



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:52 PM UTC

PDB ID : 4ZBF / pdb_00004zbf
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

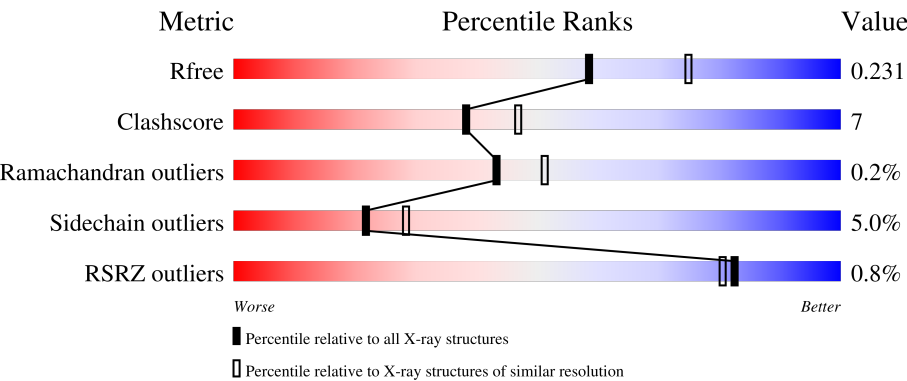
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	157	% 82%14%..
1	B	157	82%14%..
1	C	157	% 78%14%.5%
1	D	157	78%16%6%
1	E	157	77%18%..

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Mol	Chain	Length	Quality of chain
1	F	157	75% 17% • 6%
1	G	157	75% 19% • •
1	H	157	3% 80% 16% • •
1	I	157	3% 79% 16% • •
1	J	157	% 79% 15% • •
1	K	157	% 76% 18% • •
1	L	157	% 74% 20% • •

2 Entry composition

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

There are 12 discrepancies between the modelled and reference sequences:

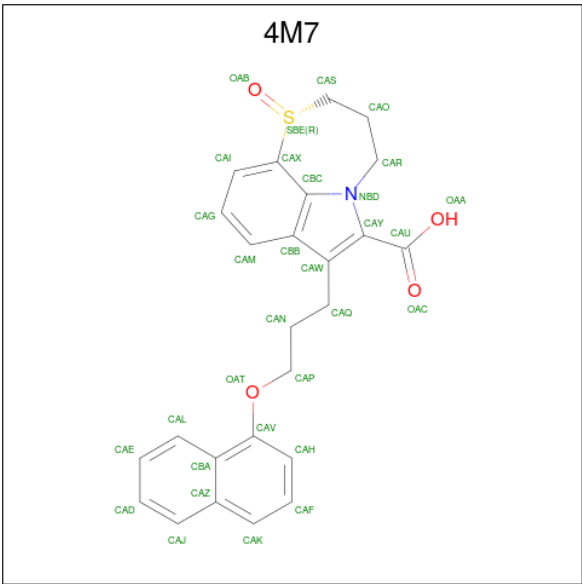
Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP Q07820
B	171	GLY	-	expression tag	UNP Q07820
C	171	GLY	-	expression tag	UNP Q07820
D	171	GLY	-	expression tag	UNP Q07820
E	171	GLY	-	expression tag	UNP Q07820

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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 (CCD ID: 4M7) (formula: C₂₅H₂₃NO₄S).



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

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

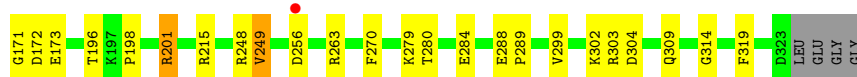
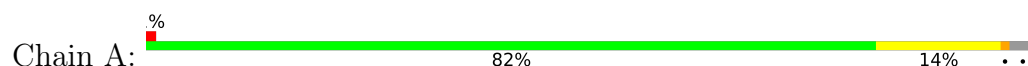
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	47	Total	O	0	0
			47	47		
3	C	29	Total	O	0	0
			29	29		
3	D	27	Total	O	0	0
			27	27		
3	E	34	Total	O	0	0
			34	34		
3	F	33	Total	O	0	0
			33	33		
3	G	32	Total	O	0	0
			32	32		
3	H	21	Total	O	0	0
			21	21		
3	I	18	Total	O	0	0
			18	18		
3	J	10	Total	O	0	0
			10	10		
3	K	21	Total	O	0	0
			21	21		
3	L	14	Total	O	0	0
			14	14		

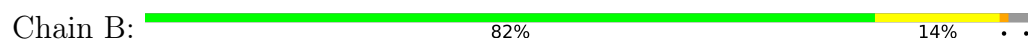
3 Residue-property plots [i](#)

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.

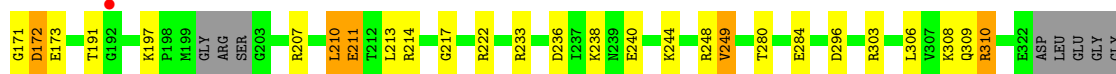
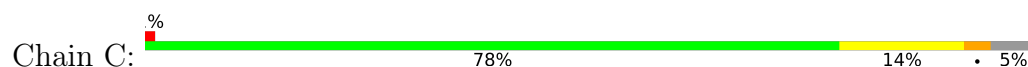
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



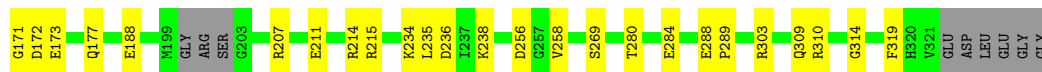
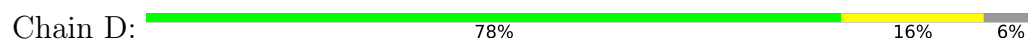
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



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



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

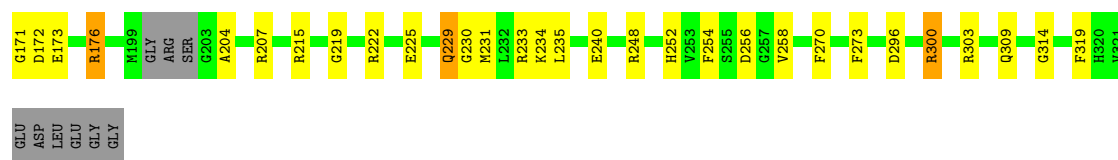


- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



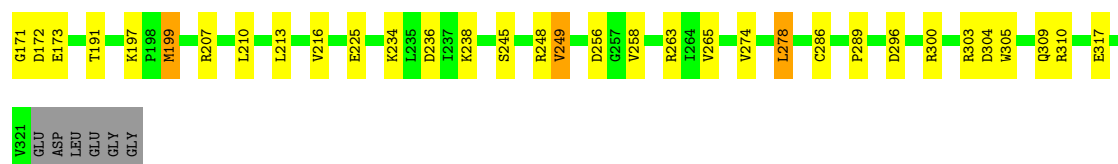
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain F: 



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

Chain G: 



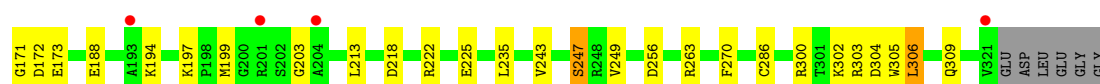
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain H: 



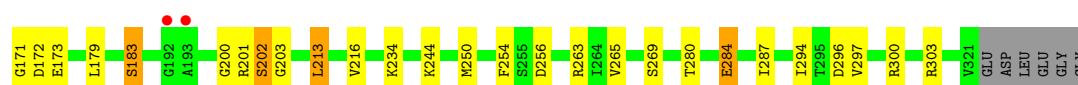
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain I: 



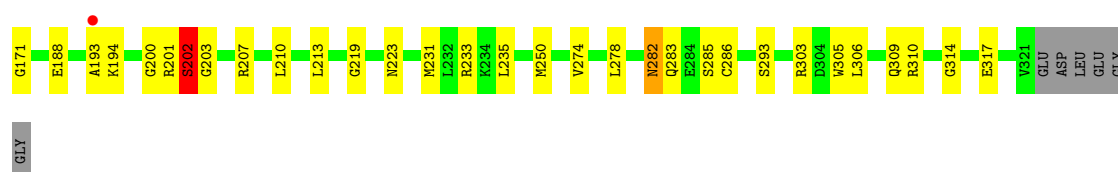
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain J: 



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

Chain K: 



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



G171	D172	E173	R176	M199	G200	G203	A204	T205	S206	R207	E211	T212	L213	R214	R215	V216	R233	K234	L235	M250	D256	V265	L278	S285	E288	P289	E292	S293	I294	T295	D296	V297	R300	R303	D304	K305	L306	V307	K308	Q309	G314	F319	H320	
GLU	ASP	LEU	GLU	GLY	GLY	GLU	ASP	LEU	GLU	GLY	GLU	ASP	LEU	GLU	GLY	GLY	GLU	ASP	LEU	GLU	GLY	GLY	GLU	ASP	LEU	GLU	GLY	GLU	ASP	LEU	GLU	GLY	GLY	GLU	ASP	LEU	GLU	GLY	GLY	GLU	ASP	LEU	GLU	GLY

4 Data and refinement statistics

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 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.00-2.20) 96.3 (30.00-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.20Å)	Xtriage
Refinement program	PHENIX dev_1951	Depositor
R, R_{free}	0.183 , 0.232 0.186 , 0.231	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 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.61	0/1242	0.92	1/1670 (0.1%)
1	B	0.64	0/1232	0.91	1/1656 (0.1%)
1	C	0.64	0/1219	0.98	4/1638 (0.2%)
1	D	0.60	0/1210	0.90	0/1626
1	E	0.60	0/1232	0.89	1/1656 (0.1%)
1	F	0.61	0/1210	0.95	3/1626 (0.2%)
1	G	0.62	0/1232	0.90	2/1656 (0.1%)
1	H	0.61	0/1232	0.94	0/1656
1	I	0.56	0/1232	0.95	1/1656 (0.1%)
1	J	0.57	0/1226	0.94	2/1649 (0.1%)
1	K	0.58	0/1222	0.91	1/1645 (0.1%)
1	L	0.54	0/1218	0.94	3/1641 (0.2%)
All	All	0.60	0/14707	0.93	19/19775 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	VAL	CB-CA-C	-7.37	102.19	112.14
1	F	231	MET	N-CA-C	-7.26	103.30	111.14
1	K	194	LYS	N-CA-C	-6.79	98.16	108.96
1	C	217	GLY	N-CA-C	6.75	121.41	112.77
1	B	191	THR	N-CA-C	-6.29	100.42	109.29
1	A	249	VAL	CB-CA-C	-6.21	103.76	112.14
1	J	254	PHE	N-CA-C	6.07	117.98	111.36
1	C	191	THR	N-CA-C	-6.00	100.52	109.94
1	I	197	LYS	N-CA-C	5.93	118.09	109.84
1	J	203	GLY	N-CA-C	5.63	120.62	113.24
1	C	172	ASP	CB-CA-C	-5.60	110.10	116.54
1	E	201	ARG	N-CA-C	5.58	122.68	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	203	GLY	N-CA-C	5.41	119.22	112.73
1	F	254	PHE	N-CA-C	5.38	117.22	111.36
1	G	191	THR	N-CA-C	5.25	120.34	113.30
1	L	233	ARG	N-CA-C	-5.17	105.64	111.28
1	F	229	GLN	N-CA-C	-5.14	102.24	109.96
1	L	292	GLU	N-CA-C	-5.14	105.68	111.28
1	G	249	VAL	CB-CA-C	-5.06	105.31	112.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1222	0	1227	24	0
1	B	1212	0	1223	22	0
1	C	1200	0	1207	13	1
1	D	1191	0	1201	12	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	16	0
1	I	1212	0	1223	20	0
1	J	1206	0	1212	15	0
1	K	1202	0	1201	19	0
1	L	1198	0	1190	23	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	31	0	22	0	0
2	L	31	0	22	1	0
3	A	61	0	0	2	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	2	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	204	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 (204) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:250:MET:HE1	1:L:294:ILE:HA	1.74	0.68
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:J:250:MET:HE1	1:J:294:ILE:HA	1.79	0.63
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: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:G:199:MET:HE3	1:G:207:ARG:HD3	1.81	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:D:234:LYS:NZ	3:D:501:HOH:O	2.33	0.56
1:B:194:LYS:HE3	1:B:214:ARG:NH2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:274:VAL:O	1:K:278:LEU:HD12	2.06	0.56
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:J:250:MET:HE2	1:J:297:VAL:HG21	1.89	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
1:D:188:GLU:OE2	1:D:214:ARG:NE	2.36	0.52
1:I:302:LYS:NZ	3:I:504:HOH:O	2.44	0.51
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:K:250:MET:HE1	1:K:293:SER:OG	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:302:LYS:NZ	3:A:503:HOH:O	2.48	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:G:286:CYS:C	1:G:289:PRO:HD2	2.40	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:L:199:MET:HE3	1:L:206:SER:HB3	1.98	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:H:310:ARG:HH22	1:H:317:GLU:CD	2.23	0.46
1:L:199:MET:HB3	1:L:203:GLY:CA	2.44	0.45
1:G:199:MET:HE1	1:G:210:LEU:HD22	1.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:LYS:NZ	1:G:256:ASP:HB2	2.32	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:K:310:ARG:HH22	1:K:317:GLU:CD	2.26	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: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:173:GLU:OE2	1:H:202:SER:OG	2.33	0.42
1:H:188:GLU:OE2	1:H:214:ARG:NE	2.52	0.42
1:K:310:ARG:NH2	1:K:317:GLU:CD	2.78	0.42
1:B:308:LYS:HD3	1:B:308:LYS:HA	1.85	0.42
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:L:250:MET:HE2	1:L:297:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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%)	18	19
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%)	18	19
1	K	149/157 (95%)	144 (97%)	3 (2%)	2 (1%)	9	8
1	L	149/157 (95%)	146 (98%)	3 (2%)	0	100	100
All	All	1776/1884 (94%)	1727 (97%)	45 (2%)	4 (0%)	43	51

