73 79	26, 52, 76, 113	12 (4%)
1	CCC	290/299 (96%)	0.72	21 (7%) 21 25	30, 60, 90, 130	16 (5%)
1	DDD	293/299 (97%)	0.73	28 (9%) 13 15	26, 57, 94, 134	15 (5%)
All	All	1159/1196 (96%)	0.64	78 (6%) 24 27	26, 58, 90, 143	55 (4%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	242	VAL	3.6
1	DDD	260	TYR	3.5
1	DDD	179	VAL	3.5
1	AAA	274	LEU	3.4
1	DDD	173	MET	3.4
1	DDD	289	LEU	3.3
1	DDD	246[A]	LYS	3.2
1	DDD	248	LEU	3.1
1	DDD	6[A]	LYS	3.1
1	BBB	291	SER	3.0
1	DDD	184	LEU	3.0
1	DDD	280	VAL	2.9
1	DDD	5	LEU	2.9
1	AAA	289	LEU	2.8
1	CCC	176[A]	GLN	2.8
1	AAA	193	VAL	2.8
1	CCC	291	SER	2.8
1	AAA	48	LEU	2.8
1	CCC	5	LEU	2.8
1	CCC	183	LEU	2.8
1	CCC	288	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	AAA	197	SER	2.7
1	DDD	250	VAL	2.7
1	CCC	260	TYR	2.7
1	DDD	178	PHE	2.7
1	CCC	174	LEU	2.7
1	DDD	183	LEU	2.7
1	CCC	12	VAL	2.7
1	DDD	291	SER	2.7
1	AAA	253[A]	GLU	2.6
1	DDD	174	LEU	2.6
1	DDD	175	ILE	2.6
1	AAA	182	ASP	2.6
1	DDD	12	VAL	2.6
1	AAA	12	VAL	2.6
1	AAA	181	ARG	2.5
1	CCC	242	VAL	2.5
1	AAA	61	GLY	2.5
1	DDD	249	ILE	2.5
1	BBB	13[A]	ASN	2.4
1	AAA	179	VAL	2.4
1	DDD	20	VAL	2.4
1	CCC	199	SER	2.4
1	AAA	192	TYR	2.4
1	DDD	21	THR	2.4
1	AAA	95	ALA	2.4
1	CCC	179	VAL	2.4
1	DDD	169	PHE	2.3
1	AAA	27	LEU	2.3
1	AAA	13[A]	ASN	2.3
1	AAA	45	ILE	2.3
1	CCC	181	ARG	2.3
1	CCC	195	ALA	2.3
1	CCC	197	SER	2.3
1	DDD	190[A]	ARG	2.2
1	AAA	250	VAL	2.2
1	AAA	222[A]	LYS	2.2
1	CCC	289	LEU	2.2
1	DDD	293	ILE	2.2
1	AAA	19	TYR	2.2
1	DDD	237	TRP	2.2
1	CCC	280	VAL	2.2
1	CCC	155	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	169	PHE	2.1
1	AAA	89	ALA	2.1
1	AAA	174	LEU	2.1
1	DDD	189	LEU	2.1
1	AAA	43	PHE	2.1
1	BBB	223	THR	2.1
1	AAA	86	LEU	2.1
1	AAA	56	ALA	2.1
1	CCC	3	GLU	2.0
1	AAA	223	THR	2.0
1	CCC	173	MET	2.0
1	DDD	277	PRO	2.0
1	CCC	190[A]	ARG	2.0
1	CCC	157	ILE	2.0
1	DDD	284	ILE	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.

