



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:38 PM UTC

PDB ID : 4ZBI / pdb_00004zbi
Title : Mcl-1 complexed with small molecules
Authors : Zhao, B.
Deposited on : 2015-04-14
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

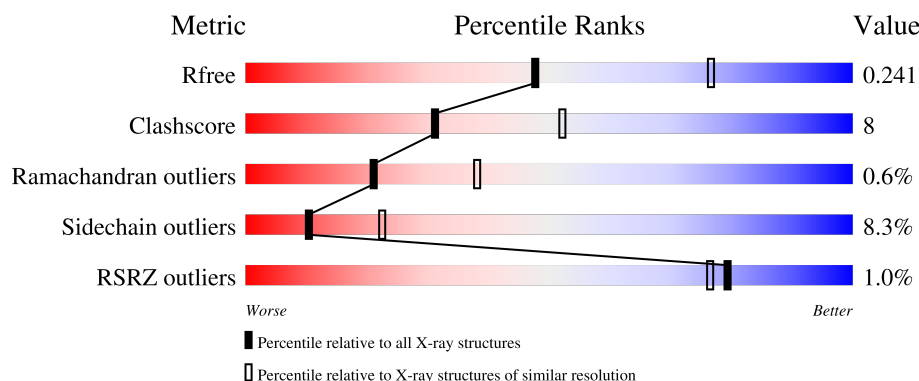
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	2% 72% 22% • •
1	B	157	% 78% 16% • •
1	C	157	4% 76% 19% • •
1	D	157	% 78% 13% 6% •
1	E	157	72% 22% • •

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Mol	Chain	Length	Quality of chain
1	F	157	73%22%
1	G	157	% 72%21%
1	H	157	65%28%
1	I	157	76%15%
1	J	157	% 76%20%
1	K	157	% 75%19%
1	L	157	% 75%20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15009 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	152	Total	C	N	O	S	0	0	0
			1215	762	225	224	4			
1	B	153	Total	C	N	O	S	0	0	0
			1218	763	224	227	4			
1	C	151	Total	C	N	O	S	0	0	0
			1198	752	219	223	4			
1	D	152	Total	C	N	O	S	0	0	0
			1221	766	225	226	4			
1	E	152	Total	C	N	O	S	0	0	0
			1215	762	224	225	4			
1	F	151	Total	C	N	O	S	0	0	0
			1202	753	222	223	4			
1	G	152	Total	C	N	O	S	0	0	0
			1211	759	224	224	4			
1	H	151	Total	C	N	O	S	0	0	0
			1208	758	223	223	4			
1	I	151	Total	C	N	O	S	0	0	0
			1206	757	223	222	4			
1	J	152	Total	C	N	O	S	0	0	0
			1199	752	220	223	4			
1	K	150	Total	C	N	O	S	0	0	0
			1195	748	221	222	4			
1	L	151	Total	C	N	O	S	0	0	0
			1196	750	219	223	4			

There are 12 discrepancies between the modelled and reference sequences:

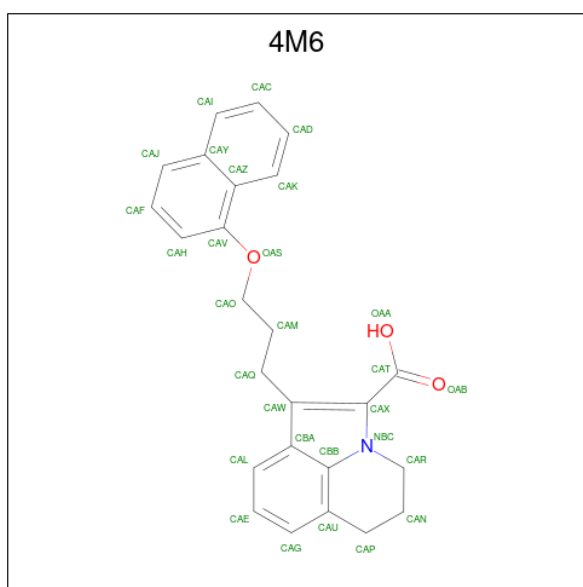
Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP Q07820
B	171	GLY	-	expression tag	UNP Q07820
C	171	GLY	-	expression tag	UNP Q07820
D	171	GLY	-	expression tag	UNP Q07820
E	171	GLY	-	expression tag	UNP Q07820

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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 1-[3-(naphthalen-1-yloxy)propyl]-5,6-dihydro-4H-pyrrolo[3,2,1-ij]quinoline-2-carboxylic acid (CCD ID: 4M6) (formula: C₂₅H₂₃NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	25	1	3		
2	B	1	Total	C	N	O	0	0
			29	25	1	3		
2	C	1	Total	C	N	O	0	0
			29	25	1	3		
2	D	1	Total	C	N	O	0	0
			29	25	1	3		
2	E	1	Total	C	N	O	0	0
			29	25	1	3		
2	F	1	Total	C	N	O	0	0
			29	25	1	3		
2	G	1	Total	C	N	O	0	0
			29	25	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	N	O	0	0
			29	25	1	3		
2	I	1	Total	C	N	O	0	0
			29	25	1	3		
2	J	1	Total	C	N	O	0	0
			29	25	1	3		
2	K	1	Total	C	N	O	0	0
			29	25	1	3		
2	L	1	Total	C	N	O	0	0
			29	25	1	3		

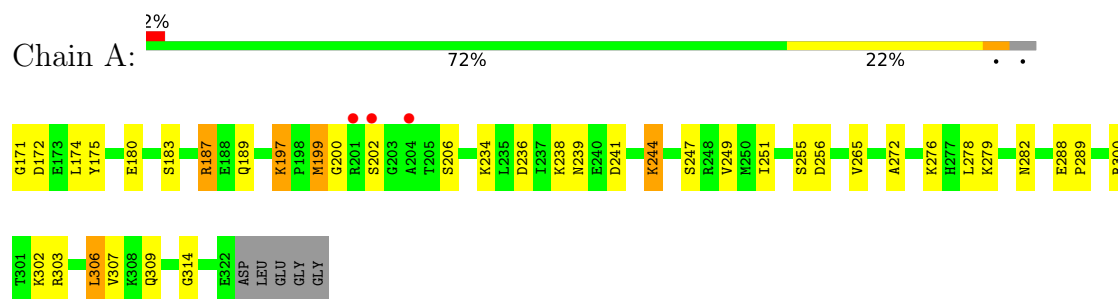
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	17	Total	O	0	0
			17	17		
3	C	16	Total	O	0	0
			16	16		
3	D	25	Total	O	0	0
			25	25		
3	E	19	Total	O	0	0
			19	19		
3	F	6	Total	O	0	0
			6	6		
3	G	8	Total	O	0	0
			8	8		
3	H	13	Total	O	0	0
			13	13		
3	I	23	Total	O	0	0
			23	23		
3	J	12	Total	O	0	0
			12	12		
3	K	11	Total	O	0	0
			11	11		
3	L	11	Total	O	0	0
			11	11		

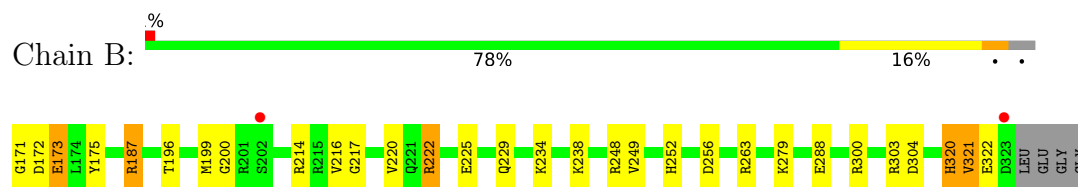
3 Residue-property plots [i](#)

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.

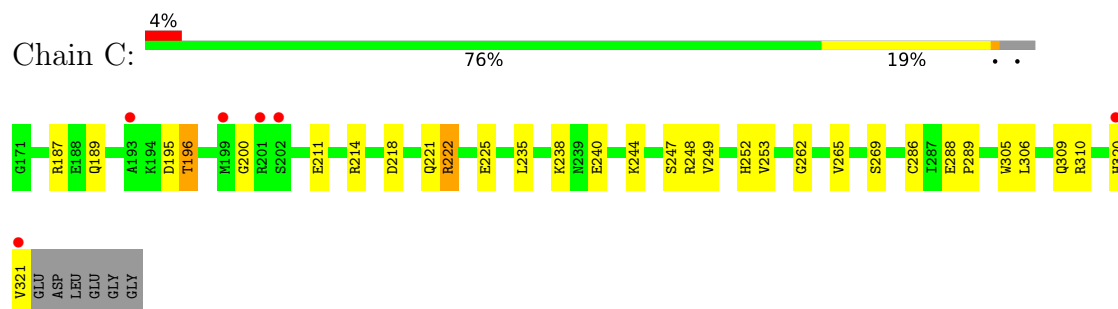
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



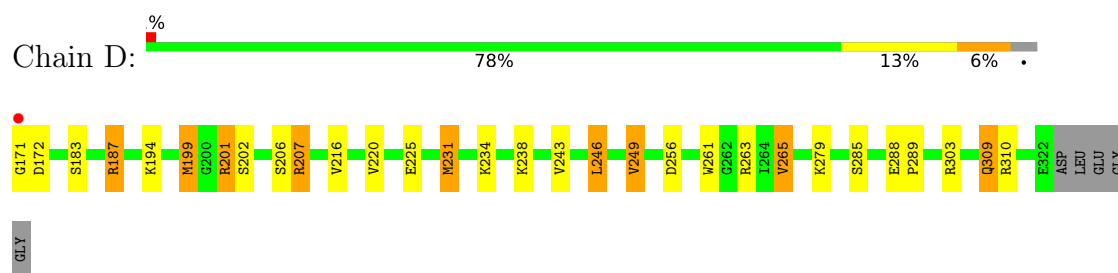
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



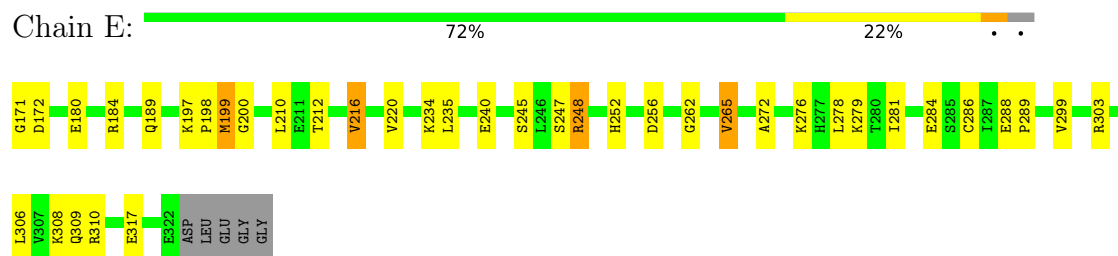
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



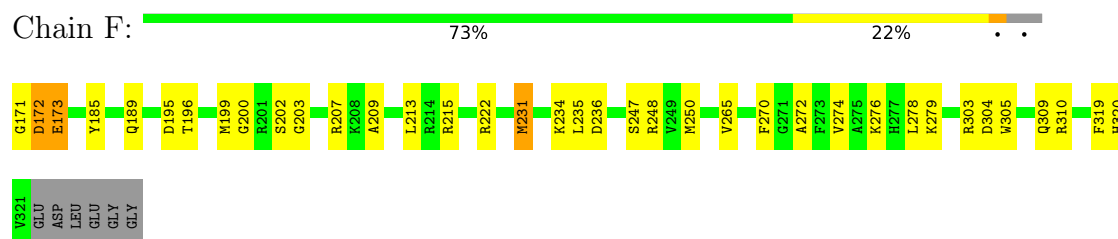
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



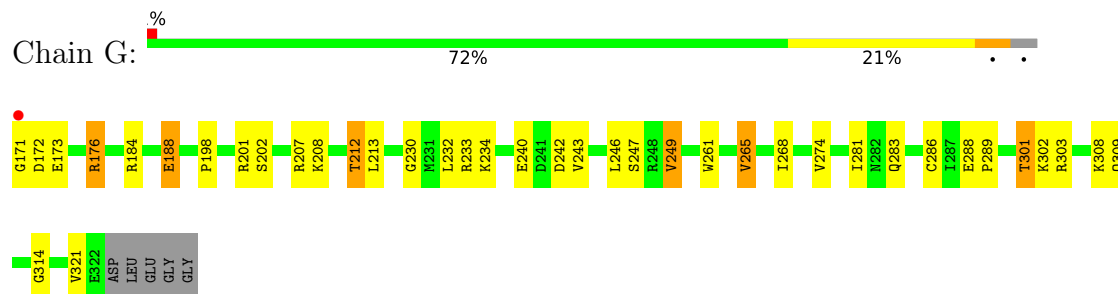
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



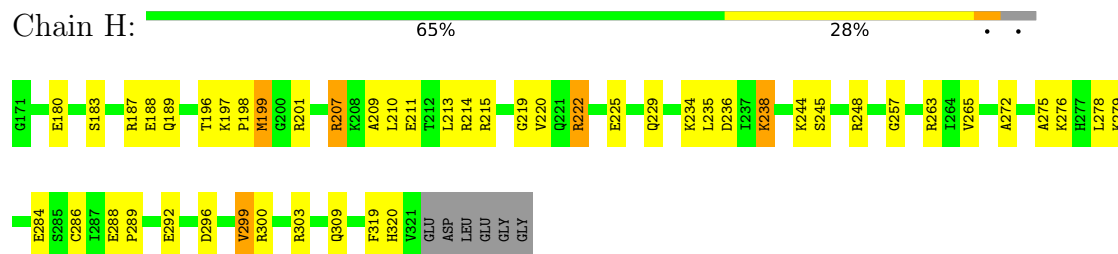
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



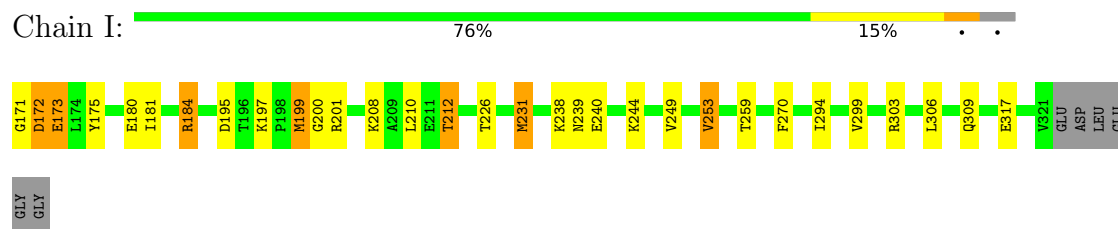
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



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

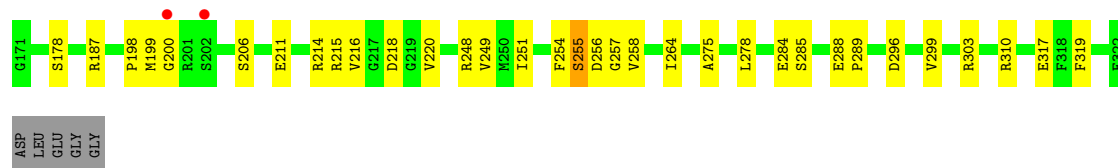


- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



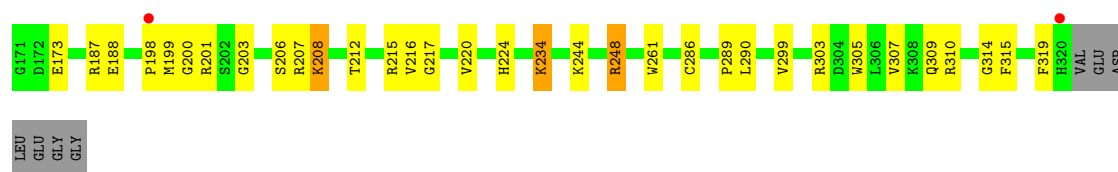
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain J:  76% 20% ..



