Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 02:32 PM EDT

PDB ID	:	4ZBF
Title	:	Mcl-1 complexed with small molecules
Authors	:	Zhao, B.
Deposited on	:	2015-04-14
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

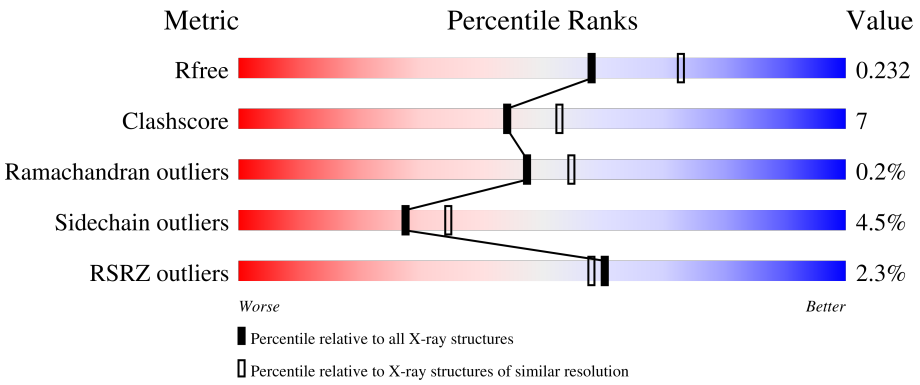
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	A	157	% 83% 13% • •
1	B	157	% 83% 13% • •
1	C	157	% 80% 13% • 5%
1	D	157	% 78% 16% 6%
1	E	157	% 78% 17% • •

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Mol	Chain	Length	Quality of chain
1	F	157	76% 18% 6%
1	G	157	3% 76% 19%
1	H	157	3% 80% 17%
1	I	157	3% 80% 15%
1	J	157	7% 82% 12%
1	K	157	2% 78% 17%
1	L	157	4% 76% 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15189 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 Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1222	767	226	225	4	0	0	0
1	B	151	1212	761	224	223	4	0	0	0
1	C	149	1200	755	219	222	4	0	0	0
1	D	148	1191	750	218	219	4	0	0	0
1	E	151	1212	761	224	223	4	0	0	0
1	F	148	1191	750	218	219	4	0	0	0
1	G	151	1212	761	224	223	4	0	0	0
1	H	151	1212	761	224	223	4	0	0	0
1	I	151	1212	761	224	223	4	0	0	0
1	J	151	1206	758	221	223	4	0	0	0
1	K	151	1202	755	220	223	4	0	0	0
1	L	151	1198	752	219	223	4	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP Q07820
B	171	GLY	-	expression tag	UNP Q07820
C	171	GLY	-	expression tag	UNP Q07820
D	171	GLY	-	expression tag	UNP Q07820
E	171	GLY	-	expression tag	UNP Q07820

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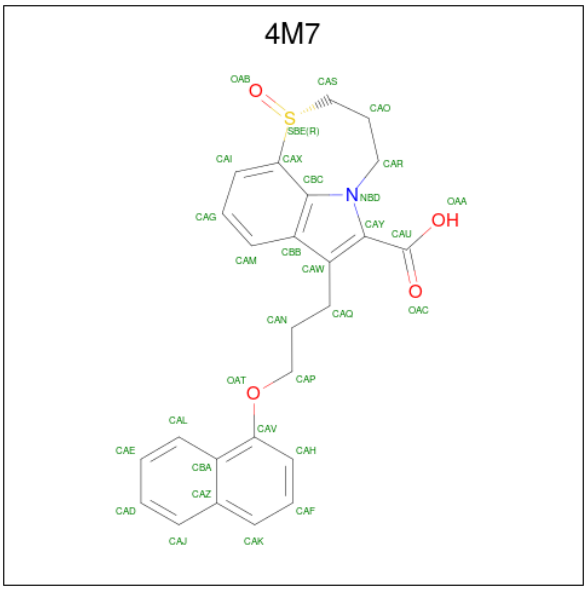
Chain	Residue	Modelled	Actual	Comment	Reference
F	171	GLY	-	expression tag	UNP Q07820
G	171	GLY	-	expression tag	UNP Q07820
H	171	GLY	-	expression tag	UNP Q07820
I	171	GLY	-	expression tag	UNP Q07820
J	171	GLY	-	expression tag	UNP Q07820
K	171	GLY	-	expression tag	UNP Q07820
L	171	GLY	-	expression tag	UNP Q07820

- Molecule 2 is (1R)-7-[3-(naphthalen-1-yloxy)propyl]-3,4-dihydro-2H-[1,4]thiazepino[2,3,4-hi]indole-6-carboxylic acid 1-oxide (three-letter code: 4M7) (formula: $C_{25}H_{23}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	31	25	1	4	1	0	0
2	B	1	31	25	1	4	1	0	0
2	C	1	31	25	1	4	1	0	0
2	D	1	31	25	1	4	1	0	0
2	E	1	31	25	1	4	1	0	0
2	F	1	31	25	1	4	1	0	0
2	G	1	31	25	1	4	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	H	1	31	25	1	4	1	0	0
			Total	C	N	O	S		
2	I	1	31	25	1	4	1	0	0
			Total	C	N	O	S		
2	J	1	31	25	1	4	1	0	0
			Total	C	N	O	S		
2	K	1	31	25	1	4	1	0	0
			Total	C	N	O	S		
2	L	1	31	25	1	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	61	61	61	0	0
			Total	O		
3	B	47	47	47	0	0
			Total	O		
3	C	29	29	29	0	0
			Total	O		
3	D	27	27	27	0	0
			Total	O		
3	E	34	34	34	0	0
			Total	O		
3	F	33	33	33	0	0
			Total	O		
3	G	32	32	32	0	0
			Total	O		
3	H	21	21	21	0	0
			Total	O		
3	I	18	18	18	0	0
			Total	O		
3	J	10	10	10	0	0
			Total	O		
3	K	21	21	21	0	0
			Total	O		
3	L	14	14	14	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: Induced myeloid leukemia cell differentiation protein Mcl-1

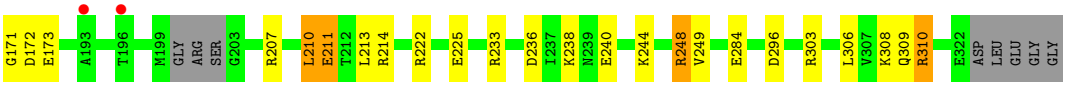
Chain A:

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain B:

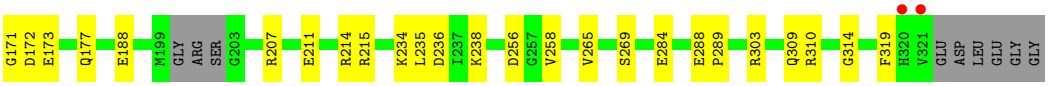
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain C:



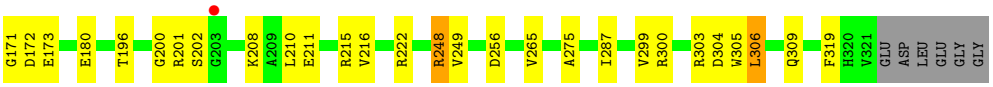
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain D:



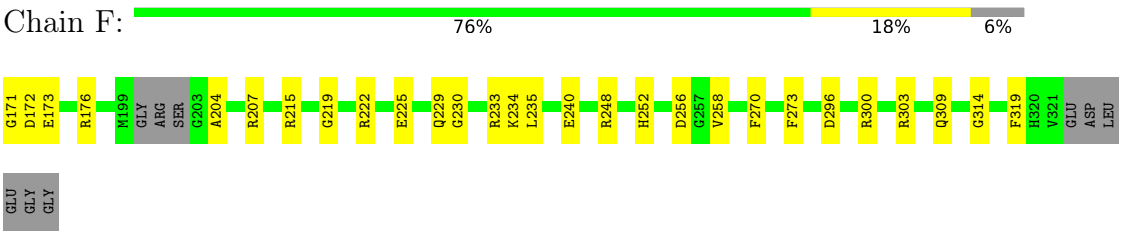
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain E:



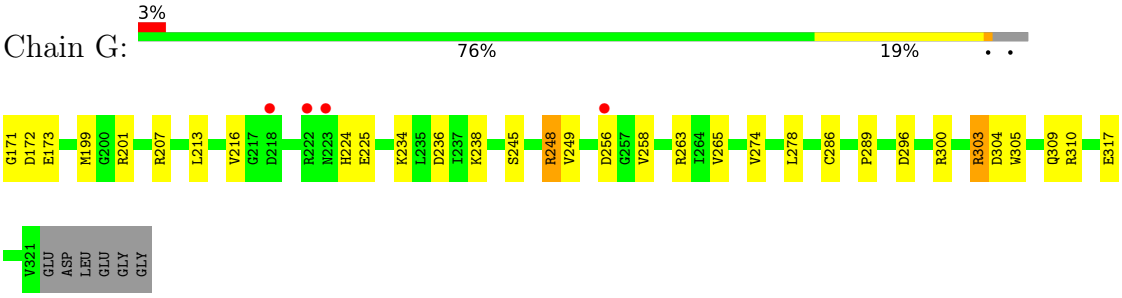
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain F:



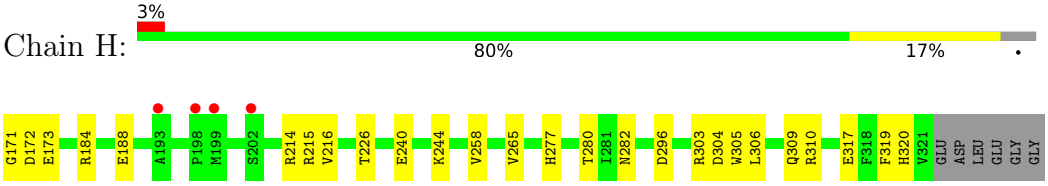
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain G:



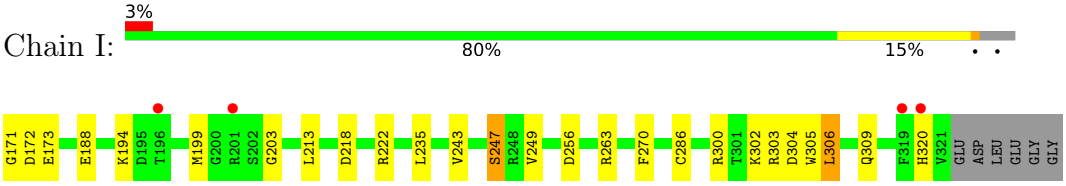
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain H:



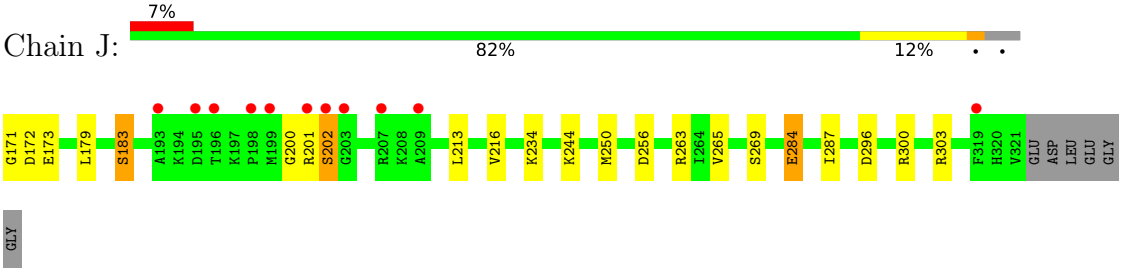
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain I:



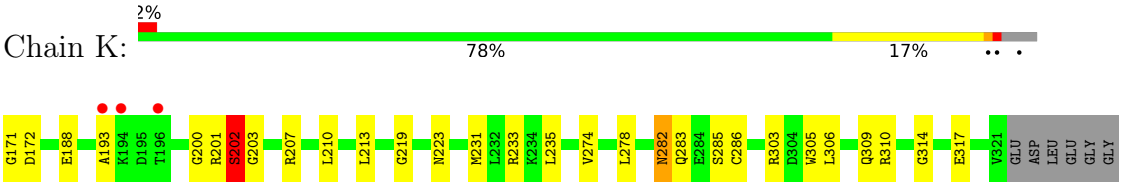
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain J:



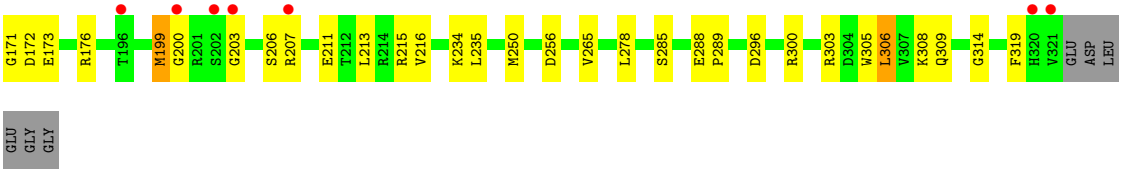
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain K:



• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.72Å 134.41Å 135.33Å 90.00° 100.27° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 48.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.00-2.20) 96.0 (48.93-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.20Å)	Xtriage
Refinement program	PHENIX dev_1951	Depositor
R, R_{free}	0.183 , 0.232 0.183 , 0.232	Depositor DCC
R_{free} test set	2023 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15189	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 4M7

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.50	0/1242	0.67	0/1670
1	B	0.52	0/1232	0.68	0/1656
1	C	0.51	0/1219	0.70	0/1638
1	D	0.47	0/1210	0.64	0/1626
1	E	0.47	0/1232	0.65	1/1656 (0.1%)
1	F	0.48	0/1210	0.67	0/1626
1	G	0.50	0/1232	0.68	1/1656 (0.1%)
1	H	0.50	0/1232	0.66	0/1656
1	I	0.46	0/1232	0.67	0/1656
1	J	0.43	0/1226	0.61	0/1649
1	K	0.44	0/1222	0.66	0/1645
1	L	0.44	0/1218	0.65	0/1641
All	All	0.48	0/14707	0.66	2/19775 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	303	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	E	306	LEU	CA-CB-CG	5.41	127.73	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1222	0	1227	23	0
1	B	1212	0	1223	22	0
1	C	1200	0	1207	13	1
1	D	1191	0	1201	13	1
1	E	1212	0	1223	21	0
1	F	1191	0	1201	20	0
1	G	1212	0	1223	25	0
1	H	1212	0	1223	15	0
1	I	1212	0	1223	19	0
1	J	1206	0	1212	14	0
1	K	1202	0	1201	16	0
1	L	1198	0	1190	21	0
2	A	31	0	22	1	0
2	B	31	0	22	1	0
2	C	31	0	22	0	0
2	D	31	0	22	0	0
2	E	31	0	22	0	0
2	F	31	0	22	1	0
2	G	31	0	22	0	0
2	H	31	0	22	0	0
2	I	31	0	22	3	0
2	J	31	0	22	0	0
2	K	31	0	22	0	0
2	L	31	0	22	1	0
3	A	61	0	0	1	0
3	B	47	0	0	0	0
3	C	29	0	0	1	0
3	D	27	0	0	2	0
3	E	34	0	0	2	0
3	F	33	0	0	2	0
3	G	32	0	0	0	0
3	H	21	0	0	0	0
3	I	18	0	0	1	0
3	J	10	0	0	1	0
3	K	21	0	0	1	0
3	L	14	0	0	0	0
All	All	15189	0	14818	196	1

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 7.