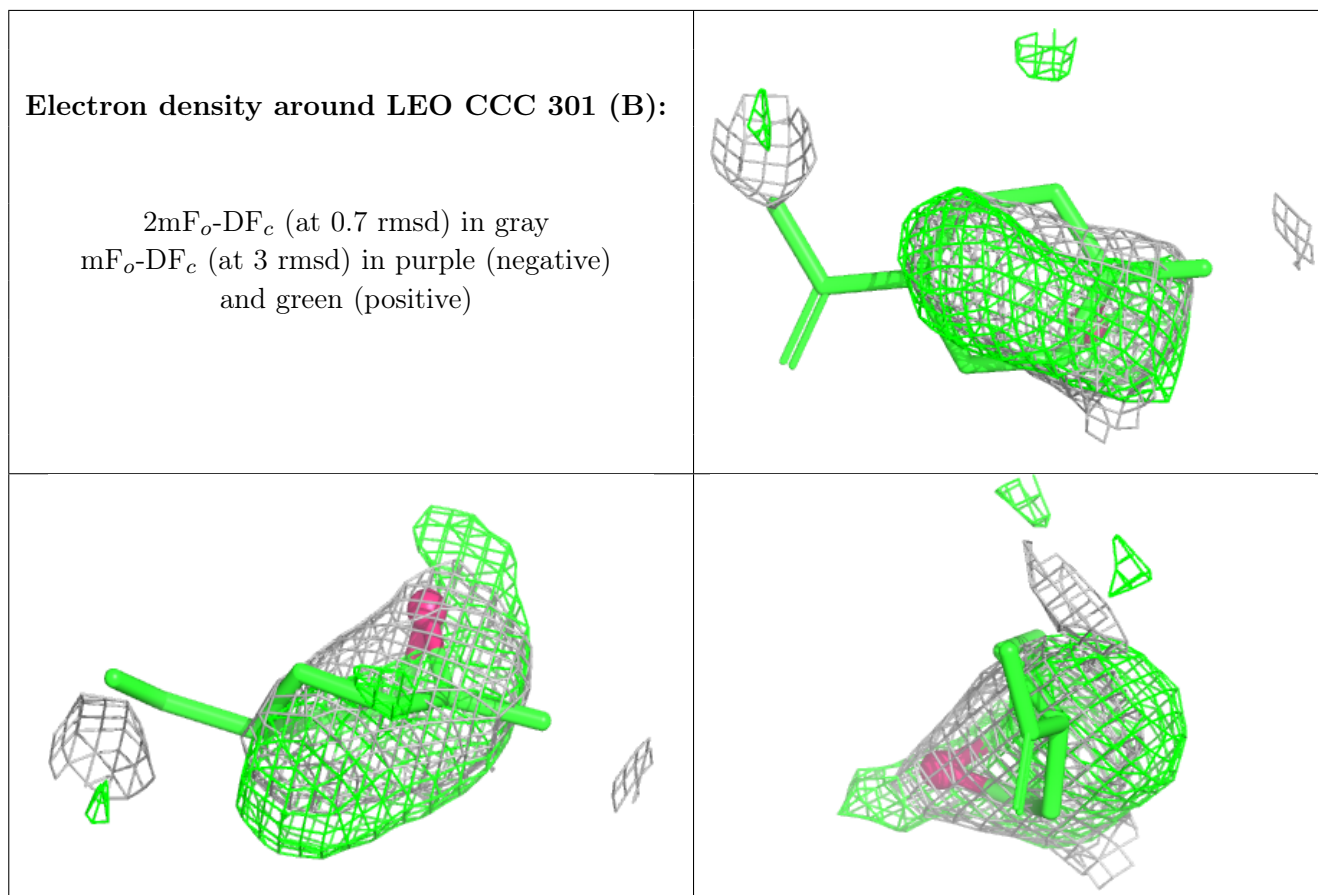
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	DDD	304	1/1	0.69	0.15	108,108,108,108	0
4	EDO	BBB	301	4/4	0.77	0.15	73,73,75,75	0
3	CL	AAA	303	1/1	0.82	0.13	101,101,101,101	0
3	CL	CCC	303	1/1	0.85	0.14	87,87,87,87	0
3	CL	DDD	303	1/1	0.86	0.15	86,86,86,86	0
2	LEO	CCC	301[B]	11/11	0.88	0.52	80,87,107,109	11
2	LEO	DDD	302	11/11	0.91	0.32	117,144,155,166	0
2	LEO	BBB	303	11/11	0.91	0.41	90,97,101,103	11