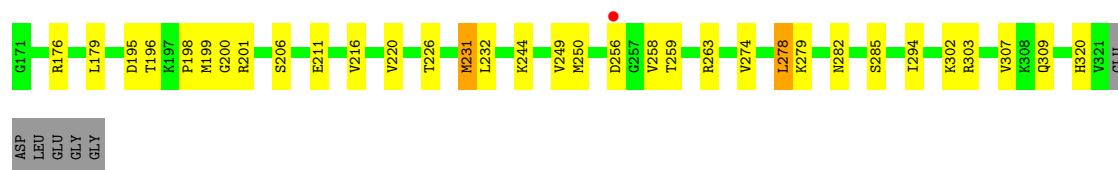
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain K:  75% 19% ..



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

Chain L:  75% 20% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.26Å 134.01Å 135.93Å 90.00° 99.65° 90.00°	Depositor
Resolution (Å)	29.97 – 2.50 29.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.4 (29.97-2.50) 90.1 (29.97-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.51Å)	Xtriage
Refinement program	PHENIX dev_1951	Depositor
R, R_{free}	0.182 , 0.239 0.184 , 0.241	Depositor DCC
R_{free} test set	1989 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15009	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: 4M6

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	0/1235	0.99	3/1660 (0.2%)
1	B	0.66	0/1238	1.01	4/1667 (0.2%)
1	C	0.64	0/1218	1.03	2/1641 (0.1%)
1	D	0.68	0/1241	0.95	1/1668 (0.1%)
1	E	0.62	0/1235	0.98	1/1661 (0.1%)
1	F	0.59	0/1222	1.04	2/1645 (0.1%)
1	G	0.64	0/1230	0.96	1/1654 (0.1%)
1	H	0.65	0/1228	0.99	2/1652 (0.1%)
1	I	0.63	0/1226	0.98	1/1649 (0.1%)
1	J	0.59	0/1218	0.96	1/1640 (0.1%)
1	K	0.58	0/1214	0.99	1/1633 (0.1%)
1	L	0.56	0/1215	0.99	2/1636 (0.1%)
All	All	0.62	0/14720	0.99	21/19806 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	217	GLY	N-CA-C	11.31	126.30	112.73
1	F	320	HIS	N-CA-C	10.21	122.00	111.07
1	G	198	PRO	N-CA-CB	8.31	110.58	103.35
1	L	198	PRO	N-CA-CB	8.13	110.42	103.35
1	J	198	PRO	N-CA-CB	8.00	110.43	103.31
1	H	257	GLY	N-CA-C	-7.68	103.80	111.56
1	C	196	THR	N-CA-C	7.53	122.46	113.28
1	K	198	PRO	N-CA-CB	7.45	110.25	103.33
1	A	172	ASP	CB-CA-C	-6.96	108.53	116.54
1	L	320	HIS	N-CA-C	6.30	118.15	111.28
1	I	173	GLU	N-CA-C	6.00	117.82	111.28
1	H	320	HIS	N-CA-C	5.63	117.50	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	LYS	CA-C-N	5.50	125.48	120.03
1	A	197	LYS	C-N-CA	5.50	125.48	120.03
1	B	320	HIS	N-CA-C	-5.45	101.58	109.59
1	B	173	GLU	N-CA-C	5.36	117.12	111.28
1	D	249	VAL	CB-CA-C	-5.35	104.92	112.14
1	F	173	GLU	N-CA-C	5.34	117.10	111.28
1	E	216	VAL	N-CA-C	5.20	116.67	111.00
1	C	253	VAL	N-CA-C	5.08	115.31	110.53
1	B	196	THR	N-CA-C	5.03	119.26	113.18

