



Full wwPDB EM Validation Report ⓘ

Mar 4, 2026 – 07:17 PM UTC

PDB ID : 8UHE / pdb_00008uhe
EMDB ID : EMD-42278
Title : Structure of the far-red light-absorbing allophycocyanin core expressed during FaRLiP
Authors : Gisriel, C.J.; Bryant, D.A.; Brudvig, G.W.; Shen, G.
Deposited on : 2023-10-09
Resolution : 2.78 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

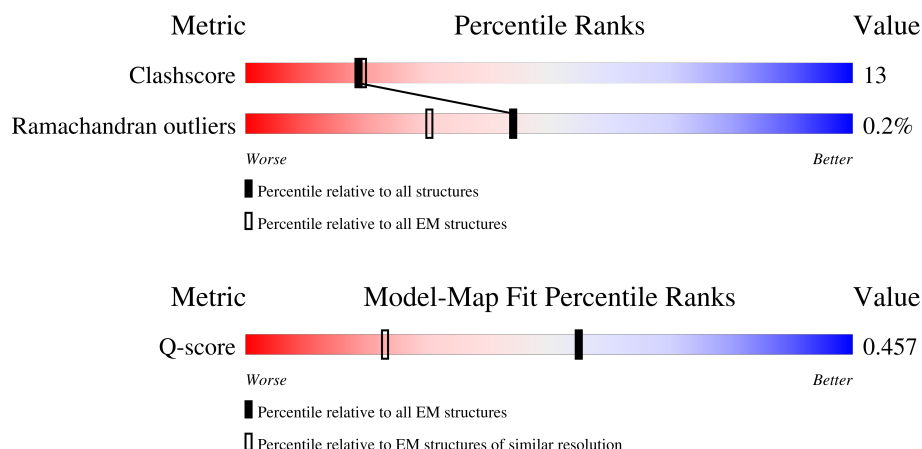
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	10754 (2.28 - 3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	158	44% 61% 37% .
1	E	158	21% 71% 28% .
1	G	158	21% 72% 27% ..
1	M	158	47% 72% 27% ..
1	O	158	38% 63% 35% .

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Mol	Chain	Length	Quality of chain
1	Q	158	
2	B	161	
2	D	161	
2	F	161	
2	H	161	
2	L	161	
2	N	161	
2	P	161	
2	R	161	
3	C	181	
4	I	159	
5	J	169	
6	K	783	
7	S	67	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 27048 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ApcD5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	156	Total	C	N	O	S	0	0
			1233	770	216	240	7		
1	E	156	Total	C	N	O	S	0	0
			1233	770	216	240	7		
1	G	156	Total	C	N	O	S	0	0
			1233	770	216	240	7		
1	M	156	Total	C	N	O	S	0	0
			1233	770	216	240	7		
1	O	156	Total	C	N	O	S	0	0
			1233	770	216	240	7		
1	Q	156	Total	C	N	O	S	0	0
			1233	770	216	240	7		

- Molecule 2 is a protein called ApcB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	161	Total	C	N	O	S	0	0
			1222	763	204	245	10		
2	D	161	Total	C	N	O	S	0	0
			1222	763	204	245	10		
2	F	160	Total	C	N	O	S	0	0
			1214	758	203	244	9		
2	H	161	Total	C	N	O	S	0	0
			1222	763	204	245	10		
2	L	159	Total	C	N	O	S	0	0
			1207	755	202	241	9		
2	N	161	Total	C	N	O	S	0	0
			1222	763	204	245	10		
2	P	161	Total	C	N	O	S	0	0
			1222	763	204	245	10		
2	R	160	Total	C	N	O	S	0	0
			1214	758	203	244	9		

- Molecule 3 is a protein called ApcD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	164	Total	C	N	O	S	0	0
			1300	828	222	243	7		

- Molecule 4 is a protein called ApcD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	158	Total	C	N	O	S	0	0
			1246	784	222	233	7		

- Molecule 5 is a protein called ApcF.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	167	Total	C	N	O	S	0	0
			1311	819	226	259	7		

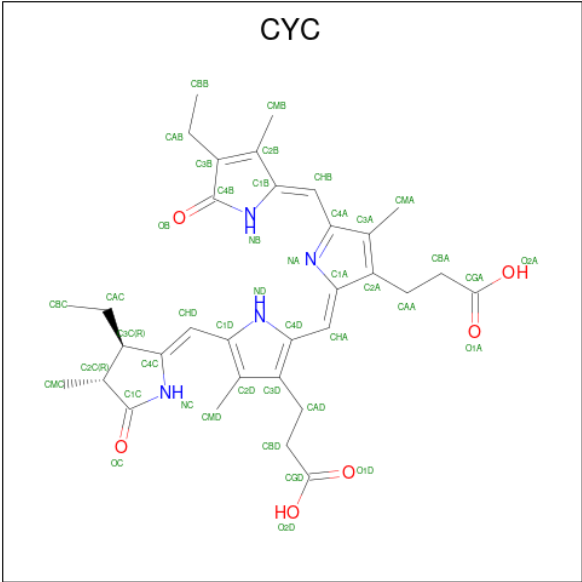
- Molecule 6 is a protein called ApcE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	593	Total	C	N	O	S	0	0
			4727	2989	849	871	18		

- Molecule 7 is a protein called ApcC.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	67	Total	C	N	O	S	0	0
			546	341	105	96	4		

- Molecule 8 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$).



