Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 10:09 pm BST

PDB ID	:	8AGM
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:

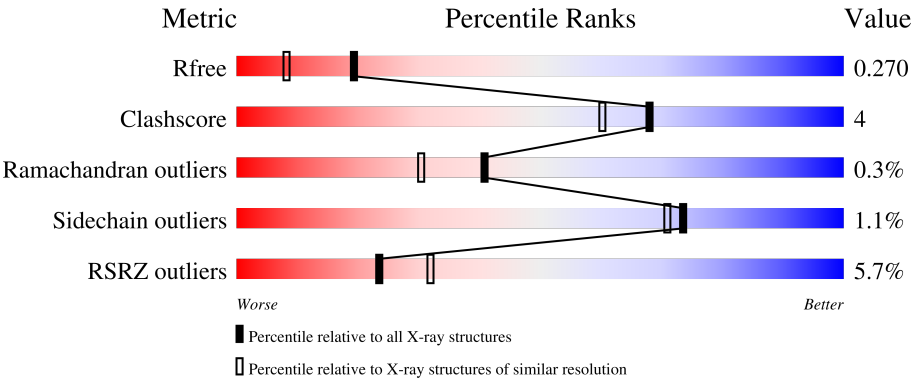
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 <=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% 87% 8% ·
1	BBB	299	% 91% 6% ·
1	CCC	299	5% 87% 10% · ·
1	DDD	299	8% 89% 8% ·

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	X
2	LEO	DDD	301[B]	-	-	X	X

2 Entry composition (i)

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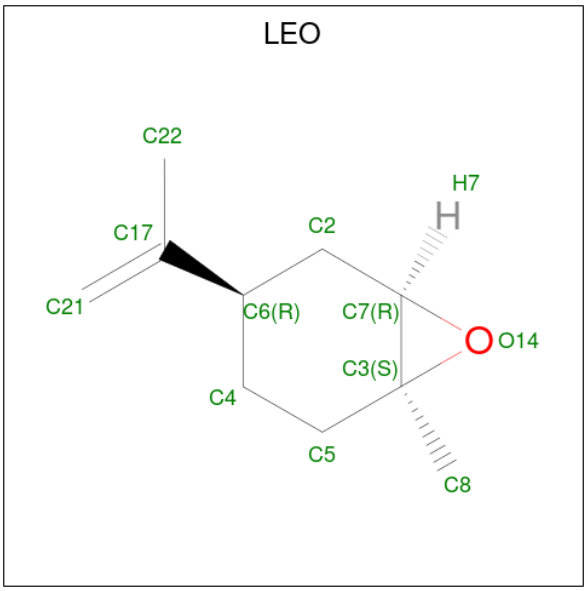
Chain	Residue	Modelled	Actual	Comment	Reference
DDD	297	HIS	-	expression tag	UNP A0A1U9WZ52
DDD	298	HIS	-	expression tag	UNP A0A1U9WZ52
DDD	299	HIS	-	expression tag	UNP A0A1U9WZ52

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

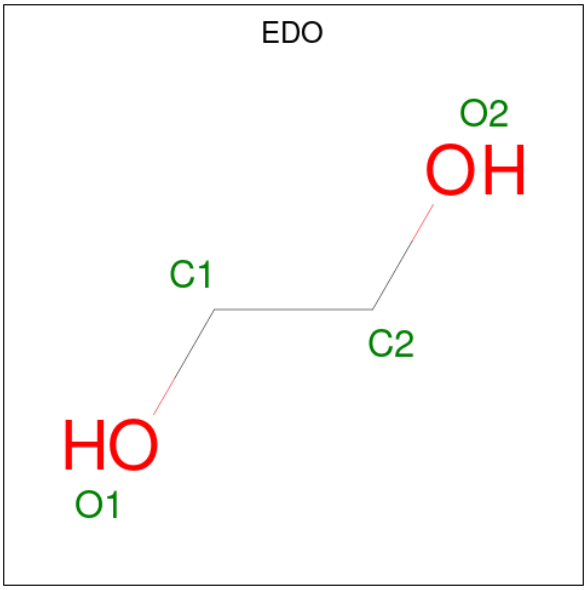


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	1
			11	10	1		
2	AAA	1	Total	C	O	0	0
			11	10	1		
2	BBB	1	Total	C	O	0	1
			11	10	1		
2	BBB	1	Total	C	O	0	0
			11	10	1		
2	CCC	1	Total	C	O	0	1
			11	10	1		
2	CCC	1	Total	C	O	0	0
			11	10	1		
2	DDD	1	Total	C	O	0	1
			11	10	1		
2	DDD	1	Total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

- Molecule 3 is CHLORIDE ION (three-letter code: 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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

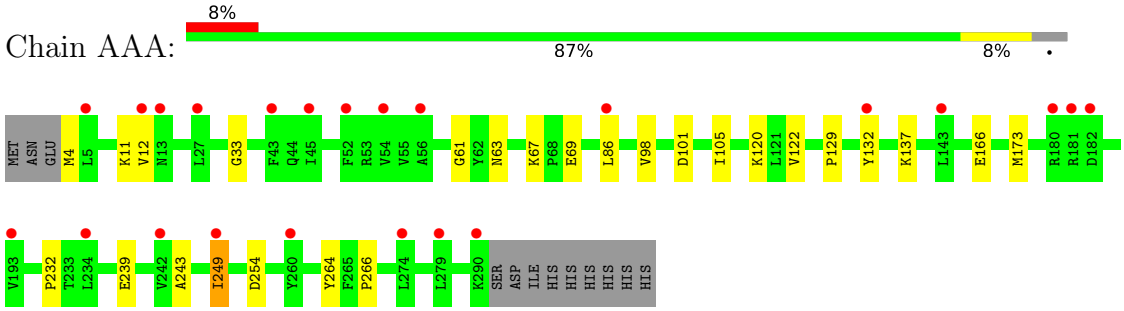
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	40	Total O 40 40	0	0
5	BBB	80	Total O 80 80	0	0
5	CCC	52	Total O 52 52	0	0
5	DDD	59	Total O 59 59	0	0

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.

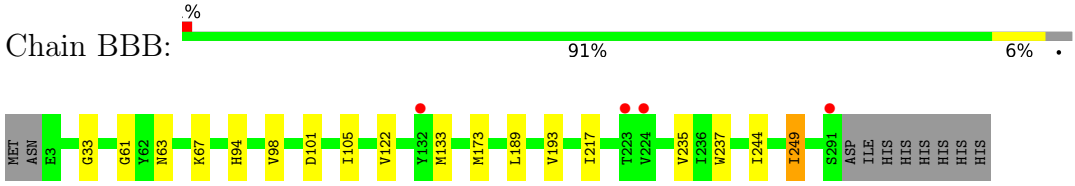
• Molecule 1: Alpha/beta epoxide hydrolase

Chain AAA:



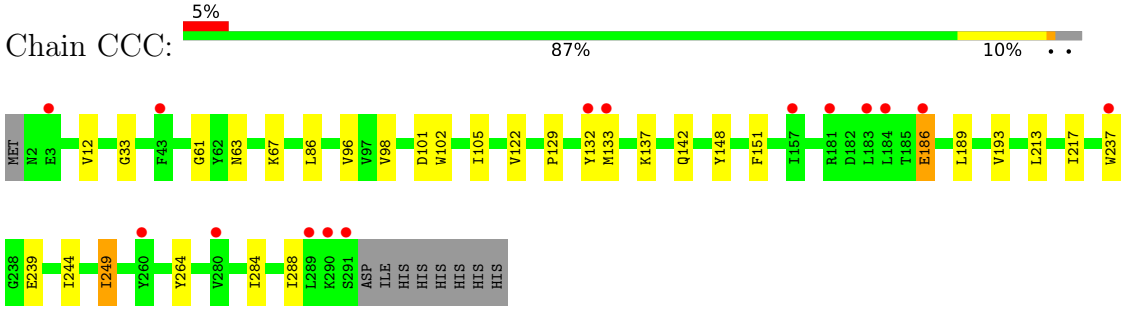
• Molecule 1: Alpha/beta epoxide hydrolase