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	1215	0	1218	22	0
1	B	1218	0	1209	24	0
1	C	1198	0	1190	18	0
1	D	1221	0	1229	22	0
1	E	1215	0	1213	22	0
1	F	1202	0	1194	31	0
1	G	1211	0	1208	21	0
1	H	1208	0	1212	33	0
1	I	1206	0	1207	24	0
1	J	1199	0	1181	16	0
1	K	1195	0	1186	21	0
1	L	1196	0	1184	12	0
2	A	29	0	22	1	0
2	B	29	0	22	0	0
2	C	29	0	22	1	0
2	D	29	0	22	4	0
2	E	29	0	22	0	0
2	F	29	0	22	0	0
2	G	29	0	22	1	0
2	H	29	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	29	0	22	3	0
2	J	29	0	22	0	0
2	K	29	0	22	1	0
2	L	29	0	22	1	0
3	A	16	0	0	0	0
3	B	17	0	0	3	0
3	C	16	0	0	1	0
3	D	25	0	0	2	0
3	E	19	0	0	1	0
3	F	6	0	0	0	0
3	G	8	0	0	1	0
3	H	13	0	0	1	0
3	I	23	0	0	1	0
3	J	12	0	0	2	0
3	K	11	0	0	0	0
3	L	11	0	0	0	0
All	All	15009	0	14695	241	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (241) 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:I:171:GLY:HA2	1:I:303:ARG:HH22	1.10	1.11
1:A:171:GLY:HA2	1:A:303:ARG:HH22	1.29	0.98
1:E:171:GLY:HA2	1:E:303:ARG:HH22	1.29	0.94
1:F:171:GLY:HA2	1:F:303:ARG:HH22	1.32	0.94
1:B:171:GLY:HA2	1:B:303:ARG:HH22	1.32	0.93
1:A:187:ARG:HH21	1:A:288:GLU:HG2	1.37	0.89
1:B:187:ARG:NH1	3:B:501:HOH:O	2.06	0.89
1:D:172:ASP:N	3:D:501:HOH:O	2.03	0.86
1:G:171:GLY:HA3	1:G:303:ARG:HH22	1.36	0.86
1:I:171:GLY:HA2	1:I:303:ARG:NH2	1.91	0.85
1:D:171:GLY:CA	1:D:303:ARG:HH22	1.89	0.85
1:E:248:ARG:NH2	1:F:235:LEU:O	2.11	0.84
1:H:199:MET:HE1	1:H:207:ARG:HG2	1.59	0.82
1:J:199:MET:HE2	1:J:206:SER:HB3	1.62	0.82
1:C:235:LEU:O	1:H:248:ARG:NH2	2.15	0.79
1:D:256:ASP:O	1:D:263:ARG:NH1	2.16	0.79
1:F:171:GLY:HA2	1:F:303:ARG:NH2	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:LYS:HG3	1:H:198:PRO:HD2	1.65	0.77
1:B:256:ASP:O	1:B:263:ARG:NH1	2.18	0.76
1:F:189:GLN:HG2	1:F:272:ALA:HB1	1.68	0.76
1:A:189:GLN:HG2	1:A:272:ALA:HB1	1.69	0.75
1:J:303:ARG:NH1	3:J:502:HOH:O	2.20	0.74
1:J:211:GLU:OE1	1:J:214:ARG:NH1	2.20	0.74
1:C:248:ARG:NH2	1:H:235:LEU:O	2.21	0.74
1:L:250:MET:HE1	1:L:294:ILE:HA	1.69	0.74
1:D:171:GLY:HA2	1:D:303:ARG:HH22	1.53	0.72
1:H:236:ASP:OD2	1:H:238:LYS:NZ	2.22	0.72
1:H:211:GLU:OE2	1:H:215:ARG:NH2	2.18	0.72
1:J:251:ILE:O	1:J:255:SER:HB2	1.91	0.71
1:I:184:ARG:HH21	1:I:199:MET:HE2	1.56	0.70
1:E:171:GLY:CA	1:E:303:ARG:HH22	2.04	0.68
1:C:189:GLN:OE1	1:C:221:GLN:NE2	2.22	0.68
1:H:300:ARG:NH1	3:H:501:HOH:O	2.26	0.68
1:G:173:GLU:OE2	1:G:176:ARG:NH1	2.27	0.67
1:A:171:GLY:HA2	1:A:303:ARG:NH2	2.07	0.66
1:D:243:VAL:HA	1:D:246:LEU:HD22	1.77	0.66
1:D:199:MET:HE3	1:D:206:SER:HB2	1.76	0.66
1:A:244:LYS:HE3	1:A:289:PRO:HB2	1.78	0.66
1:B:320:HIS:O	1:B:321:VAL:HG22	1.96	0.66
1:G:171:GLY:HA3	1:G:303:ARG:NH2	2.09	0.66
1:E:235:LEU:O	1:F:248:ARG:NH2	2.29	0.65
1:I:171:GLY:CA	1:I:303:ARG:HH22	1.99	0.65
1:J:215:ARG:NH1	1:J:319:PHE:O	2.23	0.64
1:H:199:MET:CE	1:H:207:ARG:HG2	2.26	0.64
1:F:189:GLN:HG3	1:F:276:LYS:HE3	1.79	0.64
1:H:180:GLU:HG2	1:H:199:MET:HG2	1.79	0.64
1:F:171:GLY:CA	1:F:303:ARG:HH22	2.09	0.64
1:A:183:SER:OG	1:A:288:GLU:OE2	2.15	0.64
1:B:171:GLY:HA2	1:B:303:ARG:NH2	2.09	0.64
1:H:225:GLU:O	1:H:229:GLN:HG3	1.97	0.64
1:K:199:MET:HB2	1:K:203:GLY:HA2	1.80	0.64
1:I:253:VAL:HG11	2:I:400:4M6:H23	1.81	0.63
1:L:199:MET:HE3	1:L:206:SER:HB3	1.79	0.63
1:K:248:ARG:HG3	1:K:248:ARG:HH11	1.64	0.63
1:I:173:GLU:OE1	1:I:201:ARG:NH1	2.32	0.62
1:E:262:GLY:O	1:E:265:VAL:HG12	1.99	0.62
1:J:310:ARG:NH2	1:J:317:GLU:OE1	2.35	0.60
1:I:249:VAL:O	1:I:253:VAL:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:VAL:HG21	1:E:265:VAL:HG13	1.84	0.60
1:H:201:ARG:HB3	1:I:317:GLU:OE1	2.02	0.59
1:H:279:LYS:HD2	1:H:284:GLU:OE2	2.02	0.59
1:I:180:GLU:O	1:I:184:ARG:HG2	2.03	0.59
1:H:244:LYS:NZ	1:H:289:PRO:HB3	2.17	0.59
1:D:199:MET:HE1	1:D:207:ARG:HD2	1.86	0.58
1:B:222:ARG:CZ	1:K:234:LYS:HG3	2.35	0.57
1:E:245:SER:OG	1:F:248:ARG:NH1	2.38	0.56
1:E:252:HIS:CE1	1:F:234:LYS:HE3	2.40	0.56
1:G:213:LEU:HD21	1:G:268:ILE:HG21	1.88	0.56
1:J:299:VAL:O	1:J:303:ARG:HB2	2.05	0.56
1:G:261:TRP:O	1:G:265:VAL:HG12	2.07	0.55
1:H:188:GLU:OE2	1:H:214:ARG:NE	2.36	0.55
1:H:189:GLN:HG3	1:H:276:LYS:HE2	1.88	0.55
1:E:189:GLN:HG2	1:E:272:ALA:HB1	1.88	0.55
1:I:231:MET:HG3	2:I:400:4M6:CAG	2.36	0.55
1:E:212:THR:O	1:E:216:VAL:HG22	2.07	0.54
1:F:195:ASP:OD1	1:F:196:THR:N	2.40	0.54
1:B:288:GLU:OE1	3:B:501:HOH:O	2.18	0.54
1:C:211:GLU:OE1	1:C:214:ARG:HD2	2.07	0.54
1:D:263:ARG:HH21	2:D:400:4M6:CAT	2.19	0.54
1:C:195:ASP:OD1	1:C:196:THR:N	2.39	0.54
1:C:252:HIS:HA	1:H:234:LYS:HE3	1.90	0.54
1:D:183:SER:OG	1:D:187:ARG:NH1	2.41	0.54
1:B:222:ARG:NH1	1:K:234:LYS:HG3	2.22	0.54
1:E:189:GLN:HG3	1:E:276:LYS:HE2	1.90	0.54
1:H:286:CYS:C	1:H:289:PRO:HD2	2.32	0.53
1:G:301:THR:HG23	1:G:302:LYS:HG2	1.90	0.53
1:I:240:GLU:HG2	1:I:244:LYS:HZ3	1.74	0.53
1:J:199:MET:HE2	1:J:206:SER:CB	2.37	0.53
1:J:285:SER:OG	3:J:501:HOH:O	2.19	0.53
1:D:263:ARG:NH2	2:D:400:4M6:OAB	2.27	0.53
1:G:230:GLY:O	1:G:234:LYS:HD2	2.09	0.52
1:A:302:LYS:O	1:A:306:LEU:HD22	2.10	0.52
1:A:199:MET:HG2	1:A:206:SER:HB2	1.90	0.52
1:L:256:ASP:O	1:L:263:ARG:NH1	2.31	0.52
1:L:259:THR:HG21	1:L:302:LYS:HD2	1.90	0.52
1:C:240:GLU:HG2	1:C:244:LYS:HE3	1.91	0.52
1:K:199:MET:HE2	1:K:206:SER:HB3	1.91	0.52
1:F:247:SER:HA	1:F:250:MET:HE3	1.93	0.51
1:B:171:GLY:HA3	1:B:175:TYR:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:ARG:NH2	1:F:319:PHE:O	2.43	0.51
1:E:252:HIS:O	1:F:234:LYS:NZ	2.38	0.51
1:G:301:THR:CG2	1:G:302:LYS:HG2	2.40	0.51
1:A:171:GLY:HA3	1:A:175:TYR:HB2	1.93	0.51
1:A:189:GLN:HG3	1:A:276:LYS:HE3	1.93	0.51
1:D:261:TRP:O	1:D:265:VAL:HG12	2.10	0.50
1:E:288:GLU:HB3	1:E:289:PRO:HD3	1.93	0.50
1:L:176:ARG:NH2	1:L:201:ARG:O	2.44	0.50
1:D:171:GLY:HA2	1:D:303:ARG:NH2	2.23	0.50
1:B:303:ARG:HB3	1:F:172:ASP:HB2	1.93	0.50
1:G:233:ARG:HD2	3:G:502:HOH:O	2.11	0.50
1:A:234:LYS:HE3	1:B:252:HIS:CE1	2.47	0.50
1:B:304:ASP:OD2	1:F:172:ASP:HB3	2.11	0.50
1:K:299:VAL:O	1:K:303:ARG:HB2	2.12	0.50
1:G:249:VAL:HG22	2:G:400:4M6:H22	1.93	0.49
1:J:275:ALA:HA	1:J:278:LEU:HD12	1.92	0.49
1:D:172:ASP:OD2	3:D:502:HOH:O	2.19	0.49
1:H:219:GLY:O	1:H:222:ARG:HG2	2.13	0.49
1:B:216:VAL:O	1:B:220:VAL:HG23	2.13	0.49
1:E:180:GLU:CD	1:E:199:MET:HG2	2.38	0.49
1:H:288:GLU:HB3	1:H:289:PRO:HD3	1.94	0.49
1:L:303:ARG:O	1:L:307:VAL:HG13	2.13	0.49
1:A:239:ASN:OD1	1:A:241:ASP:HB2	2.12	0.48
1:J:254:PHE:HZ	1:J:264:ILE:HD13	1.78	0.48
1:G:208:LYS:O	1:G:212:THR:HG23	2.12	0.48
1:F:274:VAL:O	1:F:278:LEU:HD13	2.13	0.48
1:I:253:VAL:HG13	2:I:400:4M6:H15	1.96	0.48
1:A:309:GLN:O	1:A:314:GLY:HA3	2.13	0.48
1:C:286:CYS:C	1:C:289:PRO:HD2	2.39	0.48
1:E:299:VAL:O	1:E:303:ARG:HB2	2.14	0.48
1:A:234:LYS:HE2	1:B:256:ASP:OD2	2.13	0.48
1:L:249:VAL:HG12	2:L:400:4M6:H22	1.95	0.48
1:K:303:ARG:O	1:K:307:VAL:HG23	2.14	0.47
1:H:279:LYS:HA	1:H:284:GLU:OE2	2.14	0.47
1:L:274:VAL:HG12	1:L:278:LEU:HD22	1.96	0.47
1:E:310:ARG:HD2	3:E:514:HOH:O	2.13	0.47
1:H:244:LYS:HZ1	1:H:289:PRO:HB3	1.78	0.47
1:B:300:ARG:HE	1:F:171:GLY:N	2.13	0.47
1:G:288:GLU:HB3	1:G:289:PRO:HD3	1.96	0.47
1:H:209:ALA:O	1:H:213:LEU:HB2	2.14	0.47
1:I:259:THR:O	3:I:501:HOH:O	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:400:4M6:OAB	2:D:400:4M6:H14	2.15	0.47
1:I:299:VAL:O	1:I:303:ARG:HB2	2.14	0.47
1:I:208:LYS:O	1:I:212:THR:HG23	2.15	0.47
1:J:187:ARG:HH22	1:J:288:GLU:HB2	1.79	0.47
1:E:256:ASP:CG	1:F:234:LYS:HE2	2.40	0.47
1:C:305:TRP:CZ2	1:C:309:GLN:HG3	2.50	0.46
1:G:208:LYS:HA	1:G:208:LYS:HD3	1.66	0.46
1:J:256:ASP:HA	1:J:257:GLY:HA2	1.63	0.46
1:K:309:GLN:O	1:K:310:ARG:HB2	2.14	0.46
1:E:256:ASP:OD2	1:F:234:LYS:HE2	2.16	0.46
1:H:180:GLU:CG	1:H:199:MET:HG2	2.45	0.46
1:D:171:GLY:HA3	1:D:303:ARG:HH22	1.76	0.46
1:H:215:ARG:NH1	1:H:319:PHE:O	2.49	0.46
1:A:244:LYS:HD2	1:A:244:LYS:HA	1.57	0.46
1:B:321:VAL:O	1:B:322:GLU:HB2	2.15	0.46
1:J:288:GLU:HB3	1:J:289:PRO:HD3	1.98	0.46
1:K:215:ARG:HH22	1:K:319:PHE:HB3	1.81	0.46
1:C:321:VAL:N	3:C:504:HOH:O	2.49	0.45
1:F:247:SER:HA	1:F:250:MET:CE	2.46	0.45
1:H:183:SER:O	1:H:187:ARG:HG2	2.16	0.45
1:H:299:VAL:O	1:H:303:ARG:HB2	2.15	0.45
1:K:212:THR:O	1:K:216:VAL:HG22	2.16	0.45
1:G:201:ARG:O	1:G:202:SER:OG	2.33	0.45
1:B:172:ASP:HB3	1:F:304:ASP:CG	2.41	0.45
1:K:261:TRP:CH2	1:K:315:PHE:HB2	2.52	0.45
1:D:171:GLY:CA	1:D:303:ARG:NH2	2.70	0.45
1:D:171:GLY:HA2	1:D:303:ARG:HH12	1.82	0.45
1:K:305:TRP:O	1:K:309:GLN:HG2	2.17	0.45
1:C:221:GLN:HG3	1:C:269:SER:HB3	1.98	0.45
1:D:231:MET:HG3	2:D:400:4M6:CAG	2.47	0.45
1:A:234:LYS:HE2	1:B:256:ASP:CG	2.42	0.44
1:I:173:GLU:CD	1:I:201:ARG:HH12	2.25	0.44
1:K:215:ARG:NH2	1:K:319:PHE:O	2.51	0.44
1:K:309:GLN:O	1:K:314:GLY:HA3	2.17	0.44
1:F:209:ALA:O	1:F:213:LEU:HB2	2.17	0.44
1:G:286:CYS:C	1:G:289:PRO:HD2	2.43	0.44
1:K:208:LYS:H	1:K:208:LYS:HG2	1.56	0.44
1:L:231:MET:HE3	1:L:231:MET:HB2	1.80	0.44
1:C:262:GLY:HA2	1:C:265:VAL:HG12	1.99	0.44
1:H:199:MET:HE2	1:H:199:MET:HB2	1.82	0.44
1:I:171:GLY:HA3	1:I:175:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:GLN:HG2	1:H:272:ALA:HB1	2.00	0.43
1:A:256:ASP:OD2	1:B:234:LYS:NZ	2.48	0.43
1:C:249:VAL:HG12	2:C:400:4M6:H22	1.98	0.43
1:A:249:VAL:HG12	2:A:400:4M6:H22	2.00	0.43
1:K:173:GLU:OE1	1:K:201:ARG:NH2	2.42	0.43
1:I:231:MET:HB3	1:I:270:PHE:CZ	2.53	0.43
1:E:184:ARG:NH2	1:E:197:LYS:O	2.52	0.43
1:I:184:ARG:NH2	1:I:199:MET:HE2	2.30	0.43
1:J:216:VAL:O	1:J:220:VAL:HG23	2.19	0.43
1:F:185:TYR:O	1:F:189:GLN:HB2	2.18	0.43
1:L:199:MET:HE3	1:L:206:SER:CB	2.48	0.43
1:A:303:ARG:O	1:A:307:VAL:HG23	2.18	0.43
1:C:305:TRP:CH2	1:C:309:GLN:HG3	2.53	0.43
1:K:220:VAL:HG23	1:K:224:HIS:CE1	2.53	0.43
1:D:199:MET:HB2	1:D:199:MET:HE2	1.64	0.43
1:E:240:GLU:HG3	1:E:286:CYS:SG	2.59	0.43
1:F:203:GLY:O	1:F:207:ARG:HG3	2.18	0.43
1:E:197:LYS:HA	1:E:198:PRO:HD3	1.87	0.42
1:G:243:VAL:HG21	1:G:286:CYS:HB3	2.01	0.42
1:K:286:CYS:C	1:K:289:PRO:HD2	2.44	0.42
1:A:251:ILE:O	1:A:255:SER:HB2	2.19	0.42
1:C:248:ARG:NH1	1:H:245:SER:OG	2.52	0.42
1:D:201:ARG:HD3	1:E:317:GLU:OE2	2.19	0.42
1:L:216:VAL:O	1:L:220:VAL:HG23	2.18	0.42
1:B:172:ASP:HB3	1:F:304:ASP:OD2	2.18	0.42
1:F:231:MET:HB3	1:F:270:PHE:CZ	2.54	0.42
1:I:195:ASP:OD1	1:I:197:LYS:HD2	2.20	0.42
1:I:210:LEU:HD12	1:I:210:LEU:HA	1.83	0.42
1:K:199:MET:HB2	1:K:203:GLY:CA	2.48	0.42
1:A:251:ILE:HD11	1:A:300:ARG:HH22	1.85	0.42
1:B:171:GLY:CA	1:B:303:ARG:HH22	2.14	0.42
1:F:305:TRP:CH2	1:F:309:GLN:HG3	2.55	0.42
1:J:284:GLU:CD	1:J:284:GLU:H	2.28	0.42
1:C:288:GLU:HB3	1:C:289:PRO:HD3	2.00	0.41
1:H:219:GLY:HA2	1:H:222:ARG:HD2	2.02	0.41
1:L:195:ASP:O	1:L:196:THR:OG1	2.30	0.41
1:D:288:GLU:HB3	1:D:289:PRO:HD3	2.02	0.41
1:H:220:VAL:HG21	1:H:265:VAL:CG1	2.50	0.41
1:I:172:ASP:HB3	1:I:173:GLU:H	1.67	0.41
1:B:304:ASP:CG	1:F:172:ASP:HB3	2.45	0.41
1:B:214:ARG:HD2	3:B:502:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:GLN:O	1:D:310:ARG:HB2	2.20	0.41
1:G:232:LEU:HD23	1:G:274:VAL:HG22	2.03	0.41
1:C:262:GLY:O	1:C:265:VAL:HG12	2.20	0.41
1:D:216:VAL:O	1:D:220:VAL:HG23	2.22	0.41
1:F:172:ASP:HB3	1:F:173:GLU:H	1.60	0.41
1:F:310:ARG:HH11	1:F:310:ARG:HG3	1.86	0.41
1:A:197:LYS:HB2	1:A:197:LYS:HE3	1.95	0.40
1:B:172:ASP:HB3	1:B:173:GLU:H	1.63	0.40
1:C:218:ASP:O	1:C:222:ARG:HG2	2.20	0.40
1:G:184:ARG:O	1:G:188:GLU:HB3	2.21	0.40
1:H:201:ARG:HA	1:I:317:GLU:O	2.22	0.40
1:K:290:LEU:HD11	2:K:400:4M6:H19	2.03	0.40
1:G:242:ASP:O	1:G:246:LEU:HG	2.22	0.40
1:G:281:ILE:HG13	1:G:283:GLN:HG2	2.03	0.40
1:H:275:ALA:HA	1:H:278:LEU:HD12	2.02	0.40
1:I:181:ILE:HG23	1:I:210:LEU:HD13	2.04	0.40
1:F:231:MET:O	1:F:235:LEU:HG	2.22	0.40
1:G:309:GLN:O	1:G:314:GLY:HA3	2.21	0.40
1:K:217:GLY:HA2	1:K:220:VAL:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/157 (96%)	145 (97%)	4 (3%)	1 (1%)	18	34
1	B	151/157 (96%)	146 (97%)	3 (2%)	2 (1%)	9	18
1	C	149/157 (95%)	145 (97%)	2 (1%)	2 (1%)	9	18
1	D	150/157 (96%)	148 (99%)	2 (1%)	0	100	100
1	E	150/157 (96%)	146 (97%)	3 (2%)	1 (1%)	18	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	149/157 (95%)	147 (99%)	1 (1%)	1 (1%)	18	34
1	G	150/157 (96%)	148 (99%)	2 (1%)	0	100	100
1	H	149/157 (95%)	146 (98%)	3 (2%)	0	100	100
1	I	149/157 (95%)	145 (97%)	3 (2%)	1 (1%)	18	34
1	J	150/157 (96%)	145 (97%)	4 (3%)	1 (1%)	18	34
1	K	148/157 (94%)	143 (97%)	4 (3%)	1 (1%)	18	34
1	L	149/157 (95%)	146 (98%)	2 (1%)	1 (1%)	18	34
All	All	1794/1884 (95%)	1750 (98%)	33 (2%)	11 (1%)	21	38

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	321	VAL
1	E	200	GLY
1	K	200	GLY
1	B	200	GLY
1	C	200	GLY
1	F	200	GLY
1	J	200	GLY
1	C	320	HIS
1	A	200	GLY
1	I	200	GLY
1	L	200	GLY

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	130/135 (96%)	116 (89%)	14 (11%)	6	13
1	B	130/135 (96%)	121 (93%)	9 (7%)	14	30
1	C	128/135 (95%)	121 (94%)	7 (6%)	19	40
1	D	132/135 (98%)	116 (88%)	16 (12%)	5	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	130/135 (96%)	116 (89%)	14 (11%)	6	13
1	F	128/135 (95%)	120 (94%)	8 (6%)	16	34
1	G	129/135 (96%)	117 (91%)	12 (9%)	8	18
1	H	130/135 (96%)	119 (92%)	11 (8%)	10	22
1	I	129/135 (96%)	117 (91%)	12 (9%)	8	18
1	J	126/135 (93%)	119 (94%)	7 (6%)	19	39
1	K	127/135 (94%)	120 (94%)	7 (6%)	19	40
1	L	127/135 (94%)	115 (91%)	12 (9%)	8	18
All	All	1546/1620 (95%)	1417 (92%)	129 (8%)	10	22

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	LEU
1	A	180	GLU
1	A	187	ARG
1	A	199	MET
1	A	202	SER
1	A	236	ASP
1	A	238	LYS
1	A	244	LYS
1	A	247	SER
1	A	265	VAL
1	A	278	LEU
1	A	279	LYS
1	A	282	ASN
1	A	306	LEU
1	B	187	ARG
1	B	199	MET
1	B	222	ARG
1	B	225	GLU
1	B	229	GLN
1	B	238	LYS
1	B	248	ARG
1	B	249	VAL
1	B	279	LYS
1	C	187	ARG
1	C	222	ARG
1	C	225	GLU

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Mol	Chain	Res	Type
1	C	238	LYS
1	C	247	SER
1	C	306	LEU
1	C	310	ARG
1	D	187	ARG
1	D	194	LYS
1	D	199	MET
1	D	201	ARG
1	D	202	SER
1	D	207	ARG
1	D	225	GLU
1	D	231	MET
1	D	234	LYS
1	D	238	LYS
1	D	246	LEU
1	D	249	VAL
1	D	265	VAL
1	D	279	LYS
1	D	285	SER
1	D	309	GLN
1	E	172	ASP
1	E	199	MET
1	E	210	LEU
1	E	234	LYS
1	E	247	SER
1	E	248	ARG
1	E	265	VAL
1	E	278	LEU
1	E	279	LYS
1	E	281	ILE
1	E	284	GLU
1	E	306	LEU
1	E	308	LYS
1	E	309	GLN
1	F	172	ASP
1	F	199	MET
1	F	202	SER
1	F	222	ARG
1	F	231	MET
1	F	236	ASP
1	F	265	VAL
1	F	279	LYS

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Mol	Chain	Res	Type
1	G	172	ASP
1	G	176	ARG
1	G	188	GLU
1	G	207	ARG
1	G	212	THR
1	G	240	GLU
1	G	247	SER
1	G	249	VAL
1	G	265	VAL
1	G	301	THR
1	G	308	LYS
1	G	321	VAL
1	H	196	THR
1	H	199	MET
1	H	207	ARG
1	H	210	LEU
1	H	222	ARG
1	H	238	LYS
1	H	263	ARG
1	H	292	GLU
1	H	296	ASP
1	H	299	VAL
1	H	309	GLN
1	I	172	ASP
1	I	184	ARG
1	I	199	MET
1	I	212	THR
1	I	226	THR
1	I	231	MET
1	I	238	LYS
1	I	239	ASN
1	I	253	VAL
1	I	294	ILE
1	I	306	LEU
1	I	309	GLN
1	J	178	SER
1	J	218	ASP
1	J	248	ARG
1	J	249	VAL
1	J	255	SER
1	J	258	VAL
1	J	296	ASP