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 ⓘ

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%)	126 (96%)	5 (4%)	29	40
1	B	131/135 (97%)	124 (95%)	7 (5%)	20	26
1	C	130/135 (96%)	120 (92%)	10 (8%)	12	13
1	D	129/135 (96%)	123 (95%)	6 (5%)	23	31
1	E	131/135 (97%)	124 (95%)	7 (5%)	20	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	129/135 (96%)	123 (95%)	6 (5%)	23	31
1	G	131/135 (97%)	123 (94%)	8 (6%)	17	20
1	H	131/135 (97%)	125 (95%)	6 (5%)	24	32
1	I	131/135 (97%)	126 (96%)	5 (4%)	29	40
1	J	130/135 (96%)	124 (95%)	6 (5%)	24	32
1	K	129/135 (96%)	123 (95%)	6 (5%)	23	31
1	L	128/135 (95%)	122 (95%)	6 (5%)	23	31
All	All	1561/1620 (96%)	1483 (95%)	78 (5%)	22	28

All (78) 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	A	280	THR
1	B	201	ARG
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	197	LYS
1	C	210	LEU
1	C	211	GLU
1	C	213	LEU
1	C	249	VAL
1	C	280	THR
1	C	284	GLU
1	C	296	ASP
1	C	306	LEU
1	C	310	ARG
1	D	177	GLN
1	D	256	ASP
1	D	258	VAL
1	D	269	SER
1	D	280	THR
1	D	284	GLU

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Mol	Chain	Res	Type
1	E	196	THR
1	E	208	LYS
1	E	222	ARG
1	E	249	VAL
1	E	269	SER
1	E	280	THR
1	E	306	LEU
1	F	176	ARG
1	F	225	GLU
1	F	240	GLU
1	F	256	ASP
1	F	258	VAL
1	F	300	ARG
1	G	197	LYS
1	G	199	MET
1	G	213	LEU
1	G	225	GLU
1	G	249	VAL
1	G	258	VAL
1	G	278	LEU
1	G	296	ASP
1	H	226	THR
1	H	240	GLU
1	H	258	VAL
1	H	282	ASN
1	H	296	ASP
1	H	306	LEU
1	I	213	LEU
1	I	225	GLU
1	I	247	SER
1	I	249	VAL
1	I	306	LEU
1	J	183	SER
1	J	202	SER
1	J	213	LEU
1	J	244	LYS
1	J	280	THR
1	J	284	GLU
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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	224	HIS
1	D	177	GLN
1	D	224	HIS
1	E	252	HIS
1	F	224	HIS
1	F	229	GLN
1	H	177	GLN
1	H	277	HIS
1	H	309	GLN
1	I	224	HIS
1	I	229	GLN
1	I	309	GLN
1	J	177	GLN
1	L	252	HIS
1	L	277	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	-	34,35,35	1.07	2 (5%)	42,50,50	1.34	4 (9%)
2	4M7	A	400	-	34,35,35	1.15	2 (5%)	42,50,50	1.23	6 (14%)
2	4M7	B	400	-	34,35,35	1.12	2 (5%)	42,50,50	1.27	6 (14%)
2	4M7	G	400	-	34,35,35	1.07	2 (5%)	42,50,50	1.10	4 (9%)
2	4M7	F	400	-	34,35,35	1.10	2 (5%)	42,50,50	1.29	6 (14%)
2	4M7	L	400	-	34,35,35	1.14	2 (5%)	42,50,50	1.14	5 (11%)
2	4M7	E	400	-	34,35,35	1.15	2 (5%)	42,50,50	1.02	3 (7%)
2	4M7	D	400	-	34,35,35	1.09	2 (5%)	42,50,50	1.24	3 (7%)
2	4M7	K	400	-	34,35,35	1.19	2 (5%)	42,50,50	1.26	6 (14%)
2	4M7	I	400	-	34,35,35	1.11	2 (5%)	42,50,50	1.21	5 (11%)
2	4M7	J	400	-	34,35,35	1.13	2 (5%)	42,50,50	1.11	4 (9%)
2	4M7	C	400	-	34,35,35	1.14	3 (8%)	42,50,50	1.06	1 (2%)

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	A	400	-	-	4/11/21/21	0/4/5/5
2	4M7	B	400	-	-	7/11/21/21	0/4/5/5
2	4M7	G	400	-	-	4/11/21/21	0/4/5/5
2	4M7	F	400	-	-	4/11/21/21	0/4/5/5
2	4M7	L	400	-	-	0/11/21/21	0/4/5/5
2	4M7	E	400	-	-	4/11/21/21	0/4/5/5
2	4M7	D	400	-	-	4/11/21/21	0/4/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4M7	K	400	-	-	8/11/21/21	0/4/5/5
2	4M7	I	400	-	-	4/11/21/21	0/4/5/5
2	4M7	J	400	-	-	4/11/21/21	0/4/5/5
2	4M7	C	400	-	-	4/11/21/21	0/4/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	400	4M7	CAY-CAW	3.07	1.41	1.37
2	E	400	4M7	CBA-CAZ	-2.98	1.37	1.43
2	K	400	4M7	CAY-CAW	2.88	1.41	1.37
2	L	400	4M7	CBA-CAZ	-2.75	1.37	1.43
2	A	400	4M7	CBA-CAZ	-2.73	1.37	1.43
2	J	400	4M7	CAY-CAW	2.67	1.41	1.37
2	J	400	4M7	CBA-CAZ	-2.67	1.38	1.43
2	I	400	4M7	CBA-CAZ	-2.65	1.38	1.43
2	H	400	4M7	CAY-CAW	2.60	1.41	1.37
2	B	400	4M7	CAY-CAW	2.58	1.41	1.37
2	C	400	4M7	CAY-CAW	2.57	1.41	1.37
2	I	400	4M7	CAY-CAW	2.56	1.41	1.37
2	D	400	4M7	CBA-CAZ	-2.51	1.38	1.43
2	G	400	4M7	CBA-CAZ	-2.36	1.38	1.43
2	A	400	4M7	CAY-CAW	2.34	1.40	1.37
2	G	400	4M7	CAY-CAW	2.33	1.40	1.37
2	C	400	4M7	CBA-CAZ	-2.31	1.38	1.43
2	C	400	4M7	CAI-CAX	2.31	1.41	1.39
2	D	400	4M7	CAS-CAO	-2.28	1.49	1.52
2	B	400	4M7	CBA-CAZ	-2.21	1.38	1.43
2	E	400	4M7	CAI-CAX	2.18	1.41	1.39
2	F	400	4M7	CAY-CAW	2.11	1.40	1.37
2	K	400	4M7	CBA-CAZ	-2.07	1.39	1.43
2	H	400	4M7	CBA-CAZ	-2.06	1.39	1.43
2	F	400	4M7	CBA-CAZ	-2.04	1.39	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	A	400	4M7	CAU-CAY-NBD	3.31	126.71	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	I	400	4M7	CAU-CAY-NBD	3.14	126.49	122.59
2	K	400	4M7	CBC-NBD-CAY	3.05	110.22	107.21
2	J	400	4M7	OAB-SBE-CAX	2.97	109.82	106.12
2	A	400	4M7	CBC-NBD-CAY	2.96	110.13	107.21
2	F	400	4M7	CAL-CBA-CAZ	2.91	121.69	117.92
2	H	400	4M7	CBC-NBD-CAY	2.90	110.07	107.21
2	L	400	4M7	CBC-NBD-CAY	2.88	110.05	107.21
2	L	400	4M7	OAA-CAU-OAC	-2.88	117.05	123.90
2	D	400	4M7	CAL-CBA-CAZ	2.84	121.59	117.92
2	B	400	4M7	CAU-CAY-NBD	2.84	126.12	122.59
2	F	400	4M7	CBC-NBD-CAY	2.82	110.00	107.21
2	E	400	4M7	CAU-CAY-NBD	2.79	126.06	122.59
2	C	400	4M7	CAU-CAY-NBD	2.74	126.00	122.59
2	F	400	4M7	CAU-CAY-NBD	2.74	126.00	122.59
2	G	400	4M7	CBC-NBD-CAY	2.71	109.89	107.21
2	J	400	4M7	CBC-NBD-CAY	2.67	109.84	107.21
2	G	400	4M7	OAB-SBE-CAX	2.66	109.43	106.12
2	A	400	4M7	OAB-SBE-CAX	2.55	109.30	106.12
2	E	400	4M7	CBC-NBD-CAY	2.44	109.61	107.21
2	G	400	4M7	CAQ-CAN-CAP	2.43	117.19	112.33
2	E	400	4M7	CAL-CBA-CAZ	2.41	121.03	117.92
2	B	400	4M7	CBC-NBD-CAY	2.40	109.58	107.21
2	K	400	4M7	OAT-CAV-CAH	-2.38	119.22	124.45
2	I	400	4M7	CBC-NBD-CAY	2.33	109.51	107.21
2	D	400	4M7	CAU-CAY-NBD	2.33	125.49	122.59
2	K	400	4M7	CAU-CAY-NBD	2.33	125.48	122.59
2	F	400	4M7	OAB-SBE-CAX	2.31	109.00	106.12
2	A	400	4M7	CAL-CBA-CAZ	2.31	120.90	117.92
2	H	400	4M7	OAT-CAV-CAH	-2.30	119.40	124.45
2	L	400	4M7	CAU-CAY-NBD	2.28	125.42	122.59
2	A	400	4M7	OAA-CAU-OAC	-2.25	118.53	123.90
2	H	400	4M7	CAU-CAY-NBD	2.22	125.35	122.59
2	F	400	4M7	CAQ-CAN-CAP	2.18	116.69	112.33
2	F	400	4M7	OAT-CAP-CAN	2.17	116.30	108.30
2	G	400	4M7	CAP-OAT-CAV	2.17	124.11	117.74
2	B	400	4M7	CAN-CAQ-CAW	2.15	116.69	113.30
2	J	400	4M7	CAU-CAY-NBD	2.15	125.26	122.59
2	A	400	4M7	CAQ-CAW-CAY	-2.14	125.68	127.46
2	B	400	4M7	OAT-CAP-CAN	2.11	116.07	108.30
2	J	400	4M7	CAQ-CAN-CAP	2.10	116.54	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	4M7	OAT-CAV-CAH	-2.09	119.85	124.45
2	L	400	4M7	OAA-CAU-CAY	2.07	122.00	116.08
2	L	400	4M7	CAQ-CAN-CAP	2.05	116.45	112.33
2	K	400	4M7	OAT-CAV-CBA	2.04	120.76	115.11
2	K	400	4M7	CAP-OAT-CAV	2.03	123.71	117.74
2	I	400	4M7	OAA-CAU-OAC	-2.03	119.07	123.90
2	I	400	4M7	OAT-CAV-CAH	-2.02	120.02	124.45

There are no chirality outliers.