Chain BBB:



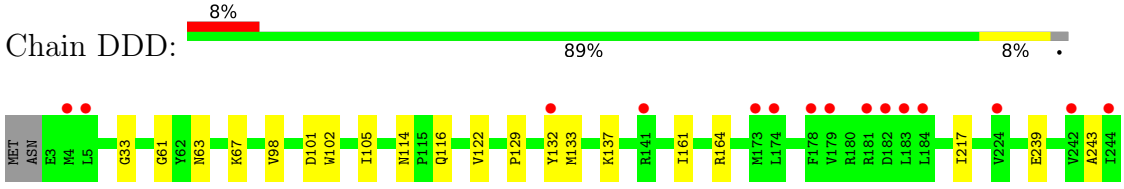
• Molecule 1: Alpha/beta epoxide hydrolase

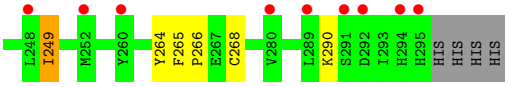
Chain CCC:



• Molecule 1: Alpha/beta epoxide hydrolase

Chain DDD:




L248
I249
M252
Y260
Y264
F265
P266
E267
C268
V280
L289
K290
S291
D292
I293
H294
H295
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

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 95.94 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.6 (96.13-1.97) 99.6 (95.94-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0267, BUSTER	Depositor
R, R_{free}	0.232 , 0.270 0.232 , 0.270	Depositor DCC
R_{free} test set	4467 reflections (4.86%)	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)	0.32 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, LEO, EDO

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	0.45	0/2539	0.62	0/3439
1	BBB	0.48	0/2553	0.62	0/3462
1	CCC	0.44	0/2612	0.61	0/3537
1	DDD	0.47	0/2630	0.60	0/3560
All	All	0.46	0/10334	0.61	0/13998

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	AAA	2442	0	2504	16	0
1	BBB	2454	0	2512	11	0
1	CCC	2495	0	2567	26	0
1	DDD	2515	0	2577	22	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	77	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 (77) 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
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:AAA:61:GLY:HA2	1:AAA:67:LYS:HG2	1.85	0.58
1:AAA:101:ASP:CG	2:AAA:301[A]:LEO:H81	2.24	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:249:ILE:HD11	1:AAA:264:TYR:HE1	1.70	0.55
1:DDD:101:ASP:CG	2:DDD:301[B]:LEO:H81	2.28	0.54
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: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: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
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: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:BBB:101:ASP:CG	2:BBB:302[A]:LEO:H81	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:186[A]:GLU:CD	1:CCC:186[A]:GLU:H	2.24	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 (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	AAA	297/299 (99%)	284 (96%)	12 (4%)	1 (0%)	41	30
1	BBB	299/299 (100%)	291 (97%)	7 (2%)	1 (0%)	41	30
1	CCC	304/299 (102%)	292 (96%)	11 (4%)	1 (0%)	41	30
1	DDD	306/299 (102%)	296 (97%)	9 (3%)	1 (0%)	41	30
All	All	1206/1196 (101%)	1163 (96%)	39 (3%)	4 (0%)	41	30

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 (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	AAA	266/267 (100%)	260 (98%)	6 (2%)	50	42
1	BBB	268/267 (100%)	265 (99%)	3 (1%)	73	71
1	CCC	274/267 (103%)	270 (98%)	4 (2%)	65	60
1	DDD	276/267 (103%)	275 (100%)	1 (0%)	91	90
All	All	1084/1068 (102%)	1070 (99%)	14 (1%)	73	65

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
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 monosaccharides 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	DDD	302	-	12,12,12	0.60	0	19,19,19	0.70	0
4	EDO	BBB	301	-	3,3,3	0.62	0	2,2,2	0.20	0
2	LEO	BBB	303	-	12,12,12	0.61	0	19,19,19	0.48	0
2	LEO	AAA	301[A]	-	12,12,12	0.70	0	19,19,19	0.94	2 (10%)
2	LEO	BBB	302[A]	-	12,12,12	0.62	0	19,19,19	0.56	0
2	LEO	AAA	302	-	12,12,12	0.63	0	19,19,19	0.46	0
2	LEO	CCC	301[B]	-	12,12,12	0.78	0	19,19,19	0.92	0
2	LEO	CCC	302	-	12,12,12	0.62	0	19,19,19	0.63	0
2	LEO	DDD	301[B]	-	12,12,12	0.72	0	19,19,19	0.86	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	DDD	302	-	-	0/4/22/22	0/2/2/2
4	EDO	BBB	301	-	-	0/1/1/1	-
2	LEO	BBB	303	-	-	0/4/22/22	0/2/2/2
2	LEO	AAA	301[A]	-	-	4/4/22/22	0/2/2/2
2	LEO	BBB	302[A]	-	-	0/4/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LEO	AAA	302	-	-	0/4/22/22	0/2/2/2
2	LEO	CCC	301[B]	-	-	0/4/22/22	0/2/2/2
2	LEO	CCC	302	-	-	4/4/22/22	0/2/2/2
2	LEO	DDD	301[B]	-	-	4/4/22/22	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	301[A]	LEO	C2-C6-C4	2.43	113.15	109.86
2	AAA	301[A]	LEO	C6-C2-C7	2.13	116.06	111.46

There are no chirality outliers.

All (12) torsion outliers are listed below:

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

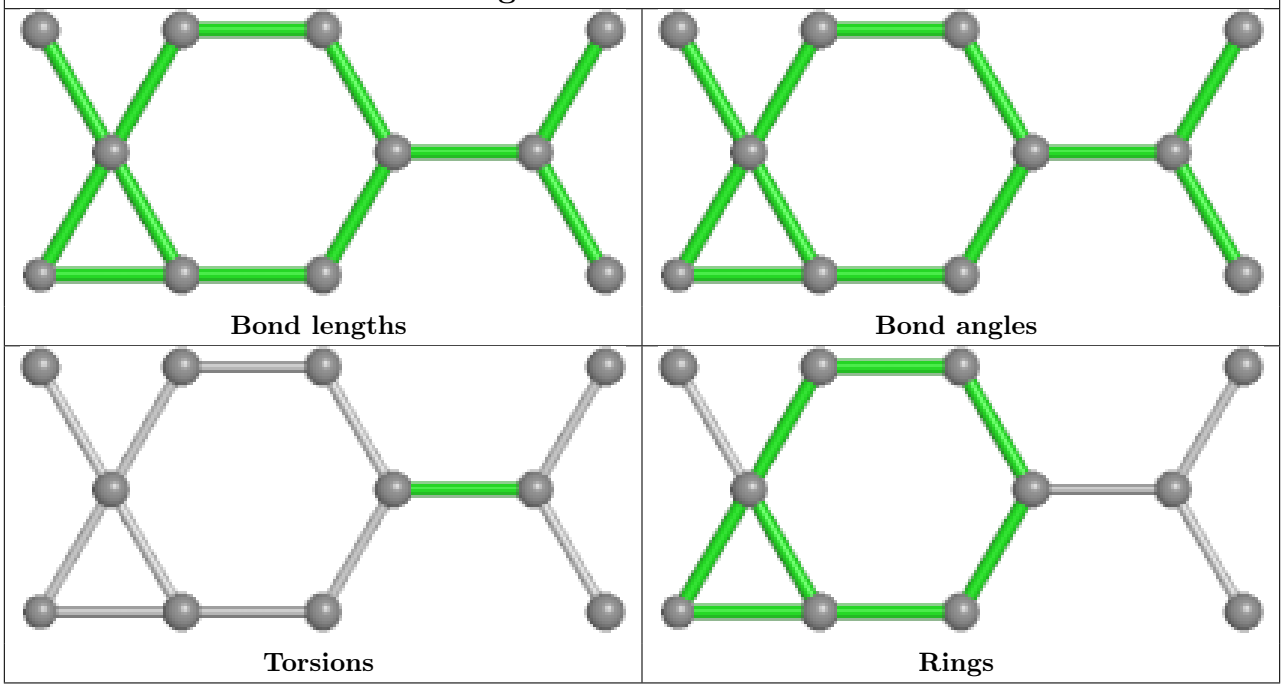
There are no ring outliers.