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Mol	Chain	Res	Type
1	K	187	ARG
1	K	188	GLU
1	K	207	ARG
1	K	208	LYS
1	K	234	LYS
1	K	244	LYS
1	K	248	ARG
1	L	179	LEU
1	L	211	GLU
1	L	226	THR
1	L	231	MET
1	L	232	LEU
1	L	244	LYS
1	L	258	VAL
1	L	278	LEU
1	L	279	LYS
1	L	282	ASN
1	L	285	SER
1	L	309	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	HIS
1	C	320	HIS
1	D	177	GLN
1	D	309	GLN
1	E	277	HIS
1	E	283	GLN
1	F	177	GLN
1	F	229	GLN
1	G	277	HIS
1	H	177	GLN
1	H	224	HIS
1	H	309	GLN
1	I	177	GLN
1	I	221	GLN
1	I	320	HIS
1	J	189	GLN
1	J	282	ASN
1	K	277	HIS
1	K	309	GLN

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Mol	Chain	Res	Type
1	L	223	ASN

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	4M6	H	400	-	33,33,33	1.37	5 (15%)	45,47,47	1.39	7 (15%)
2	4M6	E	400	-	33,33,33	1.41	5 (15%)	45,47,47	1.29	8 (17%)
2	4M6	G	400	-	33,33,33	1.37	3 (9%)	45,47,47	1.20	4 (8%)
2	4M6	A	400	-	33,33,33	1.47	5 (15%)	45,47,47	1.12	3 (6%)
2	4M6	C	400	-	33,33,33	1.39	3 (9%)	45,47,47	1.15	4 (8%)
2	4M6	B	400	-	33,33,33	1.44	4 (12%)	45,47,47	1.13	4 (8%)
2	4M6	F	400	-	33,33,33	1.40	5 (15%)	45,47,47	1.18	4 (8%)
2	4M6	L	400	-	33,33,33	1.38	3 (9%)	45,47,47	1.20	5 (11%)
2	4M6	I	400	-	33,33,33	1.47	6 (18%)	45,47,47	1.32	5 (11%)
2	4M6	J	400	-	33,33,33	1.43	4 (12%)	45,47,47	1.14	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	4M6	D	400	-	33,33,33	1.44	4 (12%)	45,47,47	1.10	4 (8%)
2	4M6	K	400	-	33,33,33	1.43	3 (9%)	45,47,47	1.07	2 (4%)

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	4M6	H	400	-	-	7/11/17/17	0/5/5/5
2	4M6	E	400	-	-	4/11/17/17	0/5/5/5
2	4M6	G	400	-	-	7/11/17/17	0/5/5/5
2	4M6	A	400	-	-	4/11/17/17	0/5/5/5
2	4M6	C	400	-	-	4/11/17/17	0/5/5/5
2	4M6	B	400	-	-	4/11/17/17	0/5/5/5
2	4M6	F	400	-	-	8/11/17/17	0/5/5/5
2	4M6	L	400	-	-	5/11/17/17	0/5/5/5
2	4M6	I	400	-	-	4/11/17/17	0/5/5/5
2	4M6	J	400	-	-	4/11/17/17	0/5/5/5
2	4M6	D	400	-	-	4/11/17/17	0/5/5/5
2	4M6	K	400	-	-	4/11/17/17	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	4M6	CBB-NBC	-3.71	1.33	1.40
2	H	400	4M6	CBB-NBC	-3.52	1.33	1.40
2	I	400	4M6	CBB-NBC	-3.48	1.33	1.40
2	F	400	4M6	CAX-CAW	3.40	1.42	1.37
2	K	400	4M6	CAX-CAW	3.36	1.42	1.37
2	K	400	4M6	CBB-NBC	-3.33	1.33	1.40
2	D	400	4M6	CAZ-CAY	-3.32	1.36	1.43
2	E	400	4M6	CBB-NBC	-3.28	1.33	1.40
2	D	400	4M6	CAX-CAW	3.24	1.42	1.37
2	J	400	4M6	CBB-NBC	-3.20	1.34	1.40
2	F	400	4M6	CBB-NBC	-3.19	1.34	1.40
2	D	400	4M6	CBB-NBC	-3.16	1.34	1.40
2	E	400	4M6	CAX-CAW	3.14	1.41	1.37
2	A	400	4M6	CBB-NBC	-3.14	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	400	4M6	CAX-CAW	3.12	1.41	1.37
2	C	400	4M6	CAX-CAW	3.10	1.41	1.37
2	C	400	4M6	CBB-NBC	-3.09	1.34	1.40
2	G	400	4M6	CBB-NBC	-3.08	1.34	1.40
2	G	400	4M6	CAX-CAW	3.08	1.41	1.37
2	L	400	4M6	CAZ-CAY	-3.02	1.37	1.43
2	A	400	4M6	CAX-CAW	3.00	1.41	1.37
2	L	400	4M6	CBB-NBC	-2.99	1.34	1.40
2	L	400	4M6	CAX-CAW	2.95	1.41	1.37
2	B	400	4M6	CAZ-CAY	-2.94	1.37	1.43
2	H	400	4M6	CAX-CAW	2.93	1.41	1.37
2	J	400	4M6	CAZ-CAY	-2.76	1.37	1.43
2	A	400	4M6	CAZ-CAY	-2.71	1.37	1.43
2	B	400	4M6	CBB-CAU	-2.69	1.36	1.40
2	I	400	4M6	CAZ-CAY	-2.69	1.38	1.43
2	I	400	4M6	CAX-CAW	2.65	1.41	1.37
2	E	400	4M6	CAZ-CAY	-2.53	1.38	1.43
2	A	400	4M6	CAG-CAU	2.50	1.43	1.39
2	F	400	4M6	CAZ-CAY	-2.48	1.38	1.43
2	F	400	4M6	CBB-CAU	-2.47	1.36	1.40
2	I	400	4M6	CBB-CAU	-2.42	1.37	1.40
2	G	400	4M6	CAZ-CAY	-2.37	1.38	1.43
2	K	400	4M6	CAZ-CAY	-2.37	1.38	1.43
2	B	400	4M6	CAX-CAW	2.36	1.40	1.37
2	J	400	4M6	CBB-CAU	-2.35	1.37	1.40
2	D	400	4M6	CBB-CAU	-2.35	1.37	1.40
2	C	400	4M6	CAZ-CAY	-2.30	1.38	1.43
2	H	400	4M6	CAZ-CAY	-2.26	1.38	1.43
2	E	400	4M6	CAX-CAT	2.22	1.53	1.48
2	A	400	4M6	CAE-CAG	2.12	1.42	1.38
2	I	400	4M6	CAX-CAT	2.11	1.53	1.48
2	E	400	4M6	CBB-CAU	-2.10	1.37	1.40
2	H	400	4M6	CAX-CAT	2.06	1.53	1.48
2	F	400	4M6	CAX-CAT	2.05	1.53	1.48
2	I	400	4M6	CAR-NBC	2.04	1.51	1.47
2	H	400	4M6	CBB-CAU	-2.01	1.37	1.40

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	400	4M6	CAT-CAX-NBC	3.95	127.51	122.59
2	B	400	4M6	CAT-CAX-NBC	3.75	127.25	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	400	4M6	CAN-CAR-NBC	3.67	116.72	109.95
2	E	400	4M6	CAN-CAR-NBC	3.50	116.40	109.95
2	H	400	4M6	OAA-CAT-CAX	3.35	125.65	116.08
2	G	400	4M6	CAN-CAR-NBC	3.32	116.06	109.95
2	L	400	4M6	CAN-CAR-NBC	3.30	116.02	109.95
2	I	400	4M6	CAM-CAQ-CAW	-3.07	108.46	113.30
2	F	400	4M6	CAN-CAR-NBC	3.06	115.59	109.95
2	D	400	4M6	CAR-NBC-CAX	3.03	132.08	127.84
2	H	400	4M6	CAM-CAQ-CAW	-2.91	108.72	113.30
2	A	400	4M6	CAT-CAX-NBC	2.88	126.17	122.59
2	E	400	4M6	OAS-CAV-CAH	-2.69	118.54	124.45
2	K	400	4M6	CAN-CAR-NBC	2.61	114.75	109.95
2	L	400	4M6	CAT-CAX-NBC	2.56	125.77	122.59
2	J	400	4M6	OAS-CAV-CAH	-2.52	118.91	124.45
2	J	400	4M6	CAT-CAX-NBC	2.50	125.70	122.59
2	A	400	4M6	CAR-NBC-CAX	2.46	131.27	127.84
2	C	400	4M6	CAR-NBC-CAX	2.40	131.19	127.84
2	B	400	4M6	CAR-NBC-CAX	2.39	131.19	127.84
2	I	400	4M6	CAK-CAZ-CAY	2.38	120.99	117.92
2	D	400	4M6	CAT-CAX-NBC	2.34	125.50	122.59
2	I	400	4M6	OAA-CAT-OAB	-2.32	118.37	123.90
2	C	400	4M6	CAV-CAZ-CAY	2.32	120.94	118.03
2	E	400	4M6	OAS-CAV-CAZ	2.32	121.53	115.11
2	I	400	4M6	CAR-NBC-CAX	2.30	131.06	127.84
2	H	400	4M6	CBB-NBC-CAX	2.30	109.47	107.21
2	G	400	4M6	CAR-CAN-CAP	2.28	119.65	111.41
2	C	400	4M6	CBB-NBC-CAX	2.27	109.45	107.21
2	L	400	4M6	CAR-CAN-CAP	2.27	119.61	111.41
2	L	400	4M6	CAU-CBB-NBC	2.26	127.73	125.50
2	E	400	4M6	OAA-CAT-CAX	2.25	122.52	116.08
2	B	400	4M6	CAK-CAZ-CAY	2.25	120.83	117.92
2	B	400	4M6	CAN-CAR-NBC	2.23	114.05	109.95
2	E	400	4M6	CAT-CAX-NBC	2.22	125.35	122.59
2	E	400	4M6	CAR-CAN-CAP	2.20	119.37	111.41
2	F	400	4M6	OAS-CAV-CAH	-2.20	119.61	124.45
2	D	400	4M6	OAA-CAT-OAB	-2.18	118.70	123.90
2	A	400	4M6	OAA-CAT-OAB	-2.18	118.71	123.90
2	C	400	4M6	OAA-CAT-OAB	-2.17	118.73	123.90
2	E	400	4M6	OAA-CAT-OAB	-2.16	118.75	123.90
2	H	400	4M6	CAR-CAN-CAP	2.14	119.17	111.41
2	H	400	4M6	OAS-CAV-CAH	-2.14	119.75	124.45
2	J	400	4M6	CAN-CAR-NBC	2.12	113.86	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	400	4M6	OAS-CAV-CAZ	2.11	120.97	115.11
2	E	400	4M6	CAM-CAQ-CAW	-2.11	109.98	113.30
2	H	400	4M6	OAA-CAT-OAB	-2.07	118.97	123.90
2	K	400	4M6	CBB-NBC-CAX	2.06	109.24	107.21
2	F	400	4M6	OAS-CAV-CAZ	2.05	120.81	115.11
2	G	400	4M6	CAV-CAZ-CAY	2.03	120.57	118.03
2	F	400	4M6	CAU-CBB-NBC	2.02	127.50	125.50
2	D	400	4M6	CAV-CAZ-CAY	2.02	120.56	118.03
2	L	400	4M6	CAK-CAZ-CAY	2.01	120.52	117.92

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	4M6	OAA-CAT-CAX-NBC
2	A	400	4M6	OAA-CAT-CAX-CAW
2	A	400	4M6	OAB-CAT-CAX-NBC
2	A	400	4M6	OAB-CAT-CAX-CAW
2	B	400	4M6	OAA-CAT-CAX-NBC
2	B	400	4M6	OAB-CAT-CAX-NBC
2	C	400	4M6	OAA-CAT-CAX-NBC
2	C	400	4M6	OAB-CAT-CAX-NBC
2	D	400	4M6	OAA-CAT-CAX-NBC
2	D	400	4M6	OAA-CAT-CAX-CAW
2	D	400	4M6	OAB-CAT-CAX-NBC
2	E	400	4M6	OAA-CAT-CAX-NBC
2	E	400	4M6	OAA-CAT-CAX-CAW
2	E	400	4M6	OAB-CAT-CAX-NBC
2	F	400	4M6	OAA-CAT-CAX-NBC
2	F	400	4M6	OAA-CAT-CAX-CAW
2	F	400	4M6	OAB-CAT-CAX-NBC
2	F	400	4M6	OAB-CAT-CAX-CAW
2	G	400	4M6	OAA-CAT-CAX-NBC
2	G	400	4M6	OAA-CAT-CAX-CAW
2	G	400	4M6	OAB-CAT-CAX-NBC
2	G	400	4M6	OAB-CAT-CAX-CAW
2	H	400	4M6	OAB-CAT-CAX-CAW
2	I	400	4M6	OAA-CAT-CAX-NBC
2	I	400	4M6	OAB-CAT-CAX-NBC
2	J	400	4M6	OAA-CAT-CAX-NBC
2	J	400	4M6	OAB-CAT-CAX-NBC
2	K	400	4M6	OAA-CAT-CAX-NBC

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Mol	Chain	Res	Type	Atoms
2	K	400	4M6	OAA-CAT-CAX-CAW
2	K	400	4M6	OAB-CAT-CAX-NBC
2	K	400	4M6	OAB-CAT-CAX-CAW
2	L	400	4M6	OAA-CAT-CAX-NBC
2	L	400	4M6	OAB-CAT-CAX-NBC
2	F	400	4M6	CAQ-CAM-CAO-OAS
2	F	400	4M6	CAZ-CAV-OAS-CAO
2	F	400	4M6	CAH-CAV-OAS-CAO
2	F	400	4M6	CAO-CAM-CAQ-CAW
2	G	400	4M6	CAQ-CAM-CAO-OAS
2	B	400	4M6	OAA-CAT-CAX-CAW
2	B	400	4M6	OAB-CAT-CAX-CAW
2	C	400	4M6	OAA-CAT-CAX-CAW
2	C	400	4M6	OAB-CAT-CAX-CAW
2	D	400	4M6	OAB-CAT-CAX-CAW
2	E	400	4M6	OAB-CAT-CAX-CAW
2	H	400	4M6	OAA-CAT-CAX-CAW
2	I	400	4M6	OAA-CAT-CAX-CAW
2	I	400	4M6	OAB-CAT-CAX-CAW
2	J	400	4M6	OAA-CAT-CAX-CAW
2	J	400	4M6	OAB-CAT-CAX-CAW
2	L	400	4M6	OAA-CAT-CAX-CAW
2	L	400	4M6	OAB-CAT-CAX-CAW
2	G	400	4M6	CAH-CAV-OAS-CAO
2	H	400	4M6	CAZ-CAV-OAS-CAO
2	G	400	4M6	CAZ-CAV-OAS-CAO
2	H	400	4M6	CAH-CAV-OAS-CAO
2	H	400	4M6	OAA-CAT-CAX-NBC
2	H	400	4M6	OAB-CAT-CAX-NBC
2	L	400	4M6	CAQ-CAM-CAO-OAS
2	H	400	4M6	CAQ-CAM-CAO-OAS

There are no ring outliers.