All (196) 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:C:171:GLY:HA2	1:C:303:ARG:HH22	1.14	1.08
1:G:171:GLY:HA2	1:G:303:ARG:HH22	1.18	1.07
1:E:171:GLY:HA2	1:E:303:ARG:HH22	1.17	1.06
1:J:171:GLY:HA3	1:J:303:ARG:HH22	1.23	0.99
1:F:171:GLY:HA3	1:F:303:ARG:HH22	1.26	0.98
1:D:171:GLY:HA3	1:D:303:ARG:HH22	1.24	0.98
1:H:171:GLY:HA2	1:H:303:ARG:HH22	1.30	0.97
1:B:171:GLY:HA2	1:B:303:ARG:HH22	1.29	0.96
1:I:171:GLY:HA3	1:I:303:ARG:HH22	1.34	0.92
1:I:256:ASP:O	1:I:263:ARG:NH2	2.05	0.88
1:K:171:GLY:HA2	1:K:303:ARG:HH22	1.38	0.87
1:L:171:GLY:HA2	1:L:303:ARG:HH22	1.38	0.86
1:F:235:LEU:O	1:G:248:ARG:NH2	2.17	0.78
1:F:248:ARG:NH1	1:G:245:SER:OG	2.19	0.77
1:E:215:ARG:NH2	1:E:319:PHE:O	2.18	0.76
1:J:179:LEU:O	1:J:183:SER:OG	2.05	0.74
1:G:256:ASP:O	1:G:263:ARG:NH2	2.21	0.73
1:C:210:LEU:HD13	1:C:214:ARG:HH21	1.54	0.73
1:L:199:MET:HB3	1:L:203:GLY:HA2	1.69	0.71
1:F:173:GLU:OE2	1:F:176:ARG:NH2	2.24	0.70
1:I:263:ARG:NH1	2:I:400:4M7:OAA	2.25	0.70
1:B:171:GLY:CA	1:B:303:ARG:HH22	2.05	0.69
1:J:200:GLY:O	1:J:202:SER:N	2.26	0.68
1:L:215:ARG:NH2	1:L:319:PHE:O	2.26	0.68
1:A:279:LYS:HD2	1:A:284:GLU:HG3	1.77	0.67
1:A:256:ASP:O	1:A:263:ARG:NH1	2.23	0.67
1:F:252:HIS:HA	1:G:234:LYS:HE3	1.77	0.67
1:G:171:GLY:CA	1:G:303:ARG:HH22	2.03	0.66
1:F:171:GLY:CA	1:F:303:ARG:HH22	2.04	0.65
1:K:219:GLY:O	1:K:223:ASN:ND2	2.26	0.65
1:L:176:ARG:NH1	1:L:200:GLY:O	2.30	0.65
1:C:233:ARG:NH1	3:C:503:HOH:O	2.31	0.64
1:B:303:ARG:HE	1:G:171:GLY:N	1.95	0.64
1:E:171:GLY:CA	1:E:303:ARG:HH22	2.02	0.63
1:D:207:ARG:NH1	1:D:211:GLU:OE2	2.31	0.63
1:F:248:ARG:HB2	3:F:504:HOH:O	1.98	0.63
1:E:172:ASP:OD1	3:E:501:HOH:O	2.16	0.63
1:F:296:ASP:OD1	1:F:300:ARG:NH1	2.32	0.63
1:C:310:ARG:O	1:C:310:ARG:HG3	2.00	0.62
1:A:171:GLY:N	1:A:303:ARG:HH22	1.98	0.62
1:D:234:LYS:NZ	3:D:501:HOH:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:310:ARG:NH2	1:G:317:GLU:OE1	2.33	0.61
1:L:171:GLY:HA2	1:L:303:ARG:NH2	2.11	0.61
1:C:171:GLY:HA2	1:C:303:ARG:NH2	1.99	0.61
1:B:172:ASP:HB3	1:G:304:ASP:OD2	2.01	0.60
1:J:284:GLU:HA	1:J:287:ILE:HD12	1.84	0.59
1:H:215:ARG:NH2	1:H:319:PHE:O	2.35	0.59
1:E:248:ARG:NH2	1:L:235:LEU:O	2.36	0.58
1:G:171:GLY:HA2	1:G:303:ARG:NH2	2.03	0.58
1:B:194:LYS:HE3	1:B:214:ARG:HH22	1.67	0.58
1:D:171:GLY:CA	1:D:303:ARG:HH22	2.10	0.58
1:K:278:LEU:HD23	1:K:286:CYS:HB2	1.85	0.58
1:A:171:GLY:CA	1:A:303:ARG:HH22	2.17	0.57
1:A:172:ASP:HB3	1:E:304:ASP:OD2	2.04	0.57
1:F:229:GLN:HG2	1:F:273:PHE:HZ	1.70	0.57
1:L:207:ARG:NH1	1:L:211:GLU:OE2	2.38	0.57
1:B:194:LYS:HE3	1:B:214:ARG:NH2	2.21	0.56
1:K:274:VAL:O	1:K:278:LEU:HD12	2.06	0.56
1:G:199:MET:HE3	1:G:207:ARG:HD3	1.87	0.55
1:I:188:GLU:HG2	1:I:194:LYS:HA	1.88	0.55
1:L:171:GLY:CA	1:L:303:ARG:HH22	2.15	0.55
1:C:207:ARG:O	1:C:211:GLU:HG2	2.06	0.55
1:F:215:ARG:NH2	1:F:319:PHE:O	2.39	0.55
1:E:171:GLY:HA2	1:E:303:ARG:NH2	2.03	0.55
1:B:216:VAL:HG12	1:B:265:VAL:HG11	1.88	0.54
1:G:274:VAL:O	1:G:278:LEU:HD13	2.07	0.54
1:K:310:ARG:NH2	1:K:317:GLU:OE2	2.40	0.54
1:A:215:ARG:NH1	3:A:501:HOH:O	2.41	0.54
1:A:171:GLY:HA3	1:A:303:ARG:HH22	1.71	0.54
1:L:296:ASP:OD2	1:L:300:ARG:NH2	2.30	0.54
1:A:303:ARG:HB3	1:E:172:ASP:HB2	1.88	0.54
1:H:171:GLY:CA	1:H:303:ARG:HH22	2.13	0.54
1:A:304:ASP:OD2	1:E:172:ASP:HB3	2.08	0.53
1:C:240:GLU:O	1:C:244:LYS:HG2	2.07	0.53
1:I:199:MET:HB2	1:I:203:GLY:HA2	1.89	0.53
1:L:199:MET:HG2	1:L:206:SER:HB2	1.89	0.53
1:B:304:ASP:OD2	1:G:172:ASP:HB3	2.07	0.53
1:J:171:GLY:N	3:J:502:HOH:O	2.41	0.53
1:L:309:GLN:O	1:L:314:GLY:HA3	2.09	0.52
1:K:305:TRP:O	1:K:309:GLN:HG2	2.10	0.52
1:K:171:GLY:CA	1:K:303:ARG:HH22	2.15	0.52
1:J:171:GLY:HA3	1:J:303:ARG:NH2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:GLU:OE2	1:D:214:ARG:NE	2.36	0.52
1:H:304:ASP:OD2	1:I:172:ASP:HB3	2.10	0.51
1:K:188:GLU:HG3	1:K:193:ALA:O	2.12	0.50
1:F:219:GLY:HA2	1:F:222:ARG:NH1	2.27	0.49
1:I:171:GLY:CA	1:I:303:ARG:HH22	2.13	0.49
1:A:171:GLY:N	1:E:300:ARG:HE	2.10	0.49
1:L:288:GLU:HB2	1:L:289:PRO:HD3	1.95	0.49
1:J:256:ASP:O	1:J:263:ARG:NH1	2.32	0.49
1:G:305:TRP:O	1:G:309:GLN:HG2	2.13	0.49
1:K:282:ASN:O	1:K:282:ASN:ND2	2.35	0.49
1:A:201:ARG:O	1:B:320:HIS:HB3	2.13	0.48
1:F:171:GLY:HA3	1:F:303:ARG:NH2	2.10	0.48
1:H:172:ASP:HB3	1:I:304:ASP:OD2	2.13	0.48
1:E:200:GLY:O	1:E:202:SER:N	2.46	0.48
1:K:283:GLN:OE1	3:K:501:HOH:O	2.20	0.48
1:A:215:ARG:NH2	1:A:319:PHE:O	2.47	0.48
1:C:308:LYS:HE3	1:C:309:GLN:HE21	1.79	0.48
1:C:222:ARG:NH1	1:J:234:LYS:HD2	2.29	0.47
1:D:310:ARG:NH2	3:D:503:HOH:O	2.46	0.47
1:H:305:TRP:O	1:H:309:GLN:HG2	2.14	0.47
1:K:309:GLN:O	1:K:314:GLY:HA3	2.14	0.47
1:A:171:GLY:HA3	1:A:303:ARG:NH2	2.28	0.47
1:L:172:ASP:HB3	1:L:173:GLU:H	1.51	0.47
1:J:216:VAL:HG12	1:J:265:VAL:HG11	1.96	0.47
1:A:173:GLU:OE2	1:A:201:ARG:HG2	2.15	0.47
1:C:172:ASP:HB3	1:C:173:GLU:H	1.58	0.47
1:E:216:VAL:HG12	1:E:265:VAL:HG11	1.98	0.46
1:H:184:ARG:O	1:H:188:GLU:HB3	2.15	0.46
1:B:171:GLY:HA3	1:G:300:ARG:HE	1.80	0.46
1:B:171:GLY:HA3	1:G:300:ARG:NE	2.30	0.46
1:G:172:ASP:HB3	1:G:173:GLU:H	1.59	0.46
1:D:172:ASP:HB3	1:D:173:GLU:H	1.42	0.46
1:F:270:PHE:CG	2:F:400:4M7:H10	2.51	0.46
1:D:215:ARG:NH2	1:D:319:PHE:O	2.48	0.46
1:E:172:ASP:HB3	1:E:173:GLU:H	1.53	0.46
1:L:216:VAL:HG12	1:L:265:VAL:HG11	1.97	0.46
1:L:199:MET:HB3	1:L:203:GLY:CA	2.44	0.45
1:E:180:GLU:OE1	3:E:502:HOH:O	2.21	0.45
1:L:171:GLY:HA2	1:L:303:ARG:HH12	1.81	0.45
1:H:277:HIS:O	1:H:280:THR:HB	2.15	0.45
1:F:204:ALA:HA	1:F:207:ARG:HE	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:240:GLU:O	1:H:244:LYS:HG3	2.16	0.45
1:F:176:ARG:NH1	3:F:503:HOH:O	2.37	0.45
1:K:231:MET:O	1:K:235:LEU:HG	2.17	0.45
1:K:274:VAL:HG12	1:K:278:LEU:CD1	2.47	0.45
1:L:305:TRP:HE3	1:L:306:LEU:HD13	1.83	0.44
1:D:236:ASP:OD2	1:D:238:LYS:HE2	2.17	0.44
1:I:270:PHE:CG	2:I:400:4M7:H10	2.52	0.44
1:I:305:TRP:O	1:I:309:GLN:HG2	2.17	0.44
1:A:172:ASP:HB3	1:A:173:GLU:H	1.53	0.44
1:F:234:LYS:NZ	1:G:256:ASP:HB2	2.32	0.44
1:G:199:MET:HE3	1:G:207:ARG:CD	2.48	0.44
1:L:296:ASP:O	1:L:300:ARG:HB2	2.17	0.44
1:A:201:ARG:HD3	1:B:320:HIS:ND1	2.33	0.44
1:J:296:ASP:OD1	1:J:300:ARG:NH2	2.51	0.44
1:G:216:VAL:HG12	1:G:265:VAL:HG11	1.99	0.43
1:C:308:LYS:HE3	1:C:309:GLN:NE2	2.32	0.43
1:G:236:ASP:OD2	1:G:238:LYS:HE3	2.17	0.43
1:J:213:LEU:HD12	1:J:213:LEU:HA	1.89	0.43
1:J:265:VAL:O	1:J:269:SER:OG	2.28	0.43
1:K:210:LEU:HA	1:K:210:LEU:HD23	1.77	0.43
1:K:203:GLY:O	1:K:207:ARG:HG3	2.19	0.43
1:K:200:GLY:O	1:K:202:SER:N	2.51	0.43
1:E:211:GLU:OE2	1:E:215:ARG:NH1	2.52	0.43
1:E:256:ASP:HB2	1:L:234:LYS:HE2	2.01	0.43
1:J:250:MET:HB3	1:J:250:MET:HE2	1.69	0.43
1:A:270:PHE:CG	2:A:400:4M7:H10	2.54	0.43
1:B:172:ASP:HB3	1:B:173:GLU:H	1.58	0.43
1:I:172:ASP:HB3	1:I:173:GLU:H	1.54	0.43
1:E:305:TRP:CZ2	1:E:309:GLN:HG3	2.54	0.42
1:H:172:ASP:HB3	1:H:173:GLU:H	1.54	0.42
1:L:250:MET:HB3	1:L:250:MET:HE2	1.70	0.42
1:A:299:VAL:O	1:A:303:ARG:HB2	2.19	0.42
1:H:216:VAL:HG12	1:H:265:VAL:HG11	2.01	0.42
1:E:275:ALA:HB1	1:E:287:ILE:HD13	2.01	0.42
1:J:172:ASP:HB3	1:J:173:GLU:H	1.60	0.42
1:A:198:PRO:HB3	1:B:309:GLN:OE1	2.19	0.42
1:B:171:GLY:N	1:G:303:ARG:HE	2.18	0.42
1:B:211:GLU:HG3	1:B:212:THR:N	2.34	0.42
1:H:188:GLU:OE2	1:H:214:ARG:NE	2.52	0.42
1:B:308:LYS:HD3	1:B:308:LYS:HA	1.85	0.42
1:D:265:VAL:O	1:D:269:SER:OG	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:286:CYS:C	1:G:289:PRO:HD2	2.40	0.41
1:A:201:ARG:HD3	1:B:320:HIS:CG	2.55	0.41
1:A:309:GLN:O	1:A:314:GLY:HA3	2.19	0.41
1:B:172:ASP:HB2	1:G:303:ARG:HB3	2.01	0.41
1:A:288:GLU:HB3	1:A:289:PRO:HD3	2.01	0.41
1:B:303:ARG:HB3	1:G:172:ASP:HB2	2.02	0.41
1:I:247:SER:HB2	3:I:501:HOH:O	2.19	0.41
1:I:263:ARG:HH11	2:I:400:4M7:CAU	2.32	0.41
1:B:270:PHE:CG	2:B:400:4M7:H10	2.54	0.41
1:F:230:GLY:HA2	1:F:233:ARG:HB3	2.02	0.41
1:C:236:ASP:OD2	1:C:238:LYS:HE2	2.20	0.41
1:H:310:ARG:NH1	1:H:317:GLU:OE1	2.42	0.41
1:I:243:VAL:HG21	1:I:286:CYS:HB3	2.02	0.41
1:C:210:LEU:HD13	1:C:214:ARG:NH2	2.29	0.41
1:D:309:GLN:O	1:D:314:GLY:HA3	2.20	0.41
1:F:309:GLN:O	1:F:314:GLY:HA3	2.21	0.41
1:H:310:ARG:HH22	1:H:317:GLU:CD	2.23	0.41
1:I:171:GLY:HA3	1:I:303:ARG:NH2	2.16	0.41
1:I:218:ASP:O	1:I:222:ARG:HG3	2.21	0.41
1:I:302:LYS:HB2	1:I:306:LEU:HD22	2.02	0.41
1:L:213:LEU:HD12	1:L:213:LEU:HA	1.96	0.41
1:D:288:GLU:HB3	1:D:289:PRO:HD3	2.03	0.41
1:E:299:VAL:O	1:E:303:ARG:HB2	2.21	0.41
1:F:229:GLN:HG2	1:F:273:PHE:CZ	2.54	0.41
1:H:171:GLY:HA3	1:I:300:ARG:NE	2.36	0.41
1:D:171:GLY:HA3	1:D:303:ARG:NH2	2.09	0.41
1:I:235:LEU:HA	1:I:235:LEU:HD23	1.89	0.41
1:B:309:GLN:O	1:B:314:GLY:HA3	2.22	0.40
1:E:210:LEU:HD23	1:E:210:LEU:HA	1.88	0.40
2:L:400:4M7:H2	2:L:400:4M7:OAA	2.21	0.40
1:A:171:GLY:HA3	1:E:303:ARG:HE	1.87	0.40
1:F:172:ASP:HB3	1:F:173:GLU:H	1.60	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ARG:NH2	1:D:235:LEU:O[1_655]	2.12	0.08