All (54) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	B	400	4M7	CAH-CAV-OAT-CAP
2	K	400	4M7	CAP-CAN-CAQ-CAW
2	A	400	4M7	OAA-CAU-CAY-CAW
2	A	400	4M7	OAC-CAU-CAY-CAW
2	B	400	4M7	OAA-CAU-CAY-CAW
2	B	400	4M7	OAC-CAU-CAY-CAW
2	C	400	4M7	OAA-CAU-CAY-CAW
2	C	400	4M7	OAC-CAU-CAY-CAW
2	E	400	4M7	OAA-CAU-CAY-CAW
2	E	400	4M7	OAC-CAU-CAY-CAW
2	G	400	4M7	OAA-CAU-CAY-CAW
2	G	400	4M7	OAC-CAU-CAY-CAW
2	I	400	4M7	OAA-CAU-CAY-CAW
2	I	400	4M7	OAC-CAU-CAY-CAW
2	J	400	4M7	OAA-CAU-CAY-CAW
2	J	400	4M7	OAC-CAU-CAY-CAW
2	A	400	4M7	OAC-CAU-CAY-NBD
2	C	400	4M7	OAC-CAU-CAY-NBD
2	E	400	4M7	OAA-CAU-CAY-NBD
2	E	400	4M7	OAC-CAU-CAY-NBD
2	G	400	4M7	OAA-CAU-CAY-NBD
2	G	400	4M7	OAC-CAU-CAY-NBD
2	J	400	4M7	OAA-CAU-CAY-NBD
2	J	400	4M7	OAC-CAU-CAY-NBD

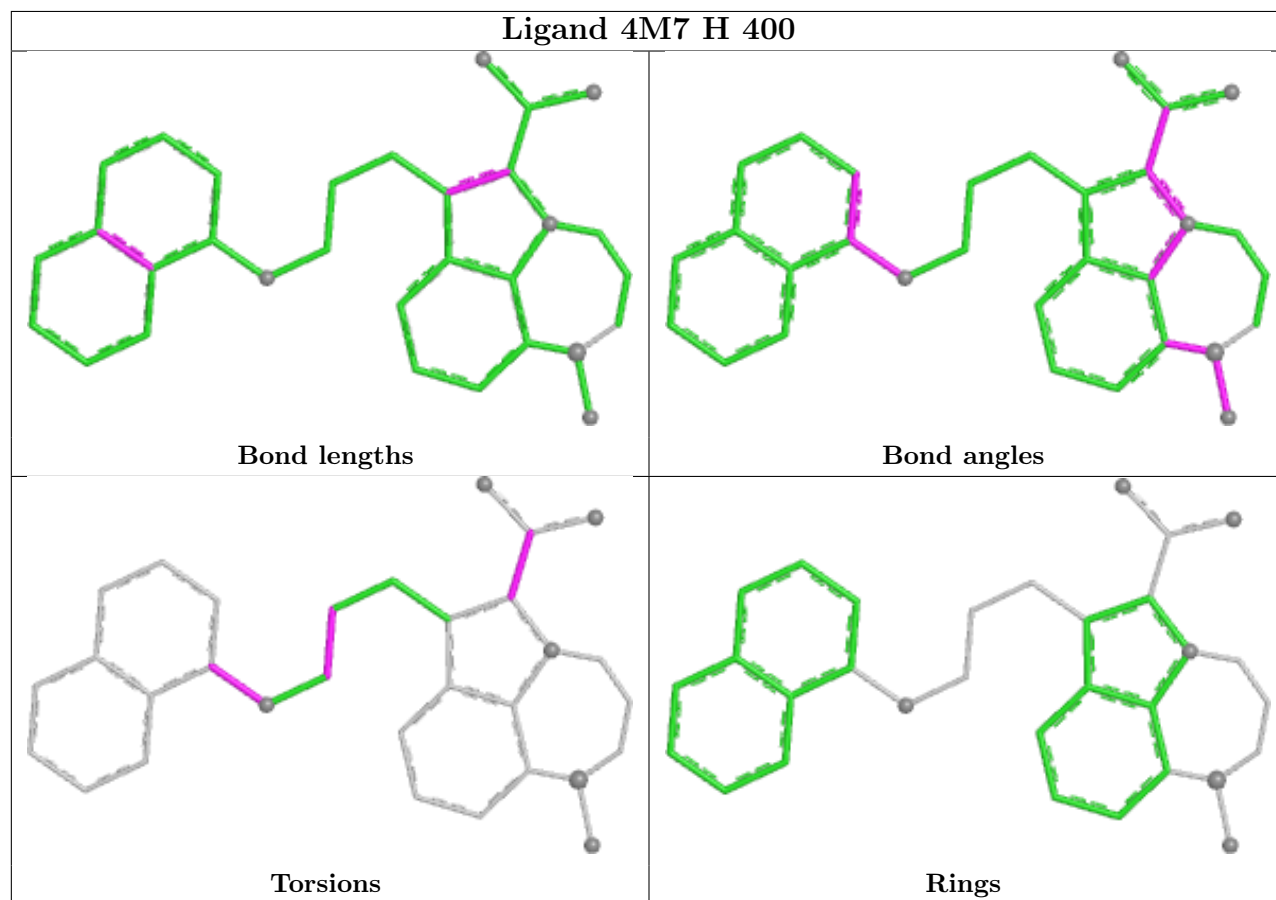
There are no ring outliers.

5 monomers are involved in 7 short contacts:

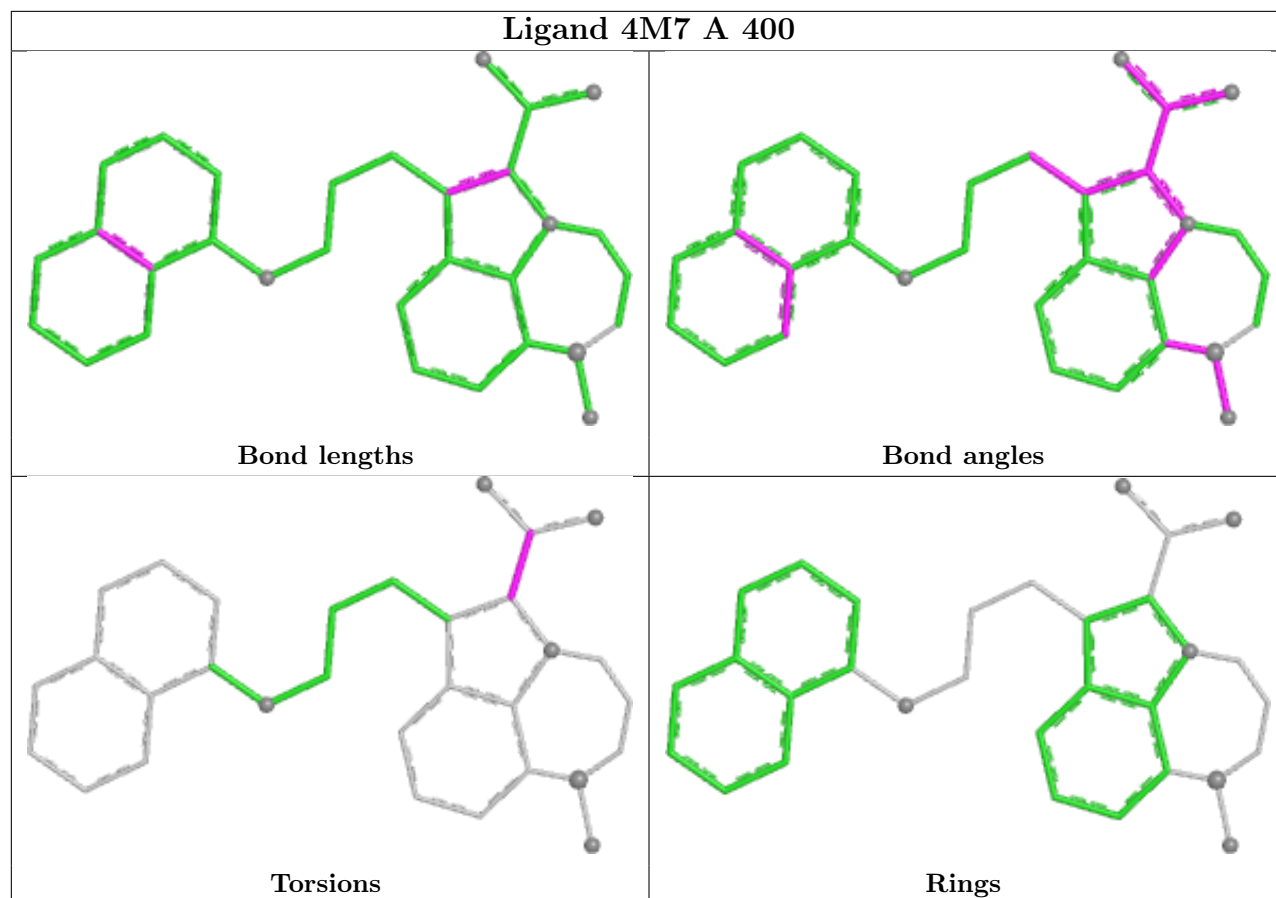
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	4M7	1	0
2	B	400	4M7	1	0
2	F	400	4M7	1	0
2	L	400	4M7	1	0
2	I	400	4M7	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