7 monomers are involved in 12 short contacts:

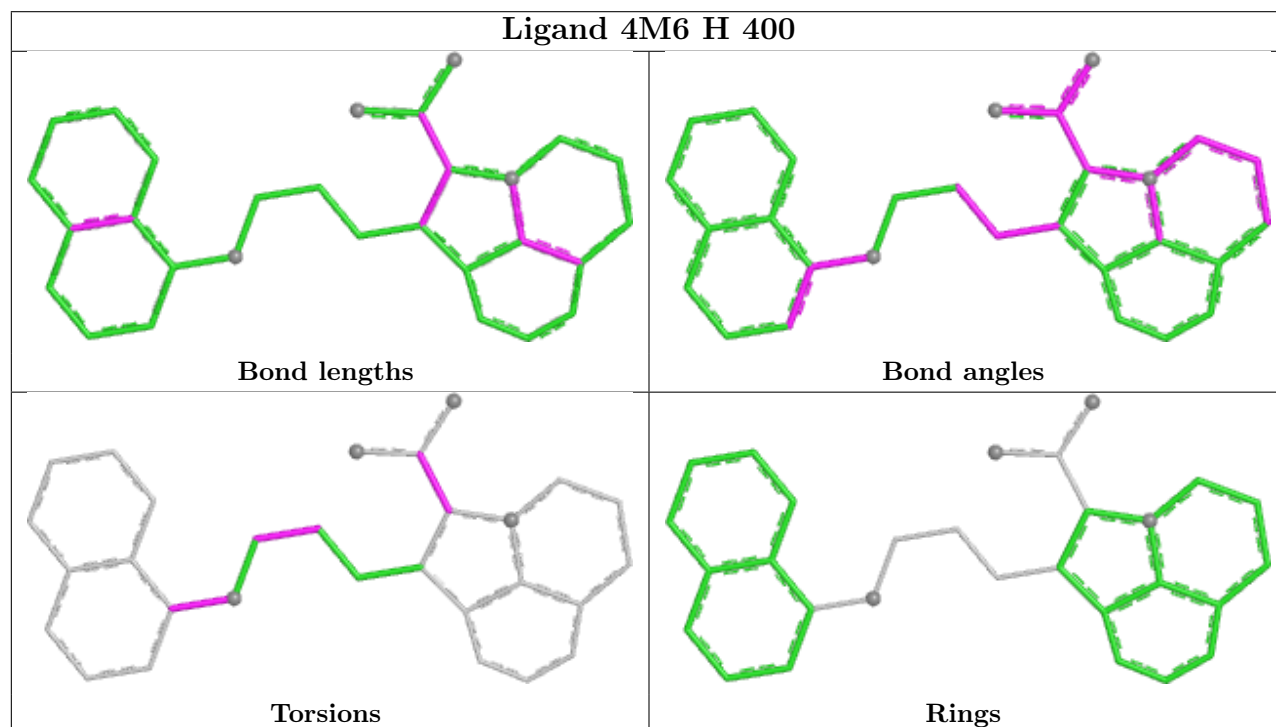
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	400	4M6	1	0
2	A	400	4M6	1	0
2	C	400	4M6	1	0
2	L	400	4M6	1	0
2	I	400	4M6	3	0
2	D	400	4M6	4	0

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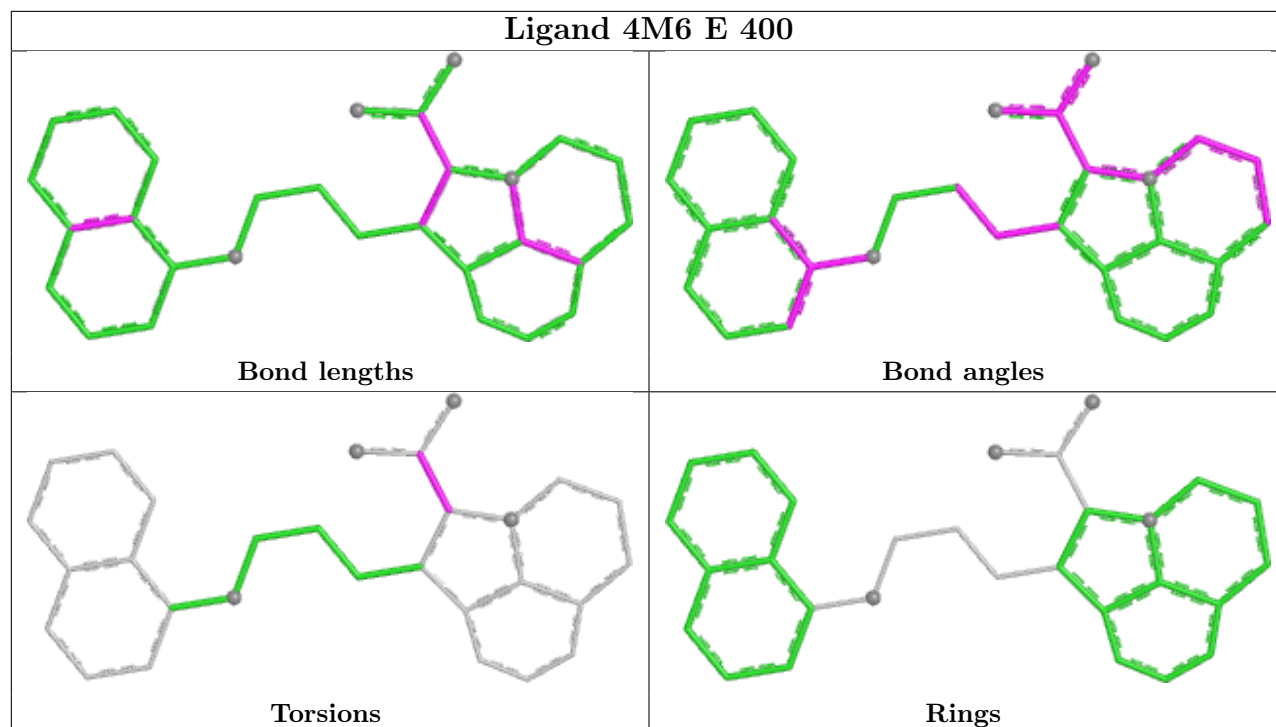
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	400	4M6	1	0

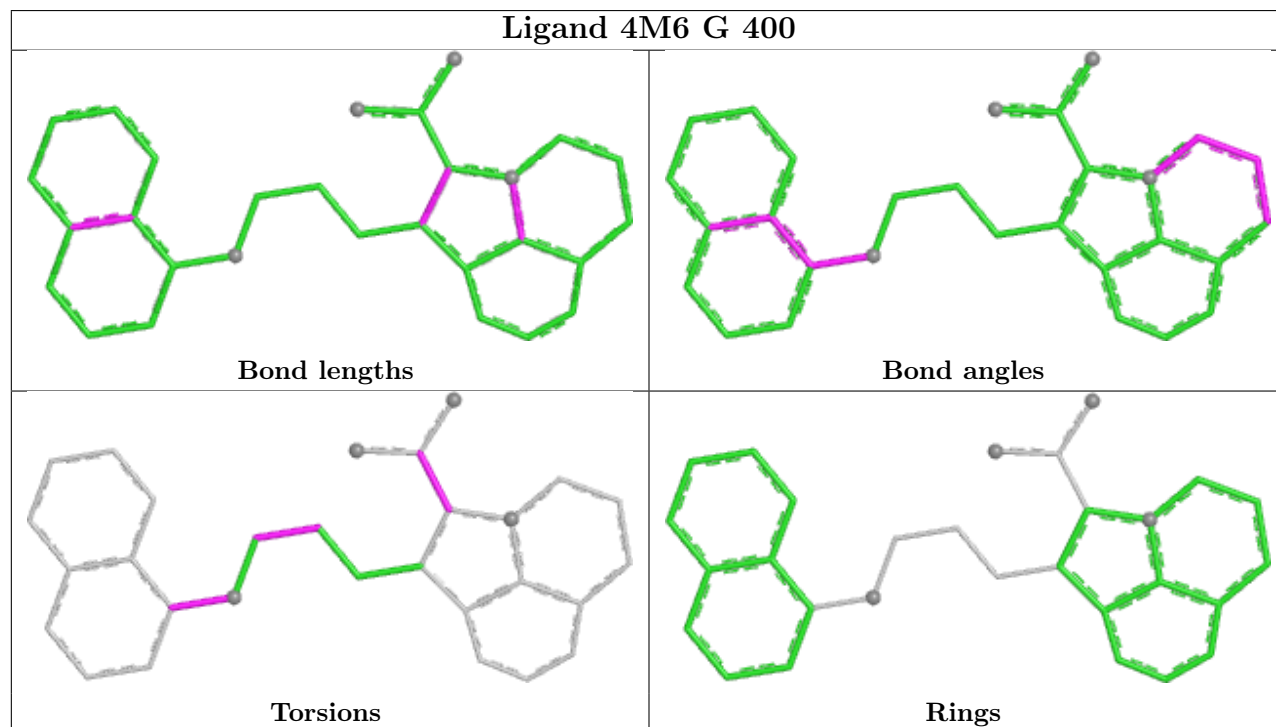
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