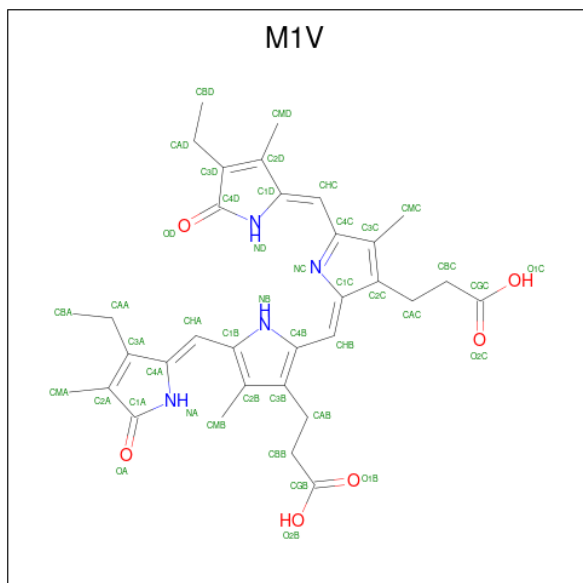
Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			43	33	4	6	
8	B	1	Total	C	N	O	0
			43	33	4	6	
8	D	1	Total	C	N	O	0
			43	33	4	6	
8	E	1	Total	C	N	O	0
			43	33	4	6	
8	F	1	Total	C	N	O	0
			43	33	4	6	
8	G	1	Total	C	N	O	0
			43	33	4	6	
8	H	1	Total	C	N	O	0
			43	33	4	6	
8	I	1	Total	C	N	O	0
			43	33	4	6	
8	J	1	Total	C	N	O	0
			43	33	4	6	
8	L	1	Total	C	N	O	0
			43	33	4	6	
8	M	1	Total	C	N	O	0
			43	33	4	6	
8	N	1	Total	C	N	O	0
			43	33	4	6	
8	O	1	Total	C	N	O	0
			43	33	4	6	
8	P	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
8	Q	1	Total	C	N	O	0
			43	33	4	6	
8	R	1	Total	C	N	O	0
			43	33	4	6	

- Molecule 9 is mesobiliverdin IX(alpha) (CCD ID: M1V) (formula: $C_{33}H_{38}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	C	1	Total	C	N	O	0
			43	33	4	6	
9	K	1	Total	C	N	O	0
			43	33	4	6	

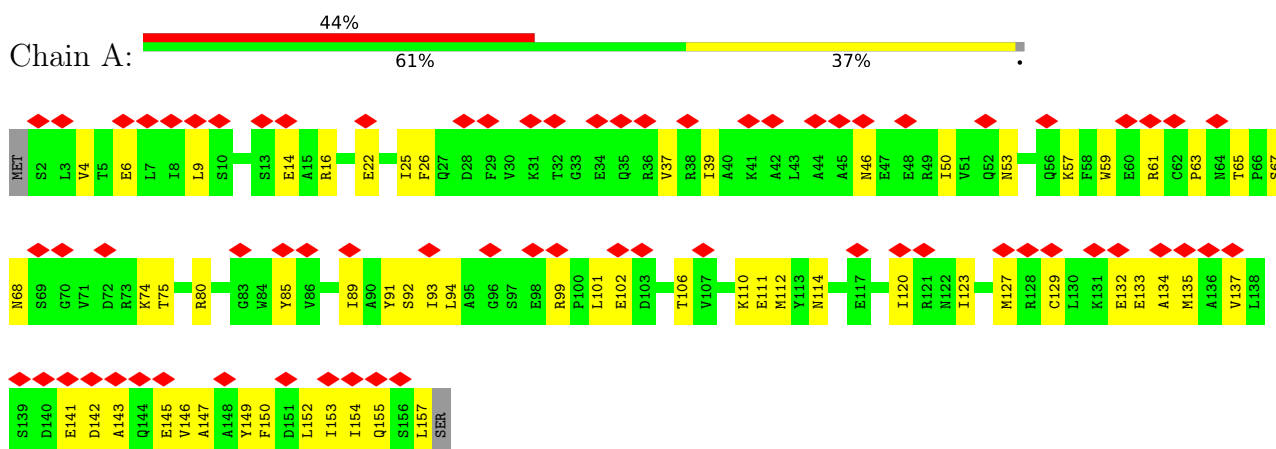
- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
10	K	1	Total	Cl	0
			1	1	

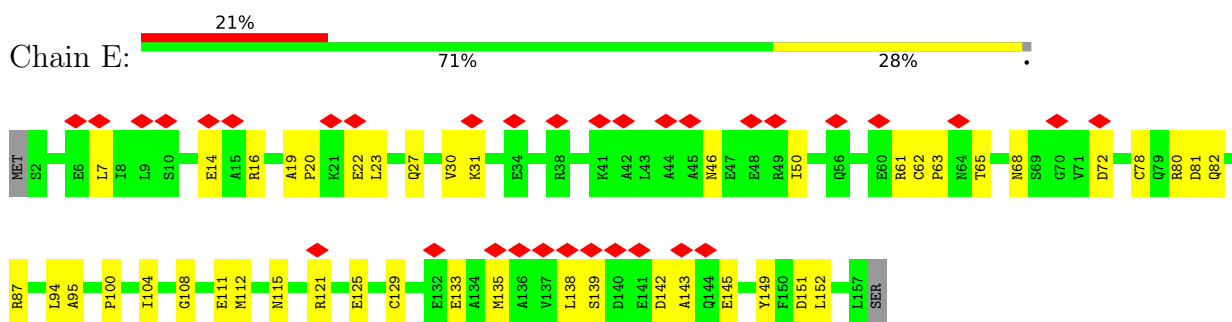
3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

