Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 06:02 pm BST

PDB ID	:	8AGN
Title	:	Cyclohexane 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	:	1.96 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:

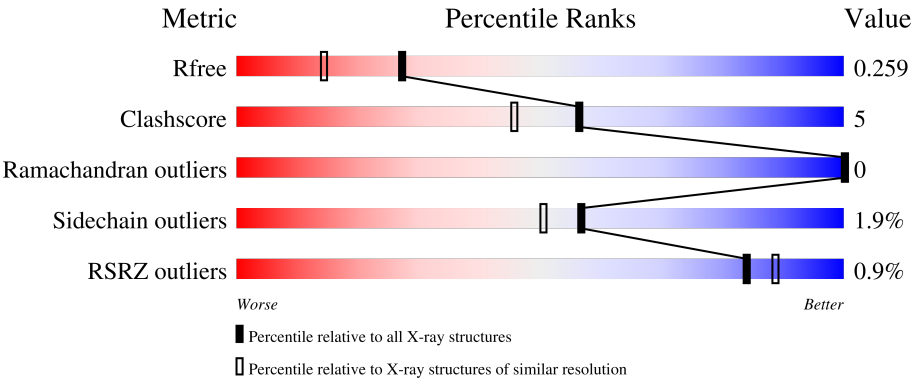
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.96 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	86% 9%
1	BBB	299	87% 9%
1	CCC	299	2% 86% 12%
1	DDD	299	% 87% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10226 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
			2439	1608	407	415	9			
1	BBB	288	Total	C	N	O	S	0	12	0
			2440	1612	400	420	8			
1	CCC	293	Total	C	N	O	S	0	13	0
			2498	1645	419	425	9			
1	DDD	290	Total	C	N	O	S	0	9	0
			2442	1606	407	421	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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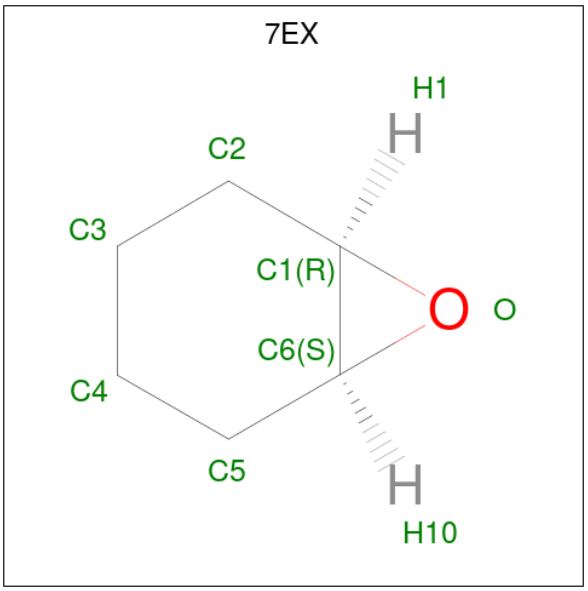
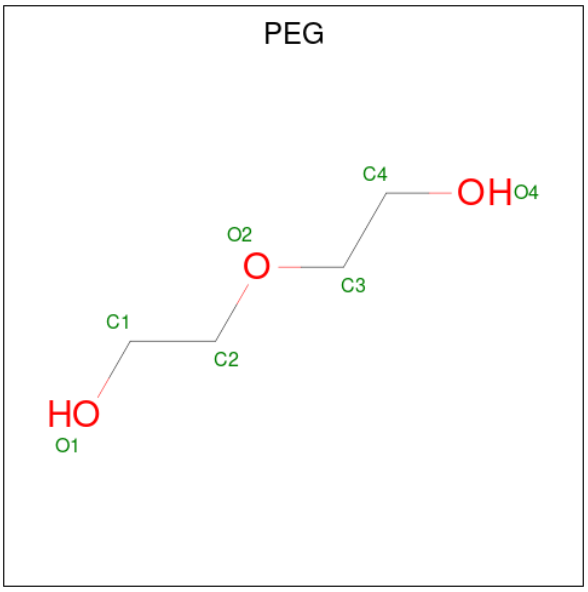
Chain	Residue	Modelled	Actual	Comment	Reference
DDD	297	HIS	-	expression tag	UNP A0A1U9WZ52
DDD	298	HIS	-	expression tag	UNP A0A1U9WZ52
DDD	299	HIS	-	expression tag	UNP A0A1U9WZ52

- Molecule 2 is (1R,6S)-7-oxabicyclo[4.1.0]heptane (three-letter code: 7EX) (formula: $C_6H_{10}O$) (labeled as "Ligand of Interest" by depositor).



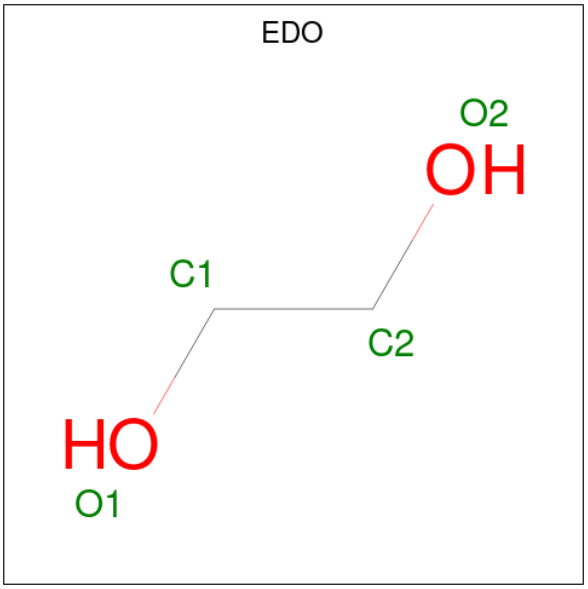
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			7	6	1		
2	AAA	1	Total	C	O	0	0
			7	6	1		
2	BBB	1	Total	C	O	0	0
			7	6	1		
2	BBB	1	Total	C	O	0	0
			7	6	1		
2	CCC	1	Total	C	O	0	0
			7	6	1		
2	CCC	1	Total	C	O	0	0
			7	6	1		
2	DDD	1	Total	C	O	0	0
			7	6	1		
2	DDD	1	Total	C	O	0	0
			7	6	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 7 4 3	0	0
3	AAA	1	Total C O 7 4 3	0	0
3	BBB	1	Total C O 7 4 3	0	0
3	DDD	1	Total C O 7 4 3	0	0
3	DDD	1	Total C O 7 4 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is water.

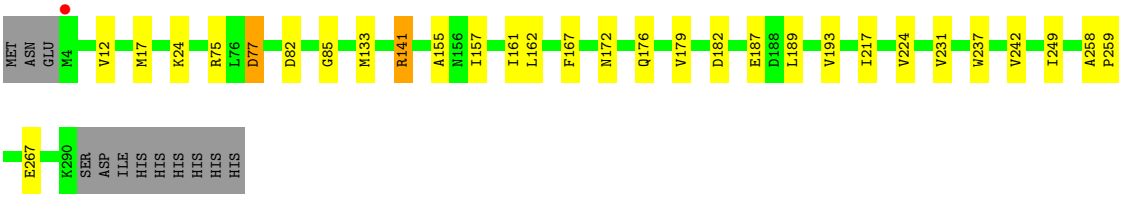
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	63	Total O 63 63	0	0
5	BBB	82	Total O 82 82	0	0
5	CCC	71	Total O 71 71	0	0
5	DDD	56	Total O 56 56	0	0

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:

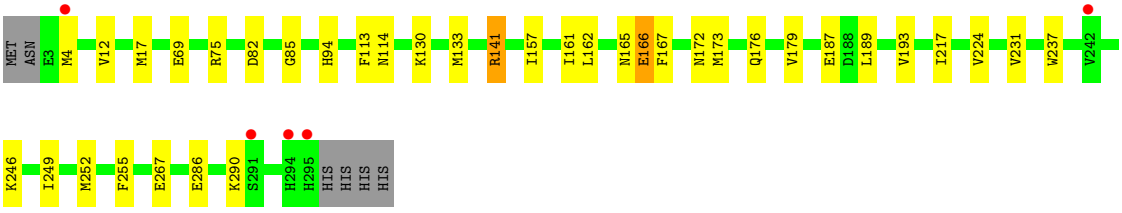


• Molecule 1: Alpha/beta epoxide hydrolase

Chain BBB:

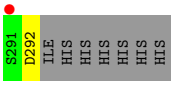
• Molecule 1: Alpha/beta epoxide hydrolase

Chain CCC:



• Molecule 1: Alpha/beta epoxide hydrolase

Chain DDD:


S291
D292
ILE
HIS
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	95.85Å 47.33Å 142.61Å 90.00° 91.71° 90.00°	Depositor
Resolution (Å)	142.55 – 1.96 142.55 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.7 (142.55-1.96) 99.7 (142.55-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0267, BUSTER	Depositor
R, R_{free}	0.205 , 0.259 0.205 , 0.259	Depositor DCC
R_{free} test set	4502 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10226	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: 7EX, PEG, 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	0.52	0/2541	0.82	0/3440
1	BBB	0.59	0/2542	0.85	1/3444 (0.0%)
1	CCC	0.54	0/2602	0.80	1/3523 (0.0%)
1	DDD	0.54	1/2535 (0.0%)	0.80	0/3434
All	All	0.55	1/10220 (0.0%)	0.82	2/13841 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	187	GLU	CD-OE2	5.52	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CCC	4	MET	CG-SD-CE	5.14	108.42	100.20
1	BBB	181	ARG	CG-CD-NE	-5.02	101.26	111.80