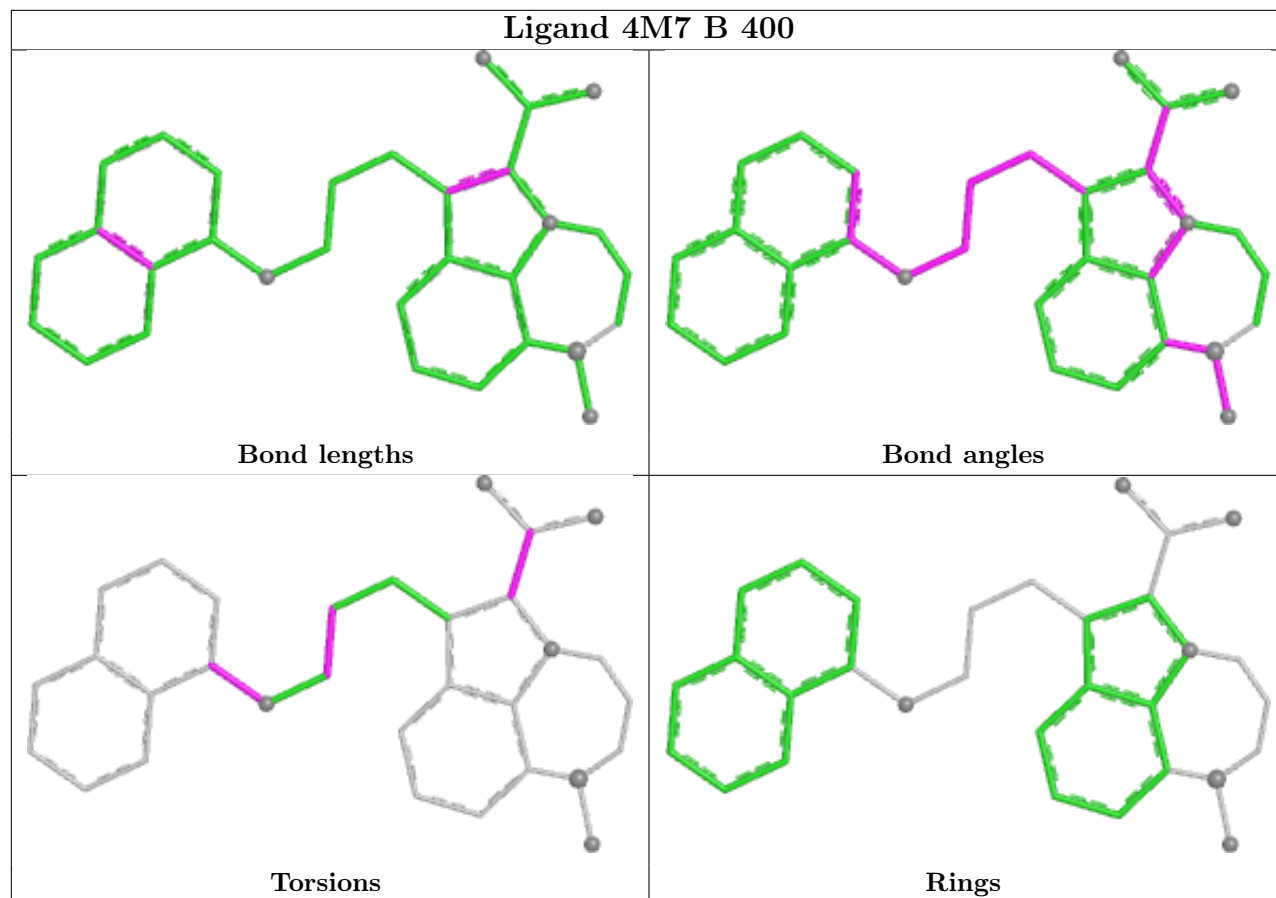
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