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	151/157 (96%)	145 (96%)	6 (4%)	0	100	100
1	B	149/157 (95%)	144 (97%)	5 (3%)	0	100	100
1	C	145/157 (92%)	142 (98%)	3 (2%)	0	100	100
1	D	144/157 (92%)	141 (98%)	3 (2%)	0	100	100
1	E	149/157 (95%)	144 (97%)	4 (3%)	1 (1%)	22	22
1	F	144/157 (92%)	141 (98%)	3 (2%)	0	100	100
1	G	149/157 (95%)	147 (99%)	2 (1%)	0	100	100
1	H	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
1	I	149/157 (95%)	143 (96%)	6 (4%)	0	100	100
1	J	149/157 (95%)	145 (97%)	3 (2%)	1 (1%)	22	22
1	K	149/157 (95%)	144 (97%)	3 (2%)	2 (1%)	12	9
1	L	149/157 (95%)	146 (98%)	3 (2%)	0	100	100
All	All	1776/1884 (94%)	1727 (97%)	45 (2%)	4 (0%)	47	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	201	ARG
1	K	201	ARG
1	J	201	ARG
1	K	202	SER

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	131/135 (97%)	127 (97%)	4 (3%)	40	51
1	B	131/135 (97%)	125 (95%)	6 (5%)	27	34
1	C	130/135 (96%)	120 (92%)	10 (8%)	13	13
1	D	129/135 (96%)	125 (97%)	4 (3%)	40	51
1	E	131/135 (97%)	125 (95%)	6 (5%)	27	34
1	F	129/135 (96%)	125 (97%)	4 (3%)	40	51
1	G	131/135 (97%)	123 (94%)	8 (6%)	18	21
1	H	131/135 (97%)	125 (95%)	6 (5%)	27	34
1	I	131/135 (97%)	126 (96%)	5 (4%)	33	42
1	J	130/135 (96%)	126 (97%)	4 (3%)	40	51
1	K	129/135 (96%)	122 (95%)	7 (5%)	22	26
1	L	128/135 (95%)	122 (95%)	6 (5%)	26	33
All	All	1561/1620 (96%)	1491 (96%)	70 (4%)	27	34

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	THR
1	A	201	ARG
1	A	248	ARG
1	A	249	VAL
1	B	211	GLU
1	B	213	LEU
1	B	234	LYS
1	B	248	ARG
1	B	249	VAL
1	B	306	LEU
1	C	210	LEU
1	C	211	GLU
1	C	213	LEU
1	C	225	GLU
1	C	248	ARG
1	C	249	VAL
1	C	284	GLU
1	C	296	ASP
1	C	306	LEU
1	C	310	ARG

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Mol	Chain	Res	Type
1	D	177	GLN
1	D	256	ASP
1	D	258	VAL
1	D	284	GLU
1	E	196	THR
1	E	208	LYS
1	E	222	ARG
1	E	248	ARG
1	E	249	VAL
1	E	306	LEU
1	F	225	GLU
1	F	240	GLU
1	F	256	ASP
1	F	258	VAL
1	G	201	ARG
1	G	213	LEU
1	G	224	HIS
1	G	225	GLU
1	G	248	ARG
1	G	249	VAL
1	G	258	VAL
1	G	296	ASP
1	H	226	THR
1	H	258	VAL
1	H	282	ASN
1	H	296	ASP
1	H	306	LEU
1	H	320	HIS
1	I	213	LEU
1	I	247	SER
1	I	249	VAL
1	I	306	LEU
1	I	320	HIS
1	J	183	SER
1	J	202	SER
1	J	244	LYS
1	J	284	GLU
1	K	172	ASP
1	K	202	SER
1	K	213	LEU
1	K	233	ARG
1	K	282	ASN

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Mol	Chain	Res	Type
1	K	285	SER
1	K	306	LEU
1	L	199	MET
1	L	256	ASP
1	L	278	LEU
1	L	285	SER
1	L	306	LEU
1	L	308	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	309	GLN
1	D	177	GLN
1	J	177	GLN

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)

12 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	$\#\|Z\| > 2$
2	4M7	H	400	-	30,35,35	1.08	2 (6%)	35,50,50	1.33	2 (5%)
2	4M7	J	400	-	30,35,35	1.22	3 (10%)	35,50,50	1.11	2 (5%)
2	4M7	E	400	-	30,35,35	1.31	3 (10%)	35,50,50	1.02	2 (5%)
2	4M7	K	400	-	30,35,35	1.29	3 (10%)	35,50,50	1.26	4 (11%)
2	4M7	C	400	-	30,35,35	1.19	2 (6%)	35,50,50	1.11	1 (2%)
2	4M7	L	400	-	30,35,35	1.19	3 (10%)	35,50,50	1.15	2 (5%)
2	4M7	A	400	-	30,35,35	1.28	3 (10%)	35,50,50	1.19	6 (17%)
2	4M7	F	400	-	30,35,35	1.27	3 (10%)	35,50,50	1.25	5 (14%)
2	4M7	D	400	-	30,35,35	1.28	4 (13%)	35,50,50	1.36	4 (11%)
2	4M7	G	400	-	30,35,35	1.18	3 (10%)	35,50,50	1.19	4 (11%)
2	4M7	I	400	-	30,35,35	1.20	3 (10%)	35,50,50	1.24	4 (11%)
2	4M7	B	400	-	30,35,35	1.17	2 (6%)	35,50,50	1.30	6 (17%)

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	4M7	H	400	-	-	7/11/21/21	0/4/5/5
2	4M7	J	400	-	-	4/11/21/21	0/4/5/5
2	4M7	E	400	-	-	4/11/21/21	0/4/5/5
2	4M7	K	400	-	-	8/11/21/21	0/4/5/5
2	4M7	C	400	-	-	4/11/21/21	0/4/5/5
2	4M7	L	400	-	-	4/11/21/21	0/4/5/5
2	4M7	A	400	-	-	4/11/21/21	0/4/5/5
2	4M7	F	400	-	-	4/11/21/21	0/4/5/5
2	4M7	D	400	-	-	4/11/21/21	0/4/5/5
2	4M7	G	400	-	-	4/11/21/21	0/4/5/5
2	4M7	I	400	-	-	4/11/21/21	0/4/5/5
2	4M7	B	400	-	-	7/11/21/21	0/4/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	400	4M7	CAR-NBD	-3.30	1.46	1.49
2	C	400	4M7	CAI-CAX	3.29	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	400	4M7	CAR-NBD	-3.19	1.46	1.49
2	E	400	4M7	CAI-CAX	3.18	1.41	1.37
2	D	400	4M7	CAR-NBD	-3.14	1.46	1.49
2	E	400	4M7	CAR-NBD	-3.09	1.46	1.49
2	E	400	4M7	CBA-CAZ	-3.03	1.37	1.43
2	D	400	4M7	CAI-CAX	2.95	1.41	1.37
2	L	400	4M7	CAI-CAX	2.87	1.41	1.37
2	B	400	4M7	CAI-CAX	2.83	1.41	1.37
2	G	400	4M7	CAR-NBD	-2.80	1.47	1.49
2	I	400	4M7	CAI-CAX	2.80	1.41	1.37
2	L	400	4M7	CBA-CAZ	-2.80	1.37	1.43
2	J	400	4M7	CAR-NBD	-2.80	1.47	1.49
2	A	400	4M7	CBA-CAZ	-2.79	1.37	1.43
2	A	400	4M7	CAR-NBD	-2.78	1.47	1.49
2	J	400	4M7	CAI-CAX	2.77	1.41	1.37
2	F	400	4M7	CAI-CAX	2.76	1.41	1.37
2	A	400	4M7	CAI-CAX	2.74	1.41	1.37
2	G	400	4M7	CAI-CAX	2.73	1.41	1.37
2	J	400	4M7	CBA-CAZ	-2.72	1.38	1.43
2	I	400	4M7	CBA-CAZ	-2.70	1.38	1.43
2	H	400	4M7	CAI-CAX	2.68	1.41	1.37
2	K	400	4M7	CAI-CAX	2.65	1.41	1.37
2	D	400	4M7	CBA-CAZ	-2.56	1.38	1.43
2	I	400	4M7	CAR-NBD	-2.48	1.47	1.49
2	G	400	4M7	CBA-CAZ	-2.41	1.38	1.43
2	C	400	4M7	CBA-CAZ	-2.35	1.38	1.43
2	D	400	4M7	CAS-CAO	-2.28	1.49	1.52
2	L	400	4M7	CAR-NBD	-2.26	1.47	1.49
2	B	400	4M7	CBA-CAZ	-2.25	1.38	1.43
2	K	400	4M7	CBA-CAZ	-2.11	1.39	1.43
2	H	400	4M7	CBA-CAZ	-2.10	1.39	1.43
2	F	400	4M7	CBA-CAZ	-2.08	1.39	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	400	4M7	OAB-SBE-CAX	3.90	110.98	106.12
2	I	400	4M7	OAB-SBE-CAX	3.62	110.63	106.12
2	B	400	4M7	OAB-SBE-CAX	3.35	110.29	106.12
2	D	400	4M7	CAS-CAO-CAR	-3.25	110.85	114.73
2	K	400	4M7	OAB-SBE-CAX	3.14	110.02	106.12
2	J	400	4M7	OAB-SBE-CAX	2.97	109.82	106.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	400	4M7	CAL-CBA-CAZ	2.93	121.69	117.89
2	D	400	4M7	CAL-CBA-CAZ	2.86	121.59	117.89
2	L	400	4M7	OAA-CAU-OAC	-2.84	117.05	123.35
2	L	400	4M7	OAA-CAU-CAY	2.72	122.00	116.40
2	G	400	4M7	OAB-SBE-CAX	2.66	109.43	106.12
2	D	400	4M7	CAM-CBB-CBC	2.63	121.65	116.73
2	A	400	4M7	OAB-SBE-CAX	2.55	109.30	106.12
2	E	400	4M7	CAL-CBA-CAZ	2.43	121.03	117.89
2	K	400	4M7	OAT-CAV-CAH	-2.38	119.22	124.46
2	A	400	4M7	OAA-CAU-CAY	2.37	121.29	116.40
2	G	400	4M7	OAA-CAU-CAY	2.36	121.27	116.40
2	C	400	4M7	CAM-CBB-CBC	2.35	121.11	116.73
2	A	400	4M7	CAL-CBA-CAZ	2.33	120.90	117.89
2	E	400	4M7	CAM-CBB-CBC	2.33	121.08	116.73
2	F	400	4M7	OAB-SBE-CAX	2.31	109.00	106.12
2	H	400	4M7	OAT-CAV-CAH	-2.30	119.40	124.46
2	K	400	4M7	CAM-CBB-CBC	2.29	121.01	116.73
2	I	400	4M7	CAM-CBB-CBC	2.26	120.96	116.73
2	D	400	4M7	CAO-CAR-NBD	2.25	112.94	111.18
2	J	400	4M7	CAM-CBB-CBC	2.20	120.84	116.73
2	B	400	4M7	CAM-CBB-CBC	2.19	120.81	116.73
2	A	400	4M7	OAA-CAU-OAC	-2.17	118.53	123.35
2	F	400	4M7	OAA-CAU-CAY	2.15	120.83	116.40
2	F	400	4M7	OAT-CAP-CAN	2.15	116.30	108.33
2	I	400	4M7	OAA-CAU-CAY	2.14	120.81	116.40
2	G	400	4M7	CAP-OAT-CAV	2.13	124.11	117.74
2	F	400	4M7	CAM-CBB-CBC	2.13	120.70	116.73
2	B	400	4M7	OAA-CAU-CAY	2.11	120.76	116.40
2	G	400	4M7	OAC-CAU-CAY	-2.10	118.41	121.30
2	A	400	4M7	CAO-CAR-NBD	2.10	112.83	111.18
2	B	400	4M7	OAT-CAV-CAH	-2.09	119.85	124.46
2	B	400	4M7	OAT-CAP-CAN	2.08	116.07	108.33
2	K	400	4M7	OAT-CAV-CBA	2.06	120.76	115.01
2	A	400	4M7	CAM-CBB-CBC	2.05	120.56	116.73
2	I	400	4M7	OAT-CAV-CAH	-2.02	120.02	124.46
2	B	400	4M7	OAT-CAV-CBA	2.00	120.61	115.01

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	4M7	OAA-CAU-CAY-NBD

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Mol	Chain	Res	Type	Atoms
2	A	400	4M7	OAA-CAU-CAY-CAW
2	A	400	4M7	OAC-CAU-CAY-NBD
2	A	400	4M7	OAC-CAU-CAY-CAW
2	B	400	4M7	OAA-CAU-CAY-NBD
2	B	400	4M7	OAA-CAU-CAY-CAW
2	B	400	4M7	OAC-CAU-CAY-NBD
2	C	400	4M7	OAA-CAU-CAY-NBD
2	C	400	4M7	OAA-CAU-CAY-CAW
2	C	400	4M7	OAC-CAU-CAY-NBD
2	C	400	4M7	OAC-CAU-CAY-CAW
2	D	400	4M7	OAA-CAU-CAY-NBD
2	D	400	4M7	OAA-CAU-CAY-CAW
2	D	400	4M7	OAC-CAU-CAY-NBD
2	D	400	4M7	OAC-CAU-CAY-CAW
2	E	400	4M7	OAA-CAU-CAY-NBD
2	E	400	4M7	OAA-CAU-CAY-CAW
2	E	400	4M7	OAC-CAU-CAY-NBD
2	E	400	4M7	OAC-CAU-CAY-CAW
2	F	400	4M7	OAA-CAU-CAY-NBD
2	F	400	4M7	OAA-CAU-CAY-CAW
2	F	400	4M7	OAC-CAU-CAY-NBD
2	F	400	4M7	OAC-CAU-CAY-CAW
2	G	400	4M7	OAA-CAU-CAY-NBD
2	G	400	4M7	OAA-CAU-CAY-CAW
2	G	400	4M7	OAC-CAU-CAY-NBD
2	G	400	4M7	OAC-CAU-CAY-CAW
2	H	400	4M7	OAA-CAU-CAY-NBD
2	H	400	4M7	OAA-CAU-CAY-CAW
2	H	400	4M7	OAC-CAU-CAY-NBD
2	H	400	4M7	OAC-CAU-CAY-CAW
2	I	400	4M7	OAA-CAU-CAY-NBD
2	I	400	4M7	OAA-CAU-CAY-CAW
2	I	400	4M7	OAC-CAU-CAY-NBD
2	I	400	4M7	OAC-CAU-CAY-CAW
2	J	400	4M7	OAA-CAU-CAY-NBD
2	J	400	4M7	OAA-CAU-CAY-CAW
2	J	400	4M7	OAC-CAU-CAY-NBD
2	J	400	4M7	OAC-CAU-CAY-CAW
2	K	400	4M7	OAA-CAU-CAY-NBD
2	K	400	4M7	OAA-CAU-CAY-CAW
2	K	400	4M7	OAC-CAU-CAY-NBD
2	K	400	4M7	OAC-CAU-CAY-CAW