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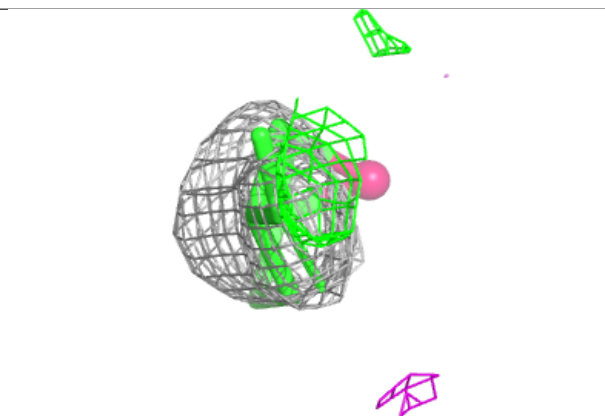
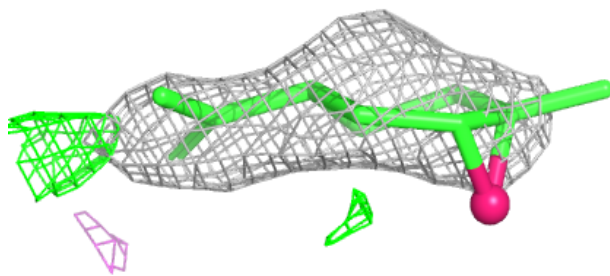
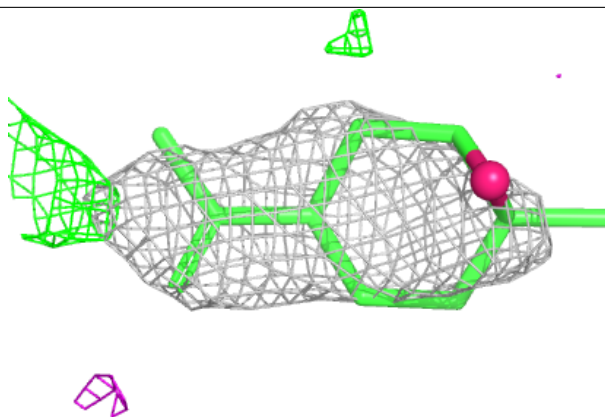
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LEO	DDD	301[B]	11/11	0.92	0.42	70,73,85,85	11
3	CL	AAA	304	1/1	0.92	0.17	74,74,74,74	0
3	CL	CCC	304	1/1	0.93	0.09	79,79,79,79	0
2	LEO	BBB	302[A]	11/11	0.93	0.42	85,91,104,107	11
2	LEO	AAA	302	11/11	0.94	0.35	103,106,111,113	11
2	LEO	AAA	301[A]	11/11	0.94	0.34	71,76,94,98	11
2	LEO	CCC	302	11/11	0.94	0.30	108,125,135,140	0
3	CL	BBB	304	1/1	0.97	0.07	59,59,59,59	0
3	CL	BBB	305	1/1	0.98	0.07	67,67,67,67	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.

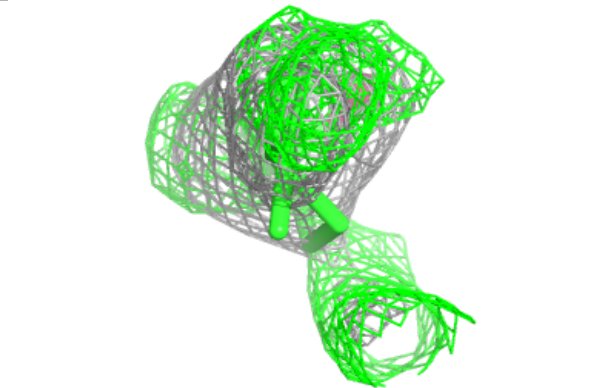
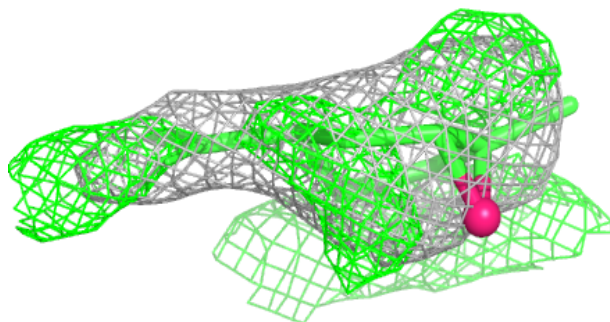
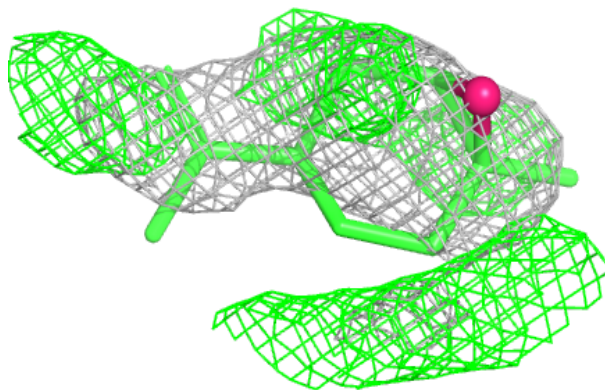