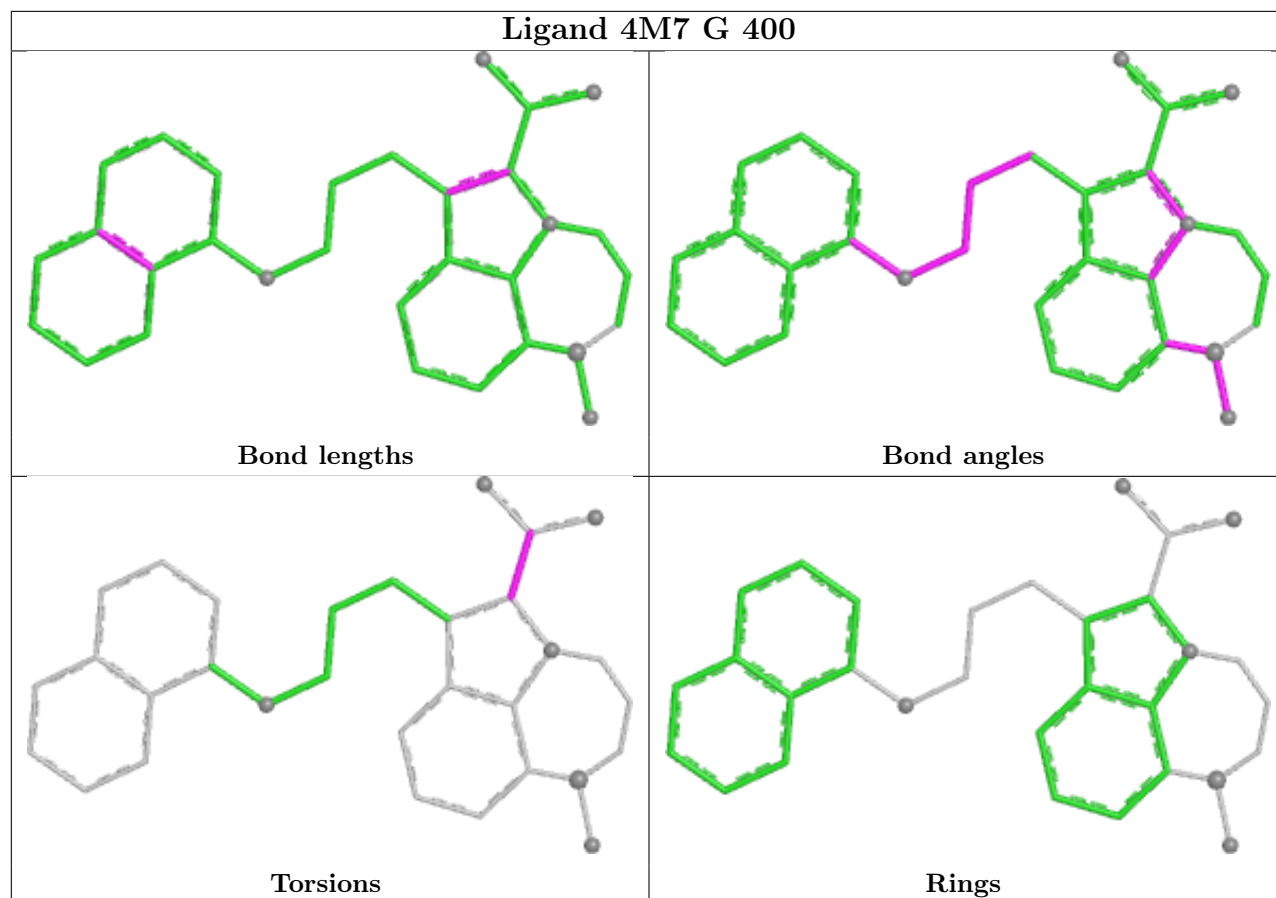
Ligand 4M7 A 400



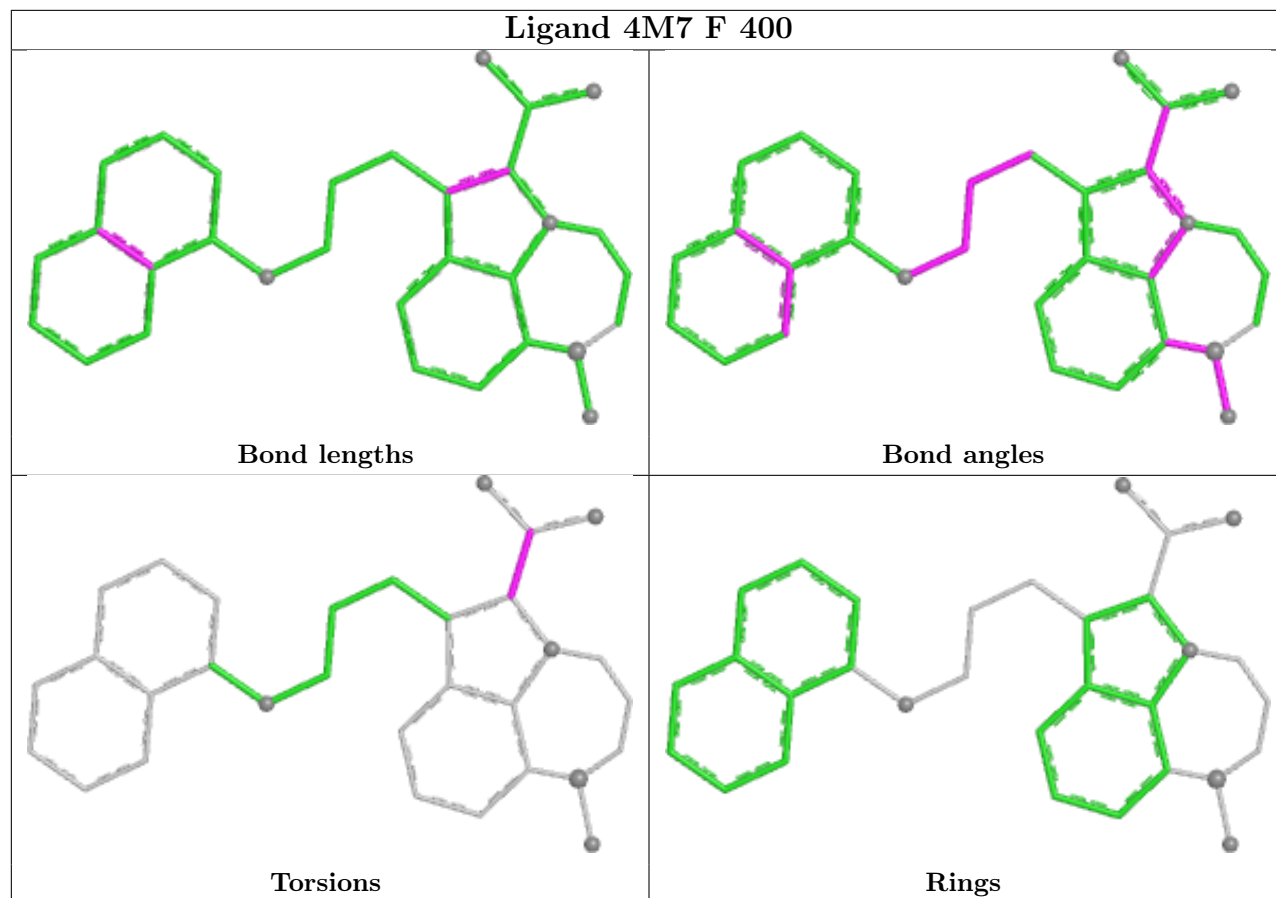
Ligand 4M7 B 400

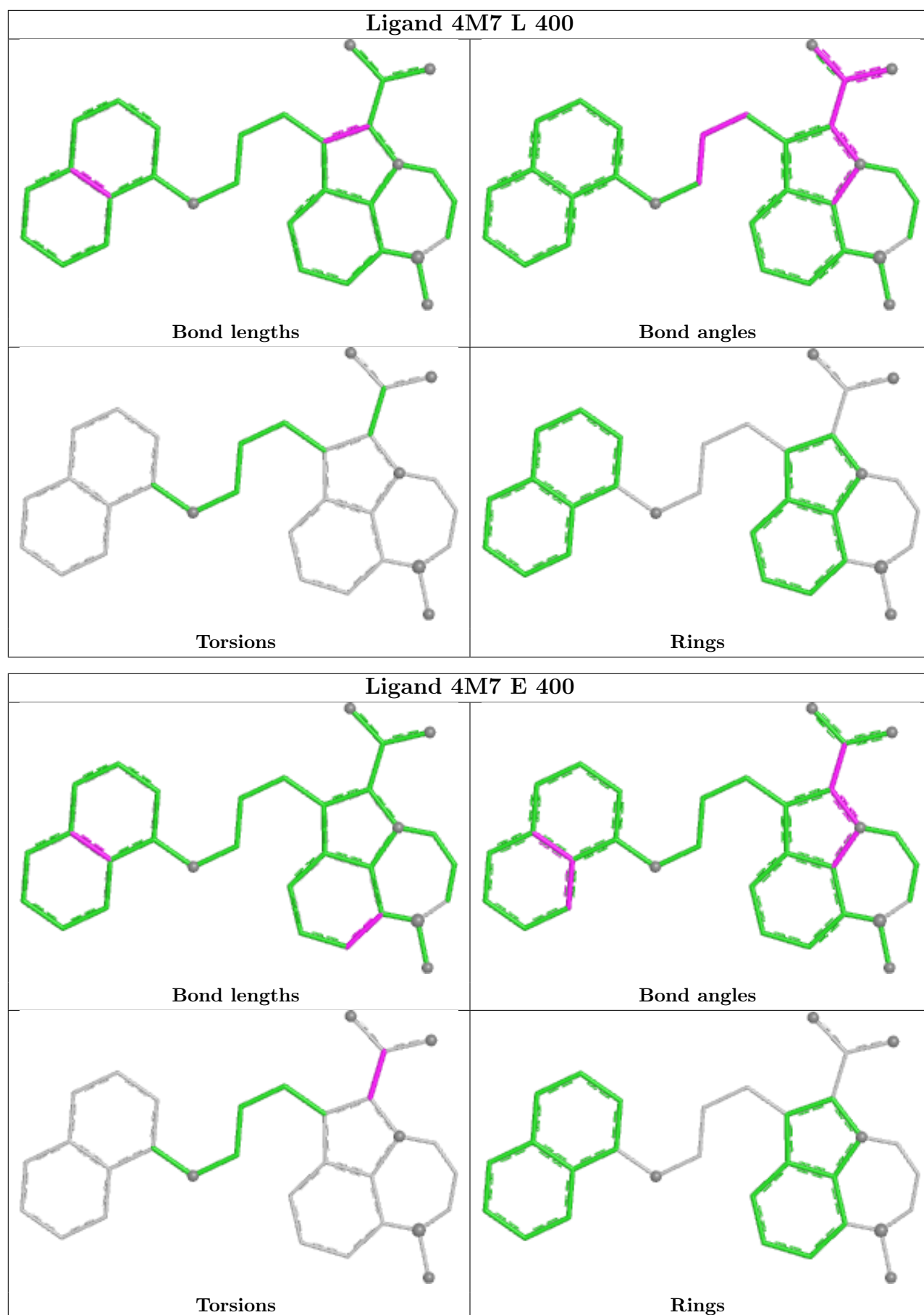


Ligand 4M7 G 400

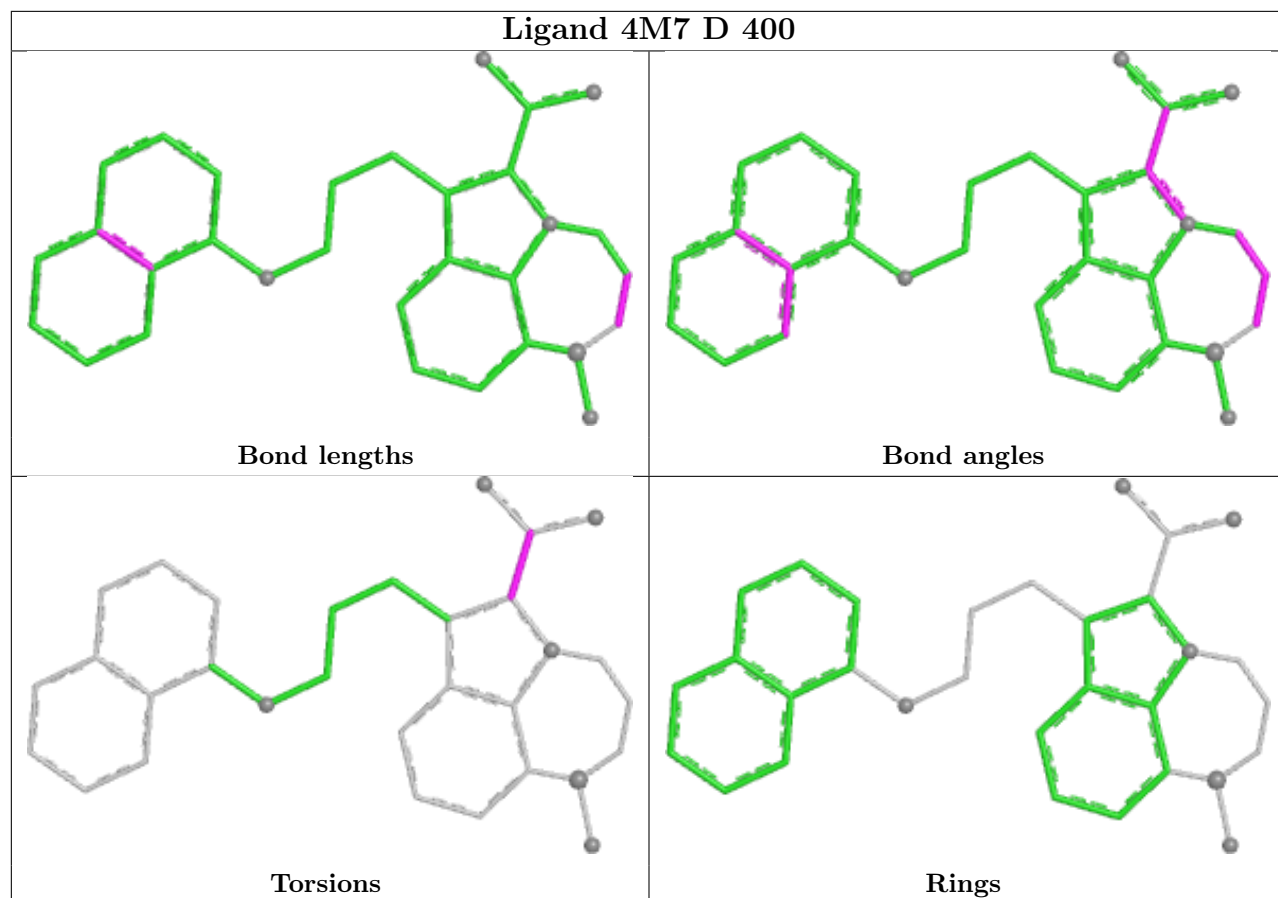


Ligand 4M7 F 400

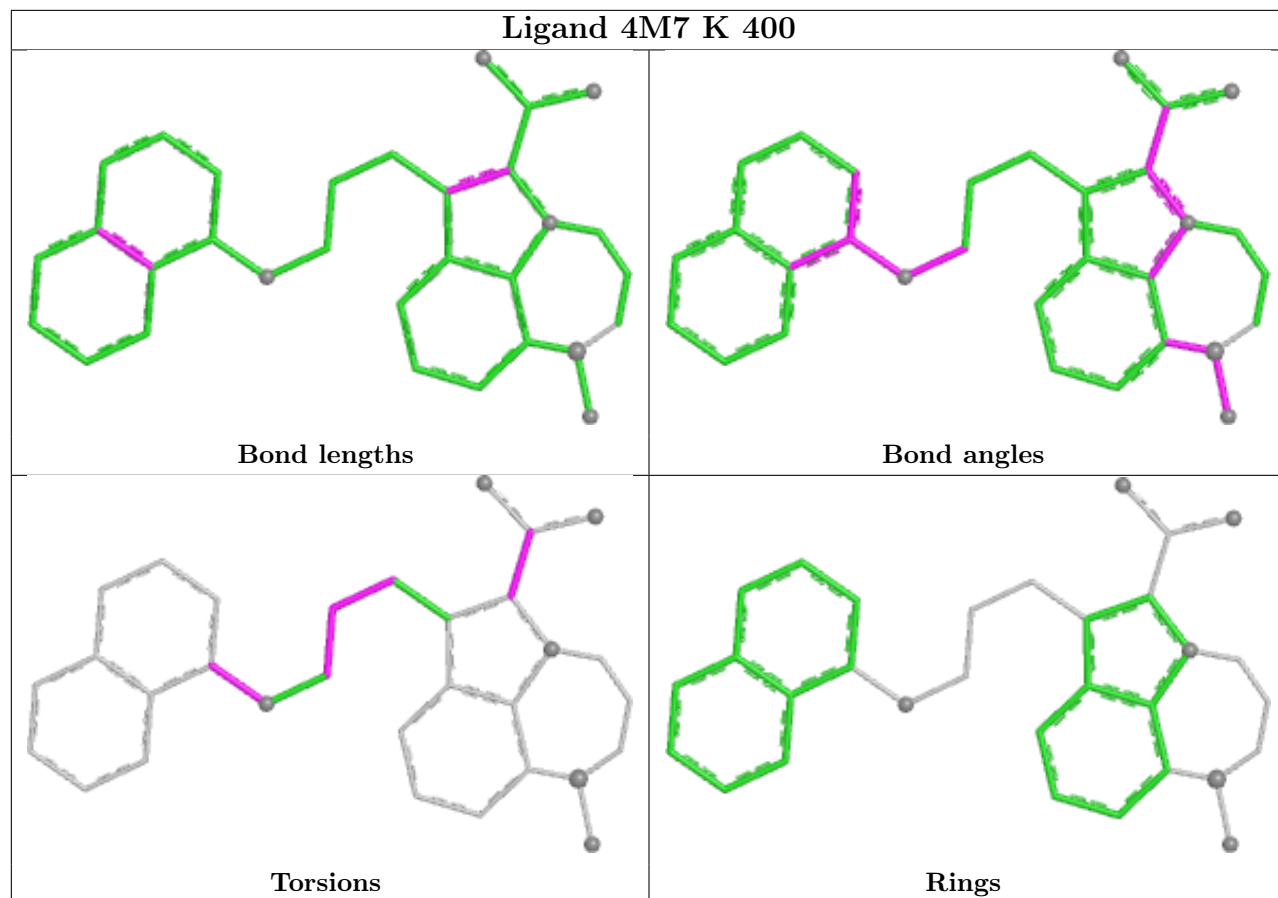


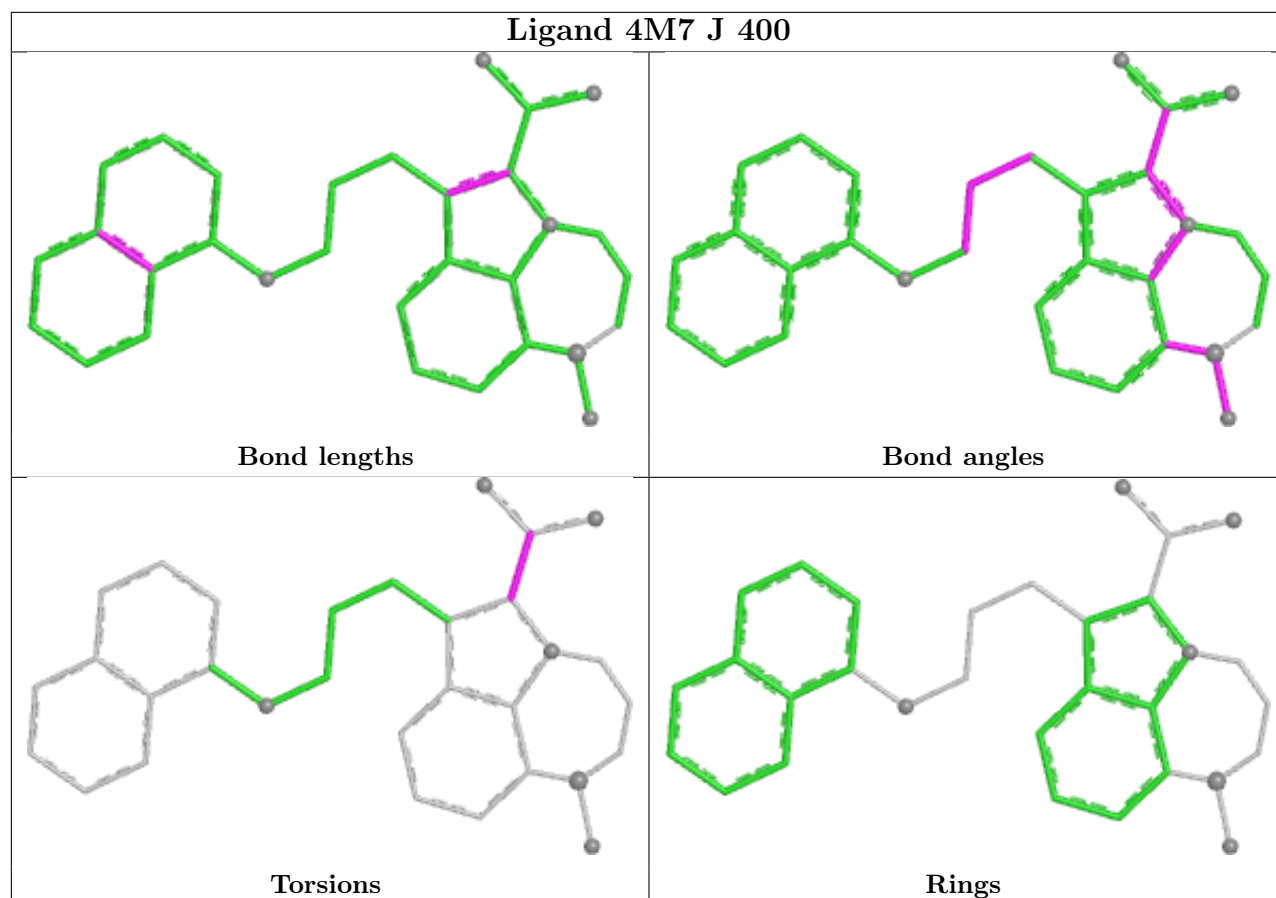
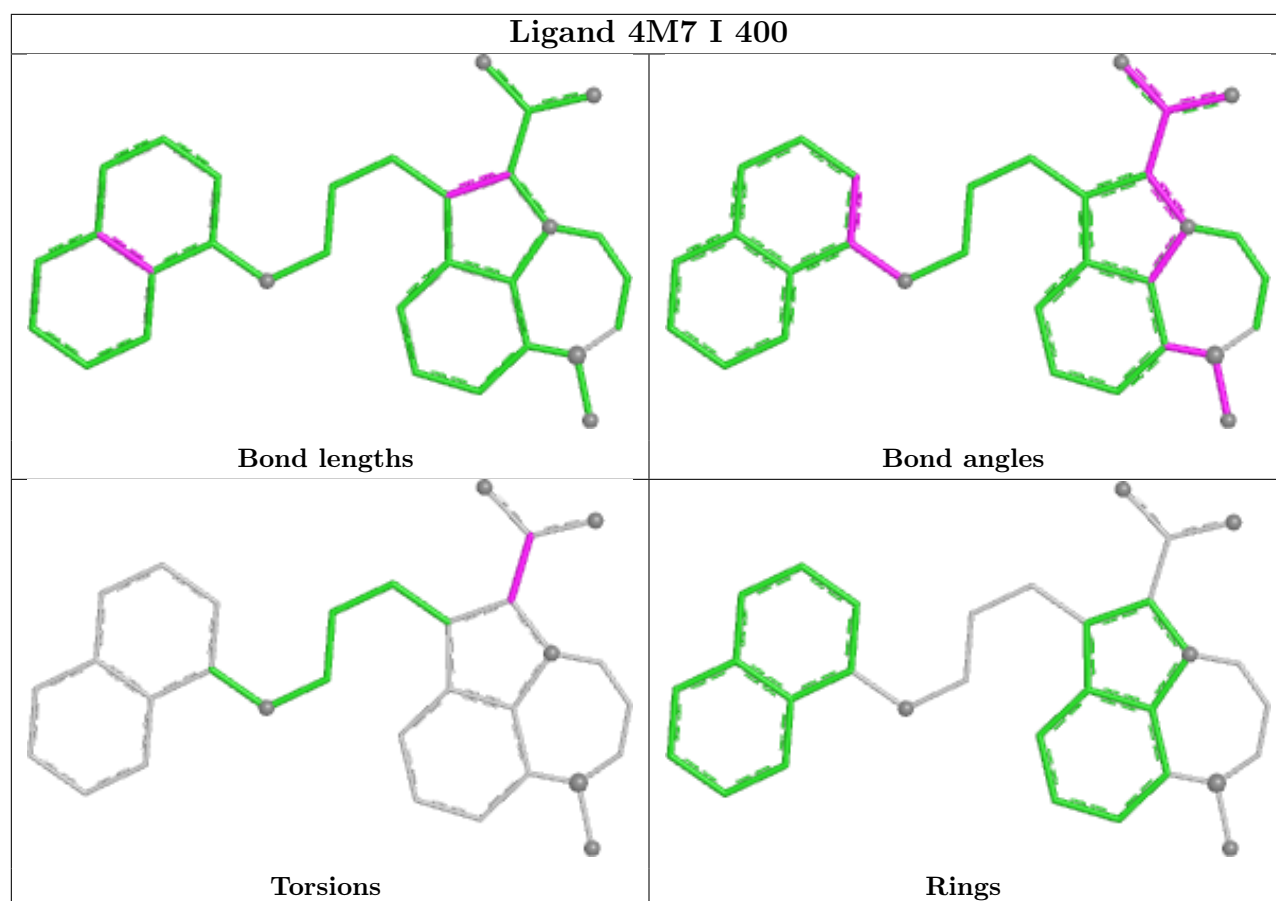


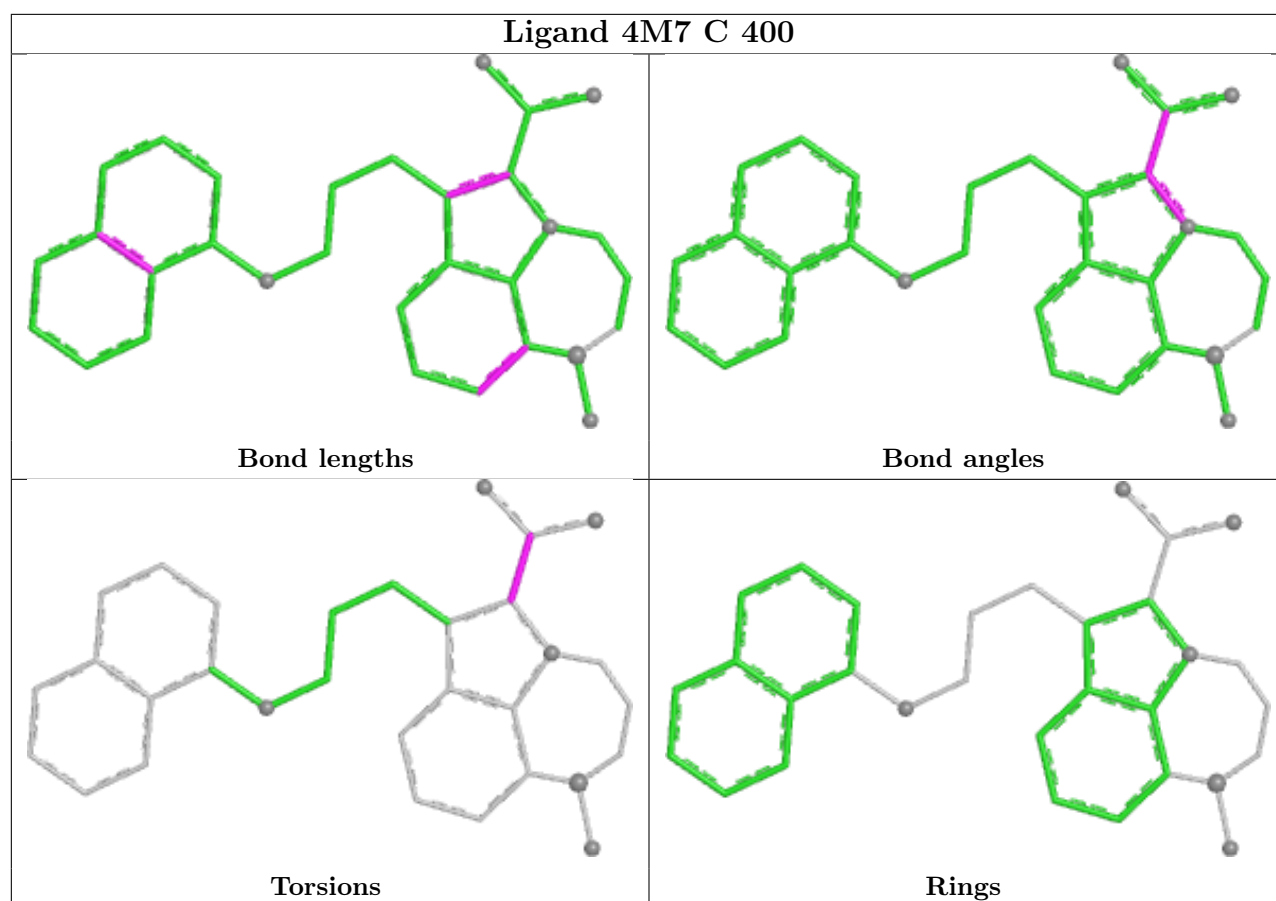
Ligand 4M7 D 400



Ligand 4M7 K 400







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	153/157 (97%)	-0.35	1 (0%) 84 82	27, 44, 67, 92	0
1	B	151/157 (96%)	-0.35	0 100 100	27, 46, 70, 81	0
1	C	149/157 (94%)	-0.32	1 (0%) 84 82	31, 44, 76, 98	0
1	D	148/157 (94%)	-0.32	0 100 100	31, 49, 77, 91	0
1	E	151/157 (96%)	-0.29	0 100 100	32, 53, 81, 91	0
1	F	148/157 (94%)	-0.27	0 100 100	32, 53, 82, 91	0
1	G	151/157 (96%)	-0.22	0 100 100	29, 50, 78, 92	0
1	H	151/157 (96%)	-0.10	4 (2%) 57 54	30, 53, 90, 104	0
1	I	151/157 (96%)	0.09	4 (2%) 57 54	38, 62, 102, 115	0
1	J	151/157 (96%)	-0.02	2 (1%) 75 73	36, 63, 102, 109	0
1	K	151/157 (96%)	-0.06	1 (0%) 84 82	34, 60, 93, 101	0
1	L	151/157 (96%)	0.01	1 (0%) 84 82	41, 60, 94, 109	0