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Mol	Chain	Res	Type	Atoms
2	K	400	4M7	CAP-CAN-CAQ-CAW
2	L	400	4M7	OAA-CAU-CAY-NBD
2	L	400	4M7	OAA-CAU-CAY-CAW
2	L	400	4M7	OAC-CAU-CAY-CAW
2	K	400	4M7	CBA-CAV-OAT-CAP
2	K	400	4M7	CAH-CAV-OAT-CAP
2	K	400	4M7	CAQ-CAN-CAP-OAT
2	B	400	4M7	CAQ-CAN-CAP-OAT
2	H	400	4M7	CAQ-CAN-CAP-OAT
2	H	400	4M7	CBA-CAV-OAT-CAP
2	H	400	4M7	CAH-CAV-OAT-CAP
2	B	400	4M7	CBA-CAV-OAT-CAP
2	B	400	4M7	CAH-CAV-OAT-CAP
2	B	400	4M7	OAC-CAU-CAY-CAW
2	L	400	4M7	OAC-CAU-CAY-NBD

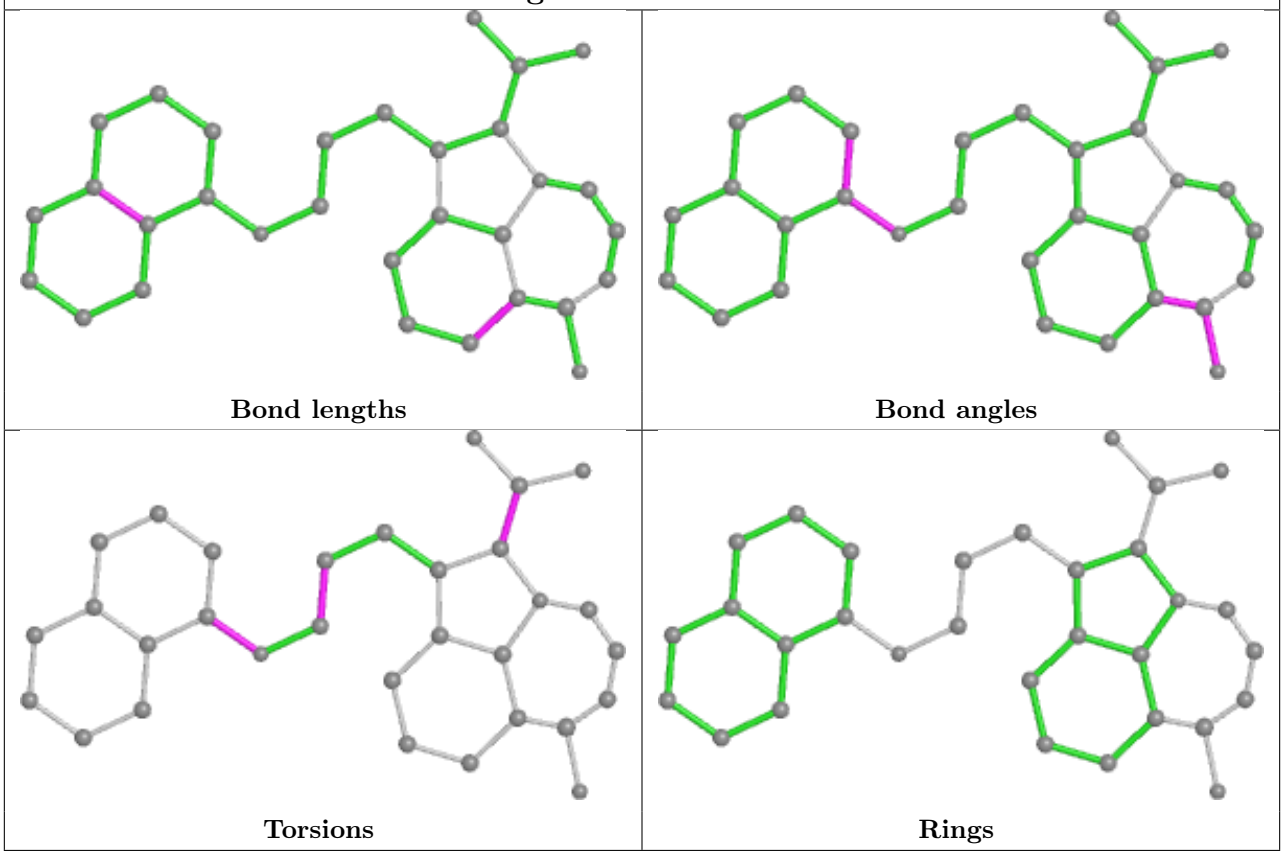
There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	400	4M7	1	0
2	A	400	4M7	1	0
2	F	400	4M7	1	0
2	I	400	4M7	3	0
2	B	400	4M7	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 4M7 H 400



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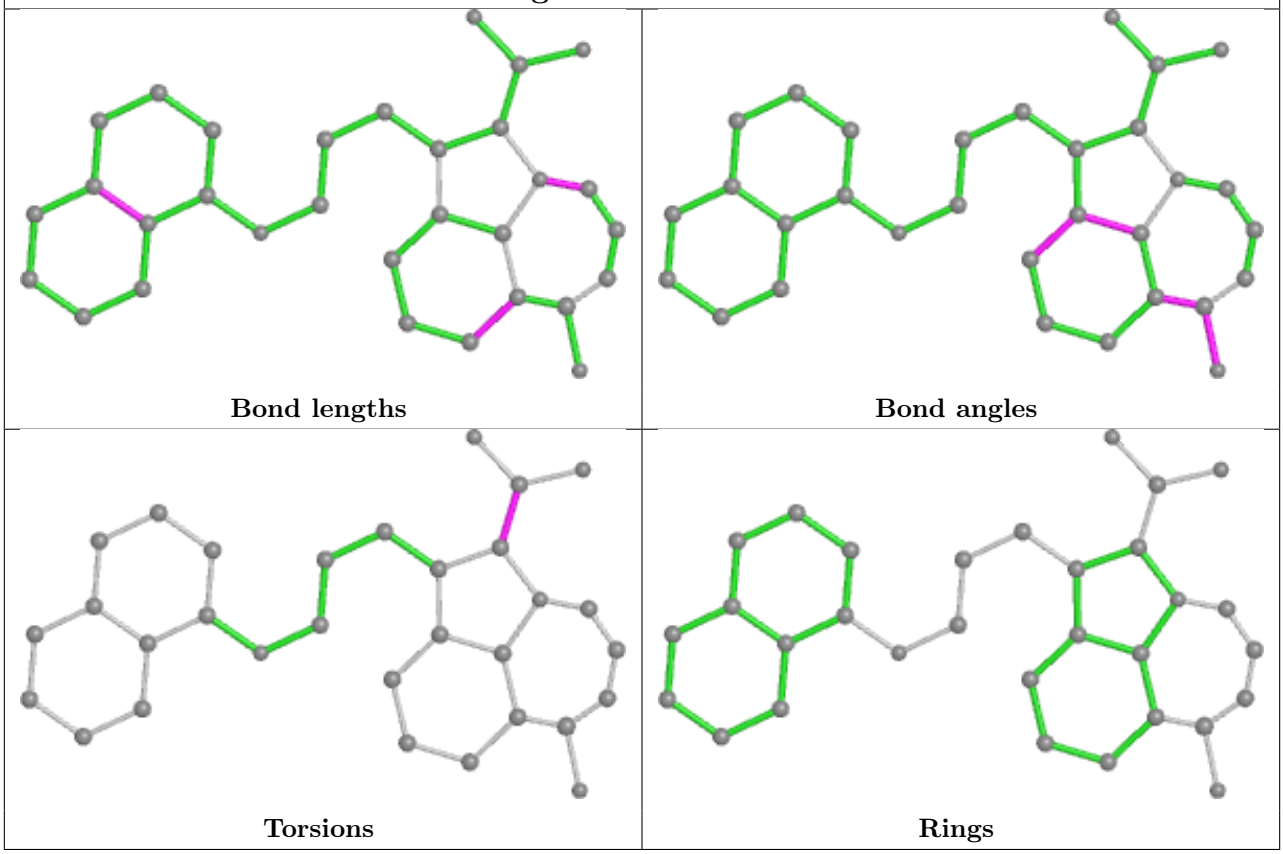

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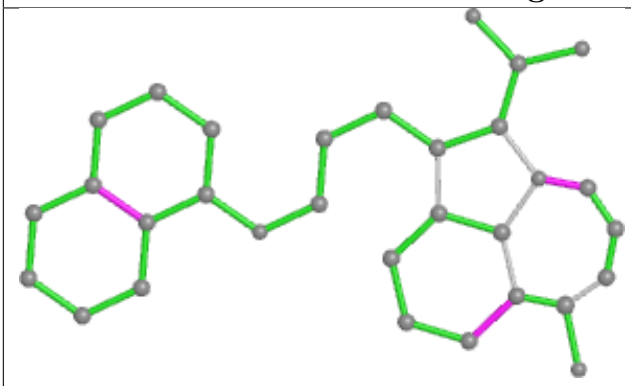

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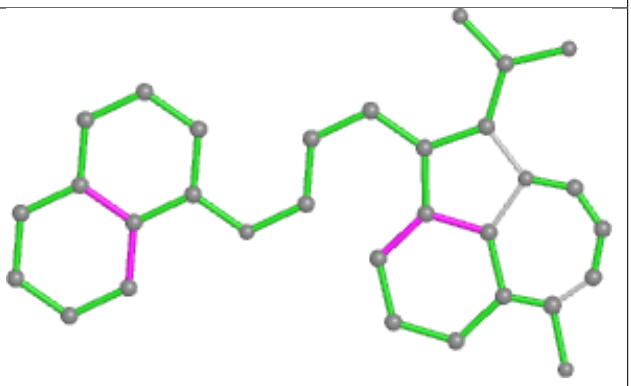
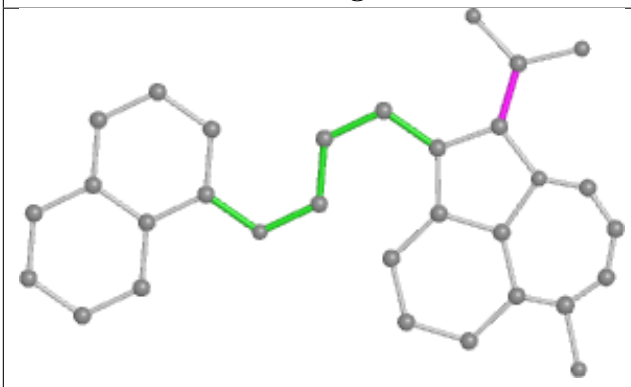
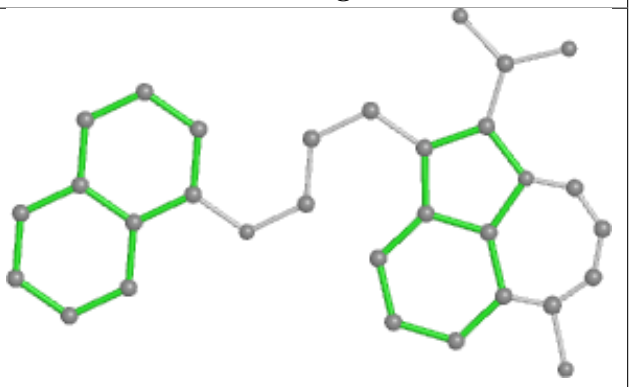


Bond angles

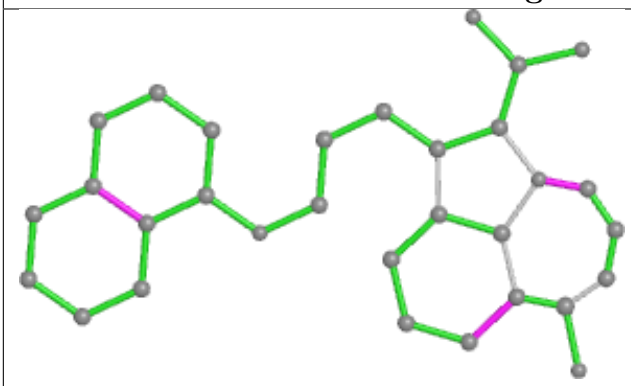


Torsions



Rings

Ligand 4M7 K 400



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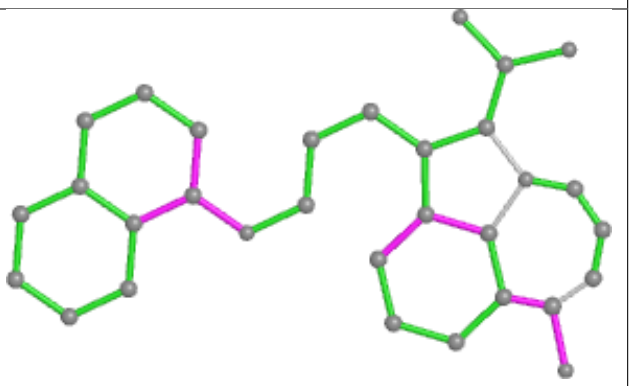

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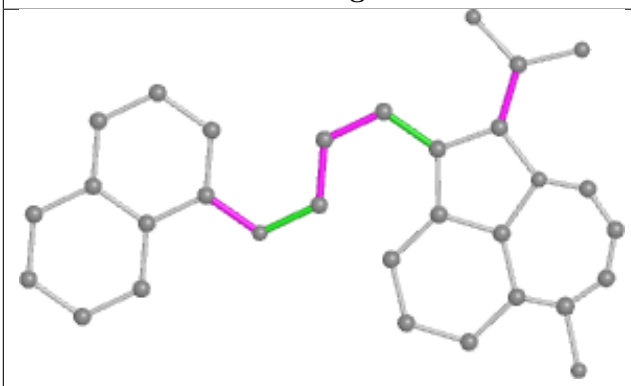

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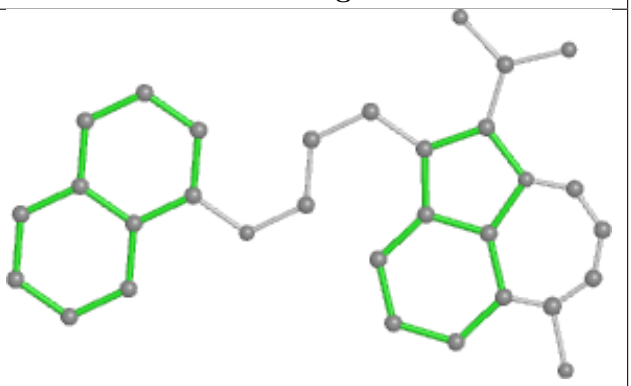
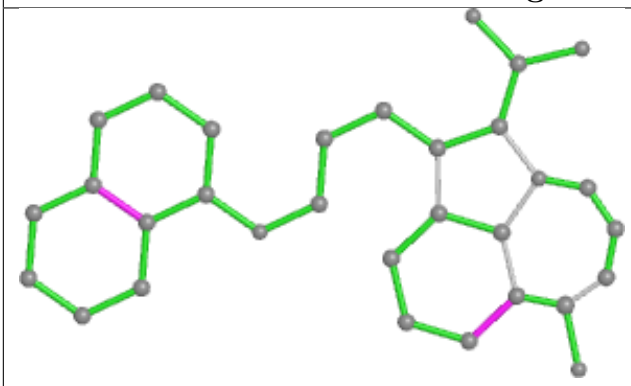