7 monomers are involved in 30 short contacts:

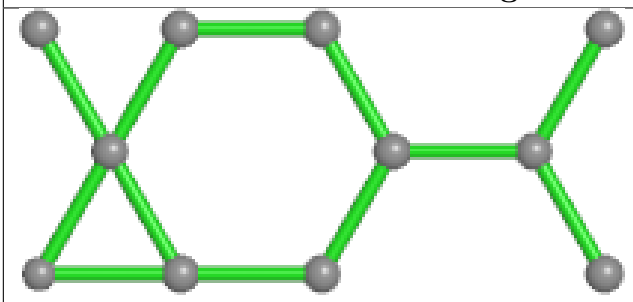
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	DDD	302	LEO	2	0
2	BBB	303	LEO	1	0
2	AAA	301[A]	LEO	3	0
2	BBB	302[A]	LEO	3	0
2	AAA	302	LEO	3	0
2	CCC	301[B]	LEO	10	0
2	DDD	301[B]	LEO	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

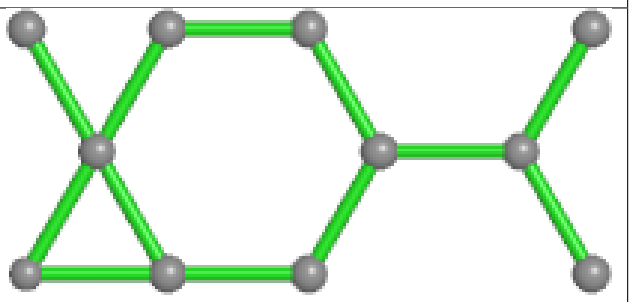
Ligand LEO DDD 302



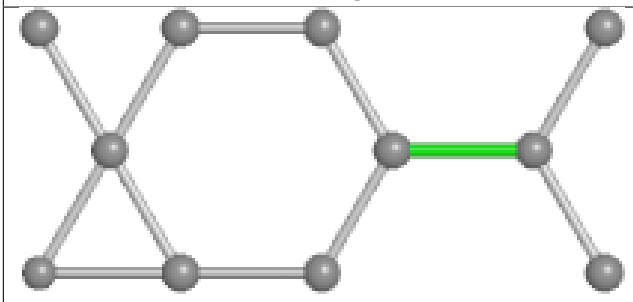
Ligand LEO BBB 303



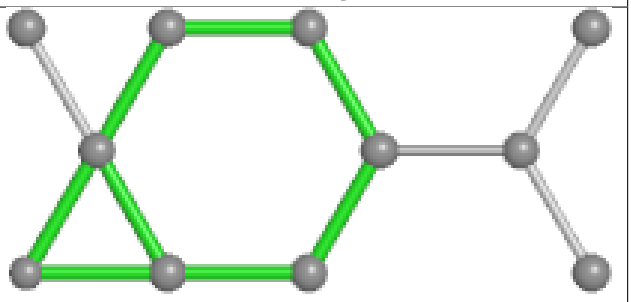
Bond lengths



Bond angles

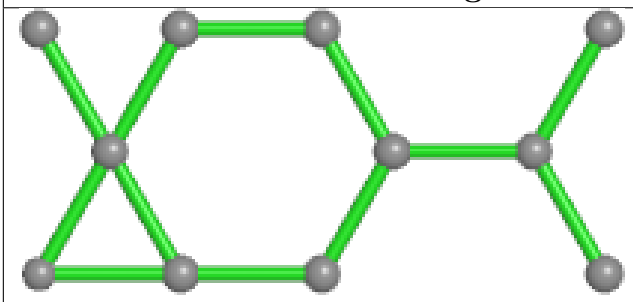


Torsions

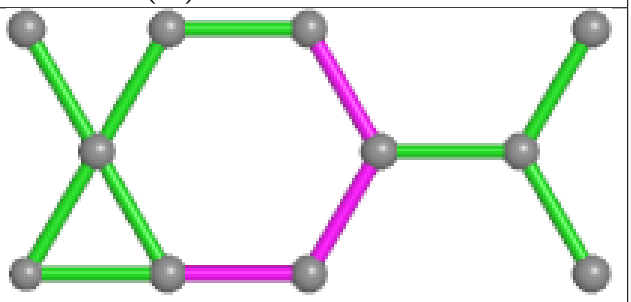


Rings

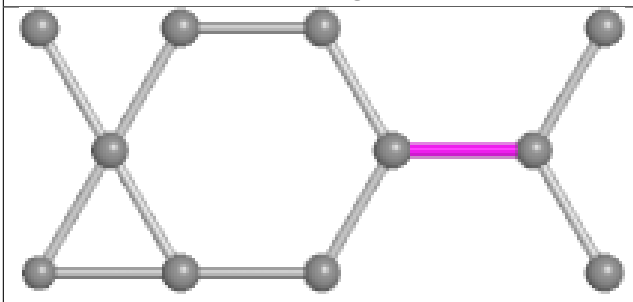
Ligand LEO AAA 301 (A)



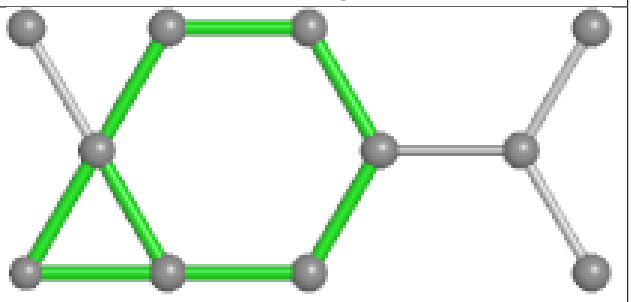
Bond lengths



Bond angles

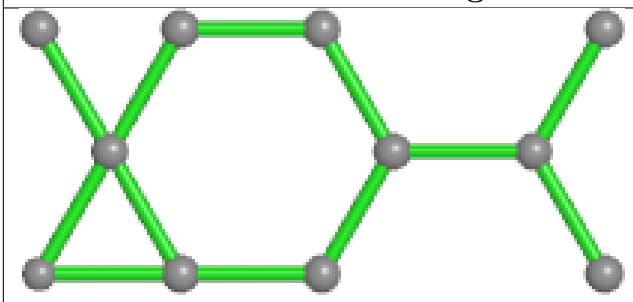


Torsions

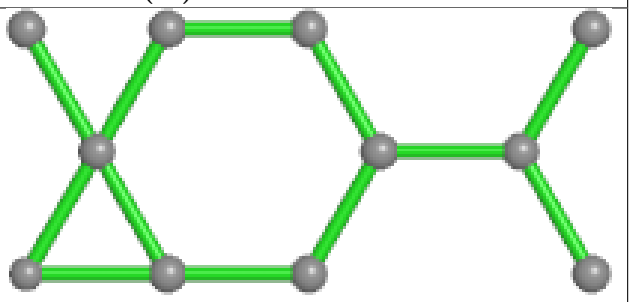


Rings

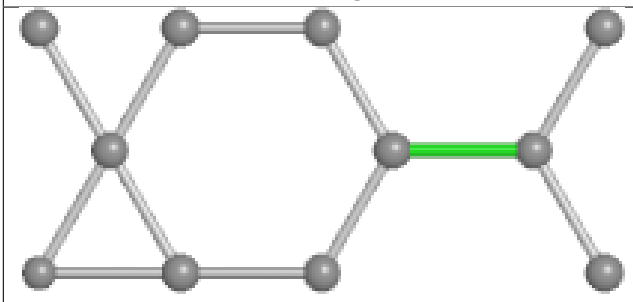
Ligand LEO BBB 302 (A)