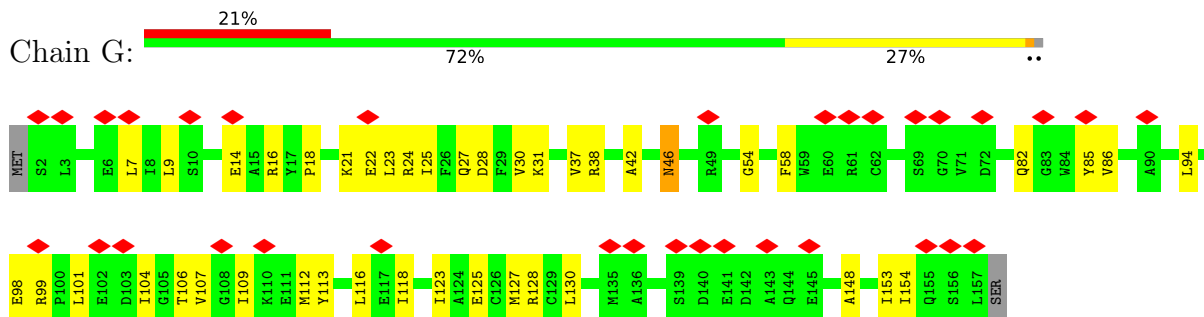
- Molecule 1: ApcD5



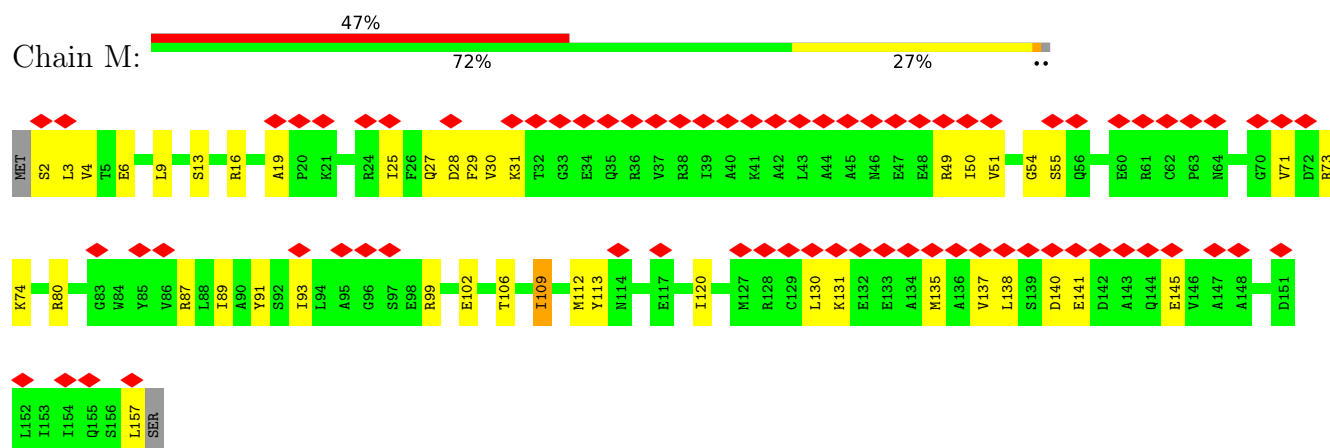
- Molecule 1: ApcD5



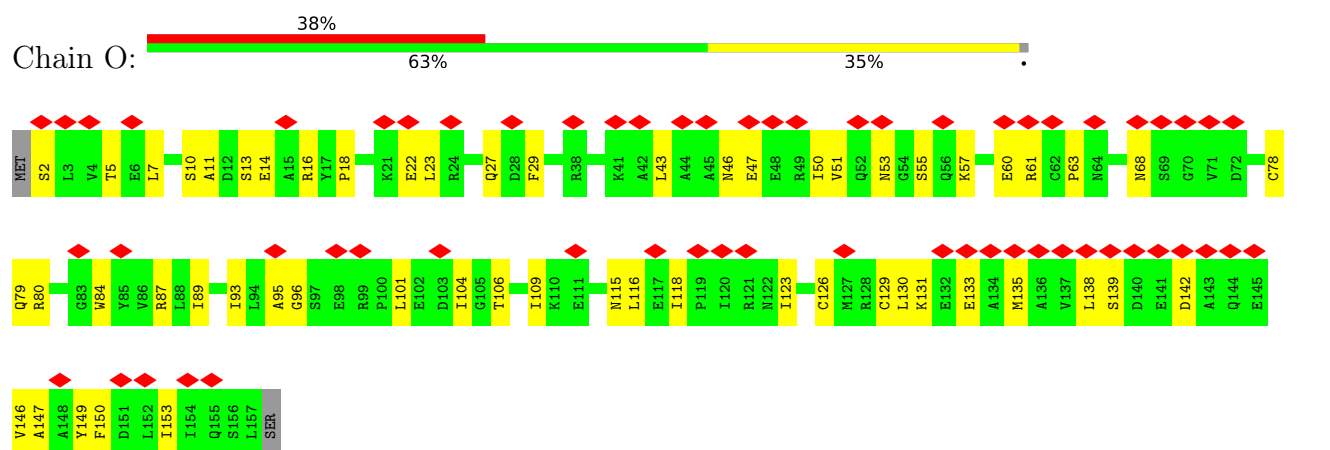
- Molecule 1: ApcD5



- Molecule 1: ApcD5



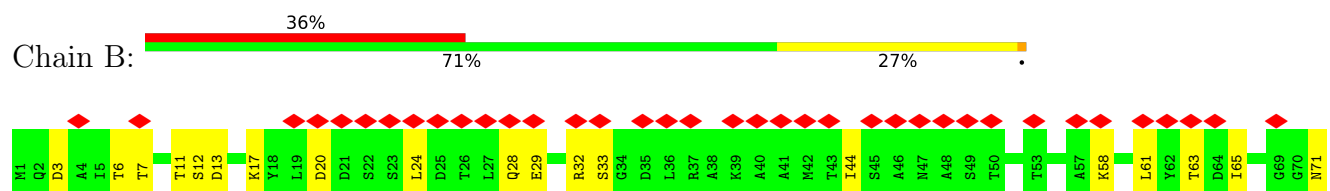
- Molecule 1: ApcD5

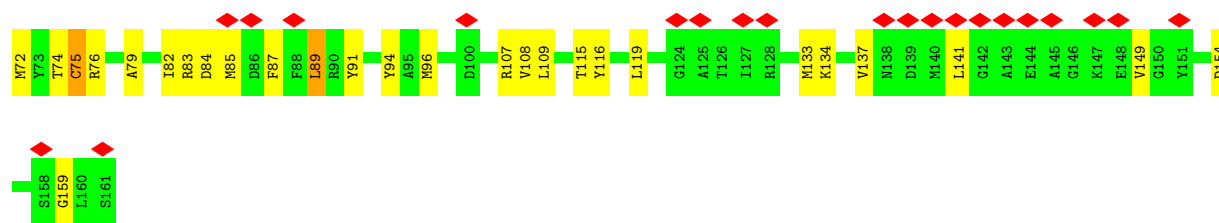