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	2439	0	2514	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	2440	0	2511	27	0
1	CCC	2498	0	2571	29	0
1	DDD	2442	0	2499	21	0
2	AAA	14	0	0	0	0
2	BBB	14	0	0	1	0
2	CCC	14	0	0	1	0
2	DDD	14	0	0	0	0
3	AAA	14	0	20	3	0
3	BBB	7	0	10	2	0
3	DDD	14	0	20	0	0
4	AAA	12	0	18	2	0
4	BBB	8	0	12	0	0
4	CCC	12	0	18	2	0
4	DDD	12	0	18	3	0
5	AAA	63	0	0	1	0
5	BBB	82	0	0	0	0
5	CCC	71	0	0	1	0
5	DDD	56	0	0	0	0
All	All	10226	0	10211	101	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (101) 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:CCC:12[B]:VAL:HG21	1:CCC:17[B]:MET:SD	1.95	1.06
1:BBB:12[B]:VAL:HG21	1:BBB:17[B]:MET:SD	1.99	1.03
1:AAA:12[B]:VAL:HG21	1:AAA:17[B]:MET:SD	2.03	0.96
1:DDD:133[B]:MET:HA	1:DDD:133[B]:MET:CE	2.06	0.85
1:CCC:12[B]:VAL:CG2	1:CCC:17[B]:MET:SD	2.68	0.81
1:BBB:234:LEU:HD11	1:BBB:263:LYS:HD2	1.62	0.81
1:BBB:237:TRP:CH2	1:BBB:249[A]:ILE:HG21	2.18	0.78
1:BBB:12[B]:VAL:CG2	1:BBB:17[B]:MET:SD	2.74	0.76
1:CCC:12[B]:VAL:HG22	1:CCC:17[B]:MET:HG3	1.70	0.73
1:AAA:12[B]:VAL:HG22	1:AAA:17[B]:MET:HG3	1.70	0.73
1:BBB:12[B]:VAL:HG22	1:BBB:17[B]:MET:HG3	1.69	0.72
1:CCC:237:TRP:CZ2	1:CCC:249:ILE:HG21	2.26	0.71
1:AAA:12[B]:VAL:CG2	1:AAA:17[B]:MET:SD	2.80	0.69
1:CCC:172:ASN:O	1:CCC:176:GLN:HG3	1.93	0.68
1:DDD:133[B]:MET:HA	1:DDD:133[B]:MET:HE1	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:237:TRP:CH2	1:CCC:249:ILE:HG21	2.31	0.65
1:BBB:237:TRP:CZ2	1:BBB:249[A]:ILE:HG21	2.32	0.64
1:BBB:237:TRP:CH2	1:BBB:249[A]:ILE:CG2	2.80	0.64
1:CCC:12[A]:VAL:HG13	1:CCC:85:GLY:HA3	1.80	0.63
1:BBB:181:ARG:NH2	1:BBB:182:ASP:OD2	2.32	0.63
1:CCC:133[B]:MET:SD	1:CCC:224:VAL:HG21	2.40	0.62
1:BBB:181:ARG:NH1	1:DDD:133[A]:MET:HE1	2.15	0.62
1:BBB:172:ASN:HD21	3:BBB:301:PEG:H12	1.64	0.61
1:DDD:133[A]:MET:HE3	4:DDD:305:EDO:O2	2.01	0.60
4:AAA:304:EDO:O2	4:AAA:307:EDO:H22	2.01	0.60
1:DDD:12[A]:VAL:HG13	1:DDD:85:GLY:HA3	1.85	0.59
1:AAA:12[A]:VAL:HG13	1:AAA:85:GLY:HA3	1.85	0.59
1:CCC:237:TRP:CH2	1:CCC:249:ILE:CG2	2.87	0.58
1:BBB:237:TRP:CZ3	1:BBB:249[A]:ILE:HG21	2.39	0.58
1:AAA:237:TRP:CZ2	1:AAA:249:ILE:HG21	2.38	0.58
1:BBB:263:LYS:HD3	1:BBB:283:HIS:ND1	2.19	0.57
1:BBB:12[A]:VAL:HG13	1:BBB:85:GLY:HA3	1.87	0.57
1:BBB:172:ASN:O	1:BBB:176:GLN:HG2	2.06	0.56
1:DDD:172:ASN:O	1:DDD:176:GLN:HG2	2.06	0.56
1:AAA:12[A]:VAL:HG11	1:AAA:82:ASP:O	2.07	0.55
1:AAA:172:ASN:O	1:AAA:176:GLN:HG2	2.07	0.55
1:AAA:133[A]:MET:SD	1:AAA:224:VAL:HG21	2.48	0.54
1:BBB:133[A]:MET:SD	1:BBB:224:VAL:HG21	2.47	0.54
1:AAA:242:VAL:CG1	4:AAA:305:EDO:H21	2.38	0.54
1:CCC:141[B]:ARG:HH12	1:CCC:246:LYS:HG2	1.73	0.53
1:CCC:12[A]:VAL:HG11	1:CCC:82:ASP:O	2.07	0.53
1:AAA:237:TRP:CH2	1:AAA:249:ILE:HG21	2.44	0.53
1:DDD:12[A]:VAL:HG11	1:DDD:82:ASP:O	2.08	0.52
1:BBB:12[A]:VAL:HG11	1:BBB:82:ASP:O	2.09	0.52
1:CCC:286:GLU:O	1:CCC:290:LYS:HB2	2.10	0.51
1:DDD:133[B]:MET:CE	1:DDD:133[B]:MET:CA	2.83	0.51
1:CCC:133[A]:MET:SD	1:CCC:217:ILE:HG22	2.52	0.50
1:BBB:181:ARG:HH12	1:DDD:133[A]:MET:HE1	1.76	0.50
1:AAA:237:TRP:CH2	1:AAA:249:ILE:CG2	2.96	0.49
1:DDD:179:VAL:HG21	1:DDD:267:GLU:O	2.13	0.49
1:BBB:173:MET:HB3	2:BBB:303:7EX:C1	2.43	0.49
1:AAA:133[B]:MET:HE3	3:AAA:306:PEG:H22	1.95	0.48
1:CCC:165:ASN:C	1:CCC:166[B]:GLU:HG2	2.34	0.47
1:CCC:179:VAL:HG21	1:CCC:267:GLU:O	2.14	0.47
1:CCC:187:GLU:HA	1:CCC:187:GLU:OE1	2.14	0.47
1:AAA:258:ALA:HB1	1:AAA:259:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:189:LEU:O	1:DDD:193:VAL:HG23	2.14	0.47
1:CCC:237:TRP:CE2	1:CCC:249:ILE:HG21	2.50	0.46
1:DDD:116:GLN:HA	4:DDD:307:EDO:H21	1.97	0.46
1:CCC:113:PHE:O	4:CCC:303:EDO:H12	2.16	0.46
1:CCC:173:MET:HB3	2:CCC:302:7EX:C1	2.45	0.46
1:CCC:249:ILE:HB	1:CCC:252[B]:MET:HE2	1.98	0.46
1:AAA:75[B]:ARG:NH2	1:AAA:77[B]:ASP:OD1	2.49	0.45
1:AAA:133[B]:MET:SD	1:AAA:217:ILE:HG22	2.55	0.45
1:AAA:179:VAL:HG21	1:AAA:267:GLU:O	2.16	0.45
1:AAA:133[B]:MET:HE3	3:AAA:306:PEG:C2	2.47	0.45
1:AAA:157:ILE:HG22	1:AAA:161:ILE:HD12	1.99	0.45
1:DDD:246:LYS:HE3	1:DDD:264:TYR:CE1	2.52	0.45
1:DDD:133[B]:MET:SD	1:DDD:217:ILE:CG2	3.05	0.44
1:DDD:12[B]:VAL:HG11	1:DDD:86:LEU:HA	1.99	0.44
1:CCC:189:LEU:O	1:CCC:193:VAL:HG23	2.18	0.44
1:AAA:155:ALA:O	1:AAA:157:ILE:HD12	2.18	0.44
1:BBB:3:GLU:HG3	1:BBB:22:GLN:HG3	1.99	0.44
1:CCC:141[A]:ARG:HD2	1:CCC:141[A]:ARG:HA	1.78	0.43
1:BBB:3:GLU:HG2	1:BBB:22:GLN:HG2	1.99	0.43
1:DDD:9:TYR:CD2	1:DDD:16:LYS:HE3	2.53	0.43
1:DDD:133[B]:MET:SD	1:DDD:217:ILE:HG22	2.59	0.43
1:DDD:162:LEU:O	1:DDD:167:PHE:HA	2.18	0.43
1:AAA:141:ARG:HA	1:AAA:141:ARG:HD2	1.74	0.43
1:DDD:258:ALA:HB1	1:DDD:259:PRO:HD2	2.00	0.43
1:AAA:187:GLU:HG3	5:AAA:445:HOH:O	2.17	0.43
1:BBB:176:GLN:NE2	3:BBB:301:PEG:H11	2.33	0.43
1:BBB:162:LEU:O	1:BBB:167:PHE:HA	2.19	0.43
1:DDD:133[A]:MET:CE	4:DDD:305:EDO:O2	2.67	0.43
1:CCC:75[A]:ARG:NE	5:CCC:405:HOH:O	2.51	0.42
1:CCC:237:TRP:CZ2	1:CCC:249:ILE:CG2	2.99	0.42
1:CCC:157[B]:ILE:HG22	1:CCC:161:ILE:HD12	2.02	0.42
1:BBB:133[B]:MET:SD	1:BBB:217:ILE:HG22	2.60	0.42
1:DDD:155:ALA:O	1:DDD:157:ILE:HD12	2.20	0.42
1:CCC:12[B]:VAL:HG22	1:CCC:17[B]:MET:CG	2.44	0.42
1:AAA:189:LEU:O	1:AAA:193:VAL:HG23	2.20	0.41
1:AAA:162:LEU:O	1:AAA:167:PHE:HA	2.20	0.41
1:BBB:12[B]:VAL:CG2	1:BBB:17[B]:MET:HG3	2.46	0.41
1:BBB:180:ARG:HB2	1:BBB:183:LEU:HD13	2.03	0.41
1:CCC:114:ASN:OD1	4:CCC:303:EDO:H11	2.21	0.41
1:BBB:12[B]:VAL:HG22	1:BBB:17[B]:MET:CG	2.46	0.41
1:BBB:187:GLU:HA	1:BBB:187:GLU:OE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:133[B]:MET:CE	3:AAA:306:PEG:H42	2.51	0.41
1:AAA:237:TRP:CE2	1:AAA:249:ILE:HG21	2.56	0.40
1:CCC:162:LEU:O	1:CCC:167:PHE:HA	2.22	0.40
1:CCC:130:LYS:HD3	1:CCC:255:PHE:HE1	1.86	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%)	288 (97%)	9 (3%)	0	100	100
1	BBB	298/299 (100%)	289 (97%)	9 (3%)	0	100	100
1	CCC	304/299 (102%)	297 (98%)	7 (2%)	0	100	100
1	DDD	297/299 (99%)	289 (97%)	8 (3%)	0	100	100
All	All	1196/1196 (100%)	1163 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	267/267 (100%)	261 (98%)	6 (2%)	52	44
1	BBB	268/267 (100%)	262 (98%)	6 (2%)	52	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	CCC	274/267 (103%)	267 (97%)	7 (3%)	46 36
1	DDD	267/267 (100%)	261 (98%)	6 (2%)	52 44
All	All	1076/1068 (101%)	1051 (98%)	25 (2%)	57 42

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	24	LYS
1	AAA	77[A]	ASP
1	AAA	77[B]	ASP
1	AAA	141	ARG
1	AAA	182	ASP
1	AAA	231	VAL
1	BBB	94	HIS
1	BBB	141	ARG
1	BBB	166[A]	GLU
1	BBB	166[B]	GLU
1	BBB	225	VAL
1	BBB	231	VAL
1	CCC	69	GLU
1	CCC	94	HIS
1	CCC	141[A]	ARG
1	CCC	141[B]	ARG
1	CCC	166[A]	GLU
1	CCC	166[B]	GLU
1	CCC	231	VAL
1	DDD	182	ASP
1	DDD	224	VAL
1	DDD	231	VAL
1	DDD	254[A]	ASP
1	DDD	254[B]	ASP
1	DDD	292	ASP