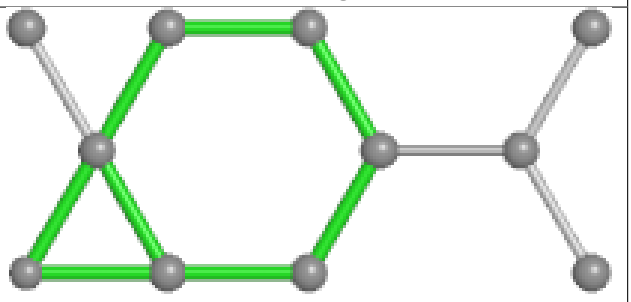
Bond lengths



Bond angles

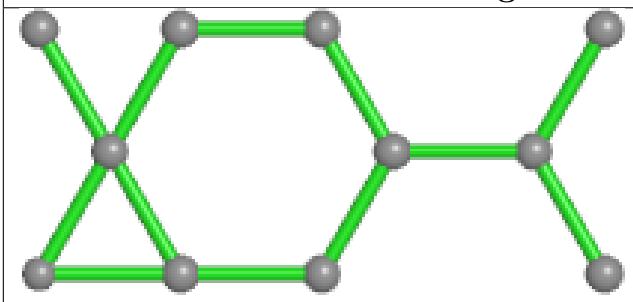


Torsions

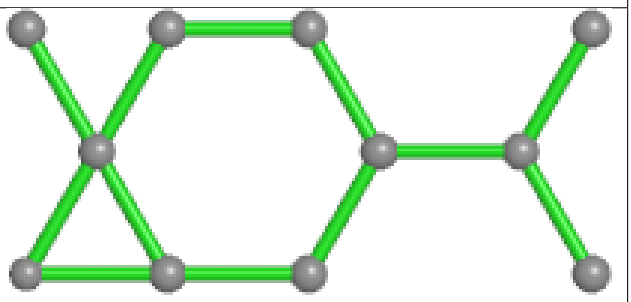


Rings

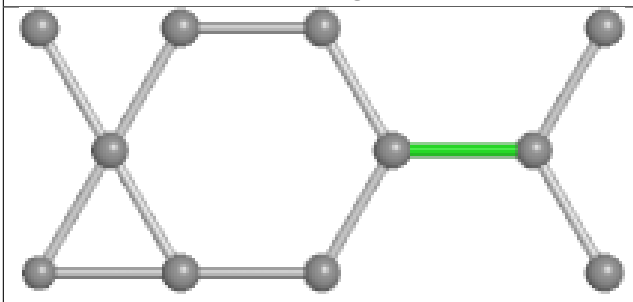
Ligand LEO AAA 302



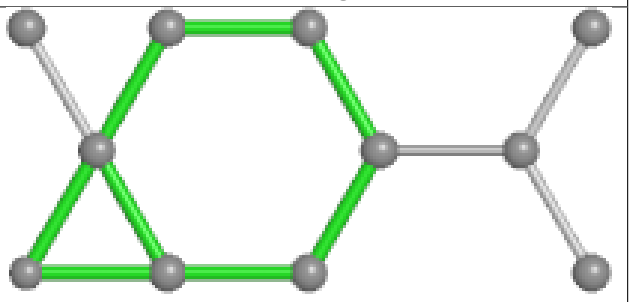
Bond lengths



Bond angles

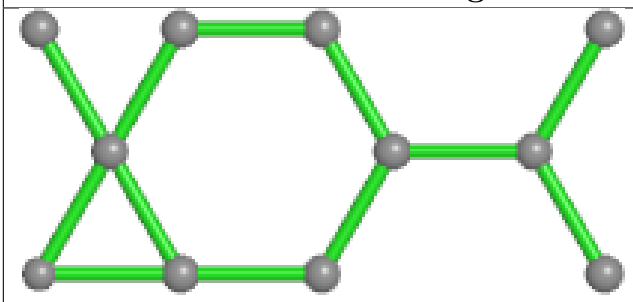


Torsions

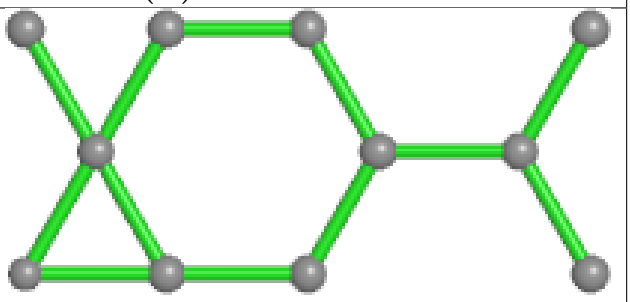


Rings

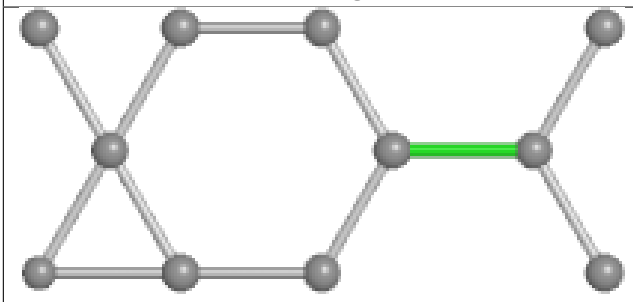
Ligand LEO CCC 301 (B)