- Molecule 1: ApcD5

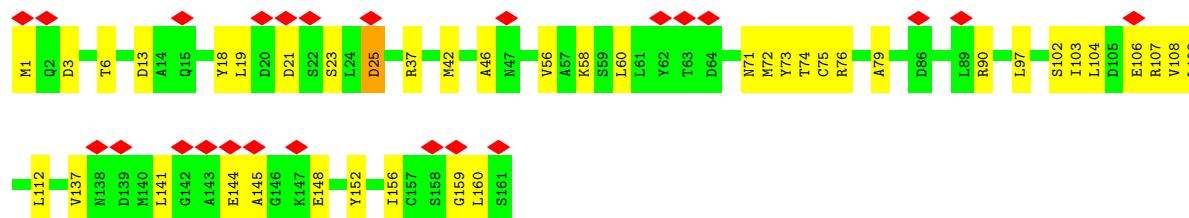
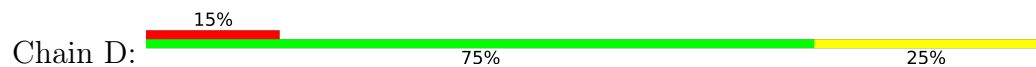


- Molecule 2: ApcB2

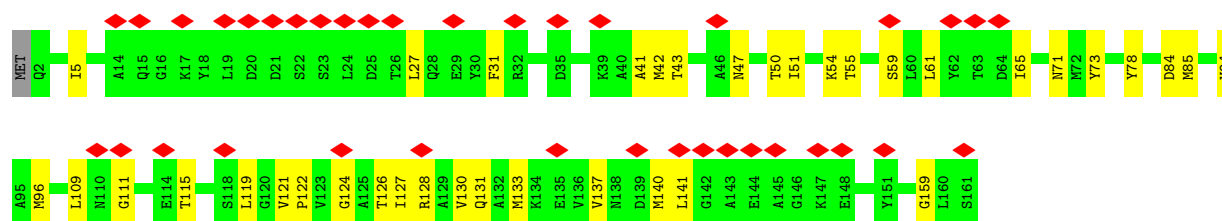
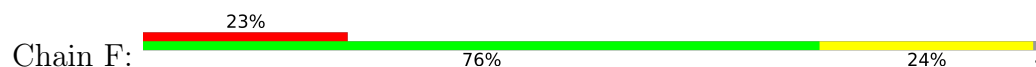




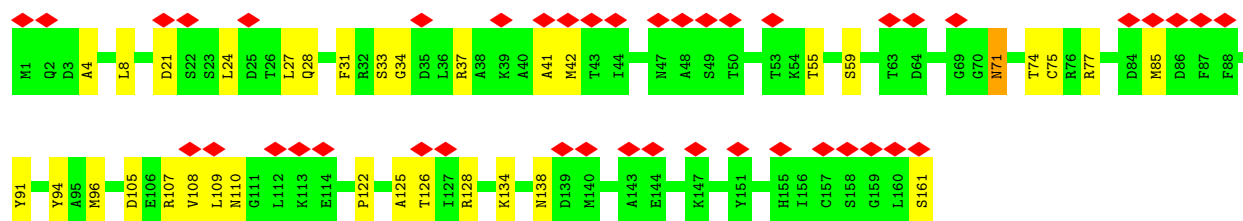
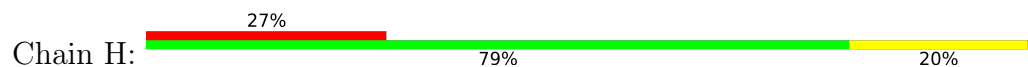
• Molecule 2: ApcB2