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

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)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	CCC	303	-	3,3,3	0.44	0	2,2,2	0.64	0
4	EDO	DDD	307	-	3,3,3	0.41	0	2,2,2	0.73	0
4	EDO	BBB	304	-	3,3,3	0.21	0	2,2,2	0.31	0
2	7EX	AAA	301	-	8,8,8	1.90	1 (12%)	11,11,11	4.59	8 (72%)
4	EDO	CCC	305	-	3,3,3	0.17	0	2,2,2	0.23	0
3	PEG	AAA	306	-	6,6,6	0.22	0	5,5,5	0.32	0
4	EDO	AAA	305	-	3,3,3	0.34	0	2,2,2	0.28	0
2	7EX	BBB	302	-	8,8,8	2.24	1 (12%)	11,11,11	3.70	7 (63%)
3	PEG	AAA	303	-	6,6,6	0.23	0	5,5,5	0.20	0
4	EDO	DDD	305	-	3,3,3	0.11	0	2,2,2	0.41	0
3	PEG	DDD	301	-	6,6,6	0.34	0	5,5,5	0.27	0
4	EDO	CCC	304	-	3,3,3	0.27	0	2,2,2	0.80	0
4	EDO	AAA	307	-	3,3,3	0.33	0	2,2,2	0.20	0
4	EDO	AAA	304	-	3,3,3	0.19	0	2,2,2	0.58	0
2	7EX	BBB	303	-	8,8,8	1.73	1 (12%)	11,11,11	3.43	7 (63%)
3	PEG	BBB	301	-	6,6,6	0.40	0	5,5,5	0.17	0
4	EDO	DDD	306	-	3,3,3	0.10	0	2,2,2	0.37	0
3	PEG	DDD	302	-	6,6,6	0.21	0	5,5,5	0.29	0
4	EDO	BBB	305	-	3,3,3	0.14	0	2,2,2	0.04	0
2	7EX	DDD	304	-	8,8,8	1.70	1 (12%)	11,11,11	4.58	7 (63%)
2	7EX	CCC	302	-	8,8,8	1.91	1 (12%)	11,11,11	3.52	7 (63%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	7EX	AAA	302	-	8,8,8	1.70	1 (12%)	11,11,11	4.01	9 (81%)
2	7EX	DDD	303	-	8,8,8	1.98	2 (25%)	11,11,11	3.93	5 (45%)
2	7EX	CCC	301	-	8,8,8	2.08	1 (12%)	11,11,11	3.76	8 (72%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	CCC	303	-	-	0/1/1/1	-
4	EDO	DDD	307	-	-	0/1/1/1	-
4	EDO	BBB	304	-	-	0/1/1/1	-
4	EDO	CCC	305	-	-	1/1/1/1	-
2	7EX	AAA	301	-	-	-	0/2/2/2
3	PEG	AAA	306	-	-	3/4/4/4	-
4	EDO	AAA	305	-	-	1/1/1/1	-
2	7EX	BBB	302	-	-	-	0/2/2/2
3	PEG	AAA	303	-	-	3/4/4/4	-
4	EDO	DDD	305	-	-	1/1/1/1	-
3	PEG	DDD	301	-	-	3/4/4/4	-
4	EDO	CCC	304	-	-	0/1/1/1	-
4	EDO	AAA	307	-	-	1/1/1/1	-
4	EDO	AAA	304	-	-	0/1/1/1	-
4	EDO	DDD	306	-	-	1/1/1/1	-
3	PEG	BBB	301	-	-	3/4/4/4	-
2	7EX	CCC	301	-	-	-	0/2/2/2
3	PEG	DDD	302	-	-	2/4/4/4	-
4	EDO	BBB	305	-	-	0/1/1/1	-
2	7EX	DDD	304	-	-	-	0/2/2/2
2	7EX	CCC	302	-	-	-	0/2/2/2
2	7EX	AAA	302	-	-	-	0/2/2/2
2	7EX	DDD	303	-	-	-	0/2/2/2
2	7EX	BBB	303	-	-	-	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	302	7EX	C6-C1	5.83	1.56	1.46
2	CCC	301	7EX	C6-C1	5.00	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	301	7EX	C6-C1	4.94	1.55	1.46
2	CCC	302	7EX	C6-C1	4.67	1.54	1.46
2	DDD	303	7EX	C6-C1	4.64	1.54	1.46
2	AAA	302	7EX	C6-C1	4.47	1.54	1.46
2	DDD	304	7EX	C6-C1	4.38	1.54	1.46
2	BBB	303	7EX	C6-C1	4.05	1.53	1.46
2	DDD	303	7EX	C2-C1	2.98	1.58	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	303	7EX	C5-C6-C1	-9.53	110.56	121.08
2	DDD	304	7EX	C5-C6-C1	-9.31	110.81	121.08
2	DDD	304	7EX	C2-C1-C6	-8.58	111.62	121.08
2	AAA	301	7EX	C5-C6-C1	-8.53	111.66	121.08
2	AAA	301	7EX	C2-C1-C6	-8.31	111.91	121.08
2	BBB	302	7EX	C6-O-C1	8.12	66.55	60.69
2	CCC	301	7EX	C6-O-C1	7.64	66.20	60.69
2	AAA	302	7EX	C2-C1-C6	-6.42	114.00	121.08
2	AAA	301	7EX	C6-O-C1	5.99	65.01	60.69
2	CCC	302	7EX	C6-O-C1	5.88	64.93	60.69
2	AAA	302	7EX	C6-O-C1	5.78	64.86	60.69
2	DDD	304	7EX	C6-O-C1	5.73	64.82	60.69
2	AAA	302	7EX	C4-C3-C2	-5.41	100.38	111.42
2	CCC	301	7EX	O-C1-C6	-5.27	56.28	59.65
2	DDD	303	7EX	C6-O-C1	5.24	64.46	60.69
2	BBB	303	7EX	C2-C1-C6	-5.21	115.33	121.08
2	CCC	301	7EX	O-C6-C5	-5.16	107.26	115.75
2	BBB	303	7EX	O-C6-C1	-5.06	56.42	59.65
2	BBB	302	7EX	O-C1-C6	-5.03	56.44	59.65
2	BBB	303	7EX	C6-O-C1	4.90	64.22	60.69
2	AAA	302	7EX	C3-C4-C5	-4.79	101.64	111.42
2	DDD	303	7EX	C2-C1-C6	-4.68	115.92	121.08
2	CCC	302	7EX	C2-C1-C6	-4.56	116.05	121.08
2	BBB	302	7EX	O-C6-C1	-4.12	57.02	59.65
2	CCC	302	7EX	C4-C5-C6	4.09	118.89	110.86
2	CCC	302	7EX	C5-C6-C1	-4.09	116.57	121.08
2	CCC	302	7EX	C3-C2-C1	4.06	118.82	110.86
2	AAA	301	7EX	O-C1-C6	-4.03	57.07	59.65
2	BBB	303	7EX	C5-C6-C1	-4.00	116.67	121.08
2	DDD	303	7EX	O-C1-C6	-3.94	57.13	59.65
2	BBB	302	7EX	C5-C6-C1	-3.67	117.03	121.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	301	7EX	C3-C2-C1	-3.66	103.67	110.86
2	BBB	303	7EX	C4-C5-C6	3.55	117.83	110.86
2	CCC	301	7EX	C5-C6-C1	-3.47	117.25	121.08
2	AAA	302	7EX	O-C6-C1	-3.43	57.46	59.65
2	CCC	302	7EX	O-C6-C1	-3.43	57.46	59.65
2	DDD	304	7EX	O-C1-C6	-3.34	57.52	59.65
2	CCC	301	7EX	O-C6-C1	-3.34	57.52	59.65
2	BBB	303	7EX	C4-C3-C2	-3.22	104.85	111.42
2	CCC	302	7EX	O-C1-C6	-3.19	57.61	59.65
2	BBB	302	7EX	O-C6-C5	-3.14	110.58	115.75
2	DDD	304	7EX	O-C6-C1	-3.10	57.67	59.65
2	AAA	302	7EX	O-C1-C6	-3.09	57.68	59.65
2	AAA	302	7EX	C5-C6-C1	-3.05	117.72	121.08
2	AAA	302	7EX	O-C6-C5	-3.01	110.80	115.75
2	BBB	302	7EX	C4-C3-C2	-3.00	105.31	111.42
2	AAA	302	7EX	O-C1-C2	-2.71	111.28	115.75
2	BBB	303	7EX	O-C1-C2	-2.71	111.28	115.75
2	AAA	301	7EX	O-C6-C1	-2.71	57.92	59.65
2	DDD	303	7EX	C3-C2-C1	2.69	116.14	110.86
2	CCC	301	7EX	C3-C2-C1	2.60	115.96	110.86
2	DDD	304	7EX	O-C1-C2	-2.49	111.66	115.75
2	BBB	302	7EX	O-C1-C2	-2.29	111.98	115.75
2	AAA	301	7EX	C3-C4-C5	2.25	115.99	111.42
2	AAA	301	7EX	C4-C5-C6	-2.18	106.59	110.86
2	DDD	304	7EX	O-C6-C5	-2.17	112.17	115.75
2	CCC	301	7EX	O-C1-C2	-2.07	112.34	115.75
2	CCC	301	7EX	C4-C3-C2	-2.02	107.30	111.42

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	306	PEG	O1-C1-C2-O2
3	DDD	302	PEG	O2-C3-C4-O4
3	DDD	301	PEG	O1-C1-C2-O2
3	DDD	302	PEG	O1-C1-C2-O2
4	AAA	305	EDO	O1-C1-C2-O2
4	AAA	307	EDO	O1-C1-C2-O2
4	DDD	305	EDO	O1-C1-C2-O2
4	DDD	306	EDO	O1-C1-C2-O2
3	AAA	306	PEG	O2-C3-C4-O4
3	BBB	301	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	DDD	301	PEG	O2-C3-C4-O4
3	AAA	303	PEG	O1-C1-C2-O2
4	CCC	305	EDO	O1-C1-C2-O2
3	AAA	303	PEG	C4-C3-O2-C2
3	BBB	301	PEG	O1-C1-C2-O2
3	BBB	301	PEG	C1-C2-O2-C3
3	AAA	306	PEG	C1-C2-O2-C3
3	DDD	301	PEG	C4-C3-O2-C2
3	AAA	303	PEG	O2-C3-C4-O4

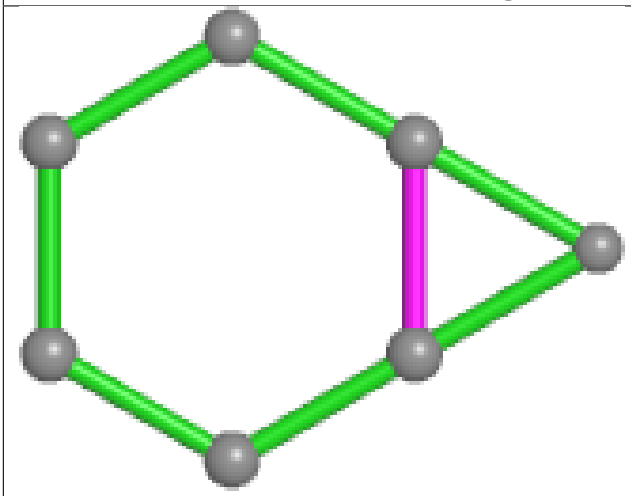
There are no ring outliers.

10 monomers are involved in 14 short contacts:

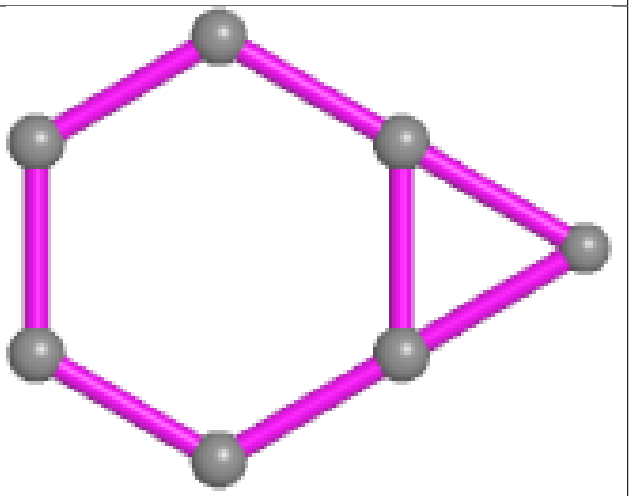
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	303	EDO	2	0
4	DDD	307	EDO	1	0
3	AAA	306	PEG	3	0
4	AAA	305	EDO	1	0
4	DDD	305	EDO	2	0
4	AAA	307	EDO	1	0
4	AAA	304	EDO	1	0
2	BBB	303	7EX	1	0
3	BBB	301	PEG	2	0
2	CCC	302	7EX	1	0

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 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.