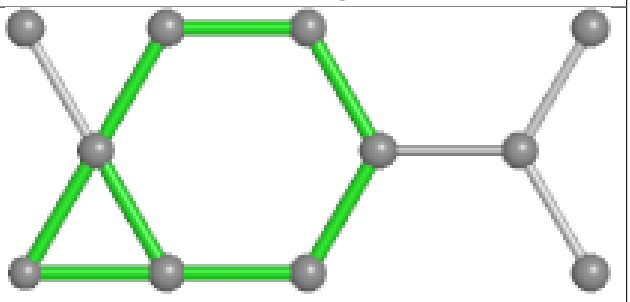
Bond lengths



Bond angles

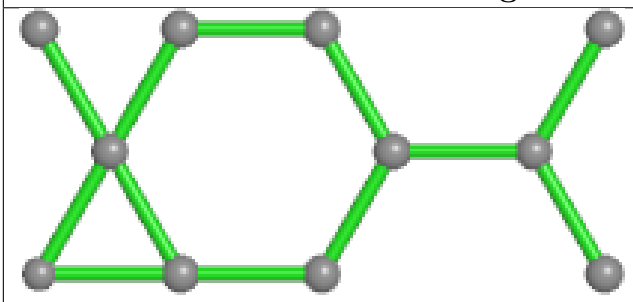


Torsions

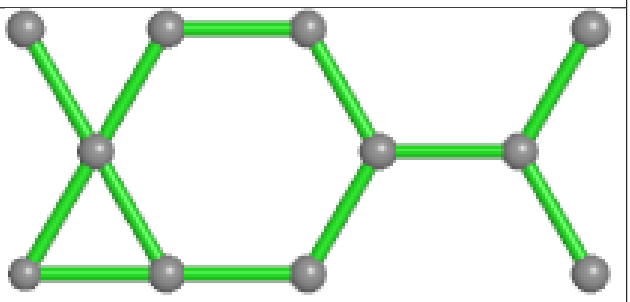


Rings

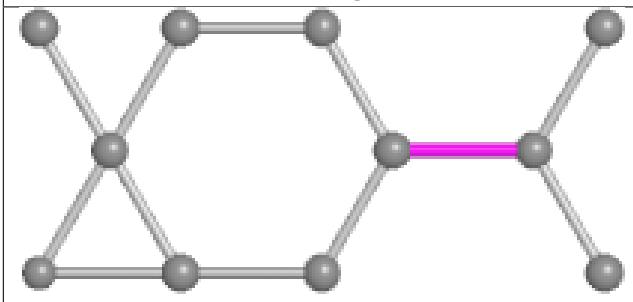
Ligand LEO CCC 302



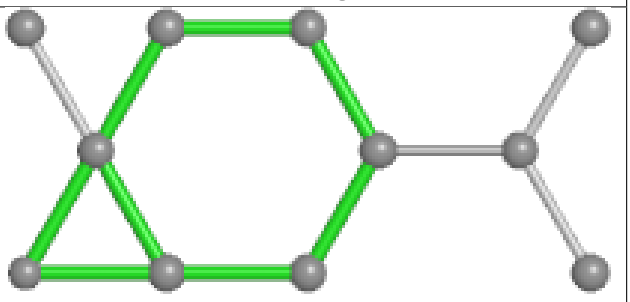
Bond lengths



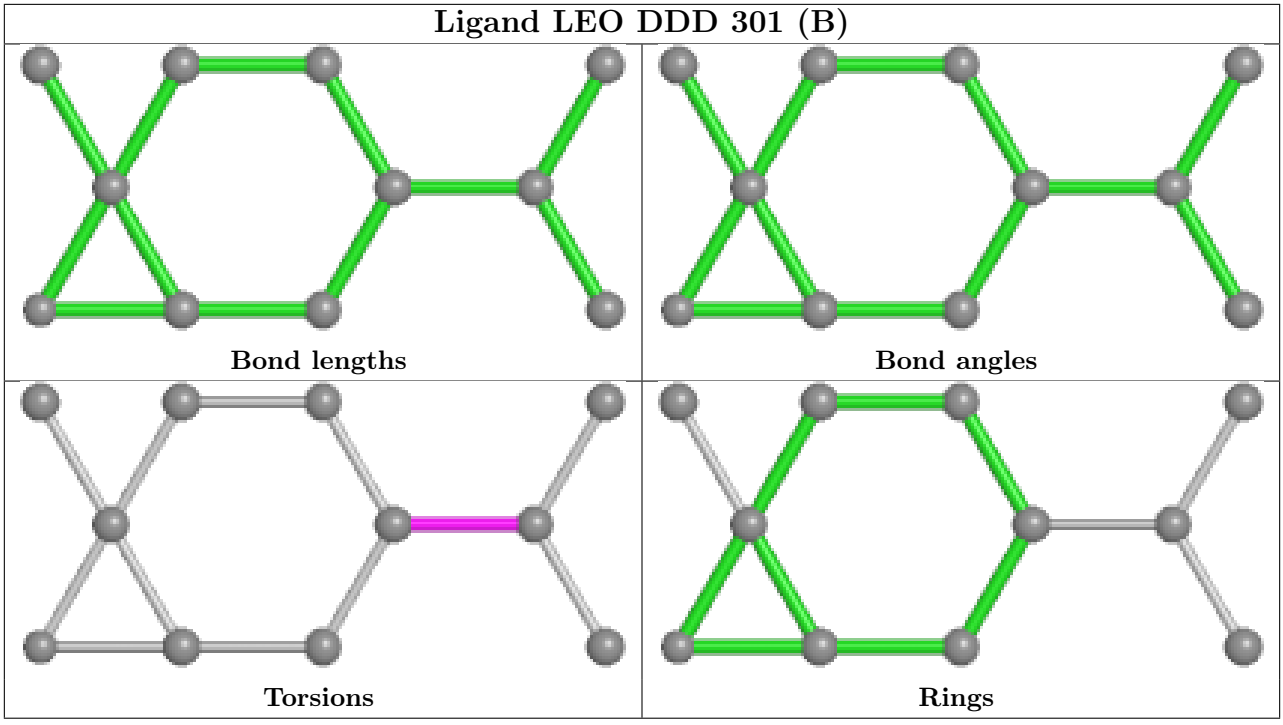
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	287/299 (95%)	0.73	23 (8%)	12	19	42, 65, 92, 143	0
1	BBB	289/299 (96%)	0.33	4 (1%)	75	82	39, 53, 77, 113	0
1	CCC	290/299 (96%)	0.54	15 (5%)	27	37	41, 61, 90, 130	0
1	DDD	293/299 (97%)	0.69	24 (8%)	11	18	40, 58, 94, 134	0
All	All	1159/1196 (96%)	0.57	66 (5%)	23	32	39, 59, 91, 143	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	179	VAL	6.6
1	DDD	181	ARG	5.8
1	DDD	291	SER	5.3
1	CCC	3	GLU	4.9
1	BBB	132[A]	TYR	4.6
1	AAA	181	ARG	4.4
1	DDD	295	HIS	4.2
1	DDD	242	VAL	4.0
1	CCC	291	SER	3.9
1	AAA	290	LYS	3.8
1	AAA	260	TYR	3.7
1	AAA	274	LEU	3.6
1	CCC	289	LEU	3.5
1	DDD	289	LEU	3.5
1	BBB	291	SER	3.4
1	DDD	280	VAL	3.3
1	CCC	290	LYS	3.2
1	DDD	173	MET	3.1
1	AAA	86	LEU	3.1
1	AAA	242	VAL	3.0
1	AAA	45	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	AAA	52	PHE	3.0
1	DDD	4	MET	2.9
1	AAA	193	VAL	2.8
1	CCC	132[A]	TYR	2.7
1	DDD	294	HIS	2.7
1	DDD	132[A]	TYR	2.7
1	AAA	13[A]	ASN	2.7
1	DDD	182	ASP	2.6
1	DDD	260	TYR	2.6
1	DDD	5	LEU	2.6
1	DDD	184	LEU	2.6
1	AAA	43	PHE	2.5
1	DDD	178	PHE	2.5
1	CCC	260	TYR	2.5
1	AAA	132[A]	TYR	2.5
1	AAA	249	ILE	2.4
1	AAA	182	ASP	2.4
1	DDD	141[A]	ARG	2.4
1	CCC	186[A]	GLU	2.4
1	BBB	224	VAL	2.4
1	AAA	5	LEU	2.4
1	AAA	27	LEU	2.4
1	CCC	181	ARG	2.4
1	DDD	248	LEU	2.3
1	AAA	12	VAL	2.3
1	DDD	244	ILE	2.3
1	CCC	43	PHE	2.3
1	CCC	280	VAL	2.3
1	DDD	183	LEU	2.3
1	CCC	237[A]	TRP	2.2
1	BBB	223	THR	2.2
1	AAA	234	LEU	2.2
1	DDD	174	LEU	2.2
1	CCC	183	LEU	2.2
1	CCC	133[A]	MET	2.2
1	AAA	279	LEU	2.1
1	DDD	252[A]	MET	2.1
1	AAA	56	ALA	2.1
1	DDD	224	VAL	2.1
1	CCC	184	LEU	2.1
1	DDD	292	ASP	2.1
1	CCC	157	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	AAA	143	LEU	2.1
1	AAA	180	ARG	2.0
1	AAA	54	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