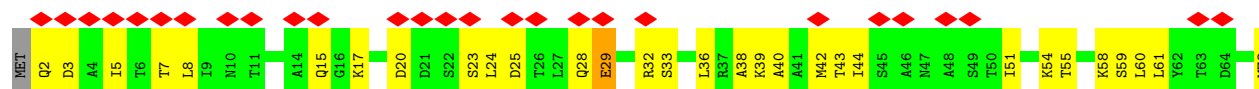
• Molecule 2: ApcB2

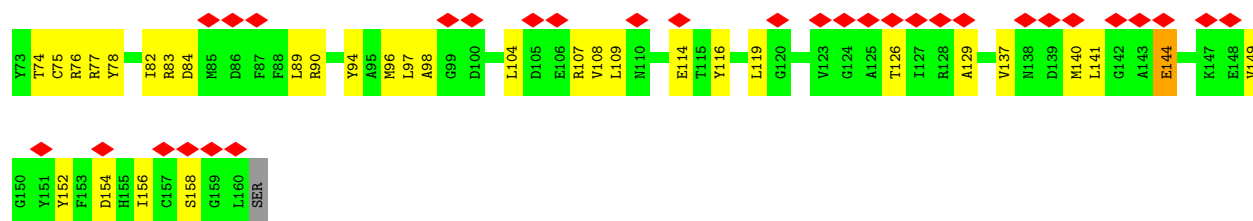


• Molecule 2: ApcB2

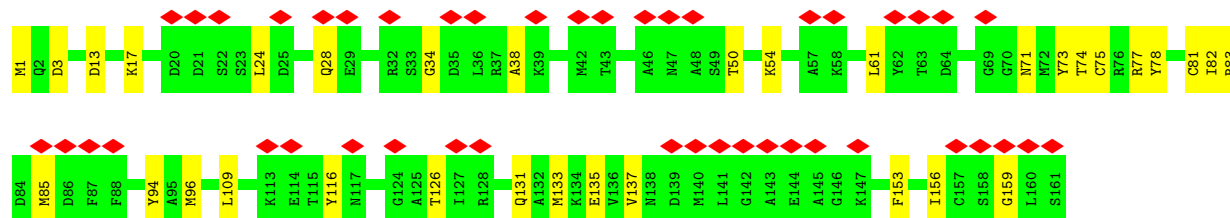
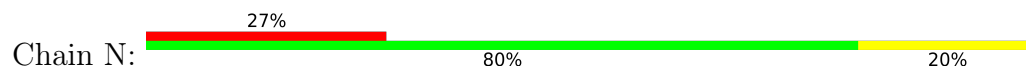


• Molecule 2: ApcB2

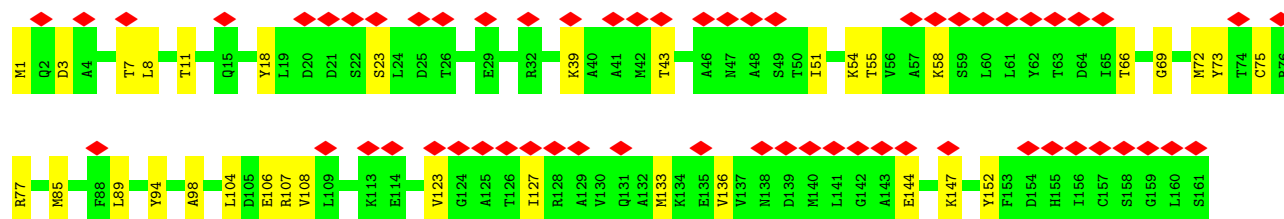
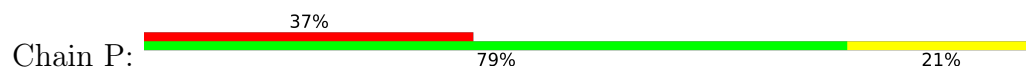




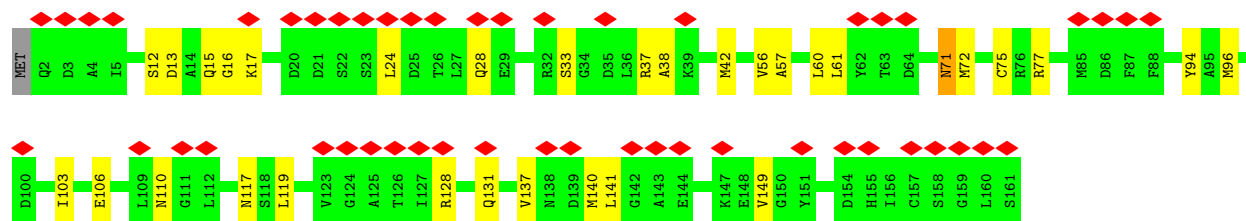
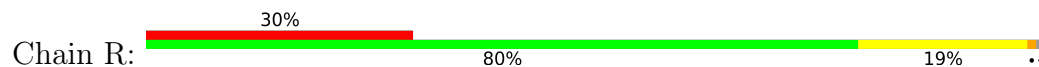
• Molecule 2: ApcB2