Rings

Ligand 4M7 C 400



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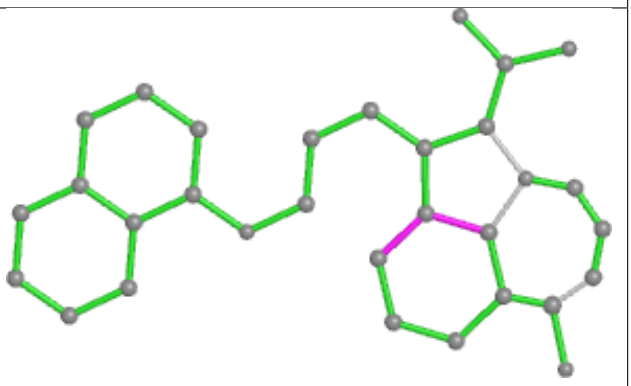

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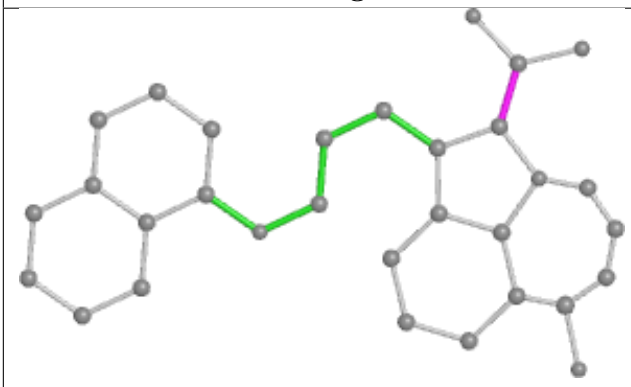

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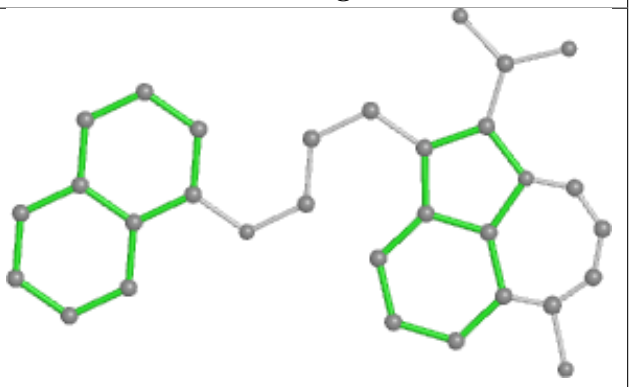
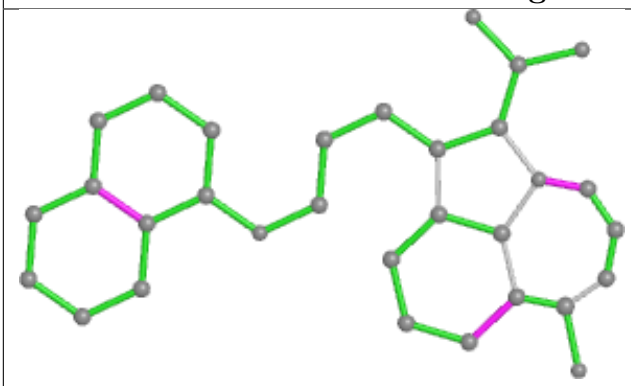


Rings

Ligand 4M7 L 400



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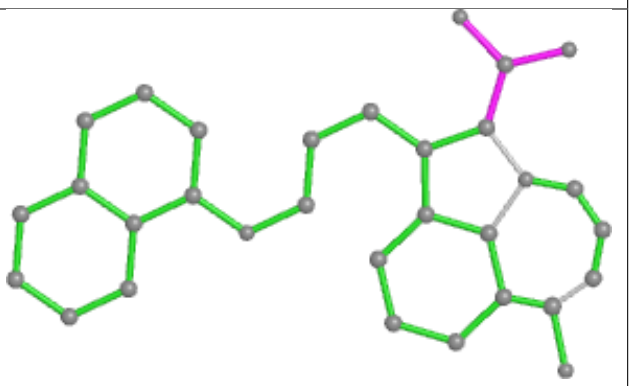

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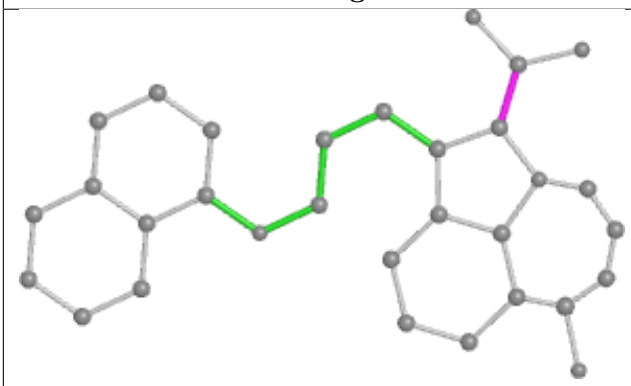

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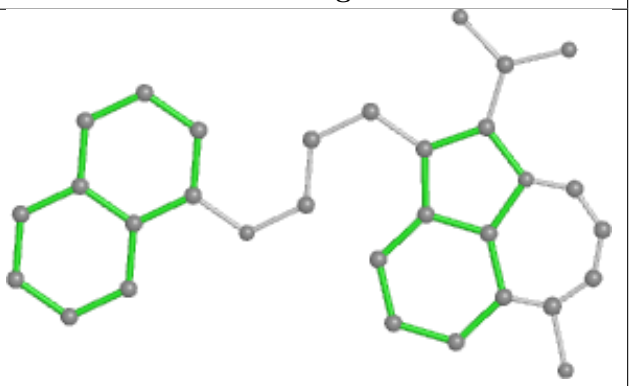
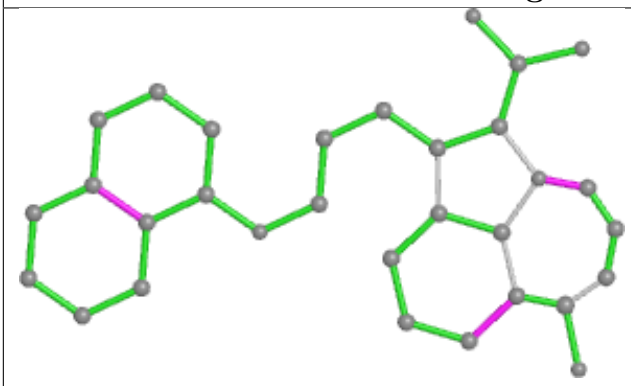


Rings

Ligand 4M7 A 400



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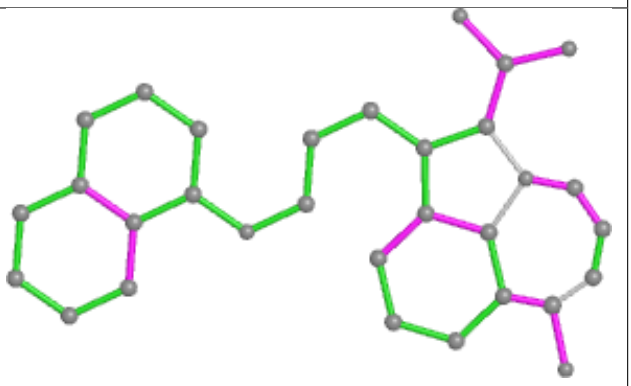

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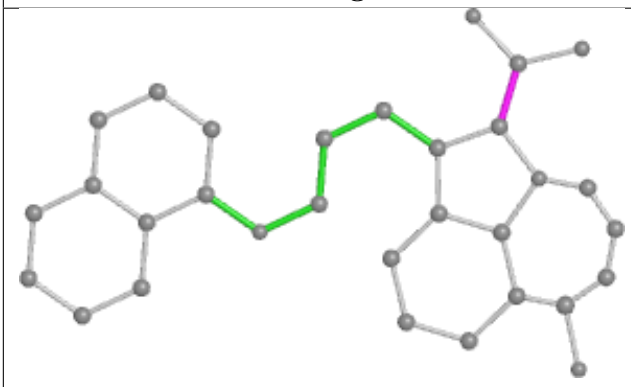

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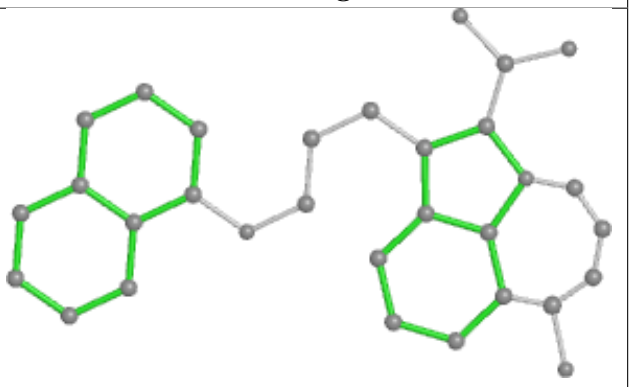
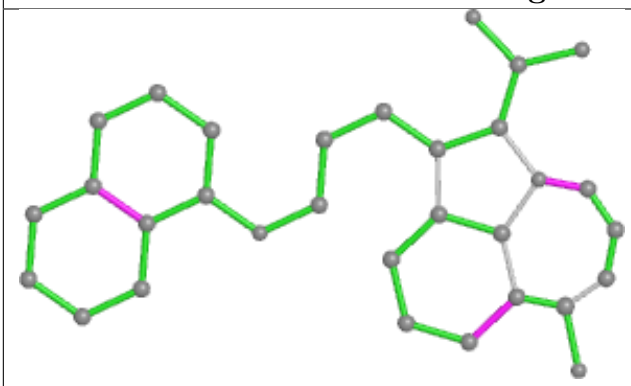


Rings

Ligand 4M7 F 400



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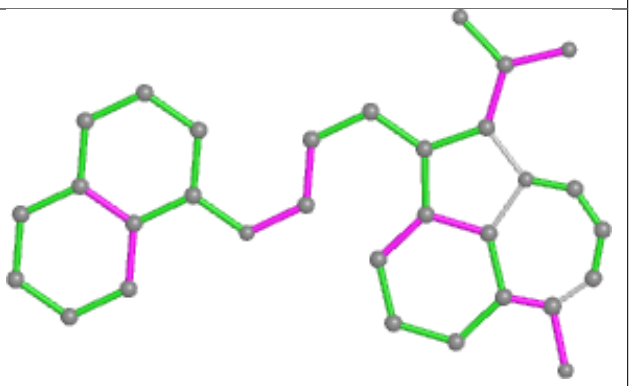

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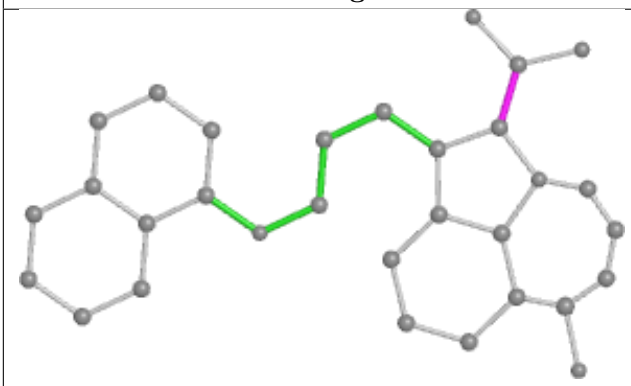

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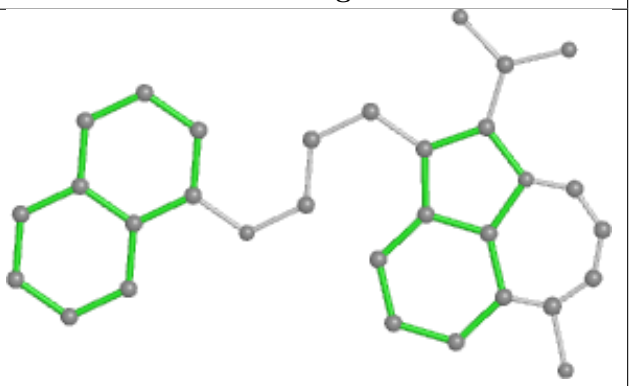
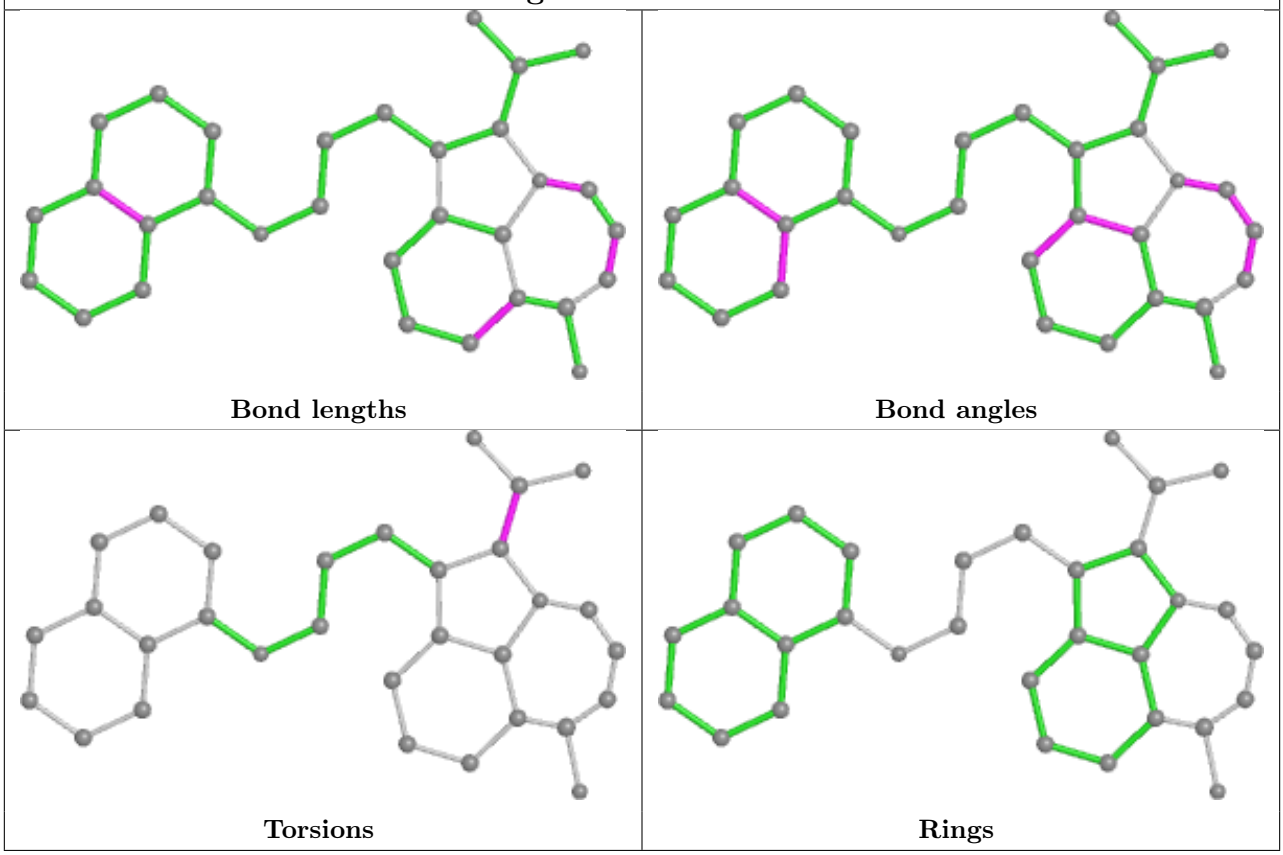
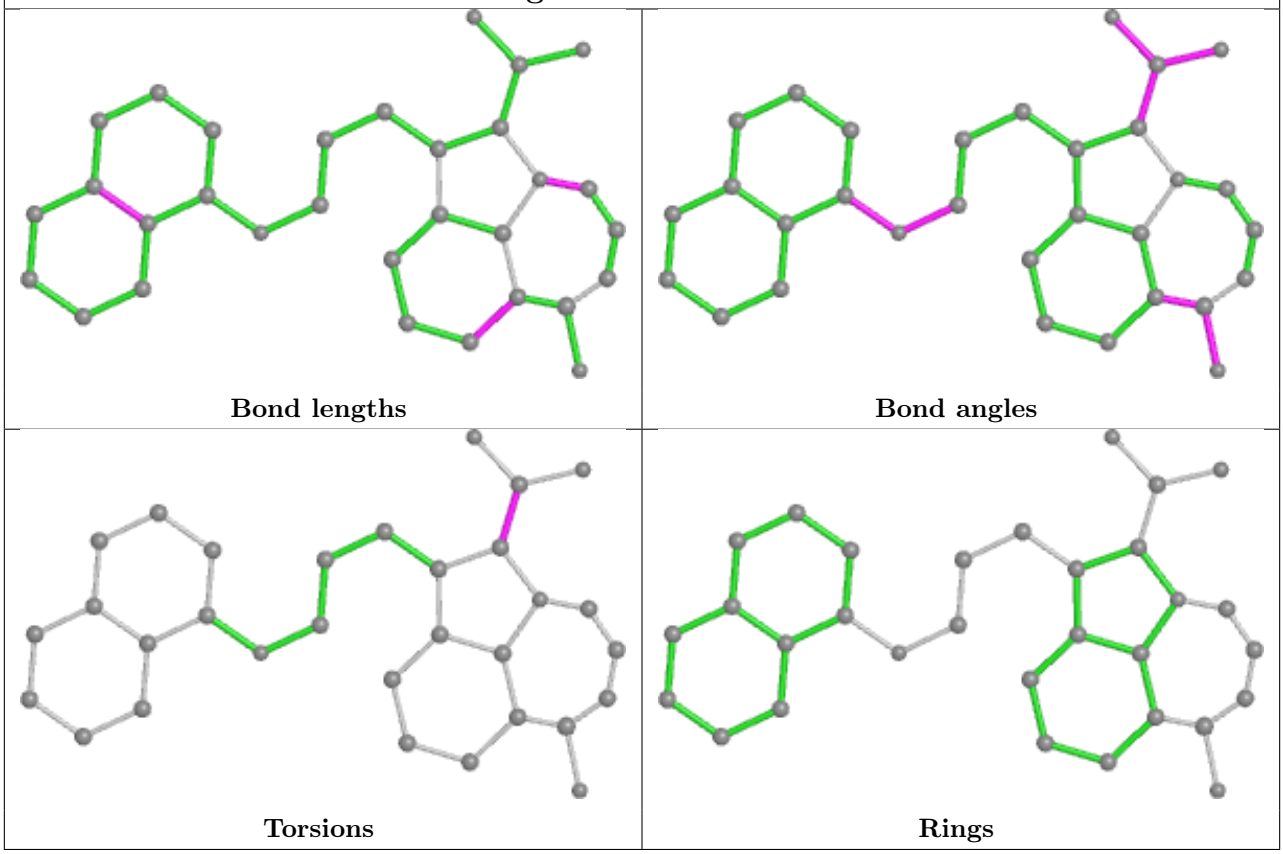