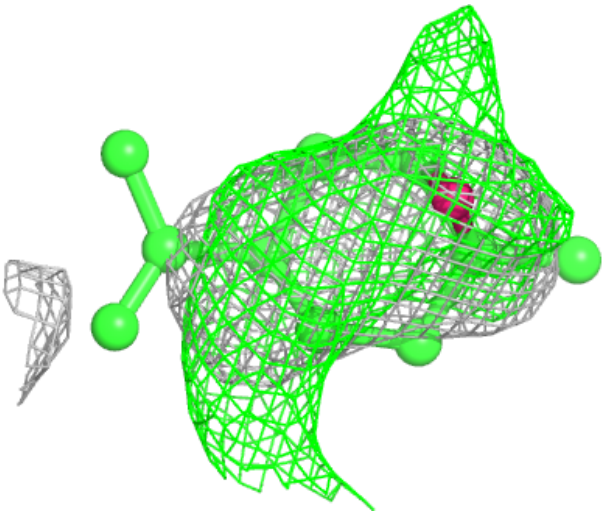
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	AAA	303	1/1	0.71	0.14	101,101,101,101	0
2	LEO	DDD	301[B]	11/11	0.72	0.52	70,73,85,85	11
2	LEO	CCC	301[B]	11/11	0.77	0.68	80,87,107,109	11
3	CL	DDD	303	1/1	0.77	0.20	86,86,86,86	0
2	LEO	DDD	302	11/11	0.78	0.27	117,144,155,166	0
4	EDO	BBB	301	4/4	0.79	0.29	73,73,75,75	0
2	LEO	BBB	303	11/11	0.80	0.40	90,97,101,103	11
3	CL	CCC	303	1/1	0.82	0.10	87,87,87,87	0
3	CL	AAA	304	1/1	0.84	0.13	74,74,74,74	0
2	LEO	AAA	301[A]	11/11	0.84	0.36	71,76,94,98	11
2	LEO	CCC	302	11/11	0.85	0.31	108,125,135,140	0
2	LEO	AAA	302	11/11	0.86	0.35	103,106,111,113	11
2	LEO	BBB	302[A]	11/11	0.87	0.53	85,91,104,107	11
3	CL	DDD	304	1/1	0.89	0.09	108,108,108,108	0
3	CL	BBB	305	1/1	0.91	0.09	67,67,67,67	0
3	CL	CCC	304	1/1	0.95	0.09	79,79,79,79	0
3	CL	BBB	304	1/1	0.98	0.07	59,59,59,59	0

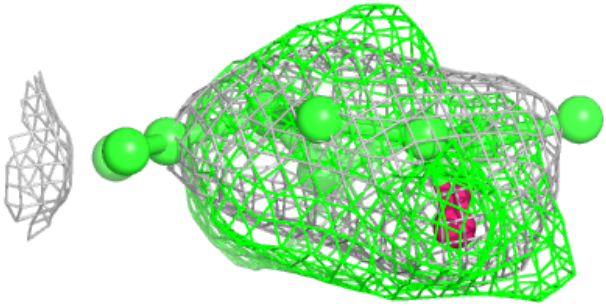
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

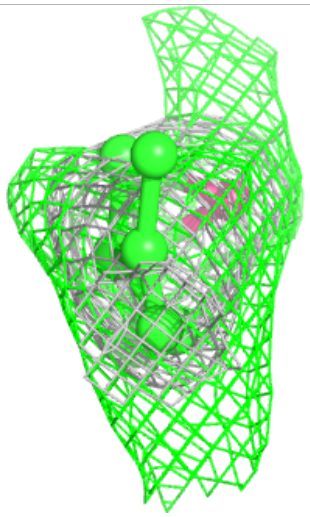
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LEO DDD 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)

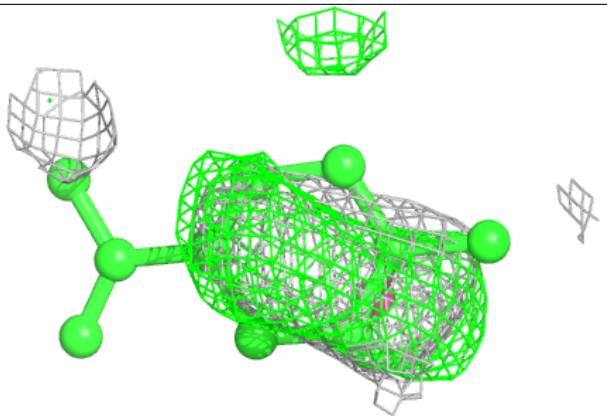


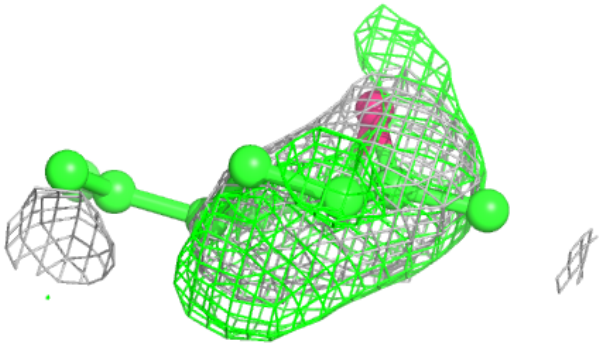


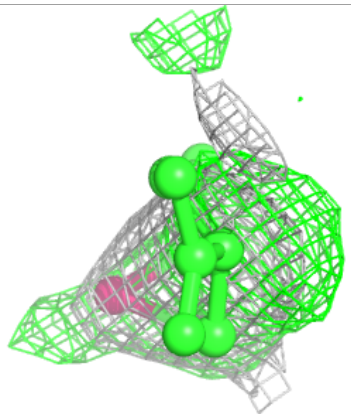


Electron density around LEO CCC 301 (B):

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

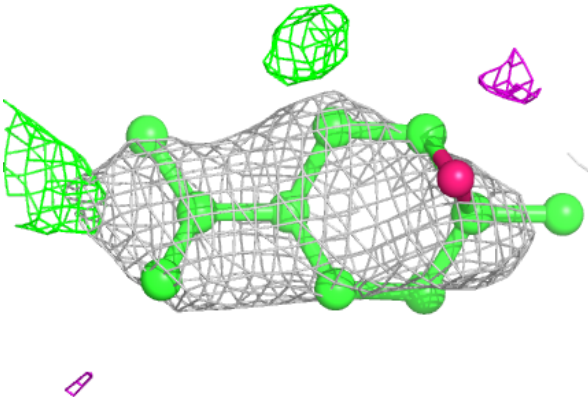


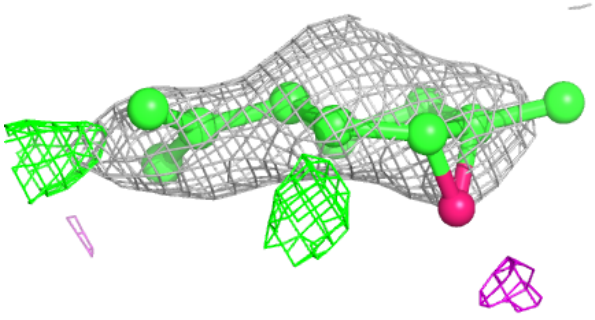


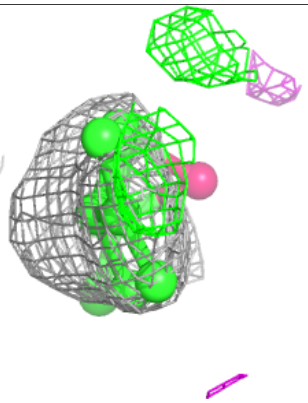


Electron density around LEO DDD 302:

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

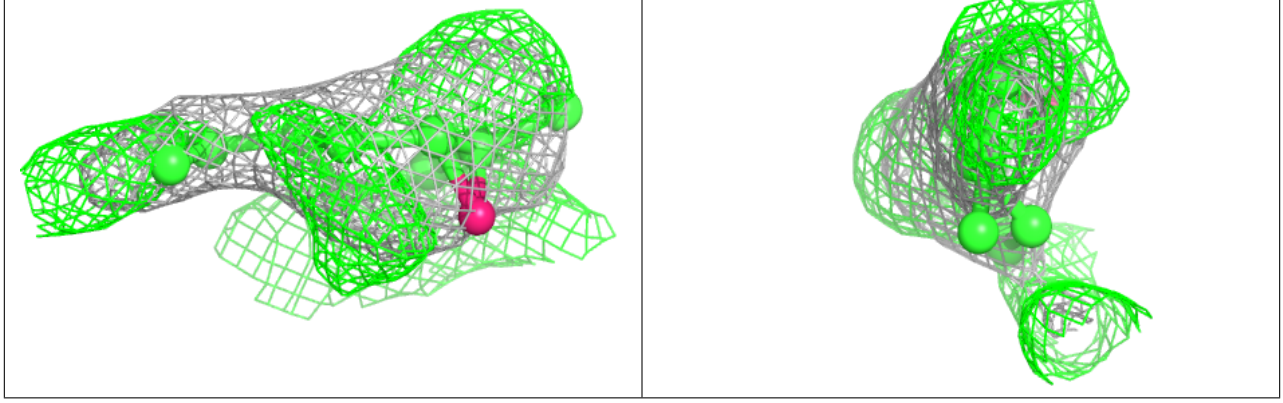






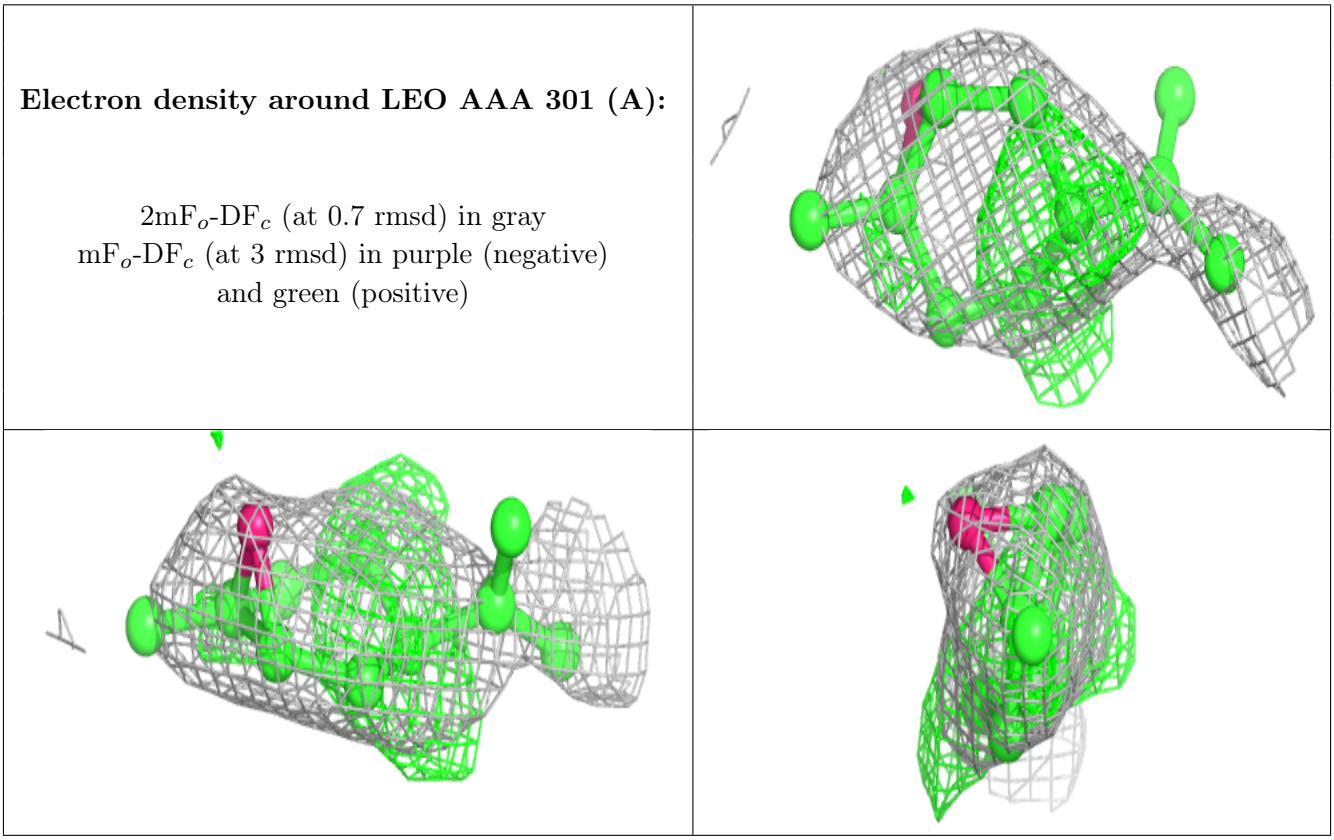
Electron density around LEO BBB 303:

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



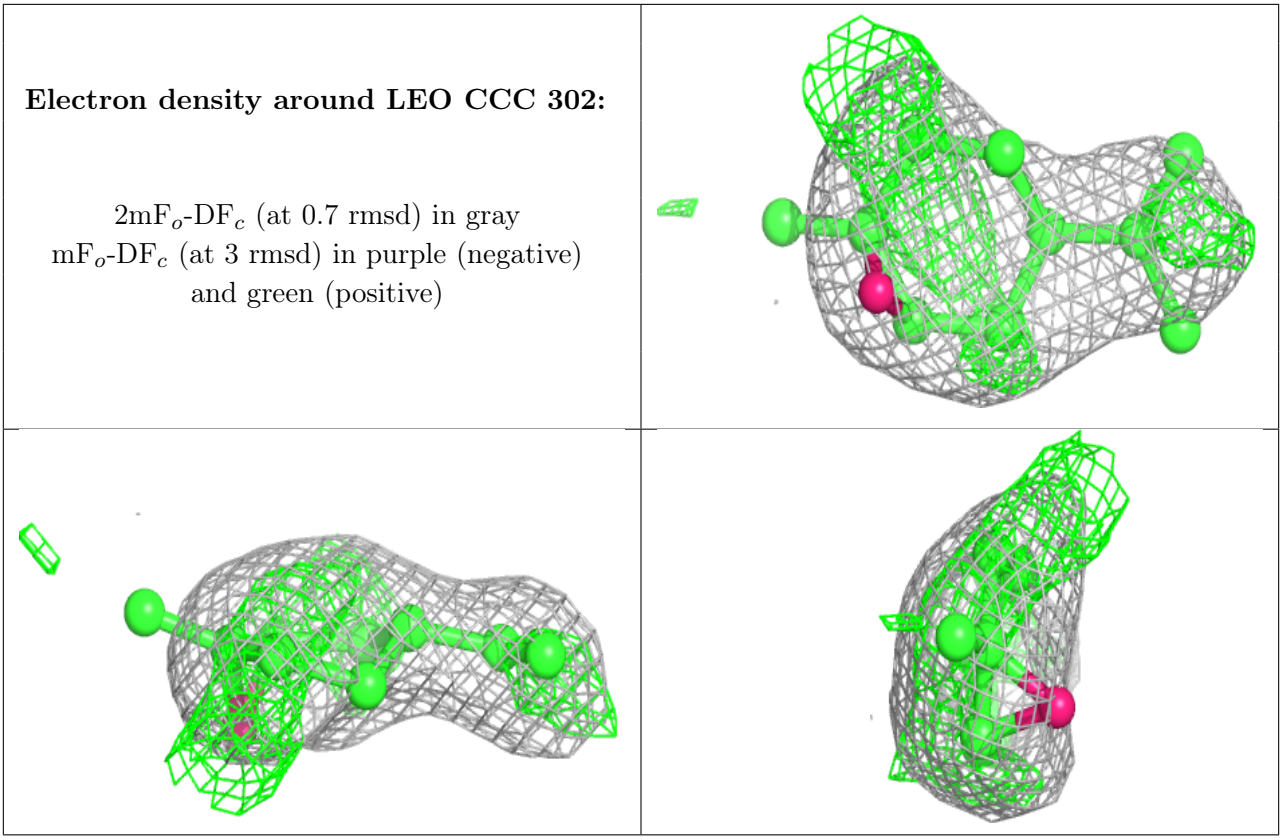
Electron density around LEO AAA 301 (A):