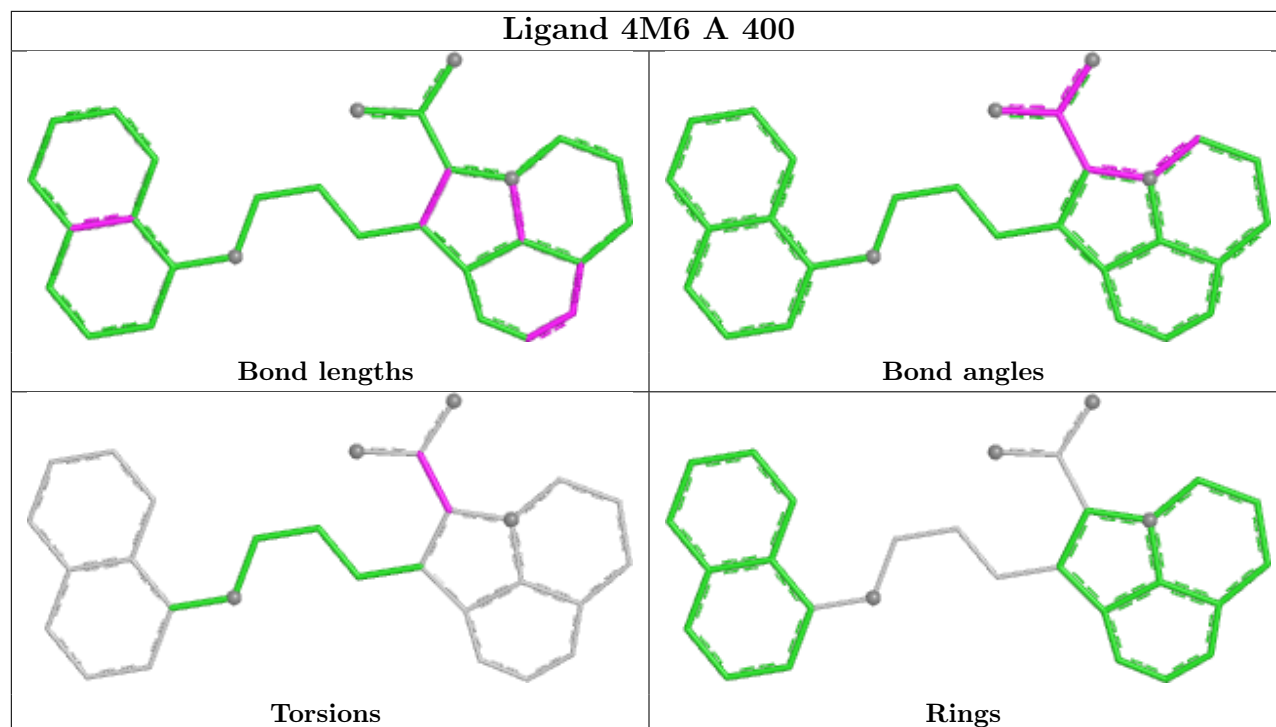
Ligand 4M6 E 400



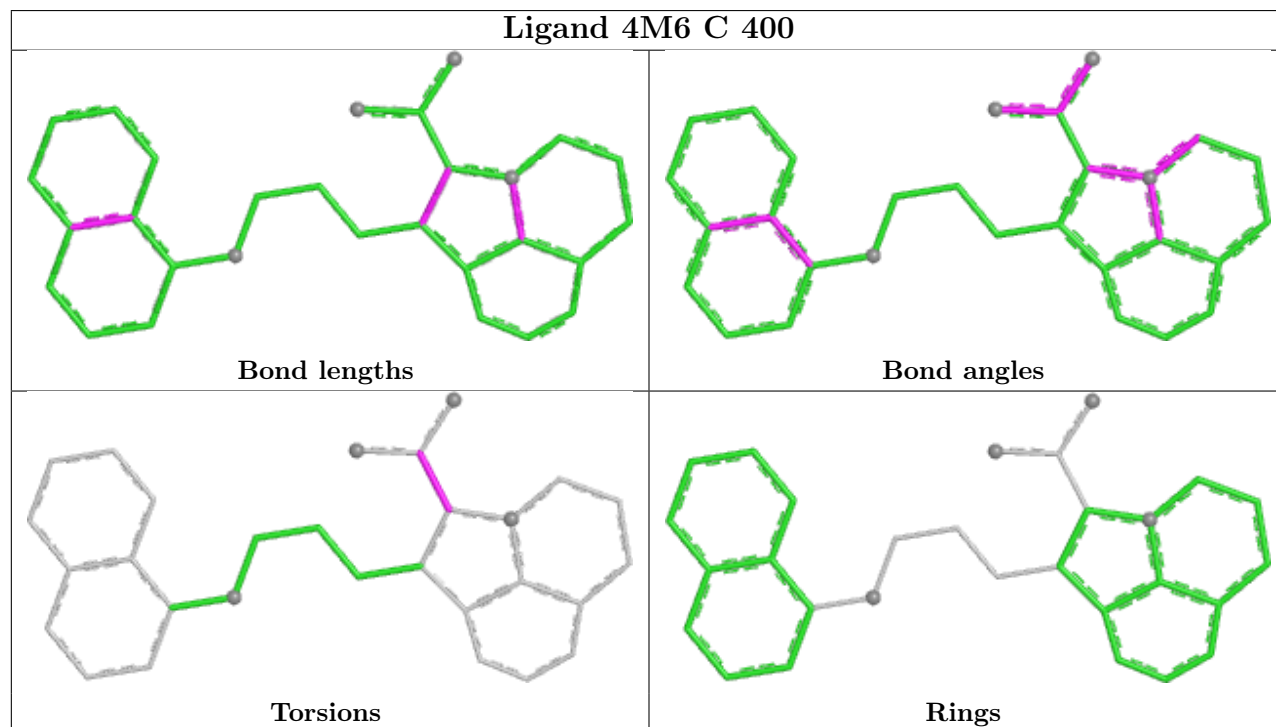
Ligand 4M6 G 400



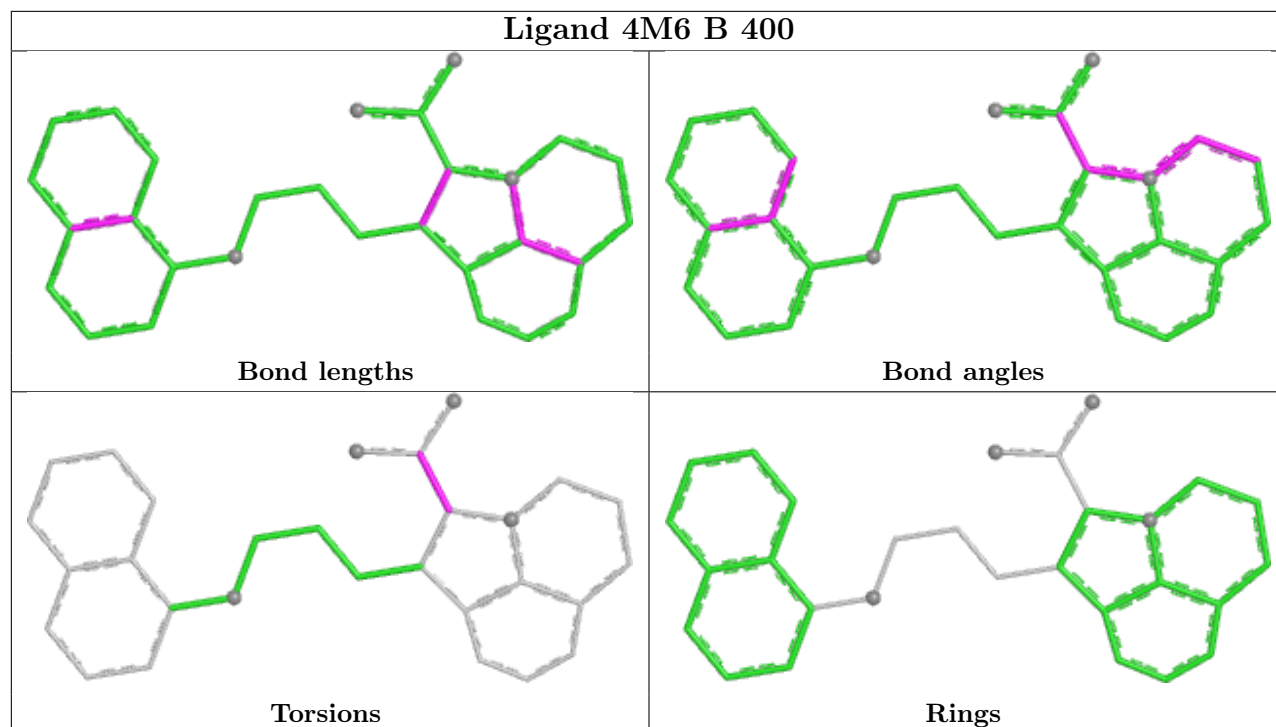
Ligand 4M6 A 400



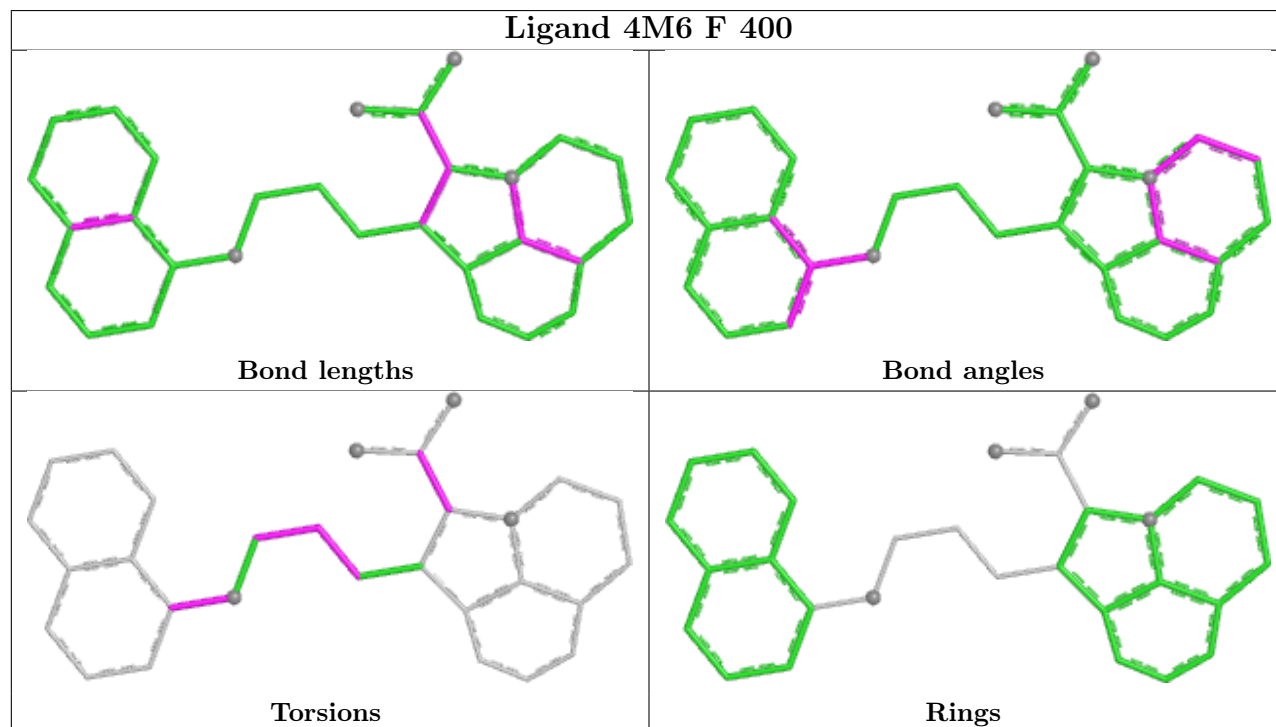
Ligand 4M6 C 400



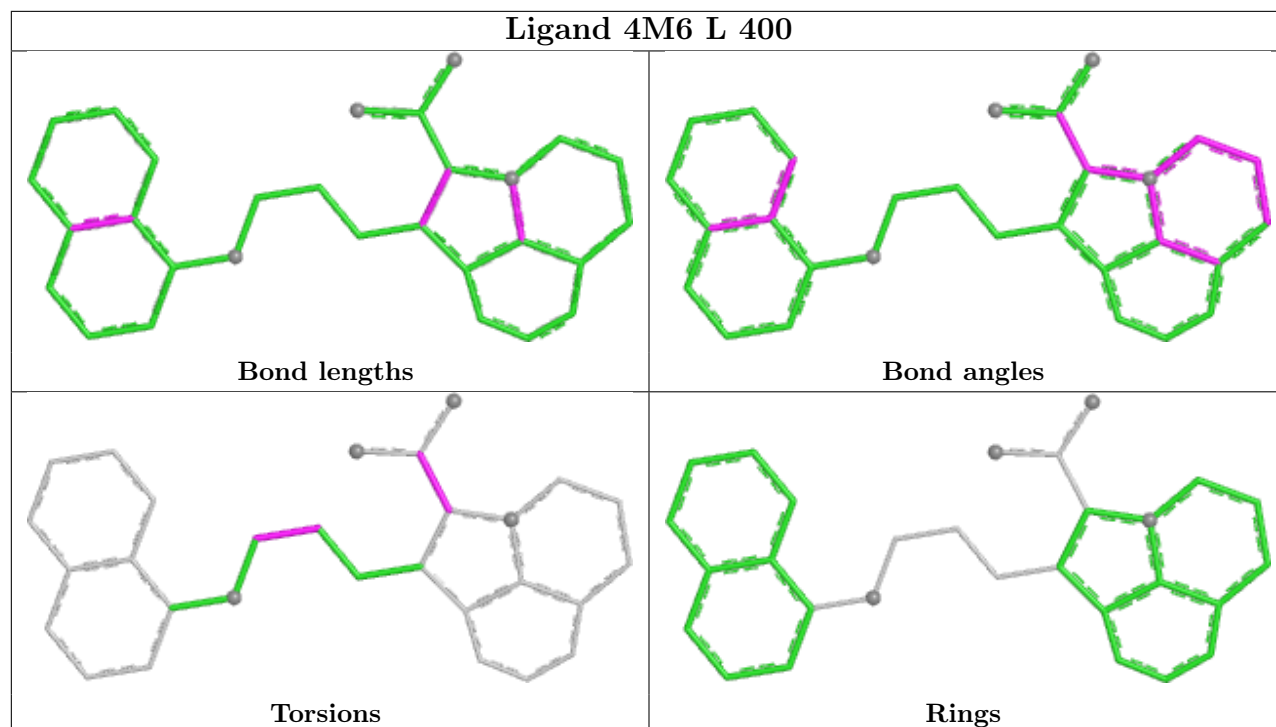
Ligand 4M6 B 400



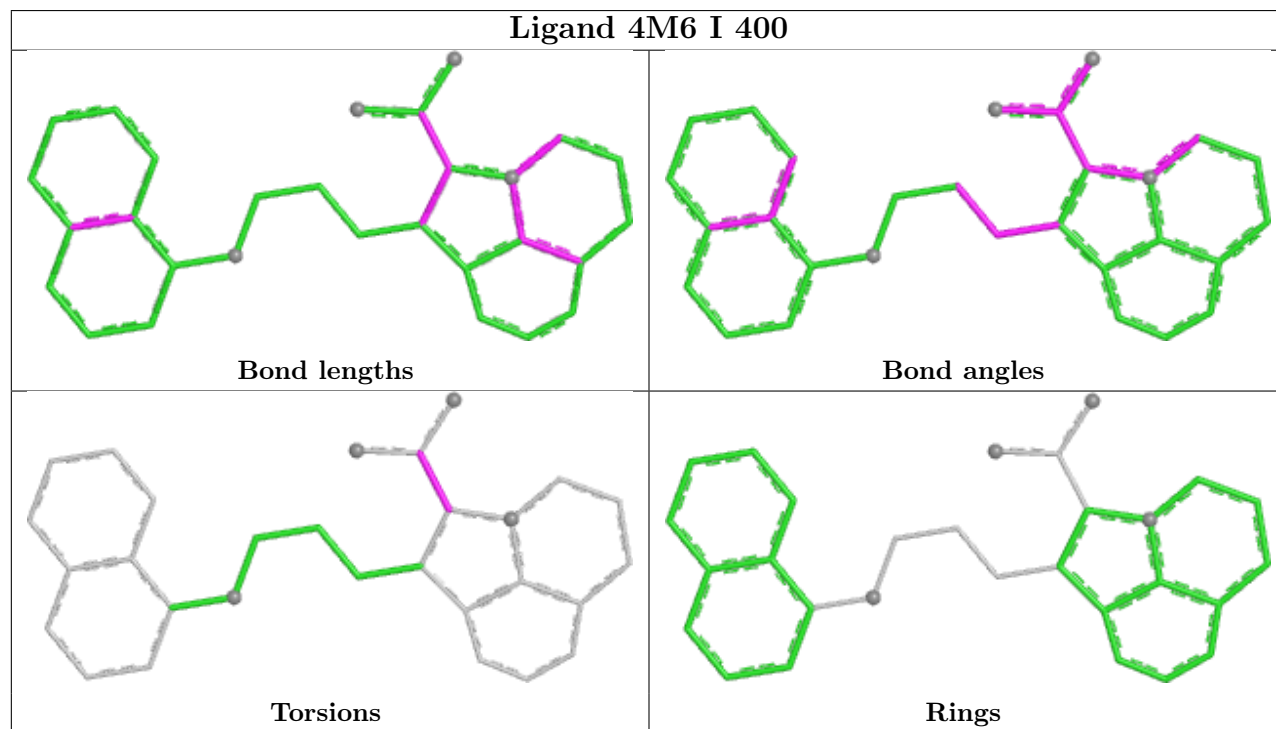
Ligand 4M6 F 400



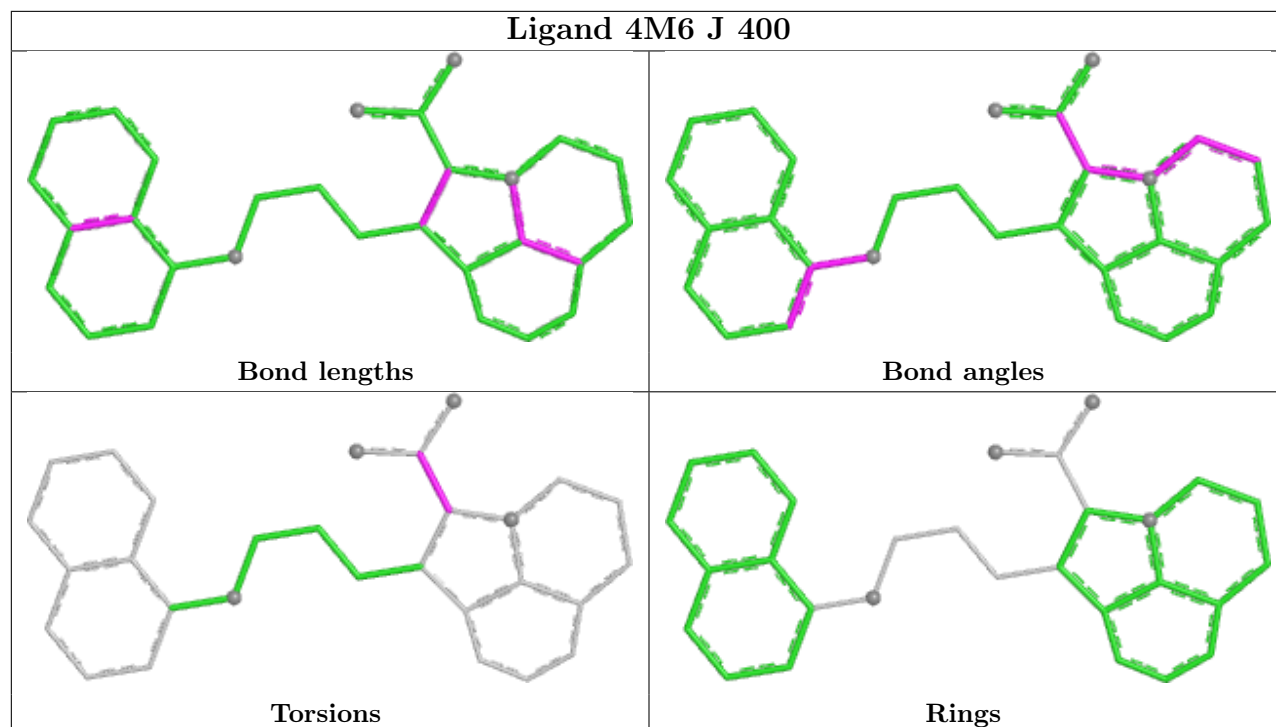
Ligand 4M6 L 400



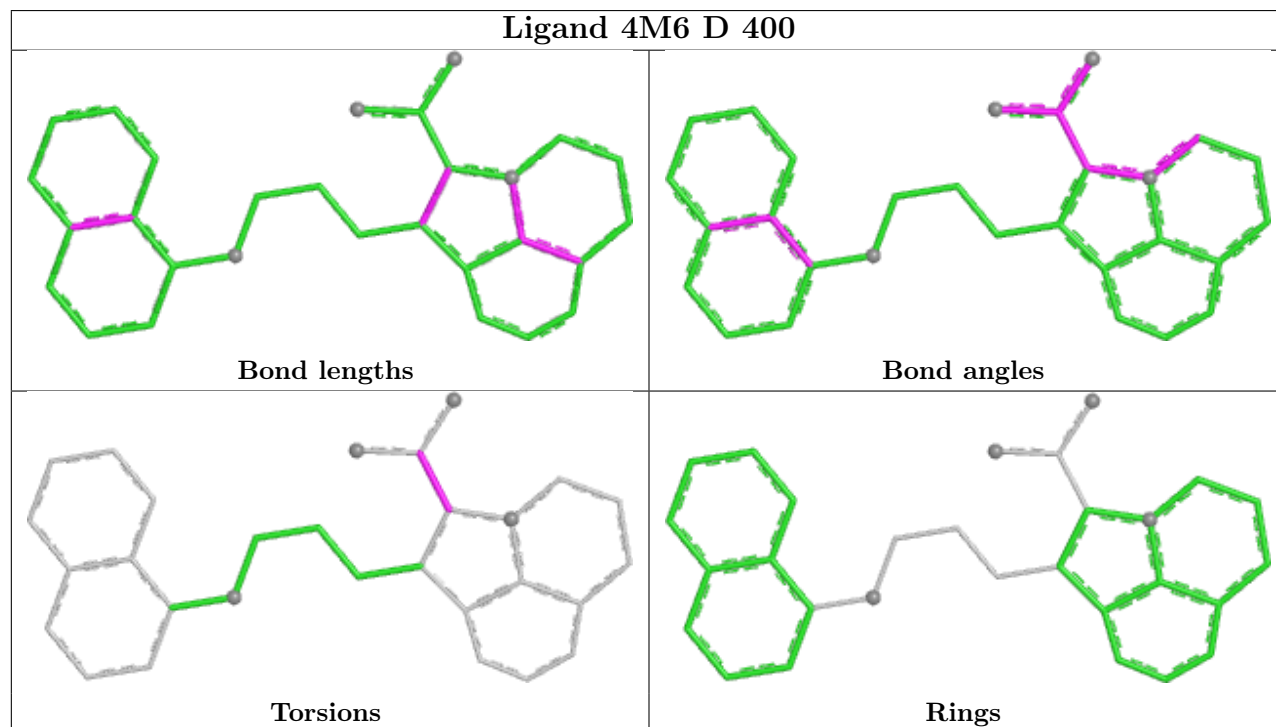
Ligand 4M6 I 400

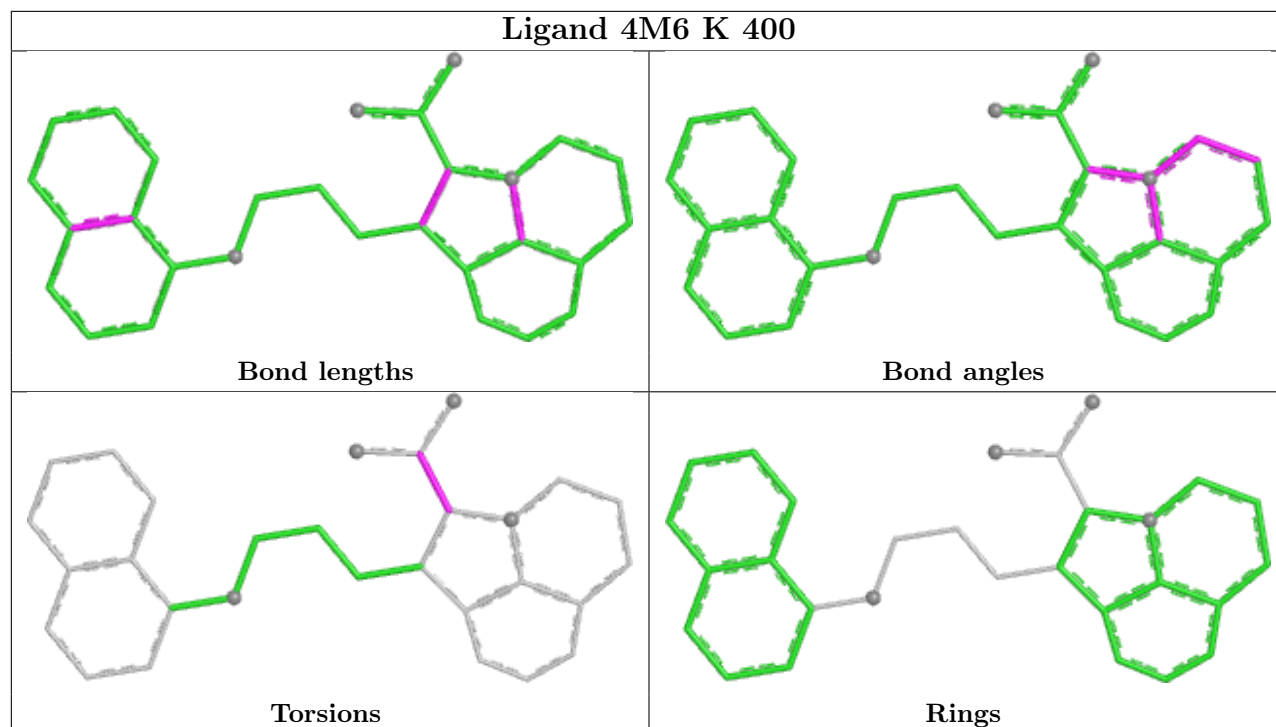


Ligand 4M6 J 400



Ligand 4M6 D 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	152/157 (96%)	-0.34	3 (1%) 65 61	26, 47, 85, 129	0
1	B	153/157 (97%)	-0.42	2 (1%) 75 71	28, 41, 83, 118	0
1	C	151/157 (96%)	-0.17	6 (3%) 42 38	28, 52, 99, 127	0
1	D	152/157 (96%)	-0.55	1 (0%) 84 81	22, 38, 62, 89	0
1	E	152/157 (96%)	-0.38	0 100 100	26, 46, 76, 110	0
1	F	151/157 (96%)	-0.16	0 100 100	31, 52, 88, 102	0
1	G	152/157 (96%)	-0.33	1 (0%) 84 81	24, 47, 83, 101	0
1	H	151/157 (96%)	-0.40	0 100 100	26, 48, 78, 95	0
1	I	151/157 (96%)	-0.42	0 100 100	26, 47, 80, 104	0
1	J	152/157 (96%)	-0.25	2 (1%) 75 71	28, 51, 95, 134	0
1	K	150/157 (95%)	-0.17	2 (1%) 75 71	31, 56, 105, 119	0
1	L	151/157 (96%)	-0.18	1 (0%) 84 81	33, 55, 92, 119	0
All	All	1818/1884 (96%)	-0.31	18 (0%) 79 76	22, 48, 89, 134	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	ASP	4.0
1	B	202	SER	3.6
1	D	171	GLY	3.6
1	A	202	SER	3.0
1	C	201	ARG	3.0
1	J	202	SER	2.9
1	K	320	HIS	2.8
1	C	202	SER	2.8
1	A	201	ARG	2.8