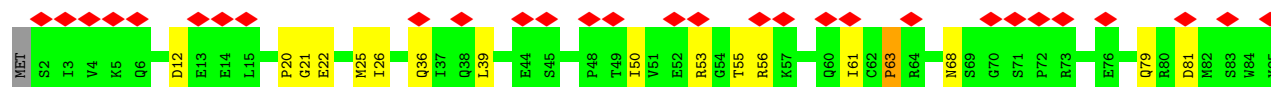
• Molecule 2: ApcB2

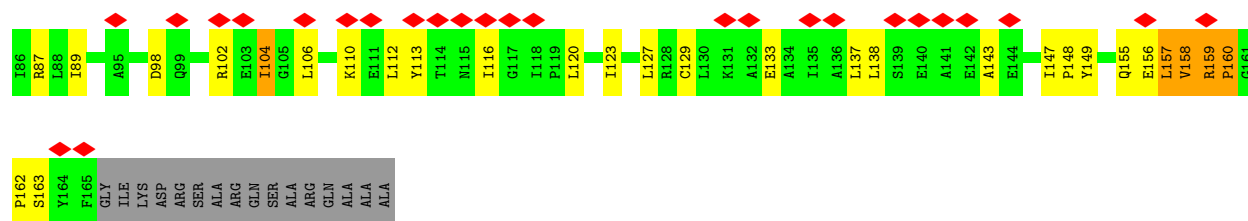


• Molecule 2: ApcB2

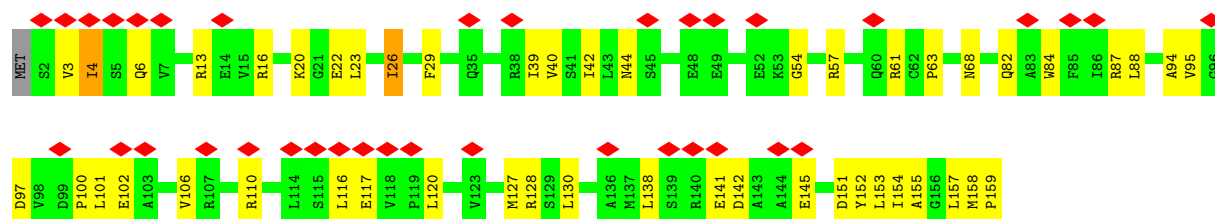


• Molecule 3: ApcD3

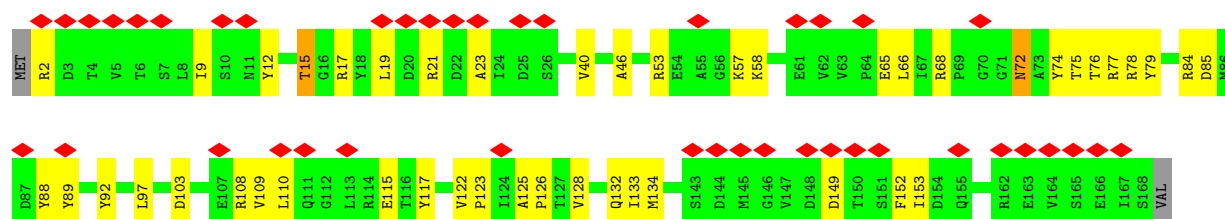




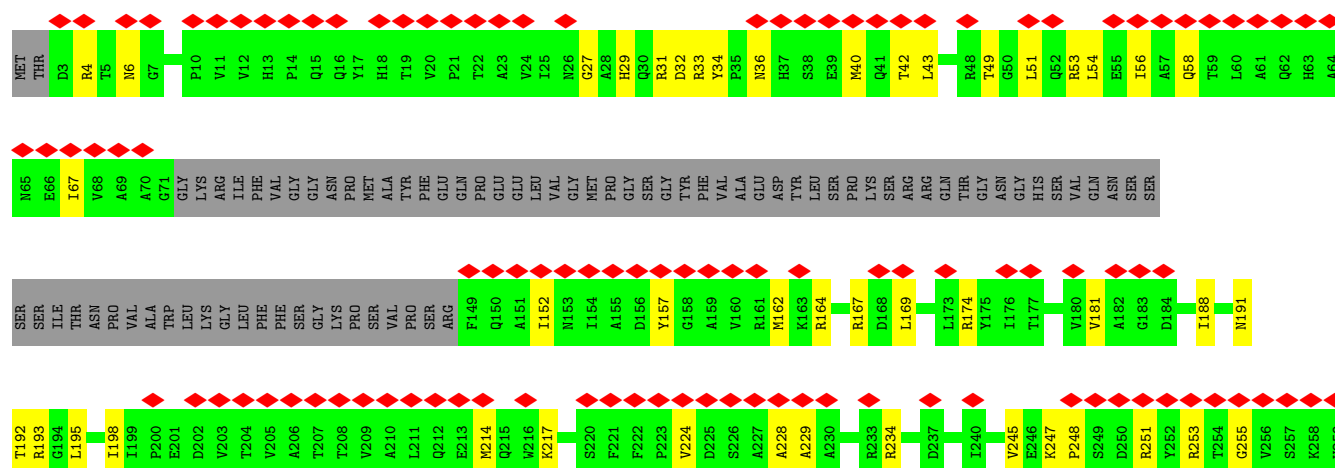
• Molecule 4: ApcD2

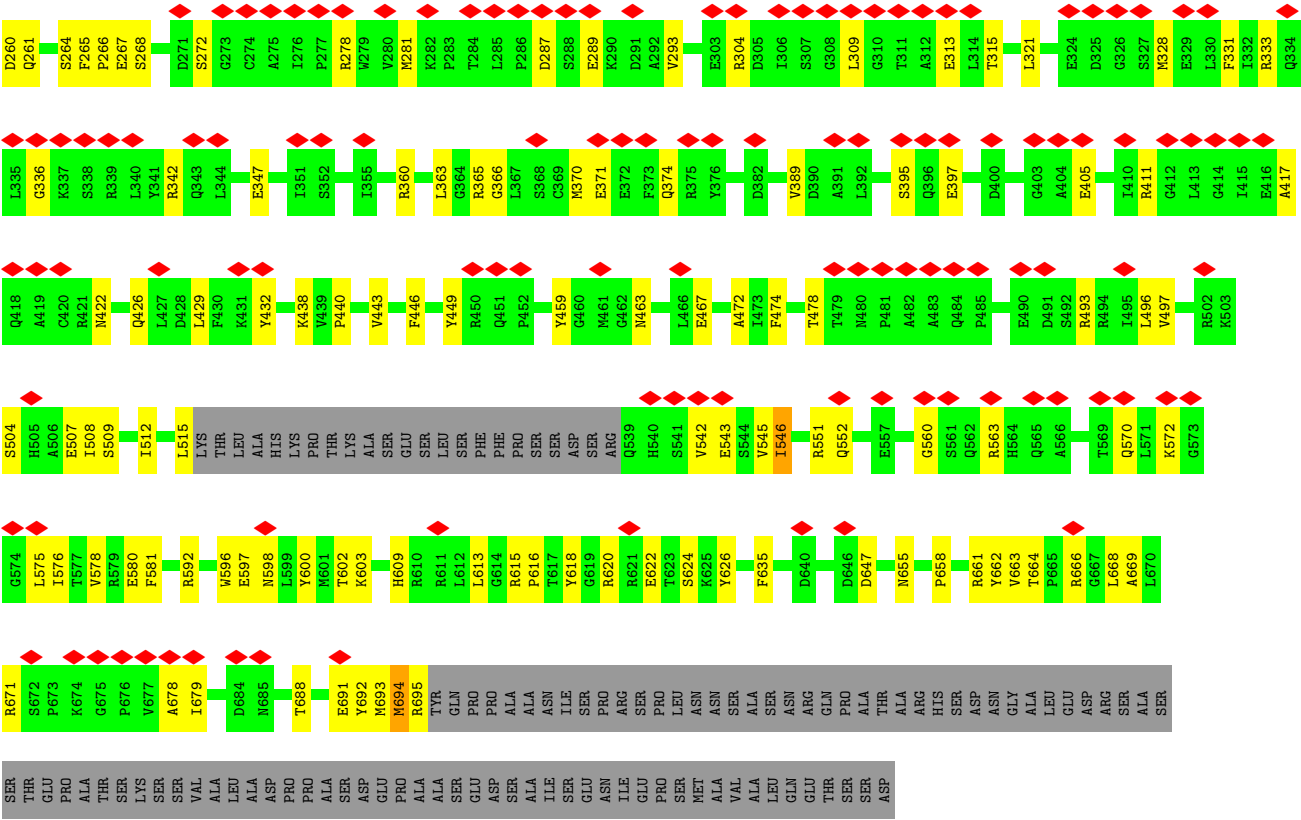


• Molecule 5: ApcF



• Molecule 6: ApcE2





• Molecule 7: ApcC



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0198	Depositor
Map size (Å)	211.2, 211.2, 211.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CYC, MEN, M1V

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	0.38	0/1251	0.60	0/1690
1	E	0.41	0/1251	0.61	0/1690
1	G	0.40	1/1251 (0.1%)	0.58	0/1690
1	M	0.49	2/1251 (0.2%)	0.60	2/1690 (0.1%)
1	O	0.35	0/1251	0.56	0/1690
1	Q	0.58	4/1251 (0.3%)	0.76	5/1690 (0.3%)
2	B	0.33	1/1228 (0.1%)	0.52	0/1656
2	D	0.44	1/1228 (0.1%)	0.62	0/1656
2	F	0.41	0/1220	0.55	0/1646
2	H	0.33	0/1228	0.54	0/1656
2	L	0.55	2/1213 (0.2%)	0.65	1/1638 (0.1%)
2	N	0.28	0/1228	0.53	0/1656
2	P	0.35	1/1228 (0.1%)	0.57	0/1656
2	R	0.28	0/1220	0.55	0/1646
3	C	0.48	1/1326 (0.1%)	0.89	11/1797 (0.6%)
4	I	0.44	1/1267 (0.1%)	0.55	2/1714 (0.1%)
5	J	0.34	0/1320	0.54	1/1783 (0.1%)
6	K	0.34	2/4838 (0.0%)	0.54	0/6553
7	S	0.44	1/554 (0.2%)	0.62	0/742
All	All	0.40	17/26604 (0.1%)	0.60	22/35939 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
6	K	0	1
All	All	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	66	PRO	CG-CD	-10.65	1.14	1.50