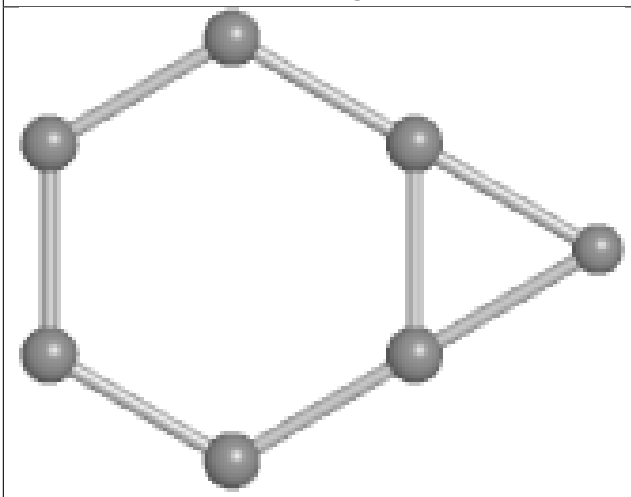
Ligand 7EX AAA 301



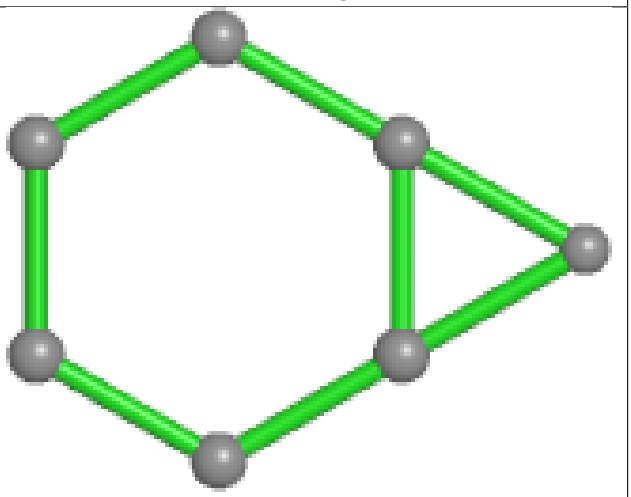
Bond lengths



Bond angles

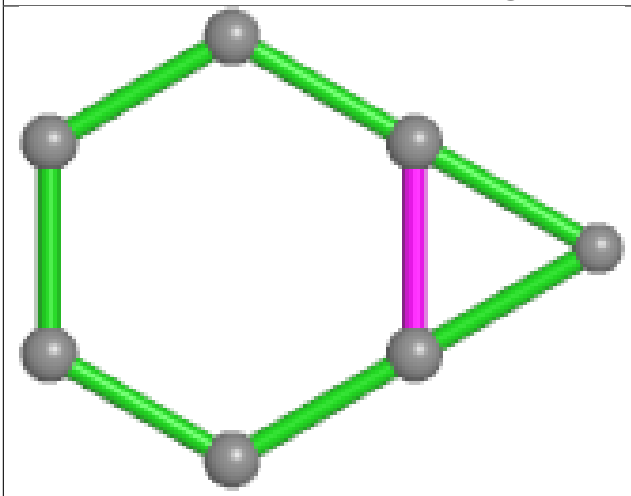


Torsions

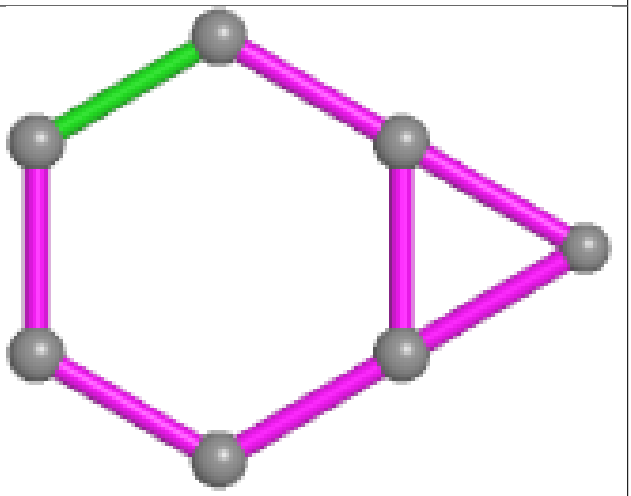


Rings

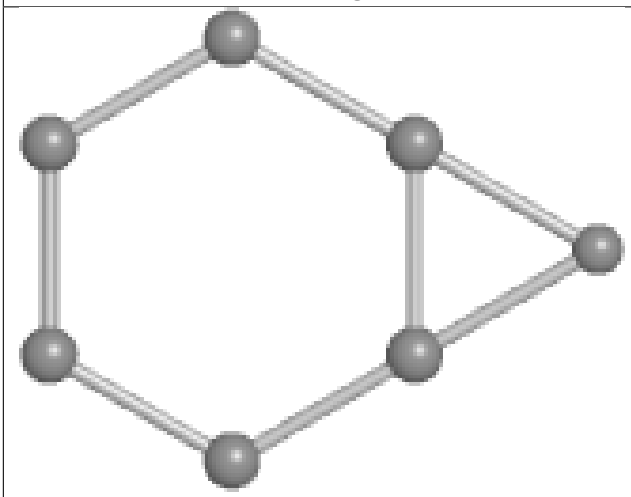
Ligand 7EX BBB 302



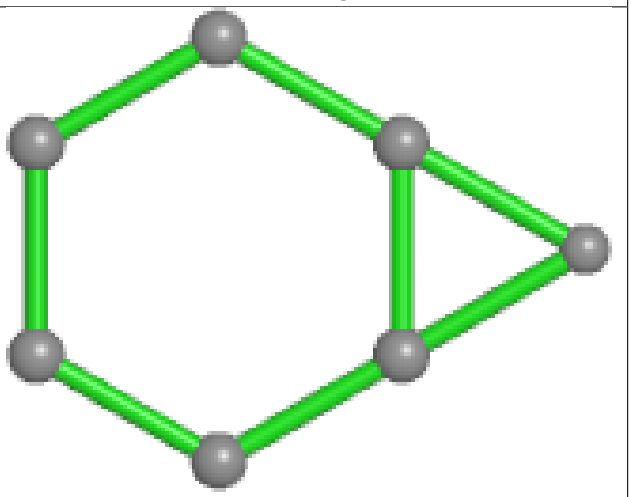
Bond lengths



Bond angles

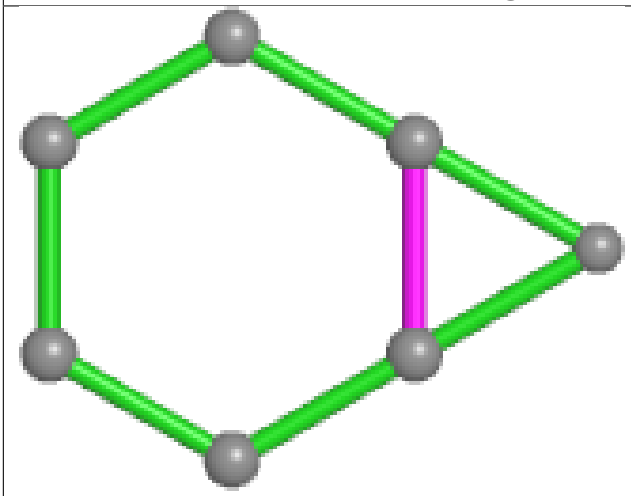


Torsions

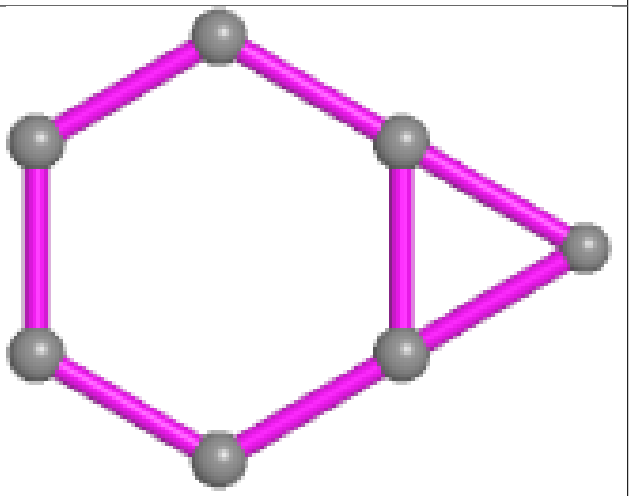


Rings

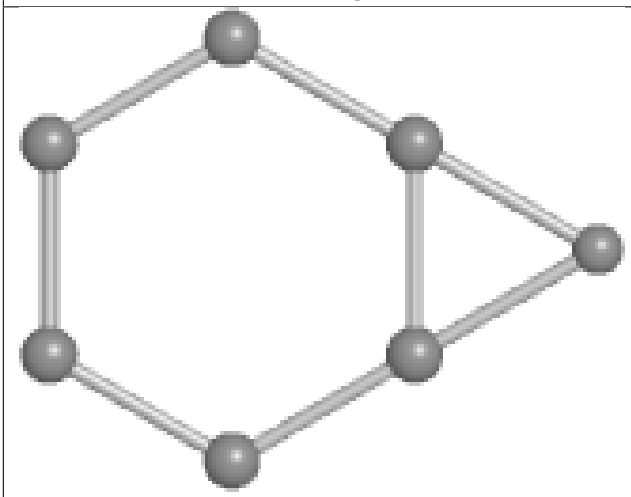
Ligand 7EX BBB 303



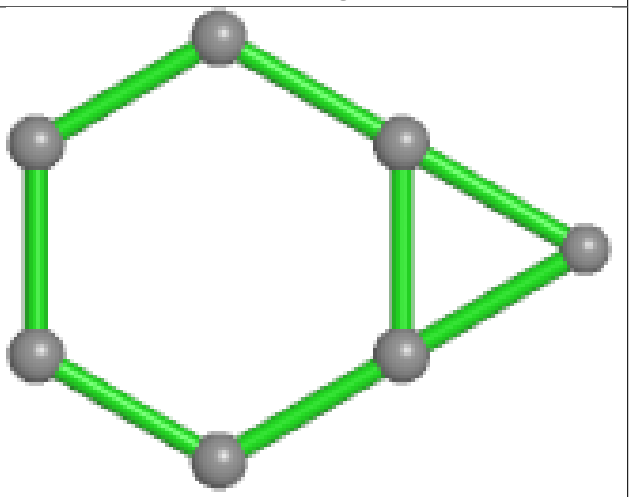
Bond lengths



Bond angles

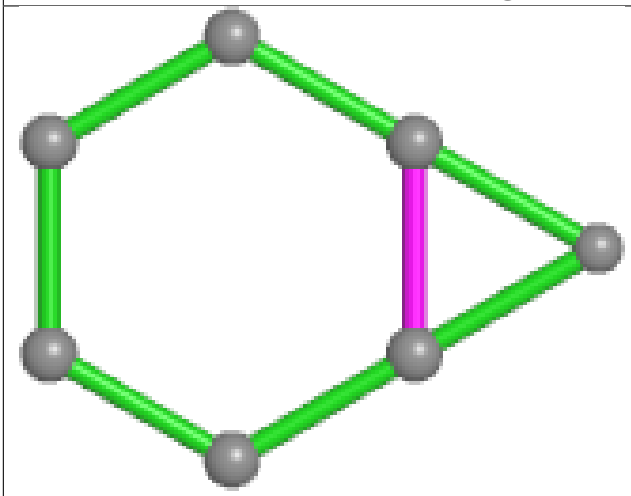


Torsions

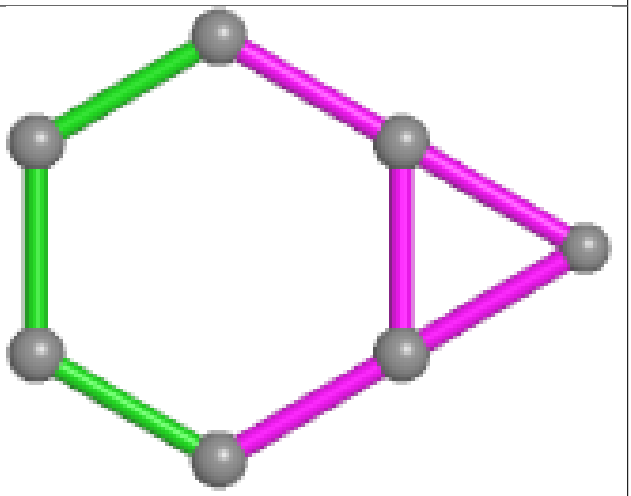


Rings

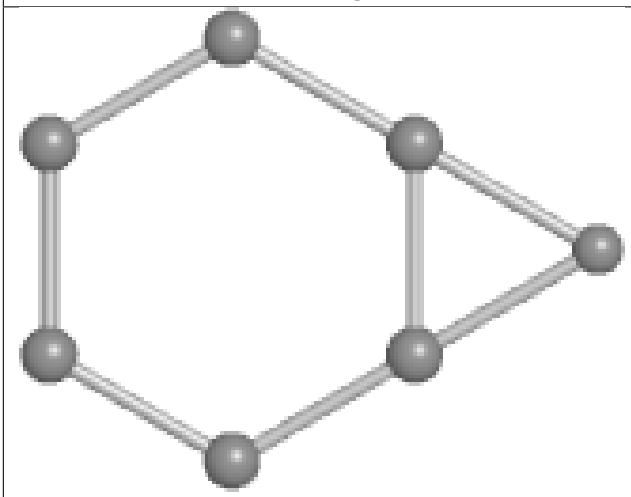
Ligand 7EX DDD 304



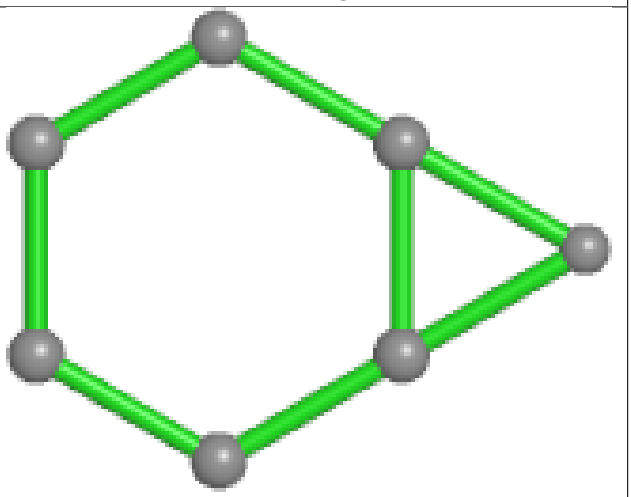
Bond lengths



Bond angles

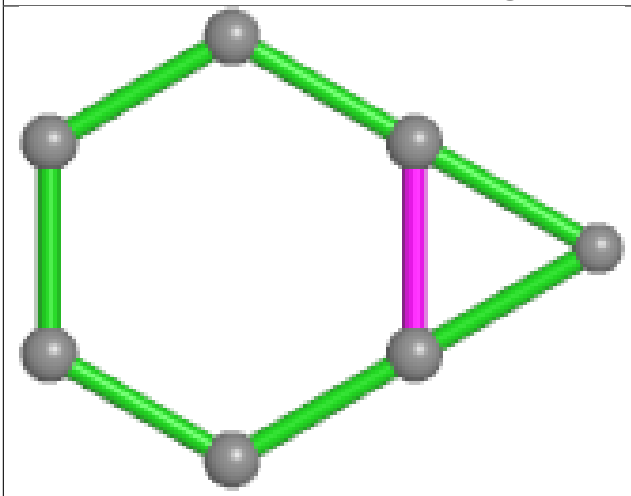


Torsions

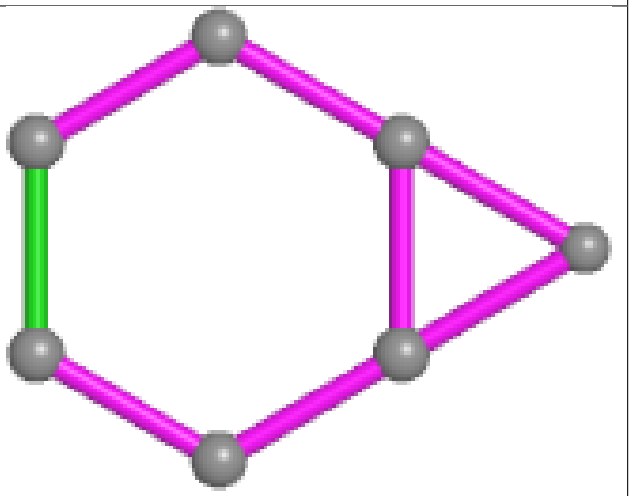


Rings

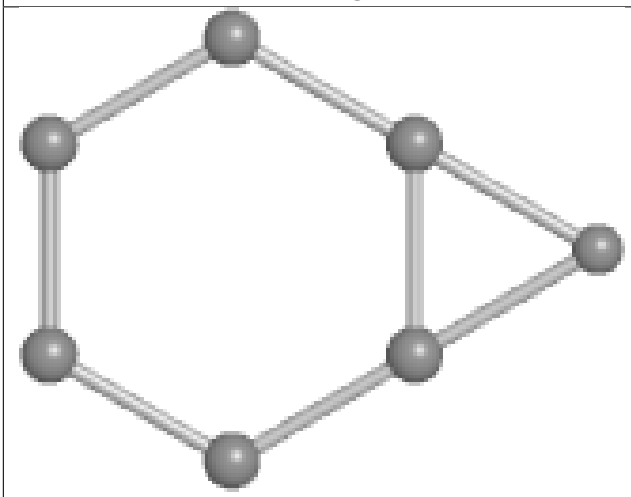
Ligand 7EX CCC 302



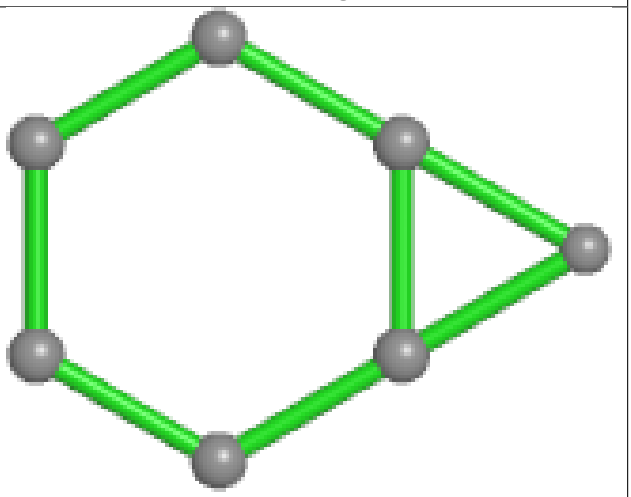
Bond lengths



Bond angles

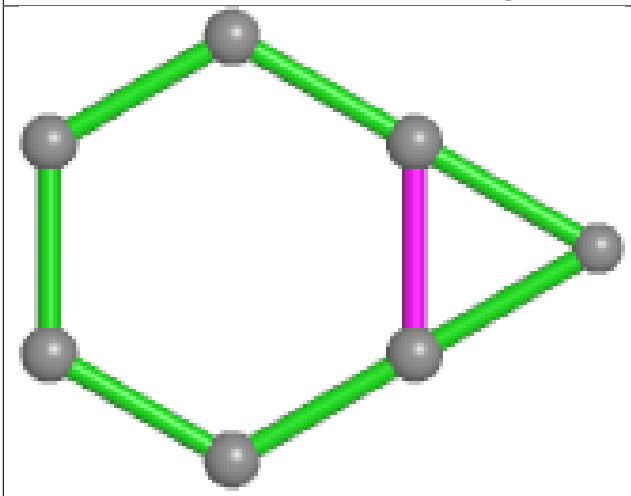


Torsions

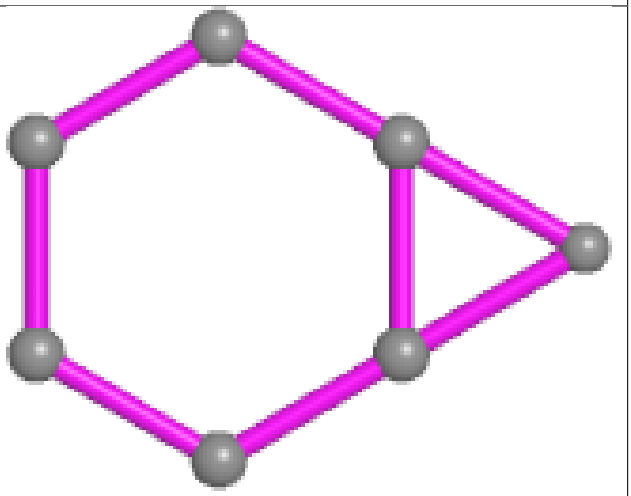


Rings

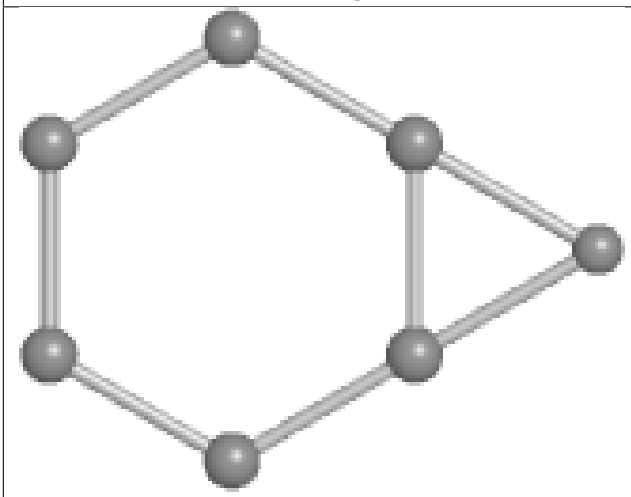