Rings

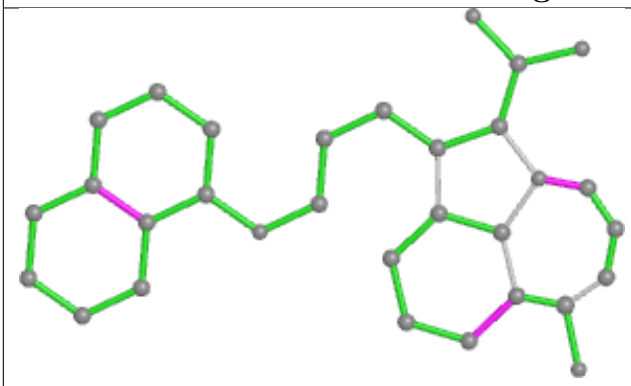
Ligand 4M7 D 400



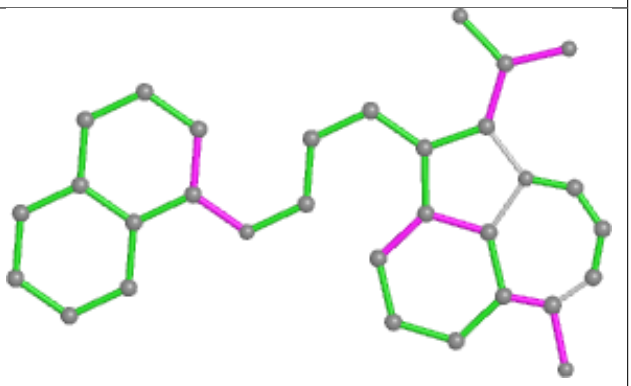
Ligand 4M7 G 400



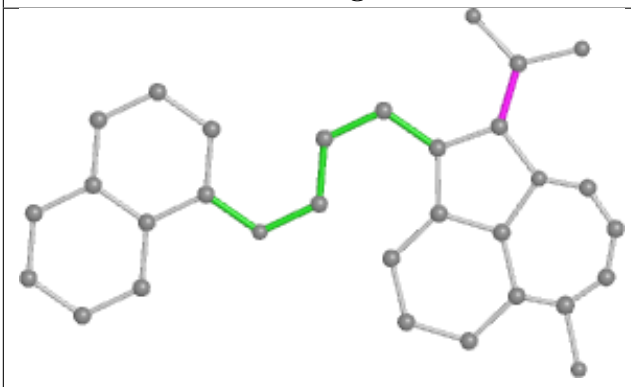
Ligand 4M7 I 400



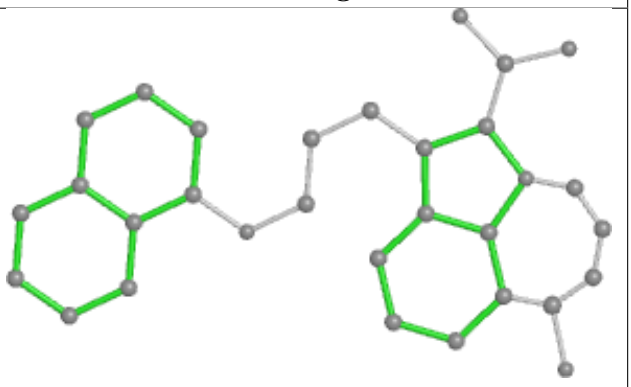
Bond lengths



Bond angles

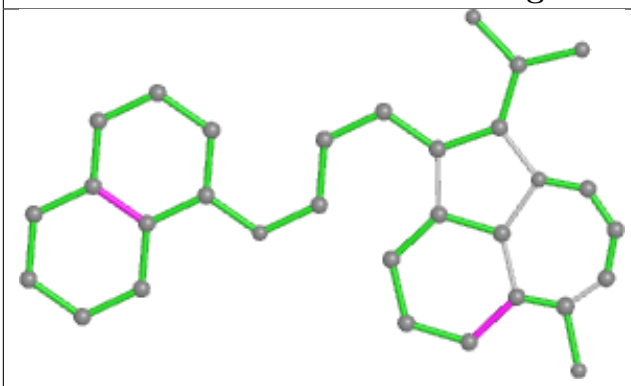


Torsions

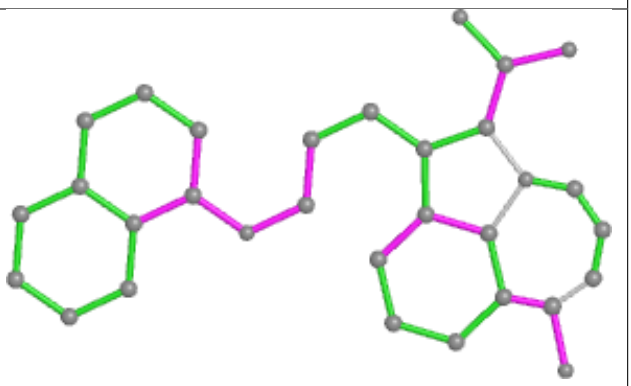


Rings

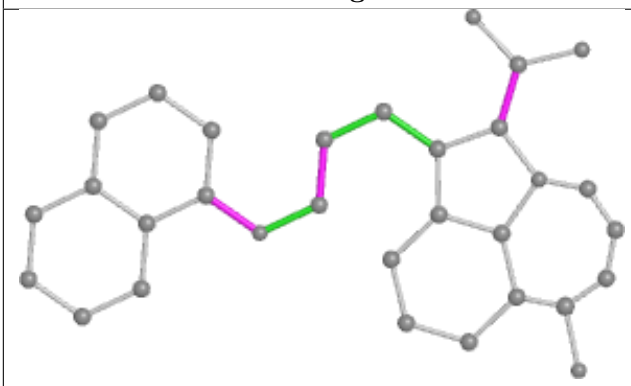
Ligand 4M7 B 400



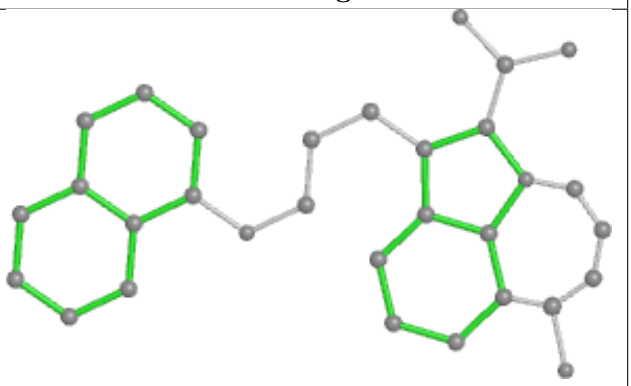
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	153/157 (97%)	-0.09	2 (1%)	77	75	27, 44, 67, 92	0
1	B	151/157 (96%)	-0.19	1 (0%)	87	86	27, 46, 70, 81	0
1	C	149/157 (94%)	0.01	2 (1%)	77	75	31, 44, 76, 98	0
1	D	148/157 (94%)	-0.12	2 (1%)	75	73	31, 49, 77, 91	0
1	E	151/157 (96%)	0.01	1 (0%)	87	86	32, 53, 81, 91	0
1	F	148/157 (94%)	-0.04	0	100	100	32, 53, 82, 91	0
1	G	151/157 (96%)	-0.03	4 (2%)	56	53	29, 50, 78, 92	0
1	H	151/157 (96%)	0.08	4 (2%)	56	53	30, 53, 90, 104	0
1	I	151/157 (96%)	0.24	4 (2%)	56	53	38, 62, 102, 115	0
1	J	151/157 (96%)	0.27	11 (7%)	15	14	36, 63, 102, 109	0
1	K	151/157 (96%)	-0.01	3 (1%)	65	63	34, 60, 93, 101	0
1	L	151/157 (96%)	0.25	7 (4%)	32	31	41, 60, 94, 109	0
All	All	1806/1884 (95%)	0.03	41 (2%)	60	58	27, 53, 87, 115	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	201	ARG	6.8
1	L	203	GLY	6.5
1	L	200	GLY	4.7
1	I	196	THR	4.1
1	D	321	VAL	3.9
1	I	320	HIS	3.4
1	L	202	SER	3.3
1	K	193	ALA	3.2
1	G	222	ARG	3.2
1	L	196	THR	3.1
1	J	193	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	202	SER	2.9
1	J	209	ALA	2.9
1	A	323	ASP	2.9
1	E	203	GLY	2.8
1	J	203	GLY	2.8
1	C	196	THR	2.8
1	H	198	PRO	2.8
1	G	223	ASN	2.8
1	J	198	PRO	2.6
1	J	199	MET	2.6
1	J	202	SER	2.5
1	L	320	HIS	2.5
1	C	193	ALA	2.4
1	D	320	HIS	2.4
1	K	194	LYS	2.3
1	J	201	ARG	2.3
1	J	319	PHE	2.2
1	A	222	ARG	2.2
1	L	321	VAL	2.2
1	J	196	THR	2.2
1	J	207	ARG	2.1
1	G	218	ASP	2.1
1	I	319	PHE	2.1
1	G	256	ASP	2.1
1	H	199	MET	2.1
1	K	196	THR	2.1
1	L	207	ARG	2.1
1	H	193	ALA	2.0
1	B	233	ARG	2.0
1	J	195	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

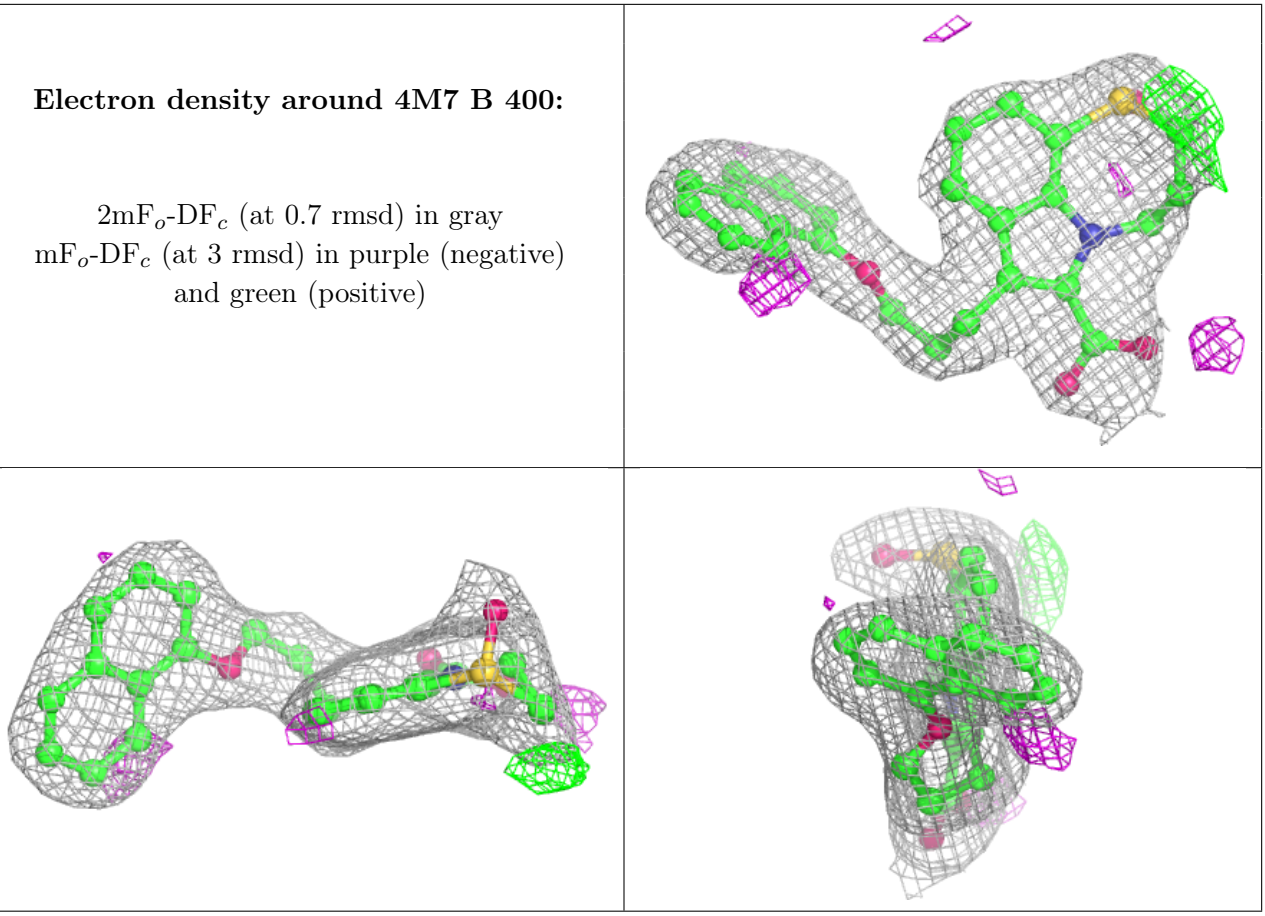
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	4M7	B	400	31/31	0.95	0.14	25,47,74,89	0
2	4M7	E	400	31/31	0.95	0.12	30,50,72,88	0
2	4M7	K	400	31/31	0.95	0.17	34,54,89,121	0
2	4M7	L	400	31/31	0.95	0.13	30,58,93,107	0
2	4M7	H	400	31/31	0.96	0.13	26,40,62,91	0
2	4M7	J	400	31/31	0.96	0.14	30,57,88,108	0
2	4M7	C	400	31/31	0.96	0.13	25,40,62,86	0
2	4M7	G	400	31/31	0.96	0.13	25,46,80,95	0
2	4M7	I	400	31/31	0.97	0.13	35,47,85,100	0
2	4M7	F	400	31/31	0.97	0.13	29,47,76,92	0
2	4M7	D	400	31/31	0.97	0.12	23,35,78,104	0
2	4M7	A	400	31/31	0.97	0.12	25,38,75,84	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.