All	All	1806/1884 (95%)	-0.18	14 (0%) 82 80	27, 53, 87, 115	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	193	ALA	2.9
1	I	193	ALA	2.8
1	I	321	VAL	2.8
1	I	204	ALA	2.8
1	L	204	ALA	2.6
1	H	200	GLY	2.5
1	I	201	ARG	2.4
1	J	192	GLY	2.3
1	H	198	PRO	2.2
1	C	192	GLY	2.1
1	J	193	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	193	ALA	2.0
1	A	256	ASP	2.0
1	H	192	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

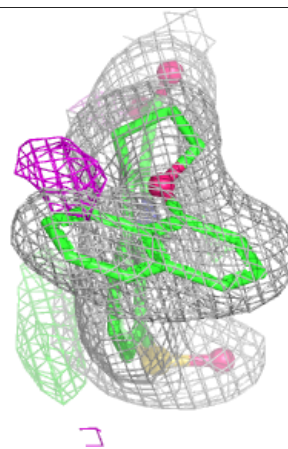
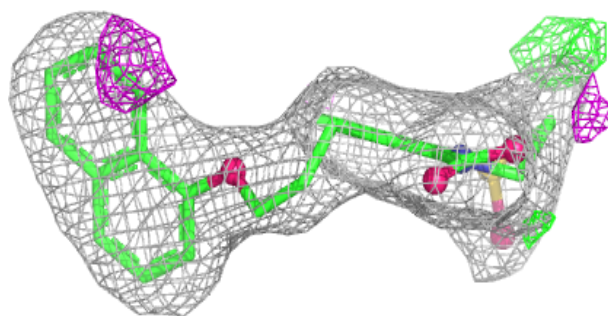
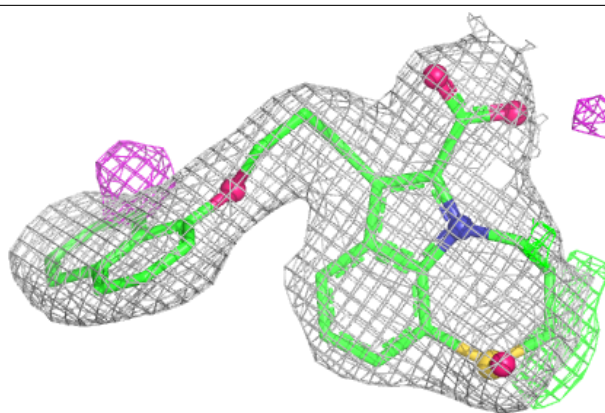
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	4M7	B	400	31/31	0.91	0.08	25,47,74,89	0
2	4M7	L	400	31/31	0.92	0.09	30,58,93,107	0
2	4M7	K	400	31/31	0.93	0.09	34,54,89,121	0
2	4M7	E	400	31/31	0.95	0.07	30,50,72,88	0
2	4M7	F	400	31/31	0.95	0.08	29,47,76,92	0
2	4M7	G	400	31/31	0.95	0.07	25,46,80,95	0
2	4M7	H	400	31/31	0.95	0.08	26,40,62,91	0
2	4M7	J	400	31/31	0.95	0.08	30,57,88,108	0
2	4M7	A	400	31/31	0.95	0.07	25,38,75,84	0
2	4M7	C	400	31/31	0.95	0.07	25,40,62,86	0
2	4M7	I	400	31/31	0.96	0.07	35,47,85,100	0
2	4M7	D	400	31/31	0.96	0.07	23,35,78,104	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.