Ligand 7EX AAA 302



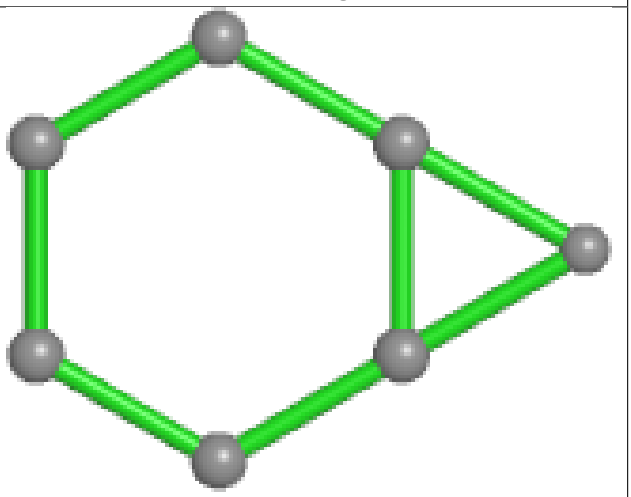
Bond lengths



Bond angles

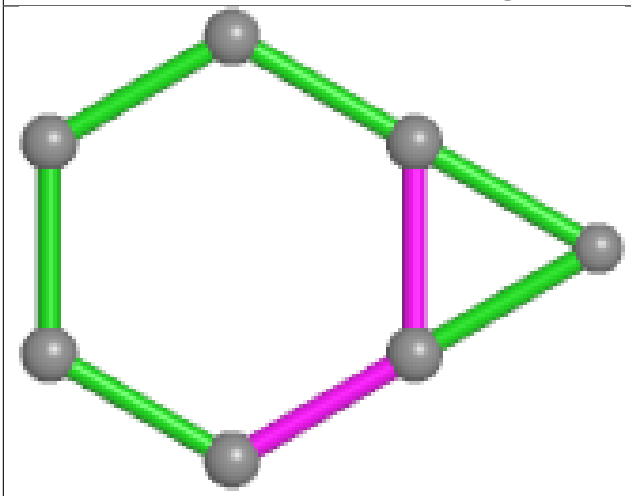


Torsions

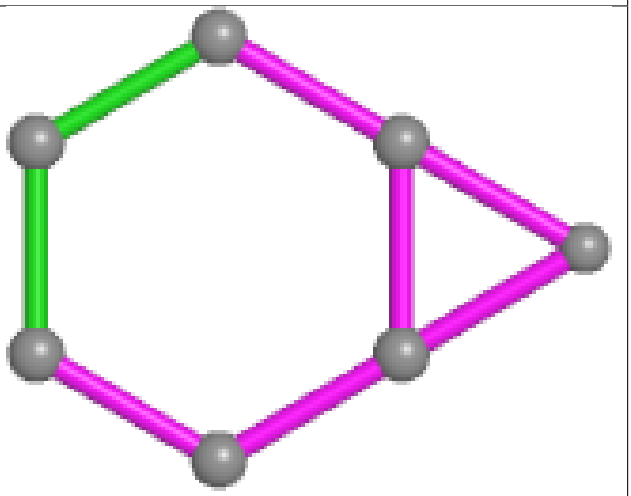


Rings

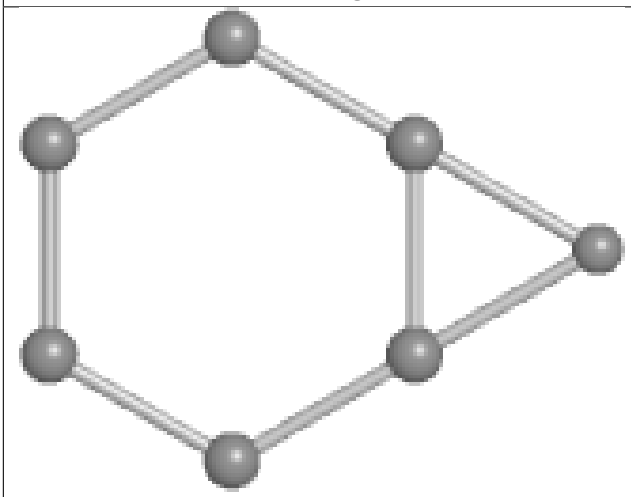
Ligand 7EX DDD 303



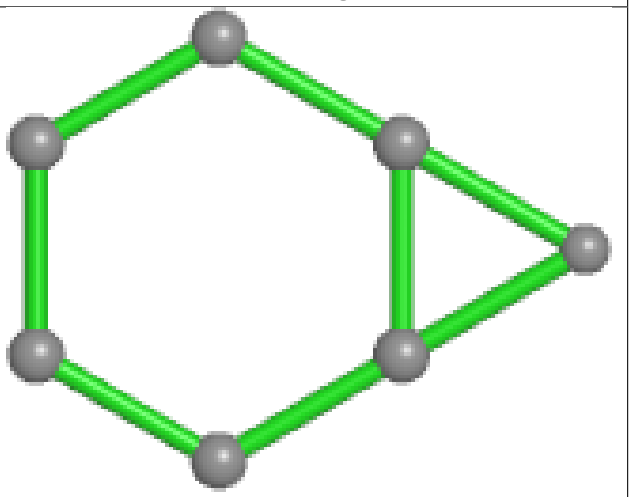
Bond lengths



Bond angles

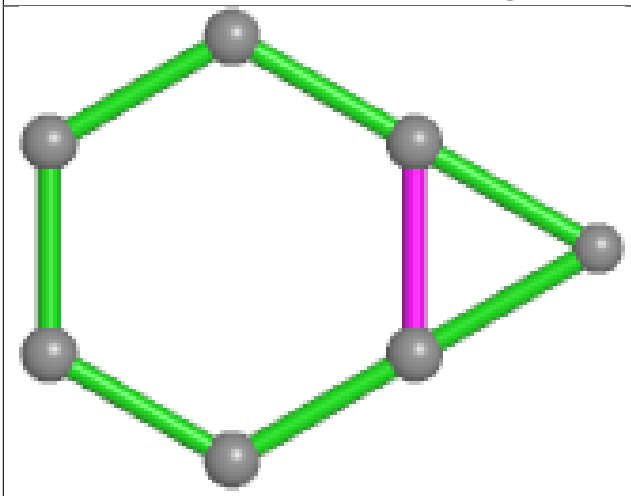


Torsions

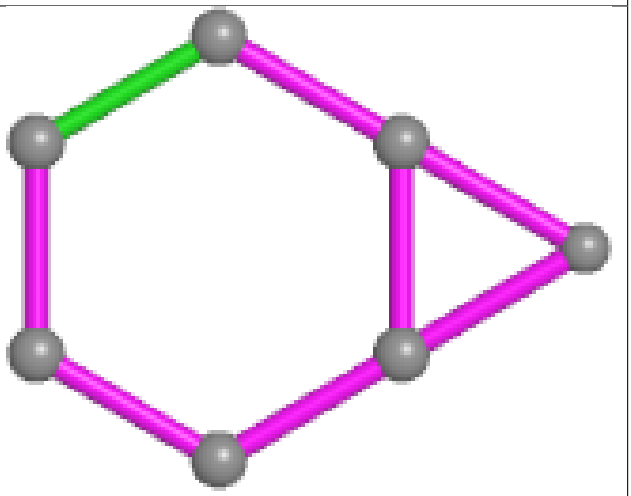


Rings

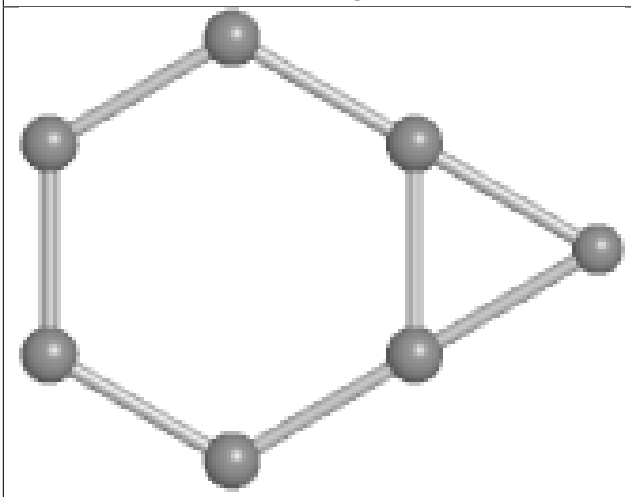
Ligand 7EX CCC 301



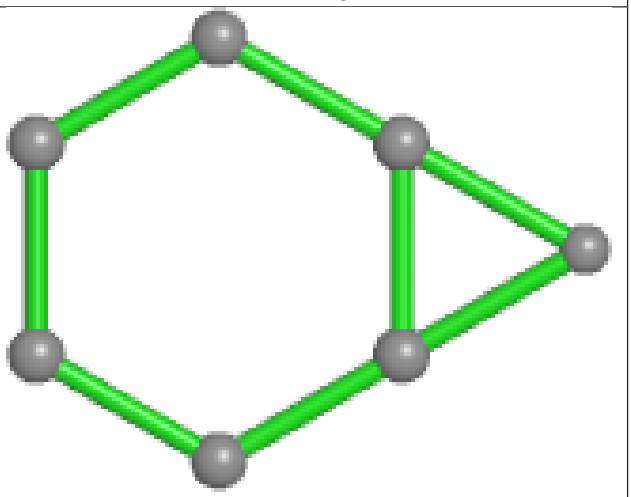
Bond lengths



Bond angles



Torsions



Rings

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, 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%)	0.10	1 (0%)	94	96	34, 53, 80, 107	0
1	BBB	288/299 (96%)	-0.04	1 (0%)	94	96	32, 46, 67, 105	0
1	CCC	293/299 (97%)	0.20	5 (1%)	70	77	33, 50, 89, 130	0
1	DDD	290/299 (96%)	0.07	3 (1%)	82	87	32, 52, 83, 131	0
All	All	1158/1196 (96%)	0.08	10 (0%)	84	89	32, 50, 81, 131	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	291	SER	3.8
1	CCC	291	SER	3.4
1	CCC	242	VAL	3.4
1	CCC	294	HIS	3.4
1	CCC	4	MET	2.6
1	CCC	295	HIS	2.5
1	AAA	4	MET	2.4
1	DDD	3	GLU	2.3
1	BBB	223	THR	2.2
1	DDD	289	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