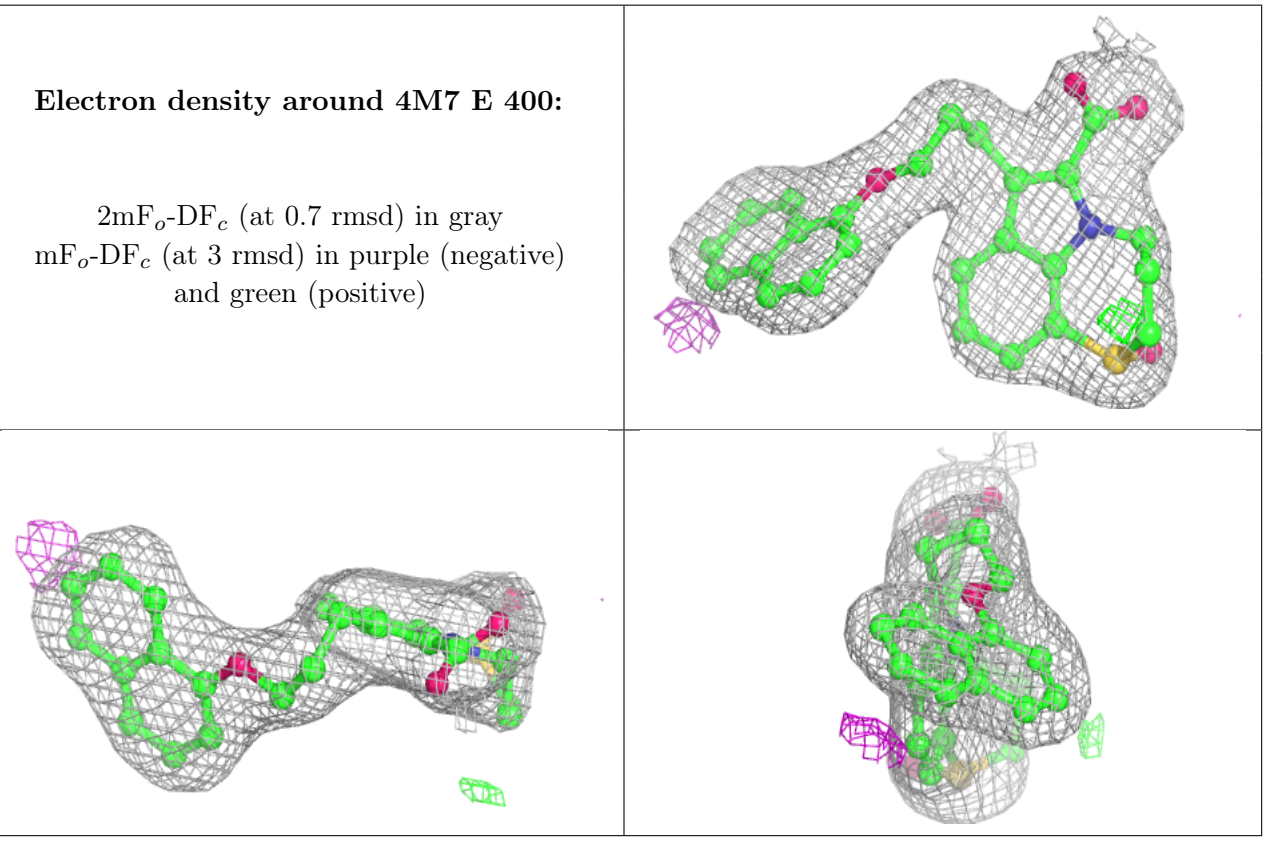
Electron density around 4M7 B 400:

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



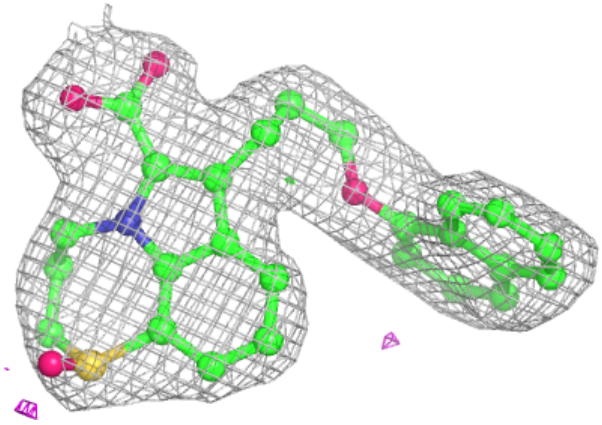
Electron density around 4M7 E 400:

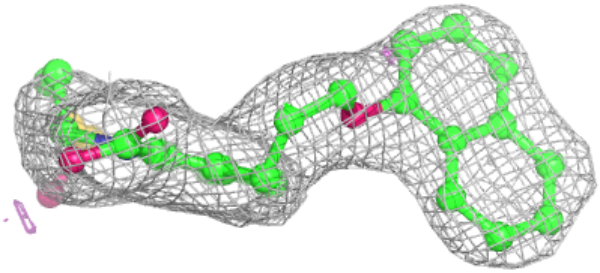
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

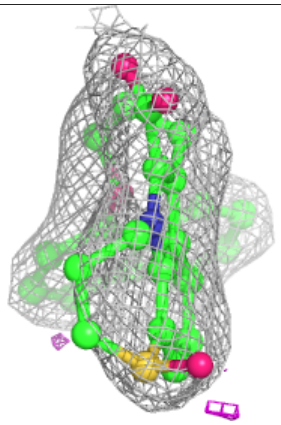


Electron density around 4M7 K 400:

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

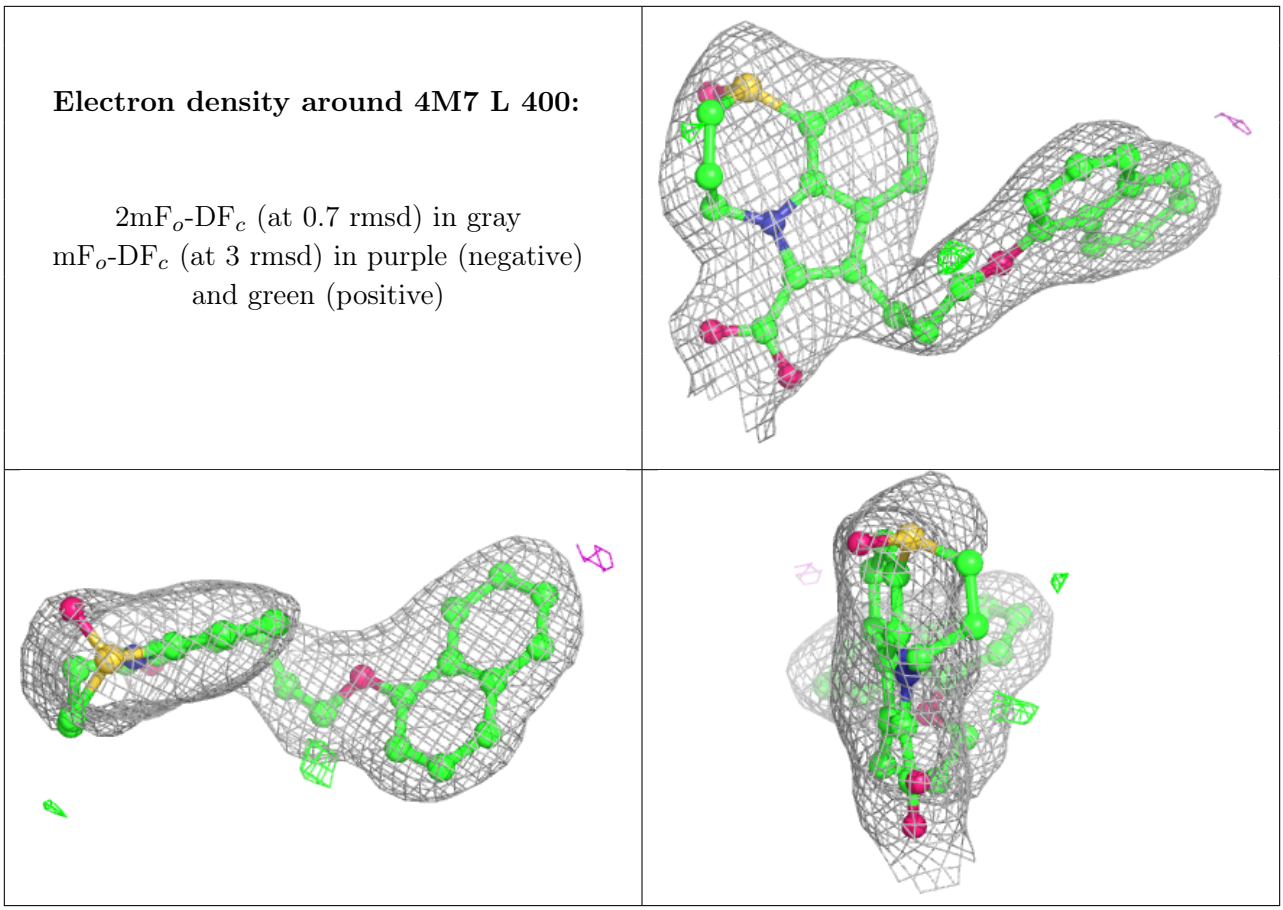






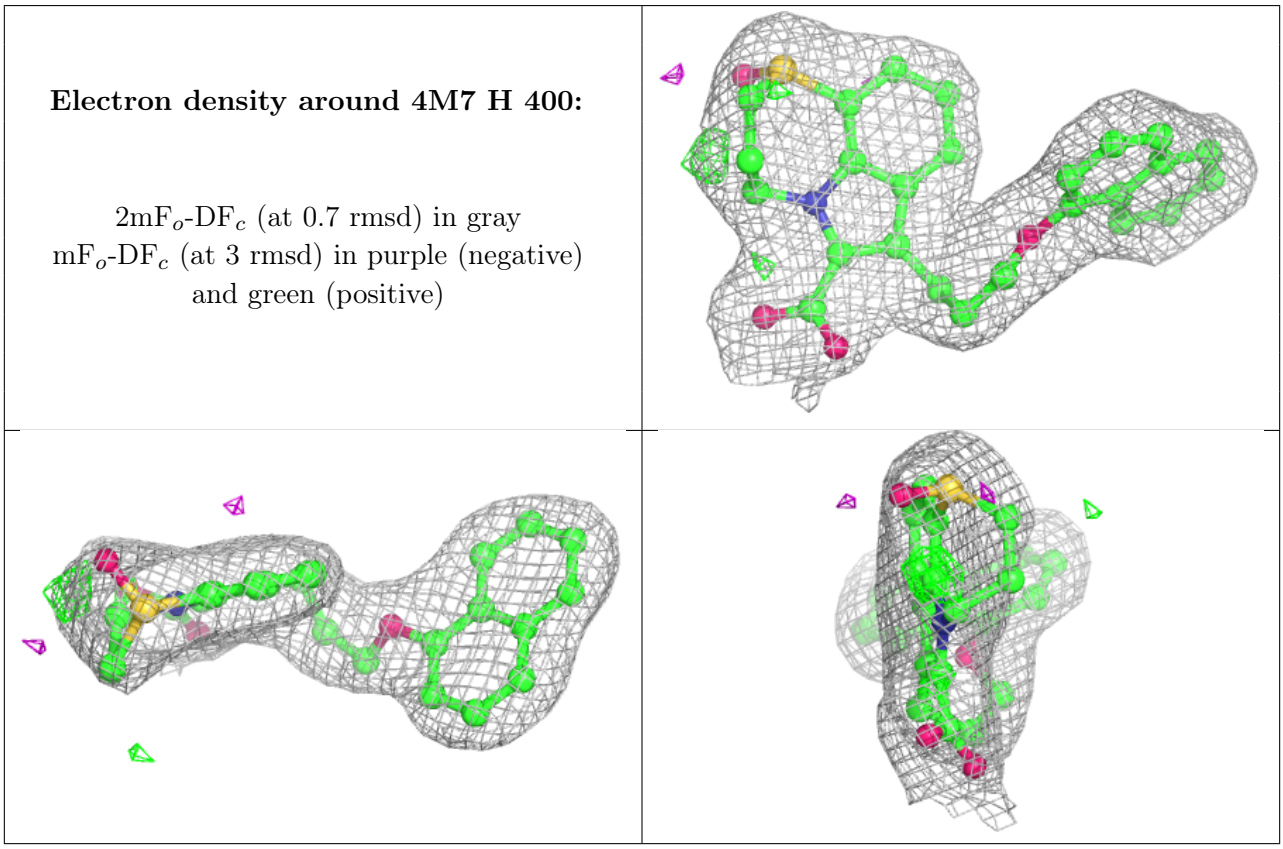
Electron density around 4M7 L 400:

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



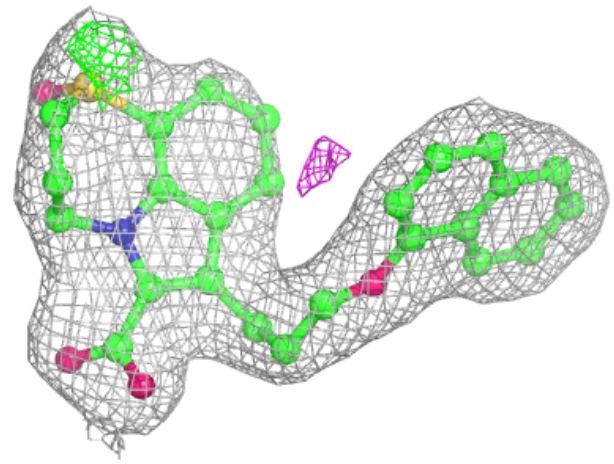
Electron density around 4M7 H 400:

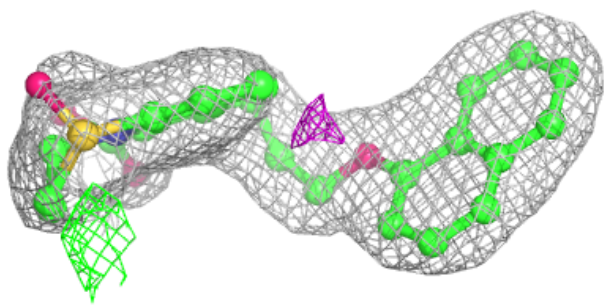
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