4	I	4	ILE	CG1-CD1	-9.98	1.12	1.51
2	L	29	GLU	CD-OE2	-9.32	1.07	1.25
1	M	25	ILE	CG1-CD1	-8.96	1.16	1.51
2	L	144	GLU	CD-OE1	-8.47	1.09	1.25
1	Q	66	PRO	N-CD	7.78	1.58	1.47
7	S	10	VAL	CA-C	-6.87	1.47	1.53
6	K	214	MET	SD-CE	-6.35	1.63	1.79
1	G	46	ASN	CG-OD1	-6.17	1.11	1.23
3	C	157	LEU	C-O	-5.75	1.16	1.24
6	K	546	ILE	CG1-CD1	-5.75	1.29	1.51
2	B	89	LEU	CG-CD2	-5.71	1.33	1.52
1	Q	65	THR	C-O	-5.41	1.18	1.24
2	P	75	CYS	CB-SG	-5.28	1.63	1.81
1	Q	22	GLU	CD-OE2	-5.25	1.15	1.25
2	D	25	ASP	CG-OD1	-5.18	1.15	1.25
1	M	109	ILE	CG1-CD1	-5.03	1.32	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	66	PRO	CA-N-CD	-13.21	93.50	112.00
3	C	163	SER	N-CA-C	10.67	125.86	109.96
1	Q	66	PRO	N-CD-CG	-10.06	88.11	103.20
3	C	157	LEU	CA-C-O	9.75	129.65	119.51
3	C	63	PRO	CA-N-CD	-7.74	101.17	112.00
1	Q	66	PRO	CA-CB-CG	-7.74	89.80	104.50
3	C	158	VAL	N-CA-C	-7.72	105.19	112.83
3	C	157	LEU	O-C-N	-7.70	111.68	122.15
2	L	144	GLU	CG-CD-OE2	7.29	135.16	118.40
1	M	25	ILE	CB-CG1-CD1	7.18	128.87	113.80
4	I	26	ILE	CG1-CB-CG2	-7.09	89.43	110.70
3	C	159	ARG	N-CA-C	6.83	124.90	109.81
3	C	160	PRO	N-CA-C	-6.83	98.41	112.47
1	Q	65	THR	C-N-CD	5.99	149.54	125.00
3	C	159	ARG	CA-C-N	-5.93	112.43	119.84
3	C	159	ARG	C-N-CA	-5.93	112.43	119.84
3	C	104	ILE	CG1-CB-CG2	-5.79	93.32	110.70
1	Q	66	PRO	CB-CG-CD	-5.50	88.50	106.10
3	C	63	PRO	N-CD-CG	-5.48	94.98	103.20
1	M	109	ILE	CB-CG1-CD1	-5.42	102.41	113.80
5	J	15	THR	CA-CB-CG2	-5.37	101.37	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	4	ILE	N-CA-C	-5.32	105.94	111.58