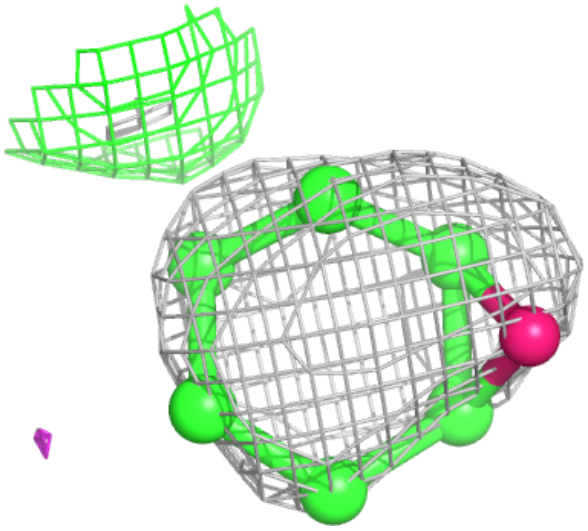
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

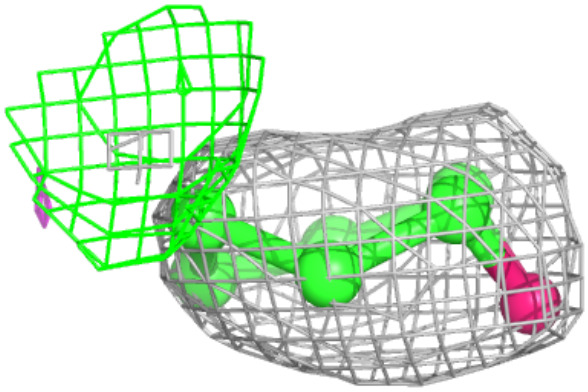
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	AAA	305	4/4	0.63	0.27	68,83,90,91	0
4	EDO	DDD	306	4/4	0.71	0.17	79,87,102,110	0
3	PEG	DDD	301	7/7	0.77	0.17	60,76,95,101	0
4	EDO	AAA	304	4/4	0.80	0.17	80,91,91,96	0
3	PEG	AAA	306	7/7	0.83	0.28	82,89,101,110	0
2	7EX	BBB	303	7/7	0.87	0.28	69,88,116,118	0
2	7EX	CCC	302	7/7	0.87	0.24	93,97,110,119	0
3	PEG	DDD	302	7/7	0.87	0.15	46,65,83,88	0
4	EDO	DDD	305	4/4	0.88	0.20	64,68,73,75	0
4	EDO	DDD	307	4/4	0.88	0.14	54,70,75,87	0
3	PEG	AAA	303	7/7	0.89	0.11	60,66,73,83	0
4	EDO	AAA	307	4/4	0.89	0.16	60,74,78,88	0
4	EDO	CCC	303	4/4	0.89	0.11	50,57,66,70	0
4	EDO	CCC	304	4/4	0.90	0.17	52,67,82,97	0
3	PEG	BBB	301	7/7	0.90	0.10	46,54,61,67	0
4	EDO	BBB	304	4/4	0.91	0.32	60,66,95,118	0
2	7EX	AAA	302	7/7	0.91	0.21	55,71,89,91	0
4	EDO	CCC	305	4/4	0.92	0.13	58,58,68,69	0
4	EDO	BBB	305	4/4	0.93	0.18	60,61,82,88	0
2	7EX	AAA	301	7/7	0.94	0.15	46,61,90,96	0
2	7EX	DDD	304	7/7	0.94	0.20	62,79,103,114	0
2	7EX	BBB	302	7/7	0.95	0.14	51,60,66,77	0
2	7EX	DDD	303	7/7	0.96	0.14	47,60,75,91	0
2	7EX	CCC	301	7/7	0.96	0.14	59,73,80,81	0