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



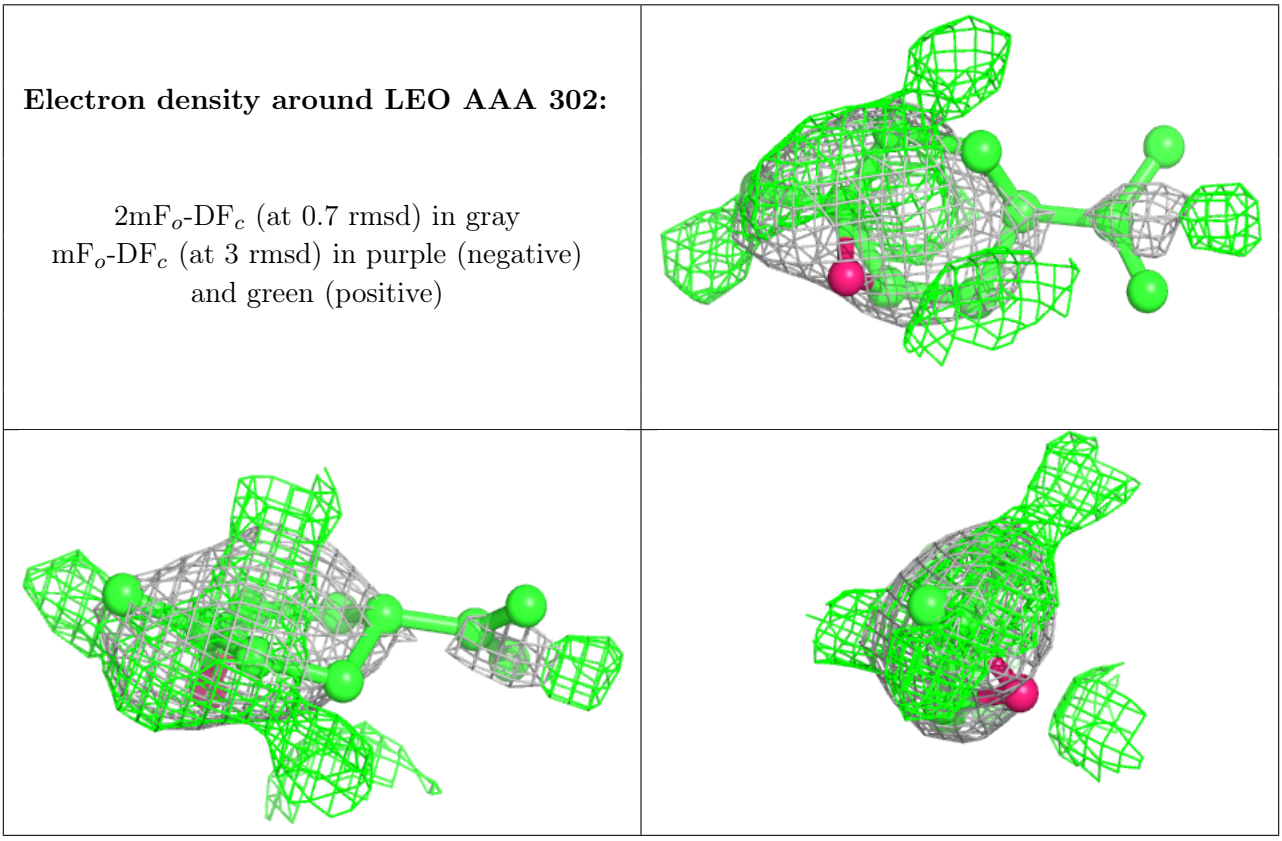
Electron density around LEO CCC 302:

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



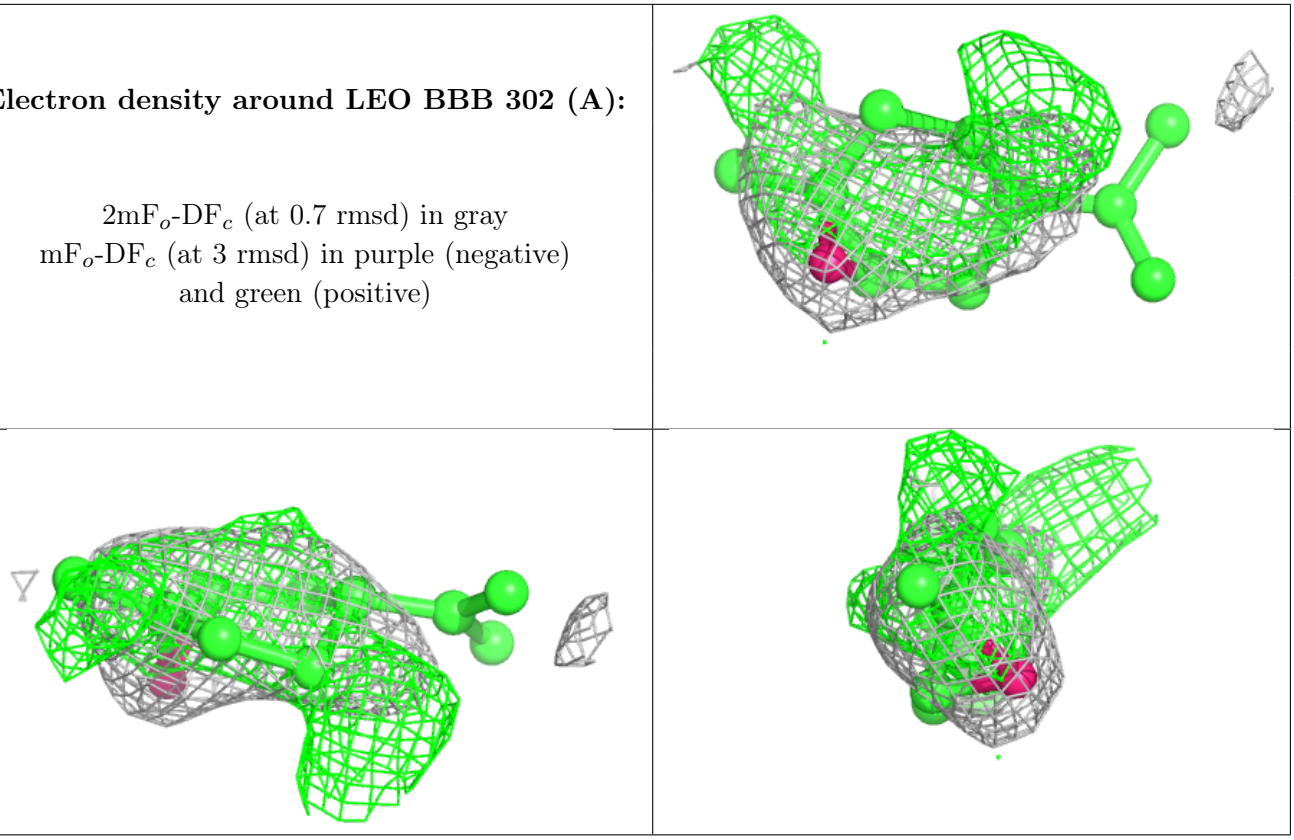
Electron density around LEO AAA 302:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.