1	G	171	GLY	2.7
1	A	204	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	256	ASP	2.4
1	K	198	PRO	2.3
1	J	200	GLY	2.3
1	C	193	ALA	2.2
1	C	321	VAL	2.2
1	C	320	HIS	2.1
1	C	199	MET	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](#)

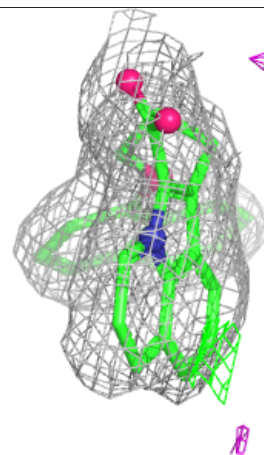
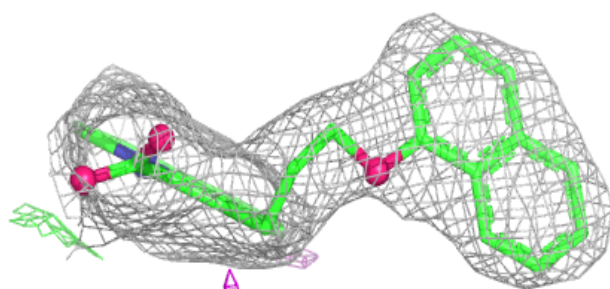
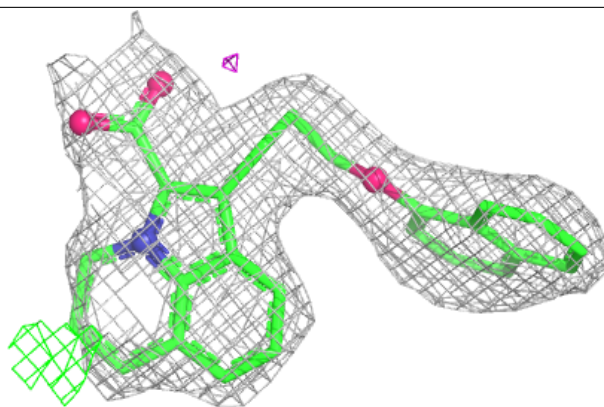
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	4M6	E	400	29/29	0.92	0.09	29,58,70,82	0
2	4M6	C	400	29/29	0.95	0.08	17,47,70,76	0
2	4M6	F	400	29/29	0.95	0.07	31,52,69,70	0
2	4M6	H	400	29/29	0.95	0.07	20,47,61,64	0
2	4M6	J	400	29/29	0.95	0.07	27,40,58,68	0
2	4M6	I	400	29/29	0.96	0.06	15,43,59,70	0
2	4M6	A	400	29/29	0.96	0.06	16,38,52,59	0
2	4M6	L	400	29/29	0.96	0.07	20,44,75,75	0
2	4M6	D	400	29/29	0.97	0.06	15,31,43,49	0
2	4M6	G	400	29/29	0.97	0.05	16,29,42,47	0
2	4M6	K	400	29/29	0.97	0.07	17,39,78,79	0
2	4M6	B	400	29/29	0.97	0.07	13,37,56,74	0

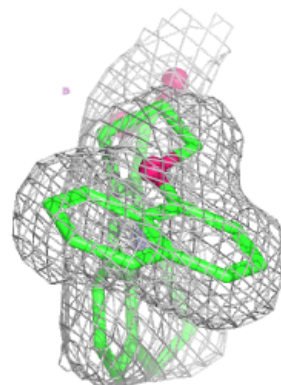
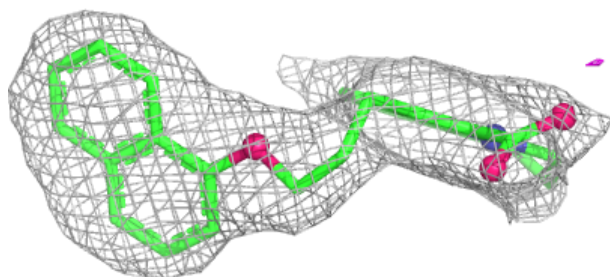
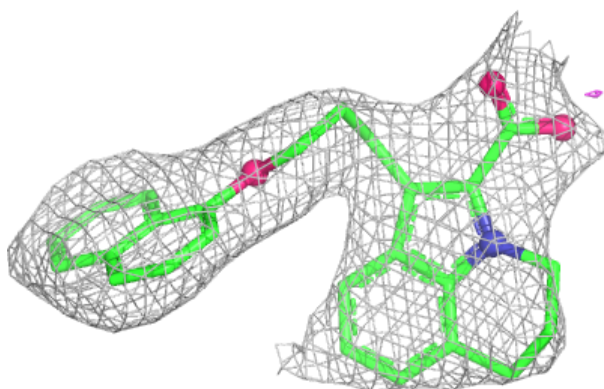
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4M6 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)

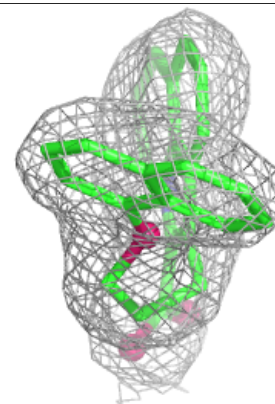
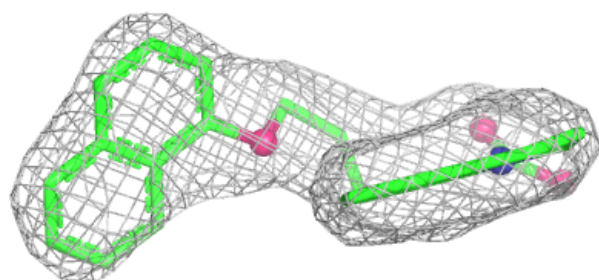
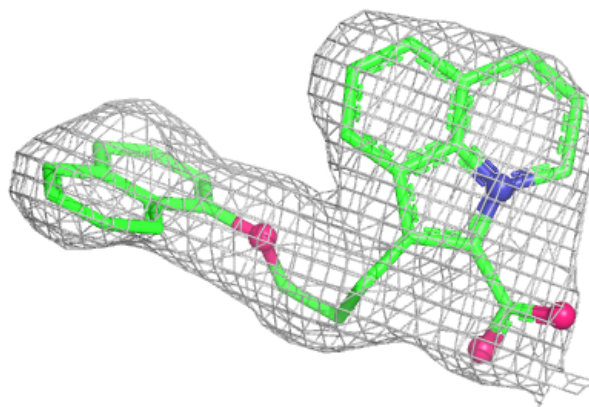
**Electron density around 4M6 C 400:**

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

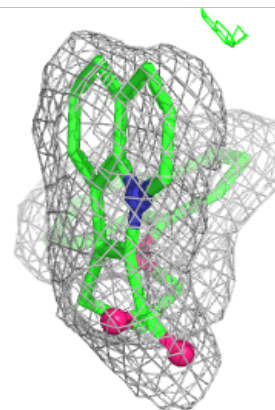
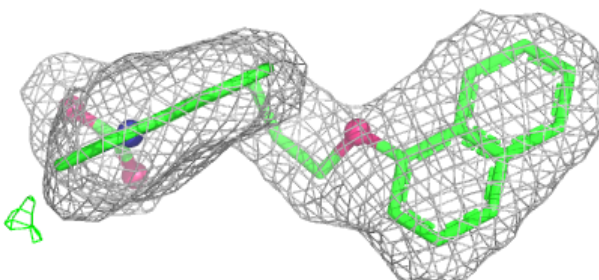
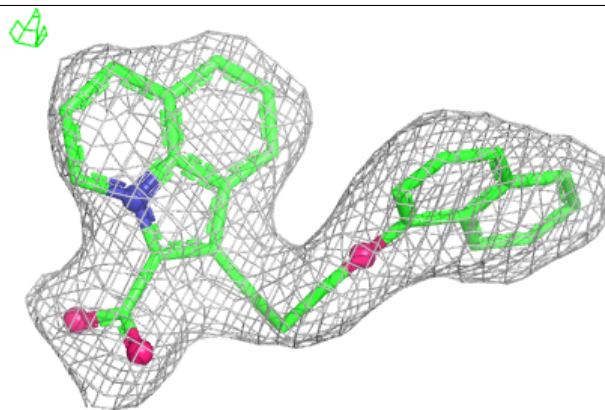