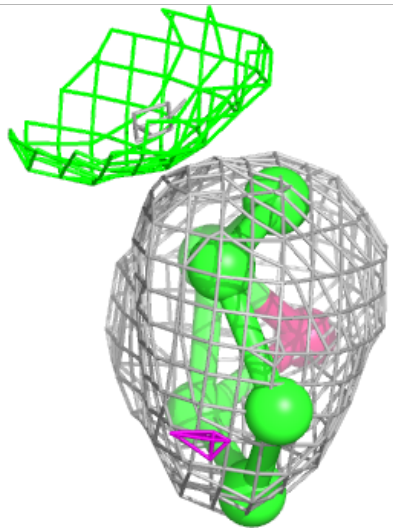
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7EX 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)

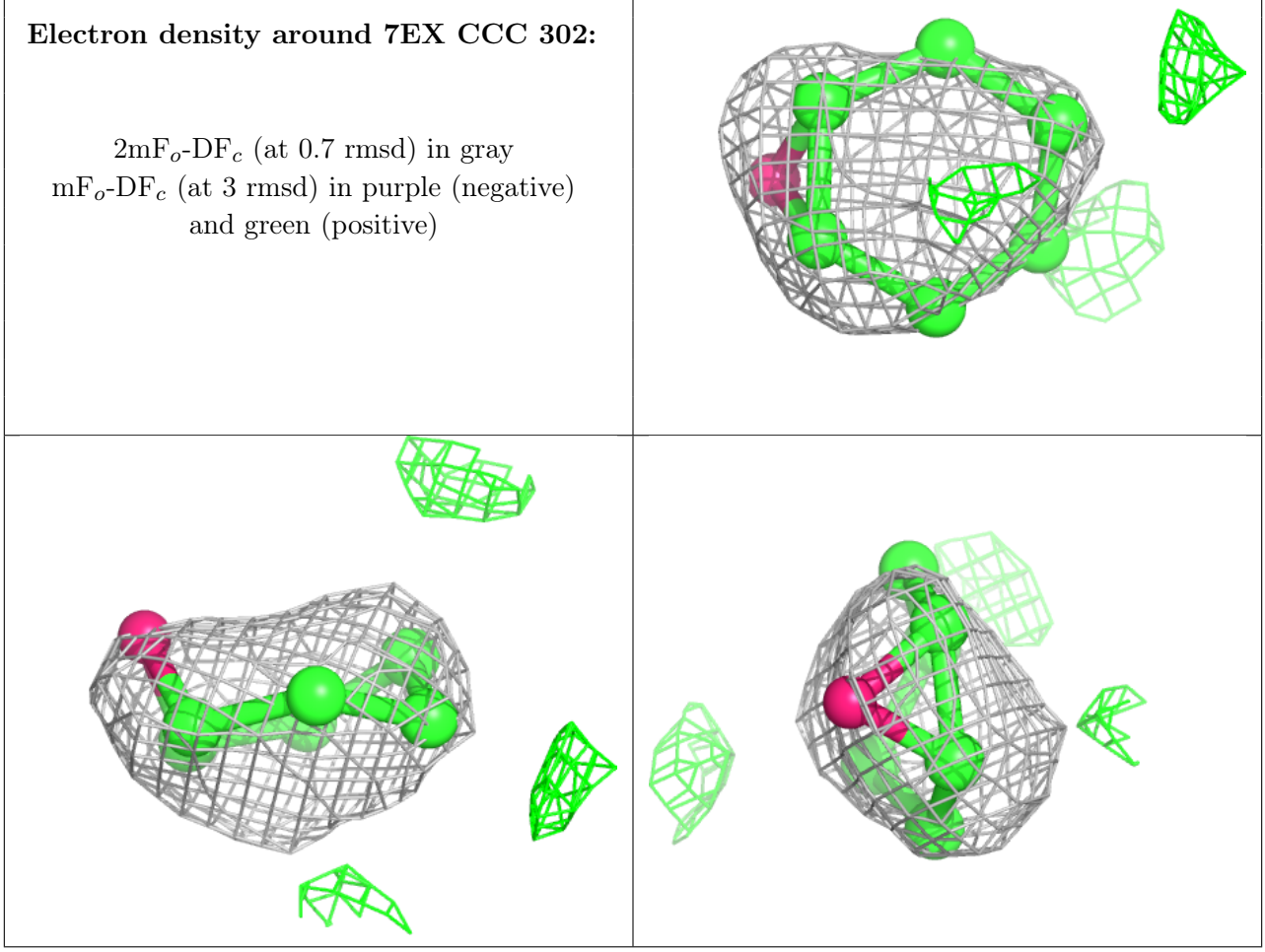






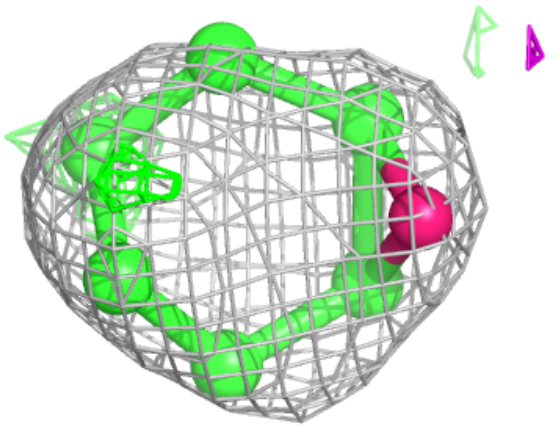
Electron density around 7EX CCC 302:

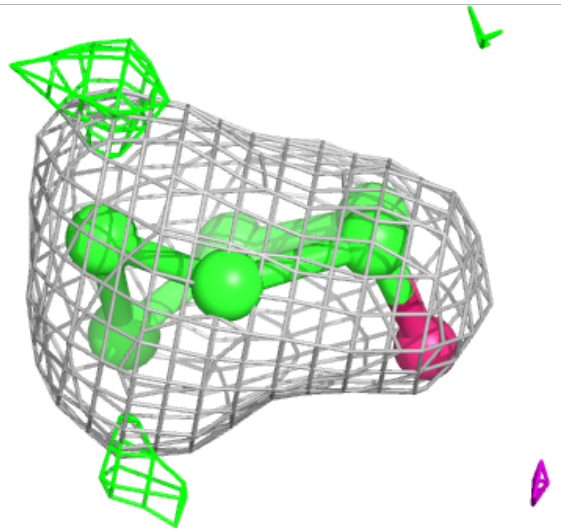
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

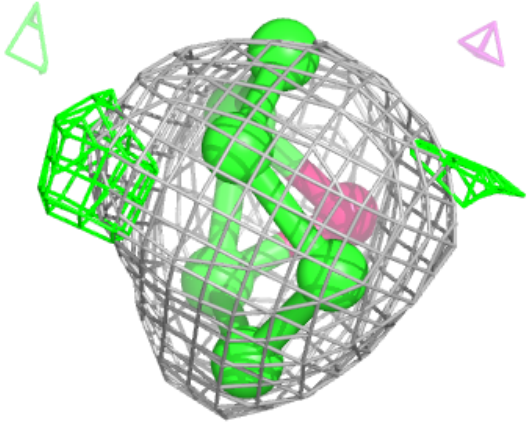


Electron density around 7EX AAA 302:

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

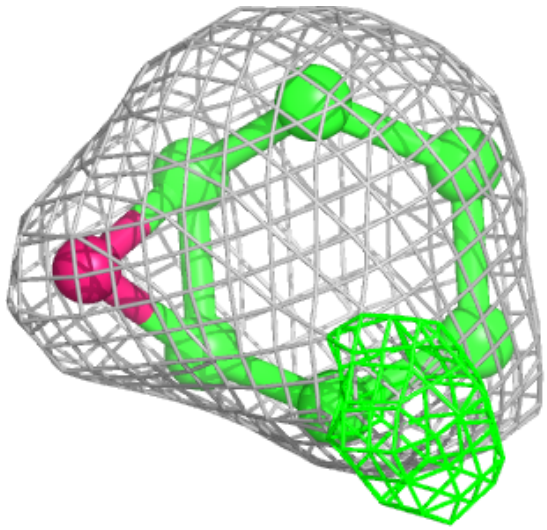


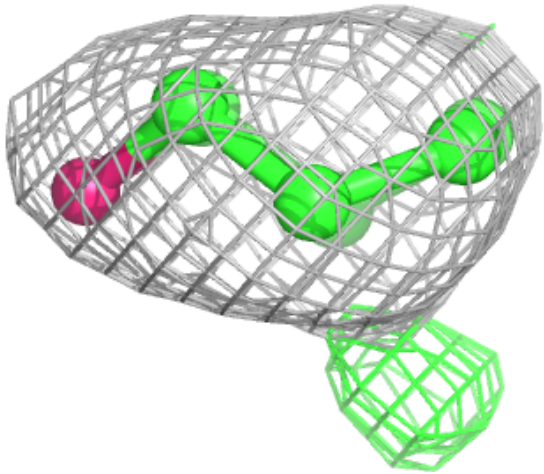


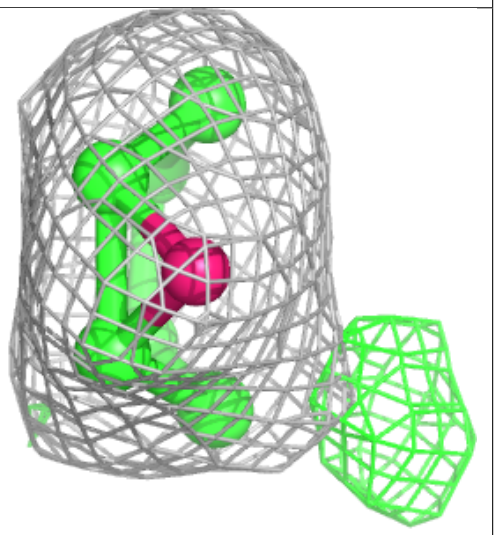


Electron density around 7EX AAA 301:

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

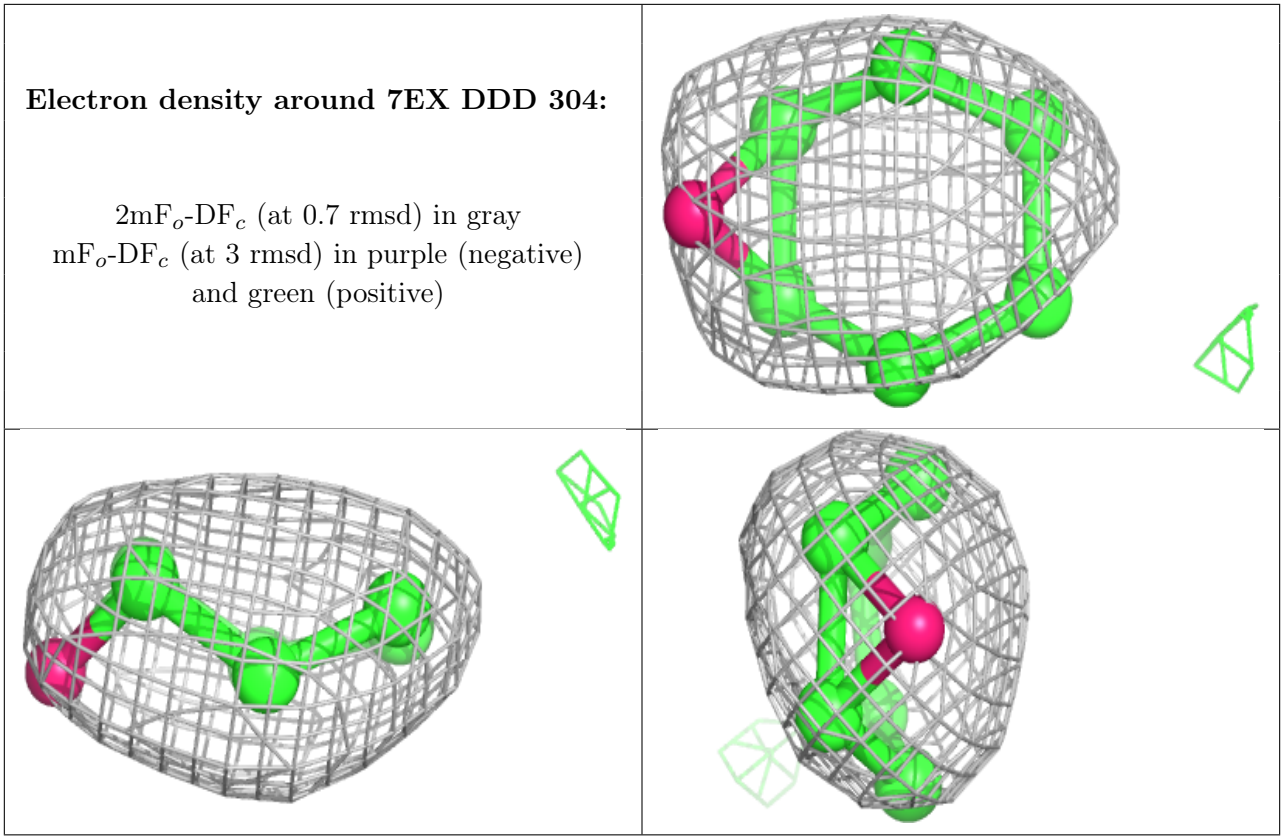






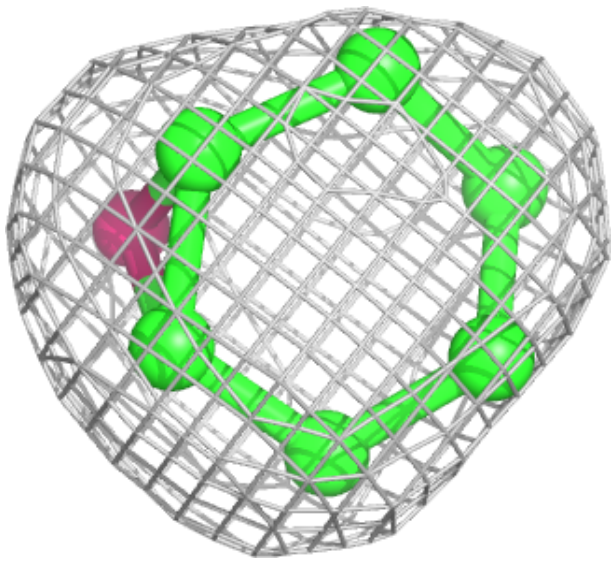
Electron density around 7EX DDD 304:

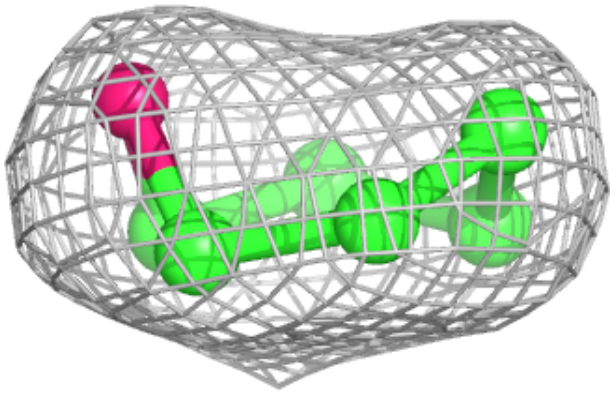
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

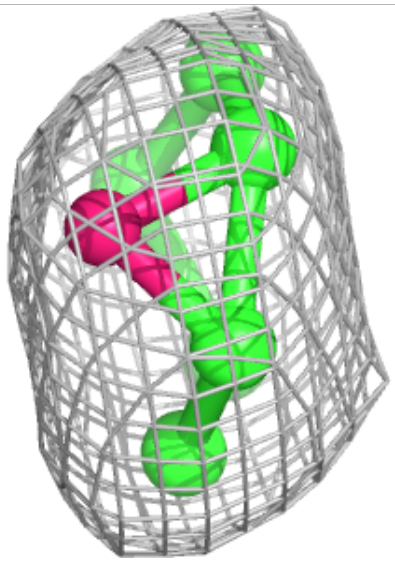


Electron density around 7EX BBB 302:

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

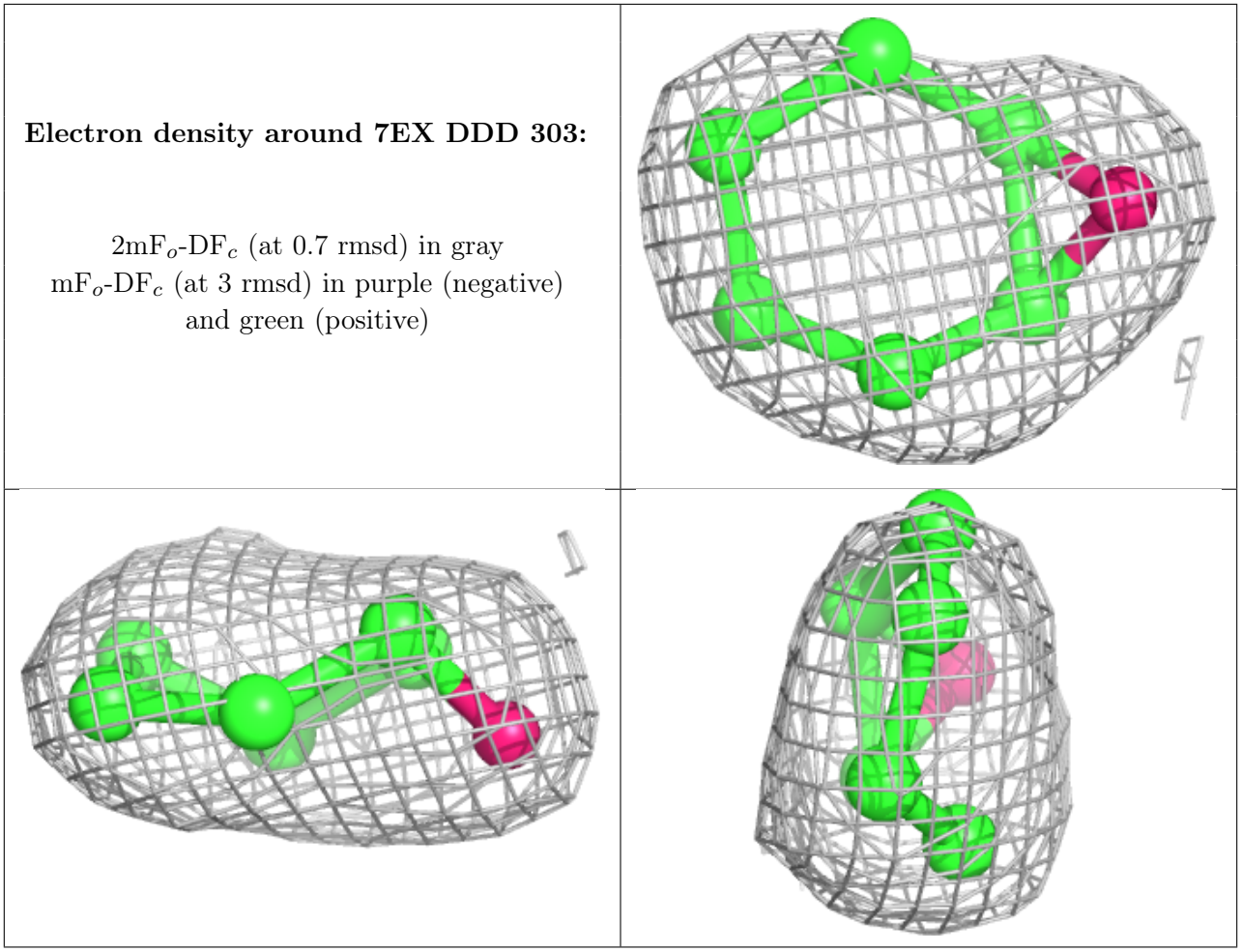






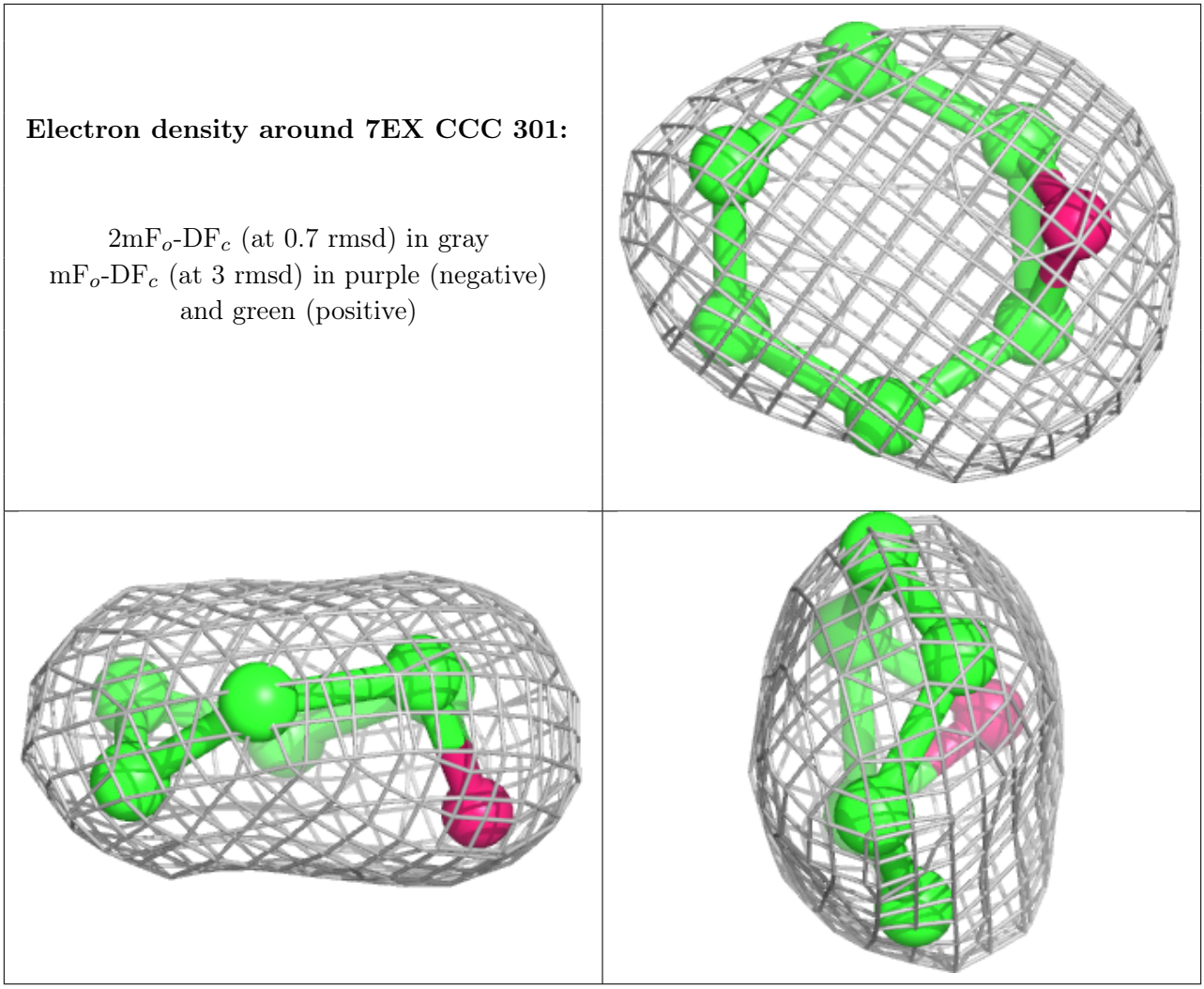
Electron density around 7EX DDD 303:

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



Electron density around 7EX CCC 301:

$2mF_o$-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.