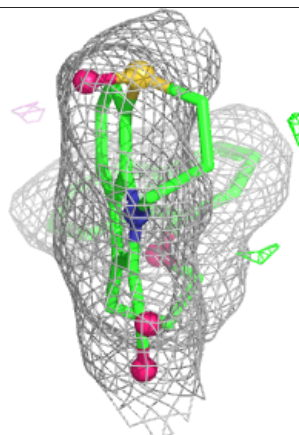
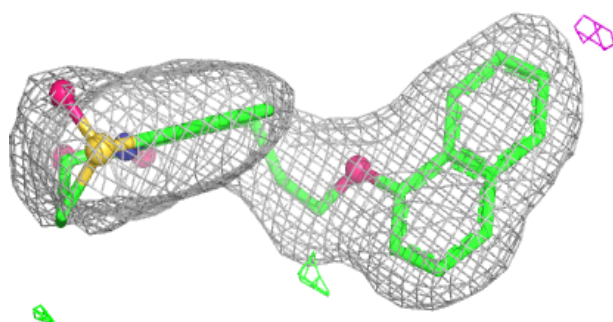
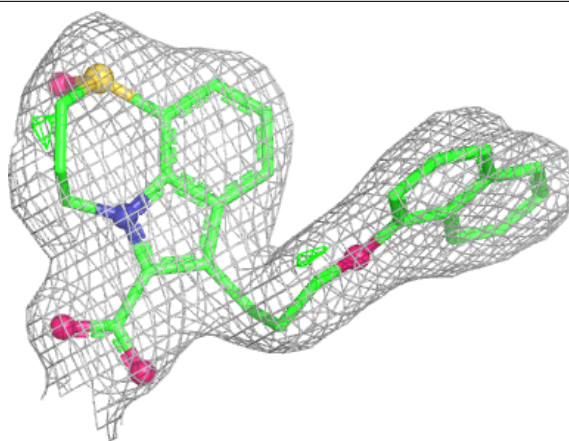
Electron density around 4M7 B 400:

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

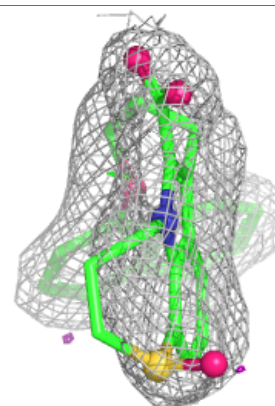
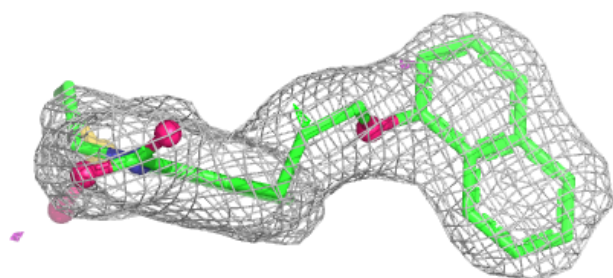
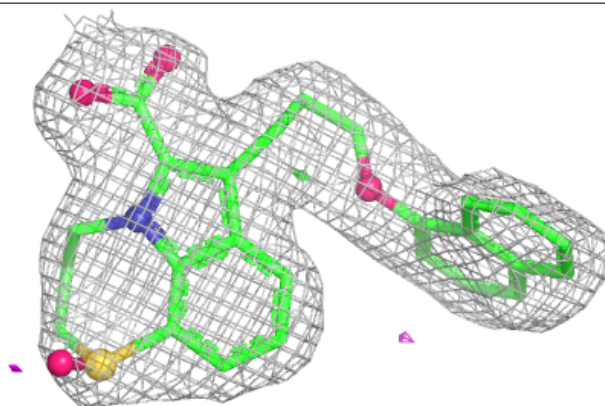


Electron density around 4M7 L 400:

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

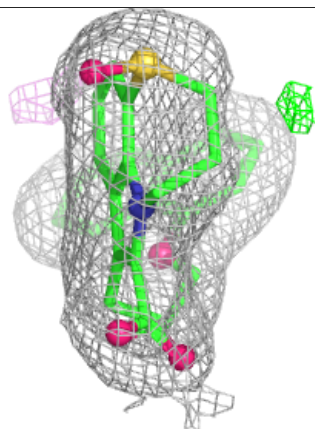
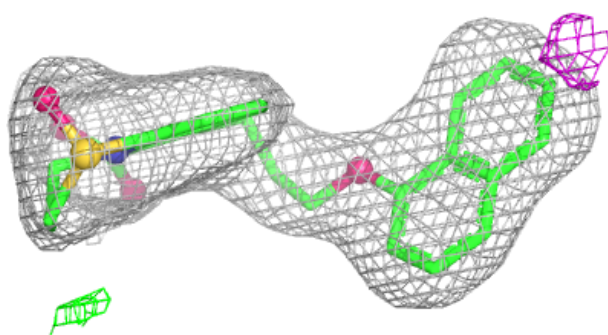
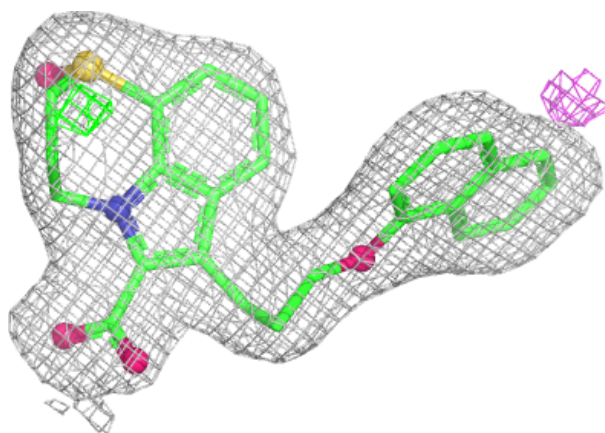
**Electron density around 4M7 K 400:**

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



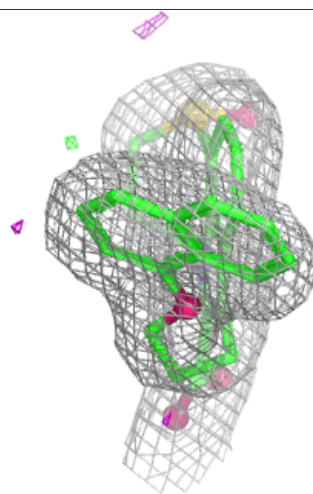
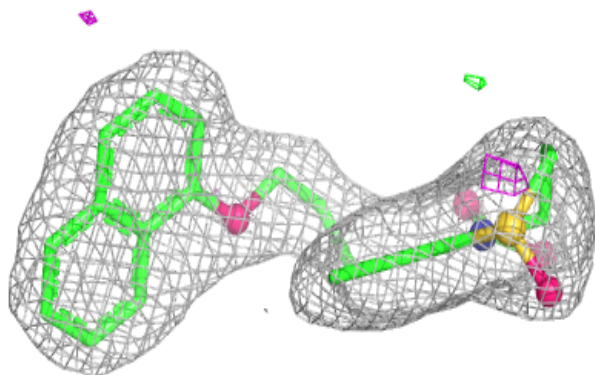
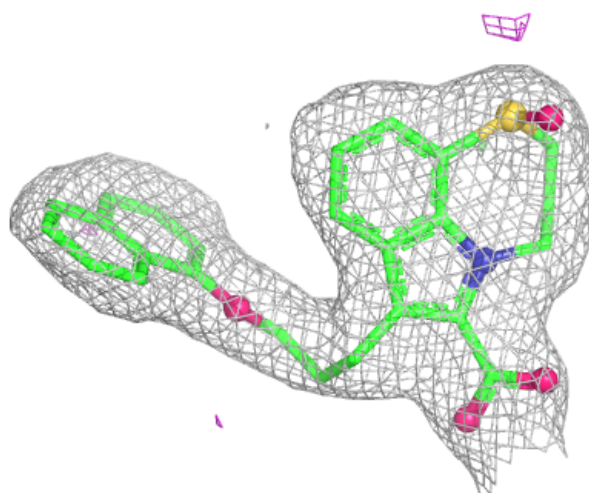
Electron density around 4M7 E 400:

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



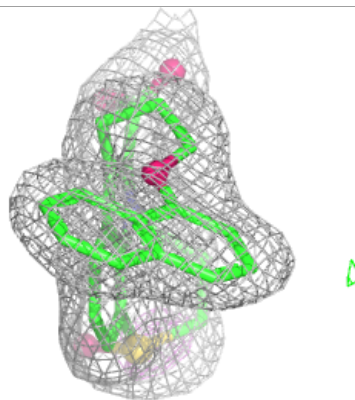
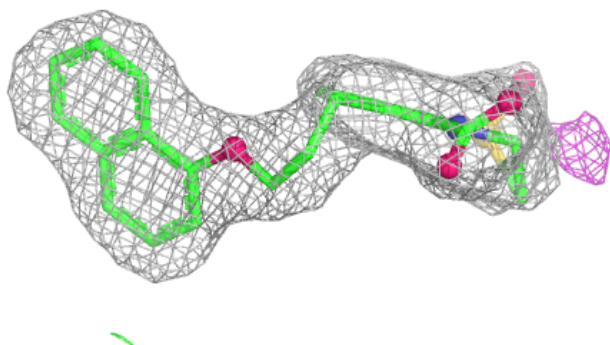
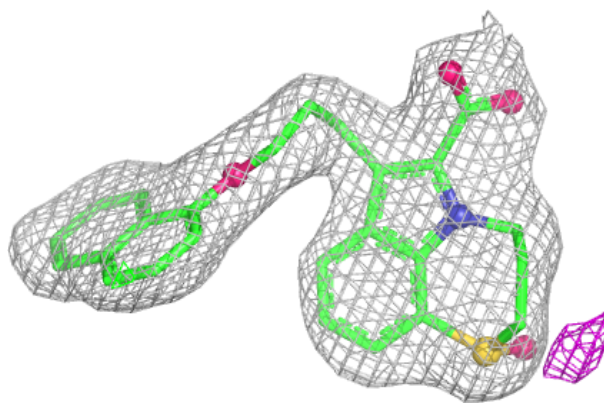
Electron density around 4M7 F 400:

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

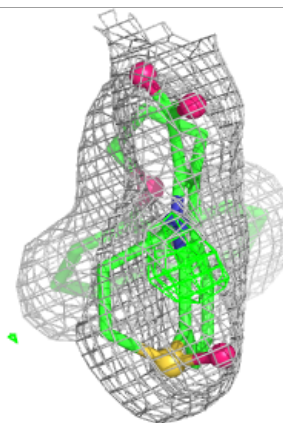
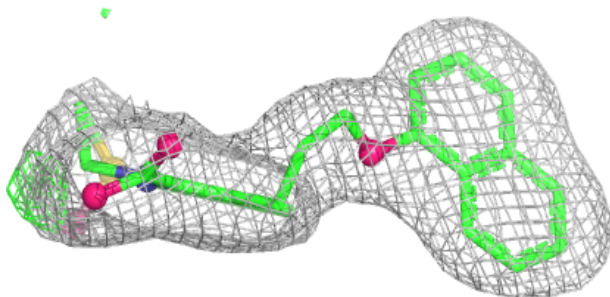
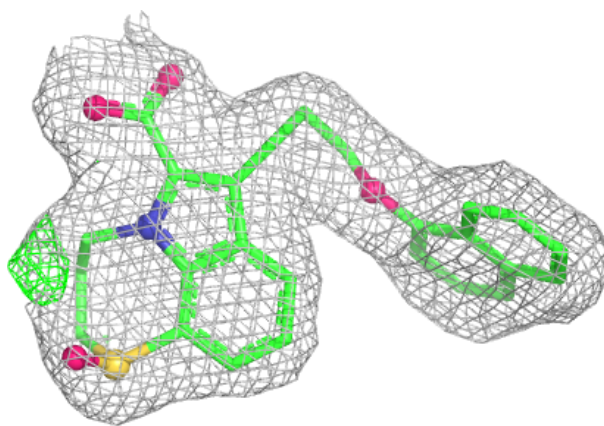


Electron density around 4M7 G 400:

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

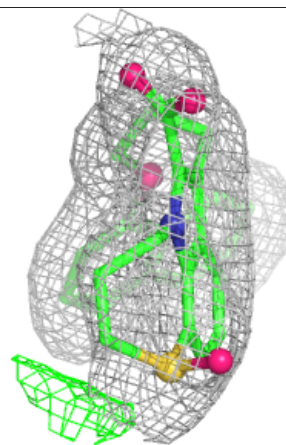
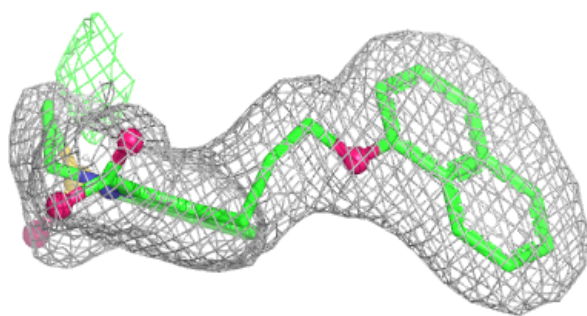
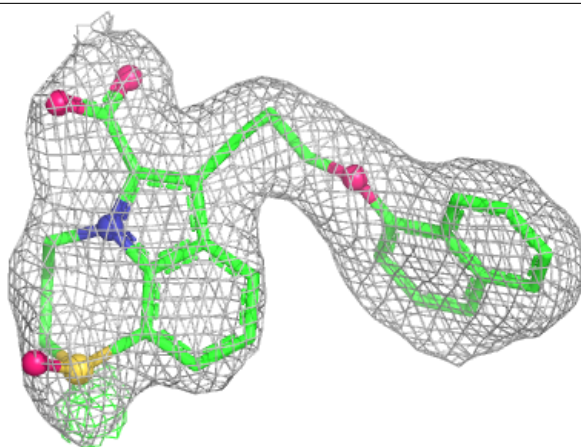
**Electron density around 4M7 H 400:**

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



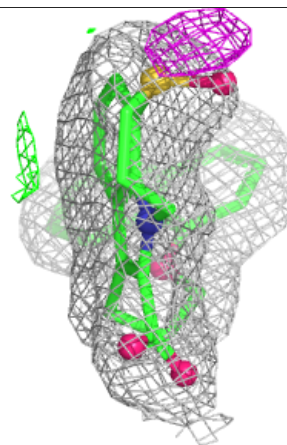
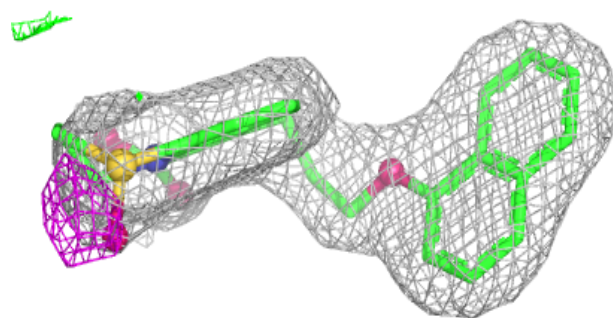
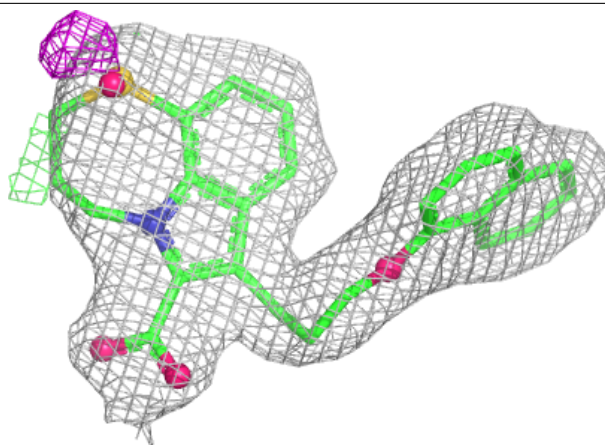
Electron density around 4M7 J 400:

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



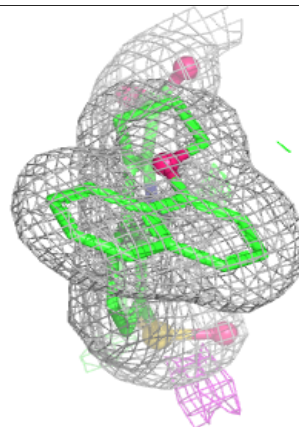
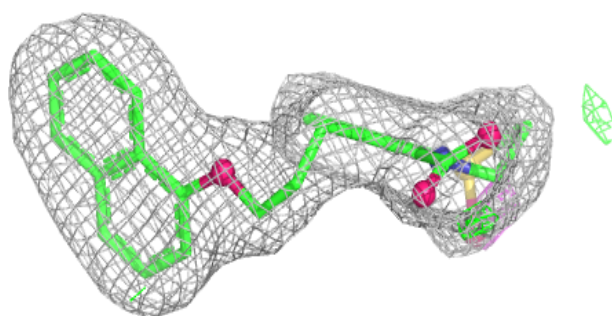
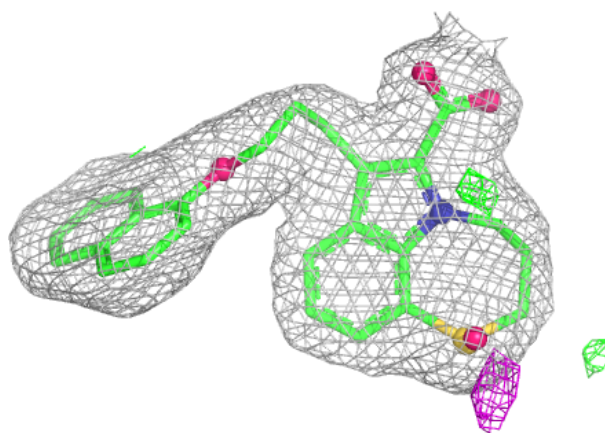
Electron density around 4M7 A 400:

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



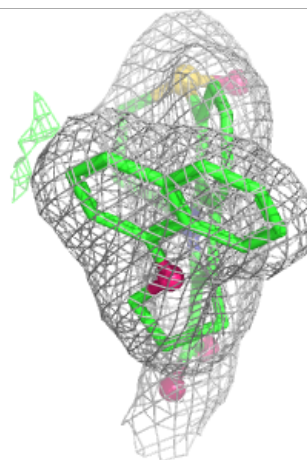
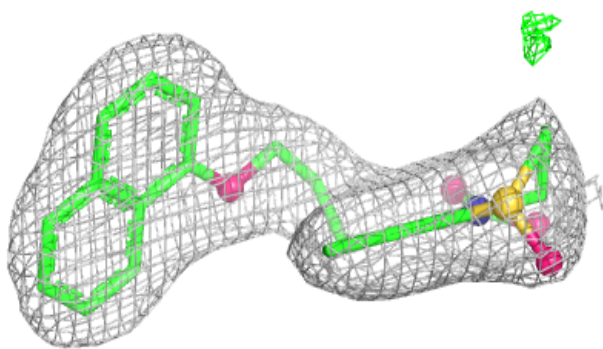
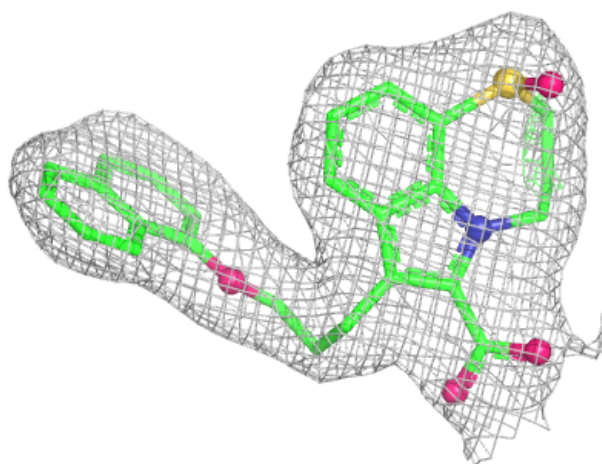
Electron density around 4M7 C 400:

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



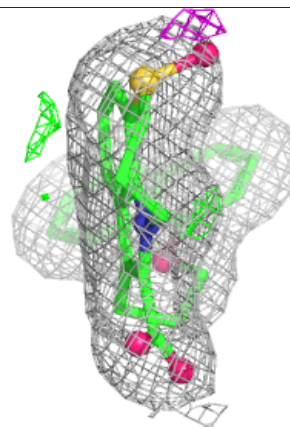
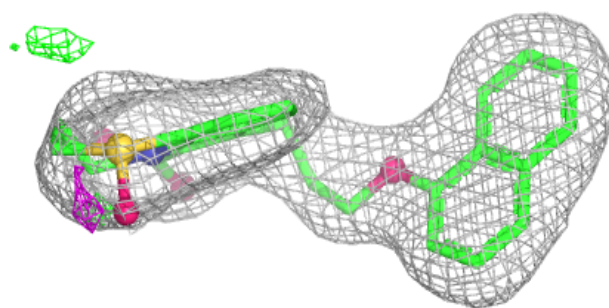
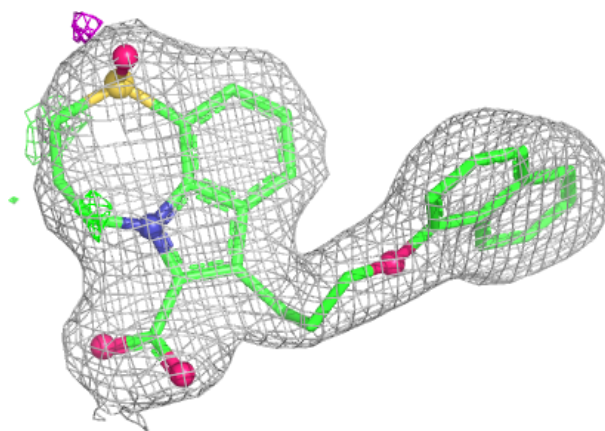
Electron density around 4M7 I 400:

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



Electron density around 4M7 D 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 ⓘ

There are no such residues in this entry.