Electron density around LEO DDD 302:

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

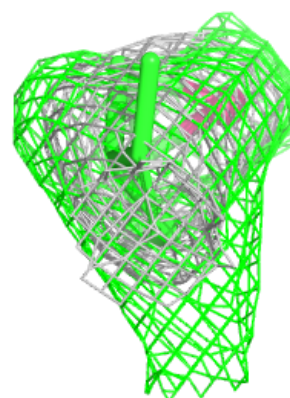
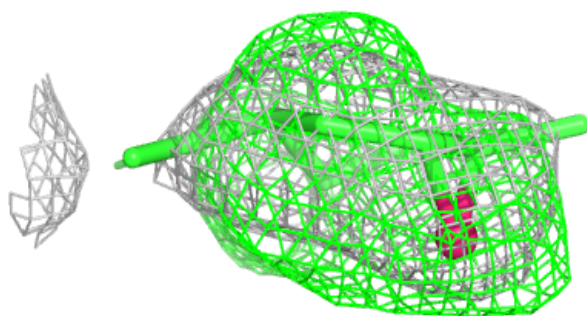
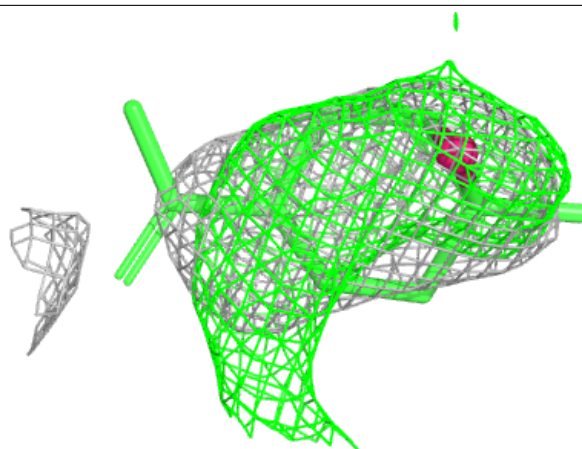
**Electron density around LEO BBB 303:**

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

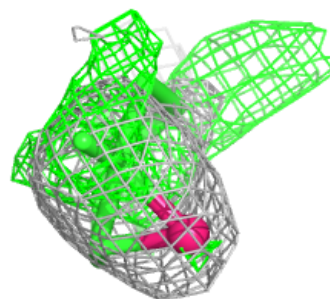
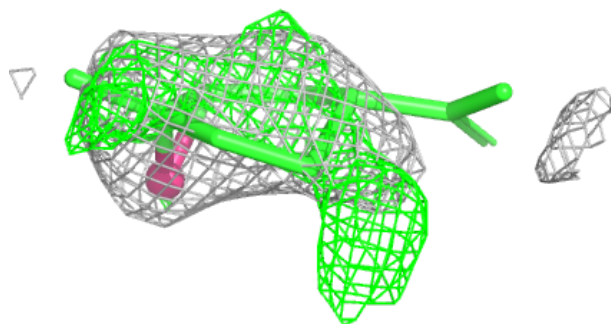
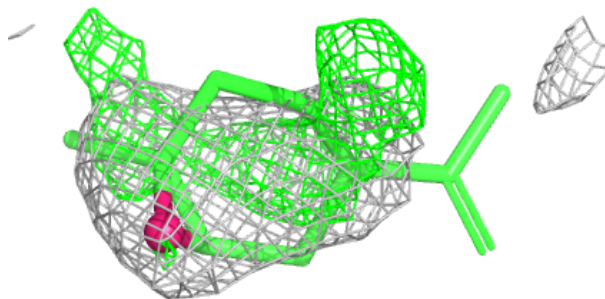


Electron density around LEO DDD 301 (B):