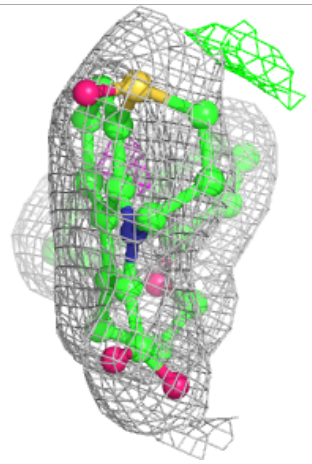


Electron density around 4M7 J 400:

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







Electron density around 4M7 C 400:

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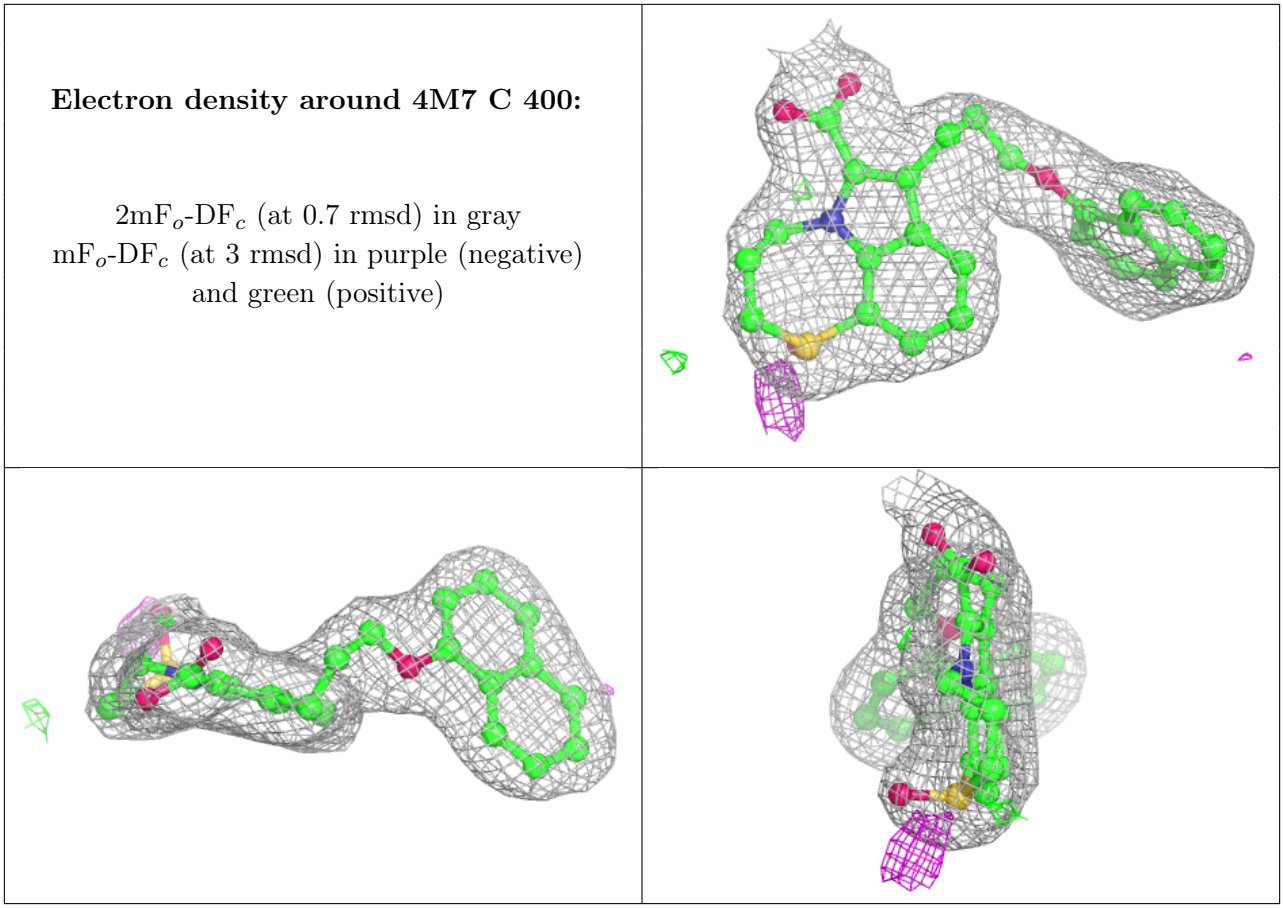
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 4M7 G 400:

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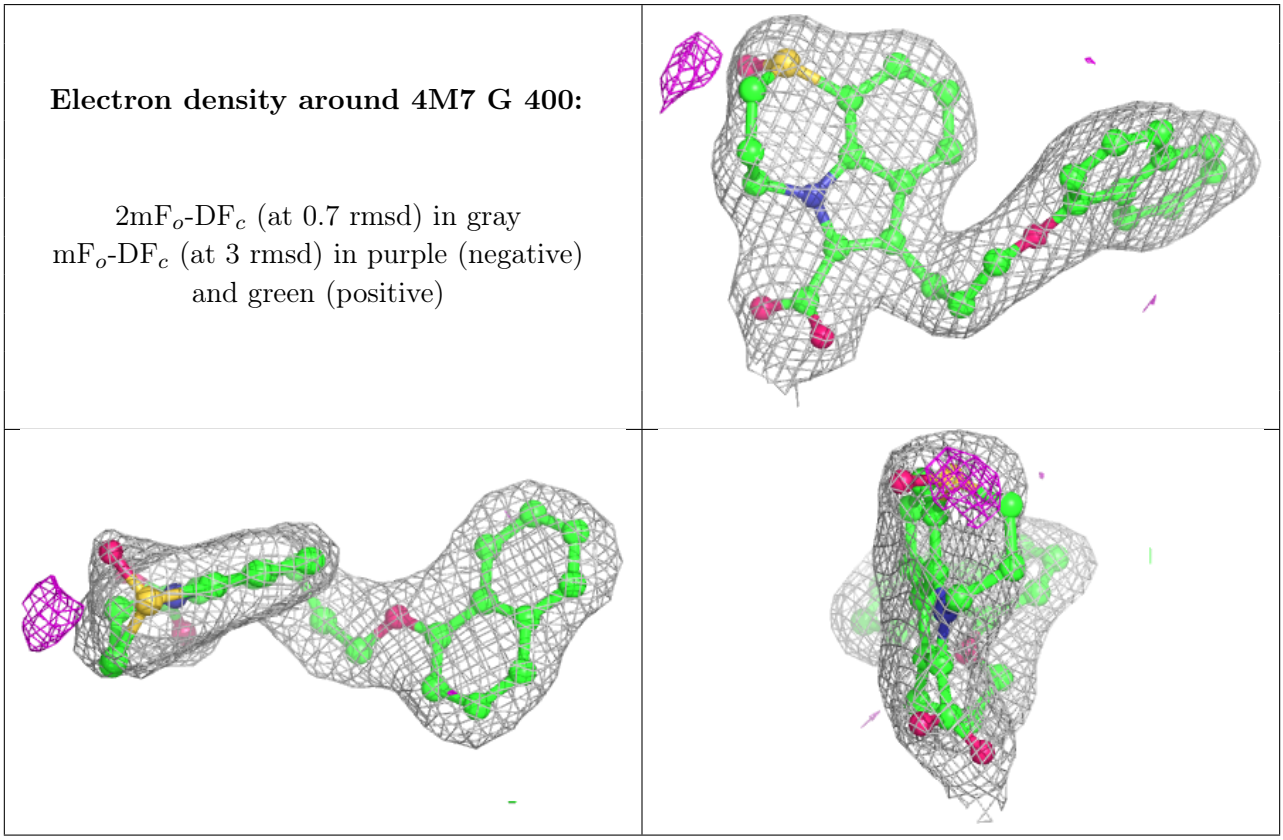
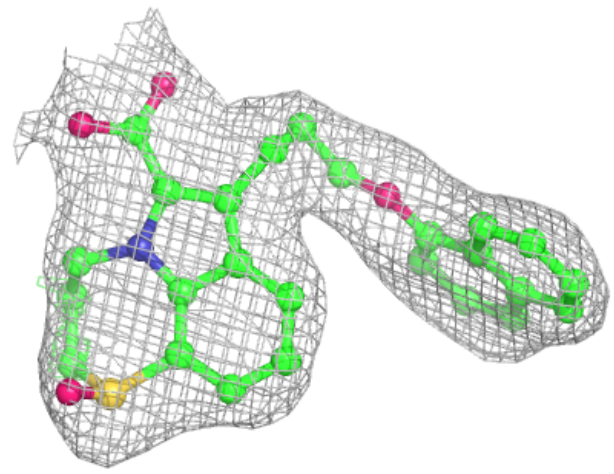
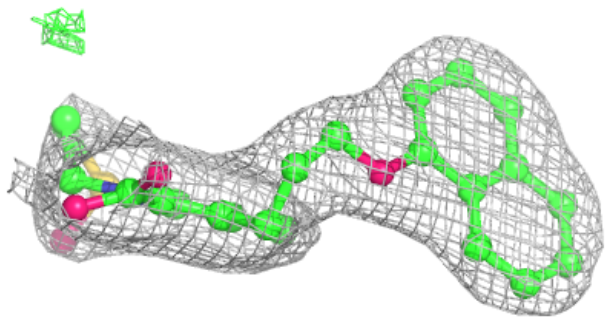
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

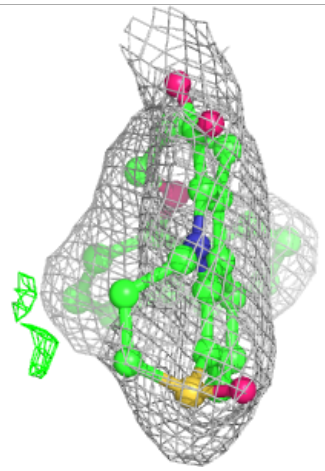


Electron density around 4M7 I 400:

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







Electron density around 4M7 F 400:

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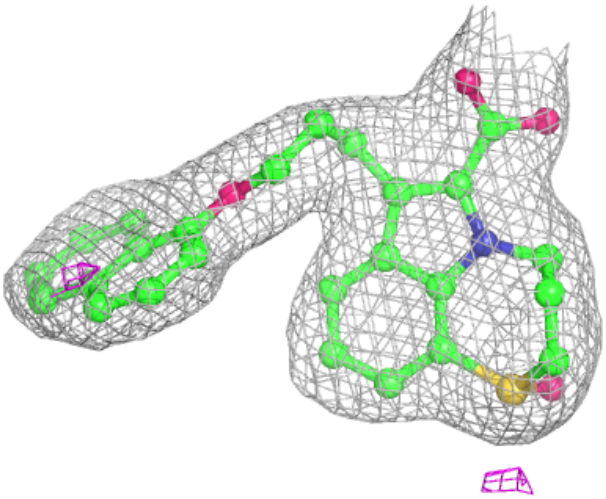
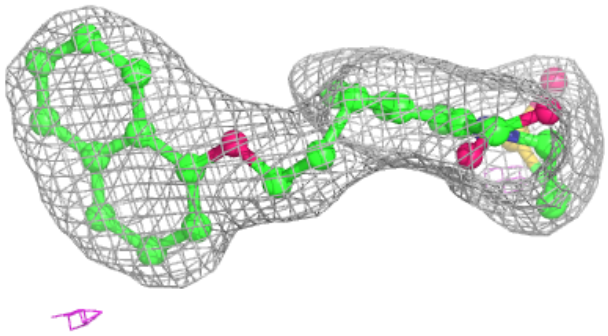
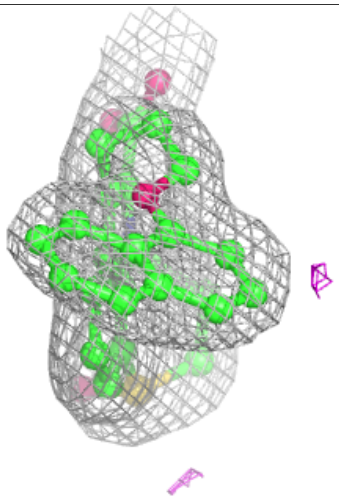
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around 4M7 D 400:

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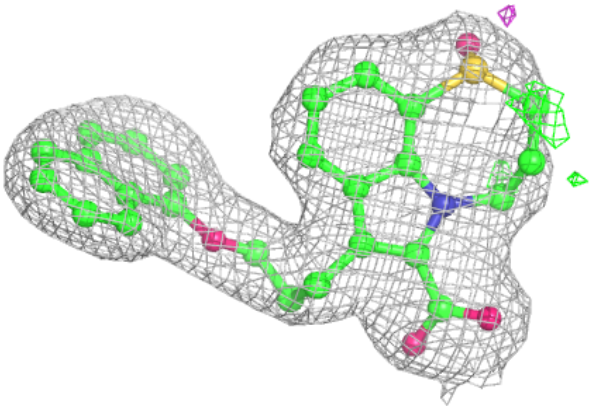
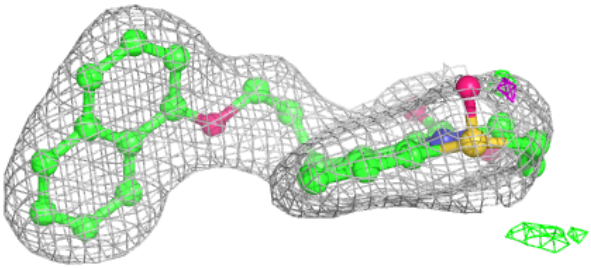
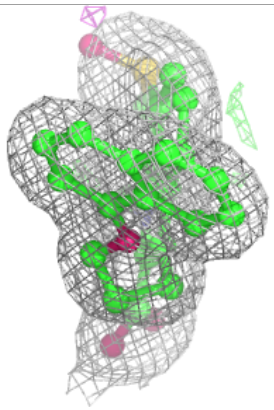
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

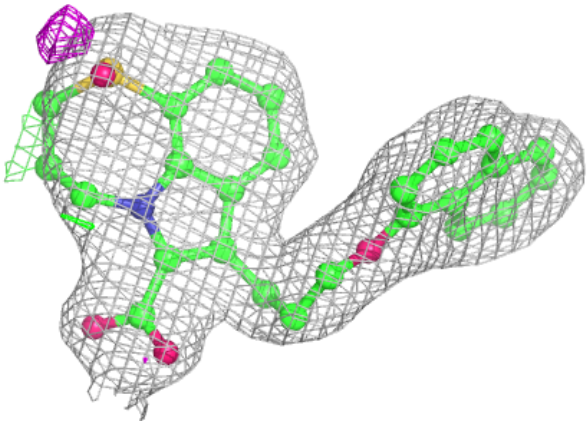


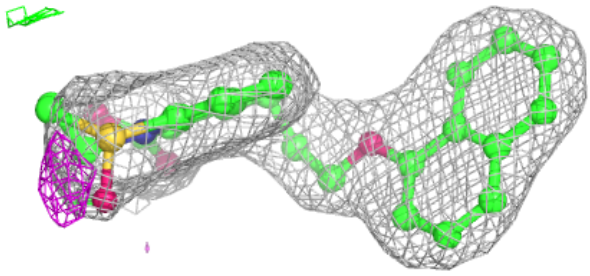


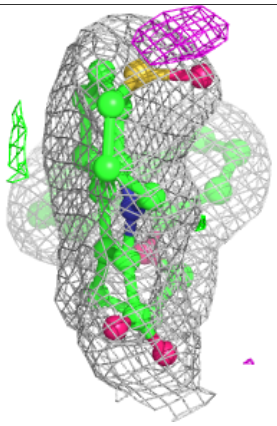


Electron density around 4M7 A 400:

$2mF_o$-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.