Electron density around 4M6 F 400:

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

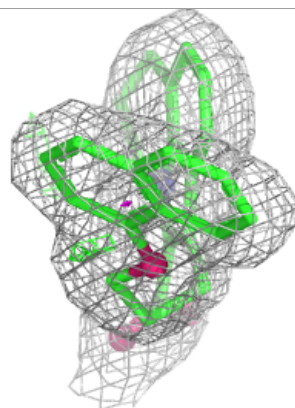
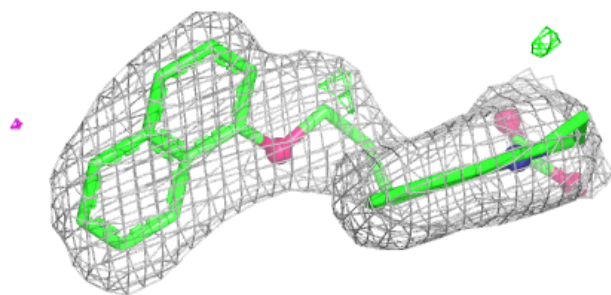
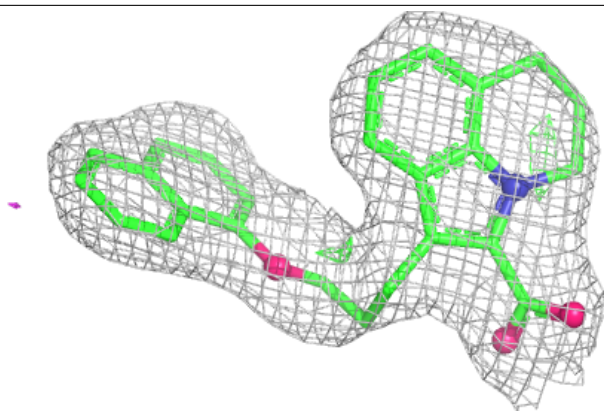
**Electron density around 4M6 H 400:**

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

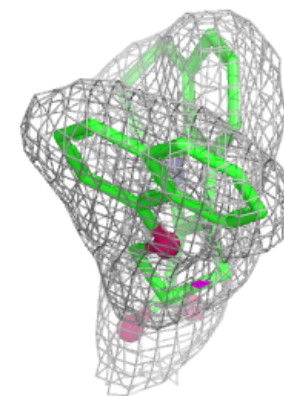
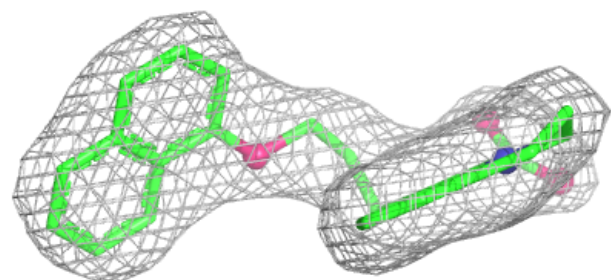
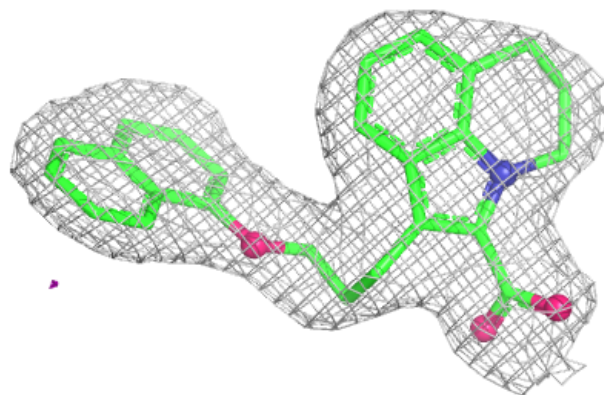


Electron density around 4M6 J 400:

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

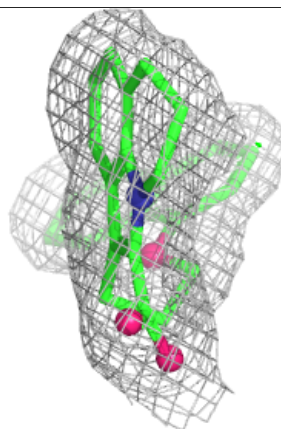
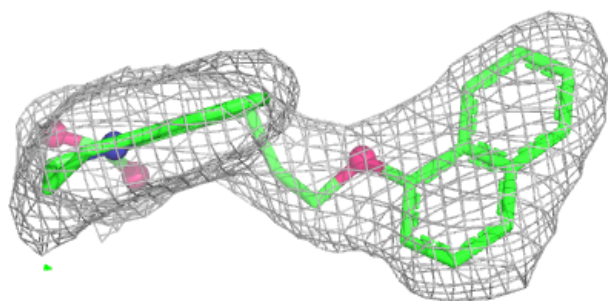
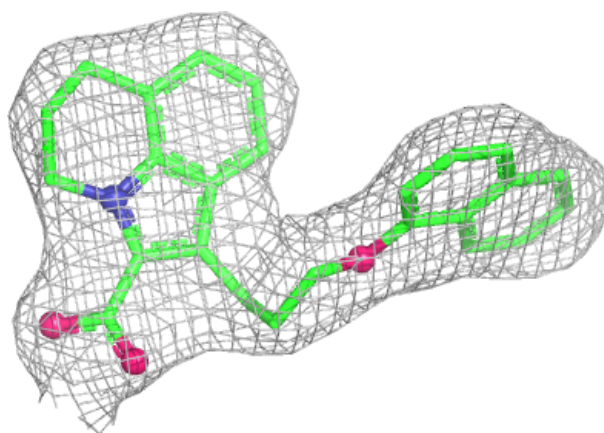
**Electron density around 4M6 I 400:**

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

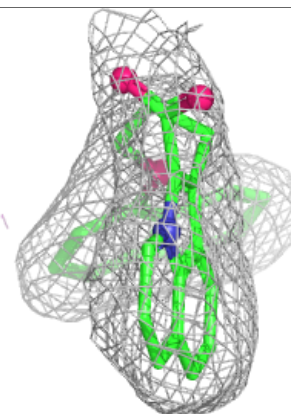
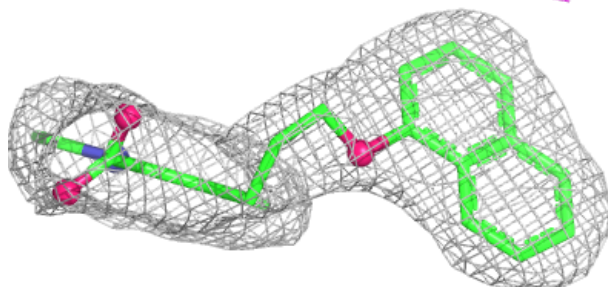
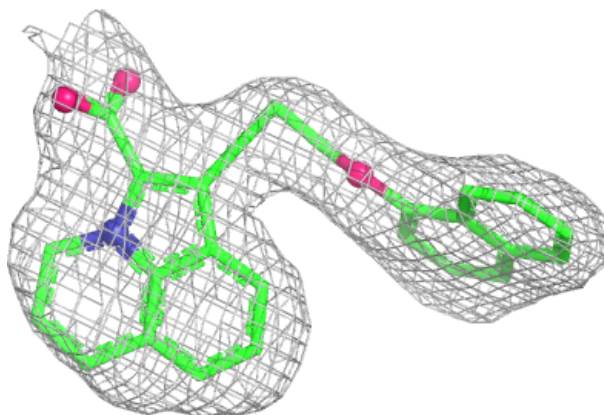


Electron density around 4M6 A 400:

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

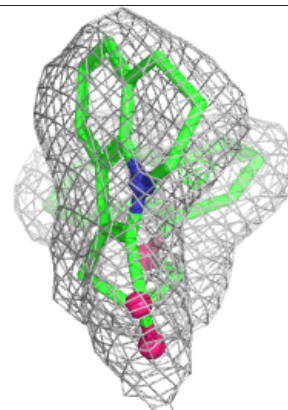
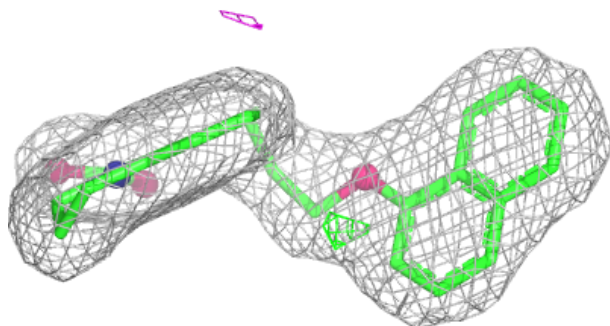
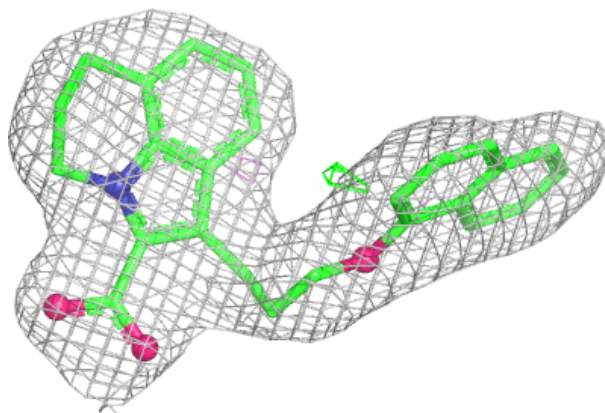
**Electron density around 4M6 L 400:**

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



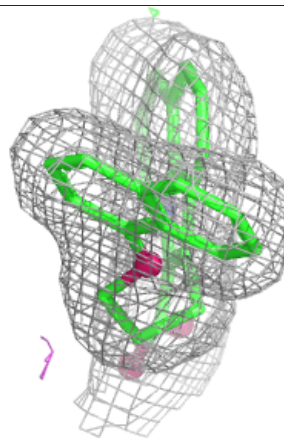
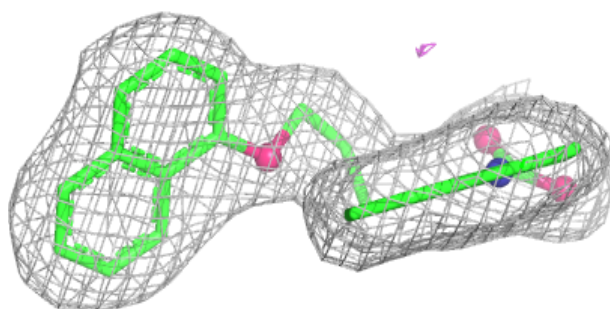
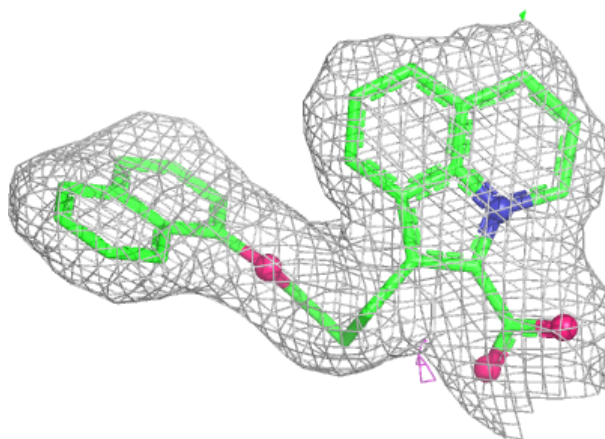
Electron density around 4M6 D 400:

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



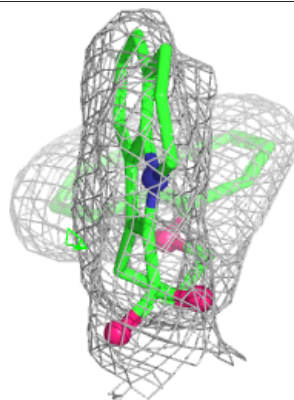
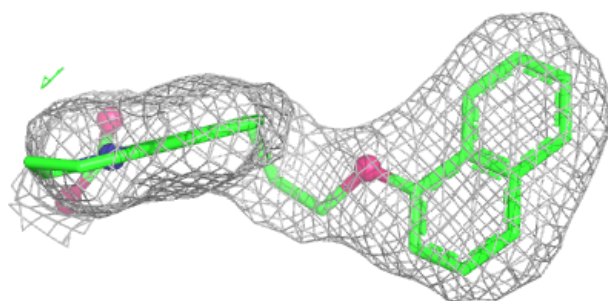
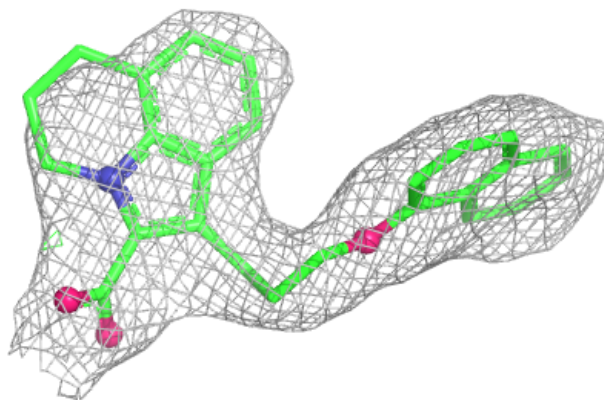
Electron density around 4M6 G 400:

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

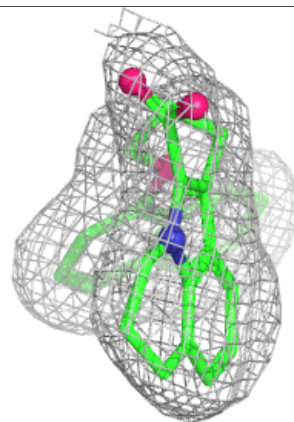
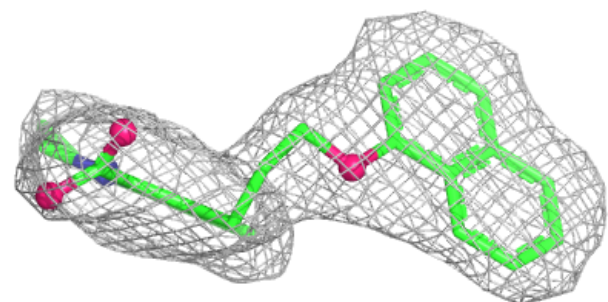
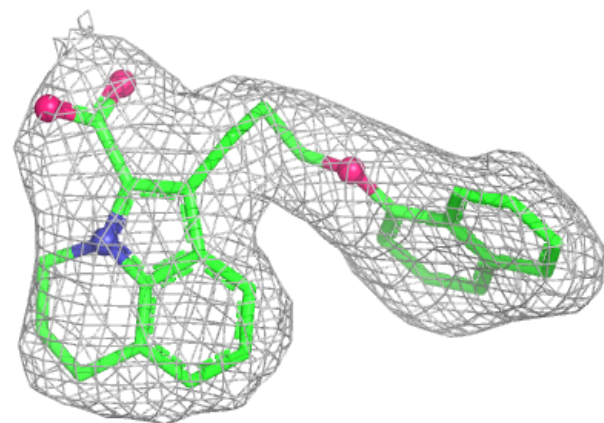


Electron density around 4M6 K 400:

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

**Electron density around 4M6 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.