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

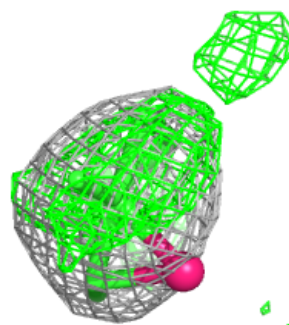
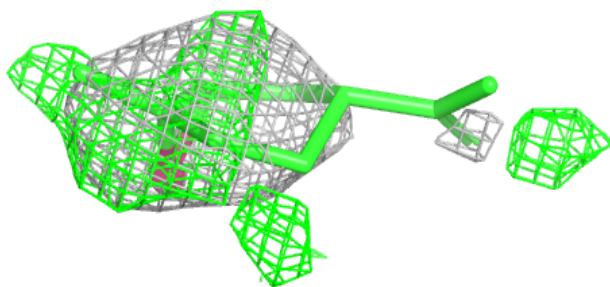
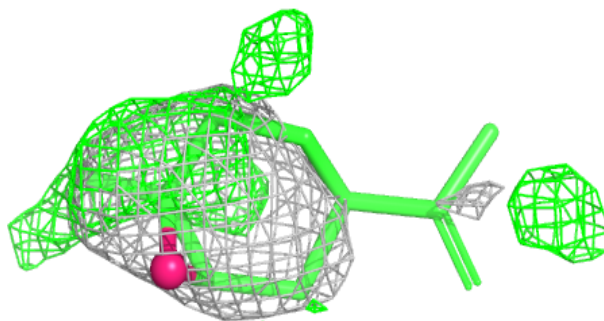
**Electron density around LEO BBB 302 (A):**

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

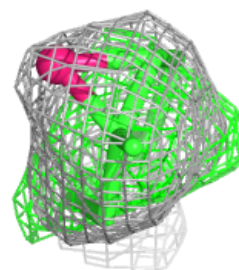
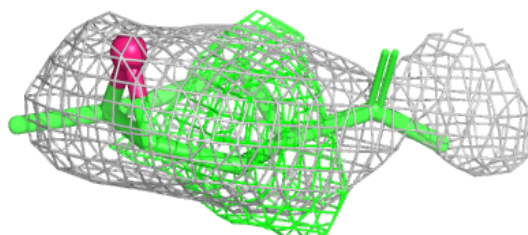
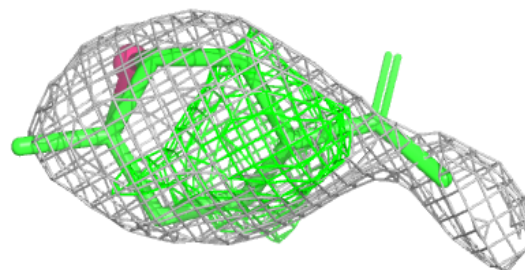


Electron density around LEO AAA 302:

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

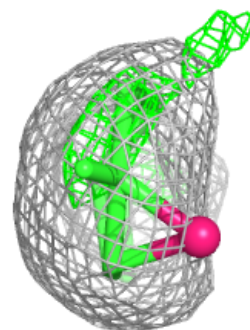
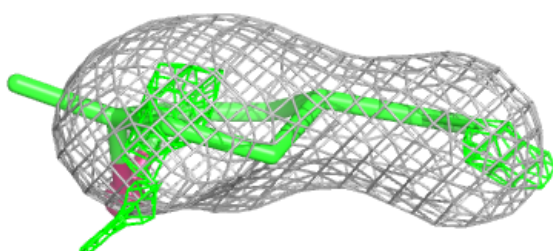
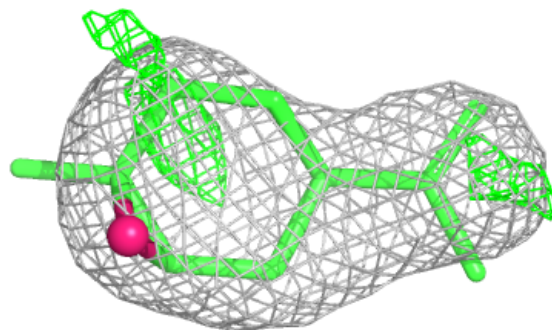
**Electron density around LEO AAA 301 (A):**

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



Electron density around LEO CCC 302:

$2mF_o-DF_c$ (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.