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	157	LEU	Mainchain
6	K	694	MET	Peptide

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	1233	0	1227	46	0
1	E	1233	0	1227	42	0
1	G	1233	0	1227	35	0
1	M	1233	0	1227	41	0
1	O	1233	0	1227	46	0
1	Q	1233	0	1227	36	0
2	B	1222	0	1208	39	0
2	D	1222	0	1208	39	0
2	F	1214	0	1196	33	0
2	H	1222	0	1208	26	0
2	L	1207	0	1191	56	0
2	N	1222	0	1208	25	0
2	P	1222	0	1208	27	0
2	R	1214	0	1196	30	0
3	C	1300	0	1320	40	0
4	I	1246	0	1249	43	0
5	J	1311	0	1295	46	0
6	K	4727	0	4631	130	0
7	S	546	0	565	26	0
8	A	43	0	37	2	0
8	B	43	0	37	3	0
8	D	43	0	37	1	0
8	E	43	0	37	4	0
8	F	43	0	37	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	43	0	37	4	0
8	H	43	0	37	4	0
8	I	43	0	37	3	0
8	J	43	0	36	2	0
8	L	43	0	37	5	0
8	M	43	0	37	3	0
8	N	43	0	37	2	0
8	O	43	0	37	3	0
8	P	43	0	37	7	0
8	Q	43	0	37	2	0
8	R	43	0	37	3	0
9	C	43	0	36	6	0
9	K	43	0	36	9	0
10	K	1	0	0	1	0
All	All	27048	0	26708	699	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 13.

All (699) 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)
9:K:801:M1V:H17	9:K:801:M1V:H20	1.36	1.05
9:C:201:M1V:H17	9:C:201:M1V:CHB	1.83	1.02
9:C:201:M1V:H20	9:C:201:M1V:CBB	1.93	0.99
9:C:201:M1V:H17	9:C:201:M1V:H20	0.97	0.94
5:J:97:LEU:HD11	5:J:153:ILE:HG23	1.55	0.88
1:Q:101:LEU:HD23	1:Q:152:LEU:HD23	1.55	0.88
3:C:106:LEU:HD22	3:C:156:GLU:HG3	1.55	0.87
1:O:14:GLU:HB2	1:O:16:ARG:HE	1.41	0.85
5:J:40:VAL:HG21	5:J:152:PHE:CZ	2.15	0.81
3:C:102:ARG:HA	3:C:106:LEU:HB2	1.64	0.78
1:A:39:ILE:HD11	1:A:142:ASP:HB3	1.68	0.75
9:C:201:M1V:H9	9:C:201:M1V:H8	1.69	0.74
1:E:149:TYR:HA	1:E:152:LEU:HD23	1.69	0.74
6:K:195:LEU:HD21	9:K:801:M1V:CHC	2.18	0.74
4:I:4:ILE:HD12	4:I:26:ILE:HG22	1.69	0.73
6:K:234:ARG:NH2	10:K:802:CL:CL	2.53	0.73
2:D:56:VAL:HG11	1:E:115:ASN:HD21	1.52	0.73
2:P:66:THR:HA	2:P:72:MET:HB2	1.71	0.73
2:D:1:MET:SD	2:D:107:ARG:NH2	2.62	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:LEU:HD21	1:G:153:ILE:HD11	1.72	0.72
4:I:110:ARG:HD3	4:I:159:PRO:HG2	1.70	0.71
1:E:61:ARG:HH11	1:E:125:GLU:CD	1.97	0.71
1:Q:55:SER:OG	1:Q:79:GLN:NE2	2.24	0.71
1:E:30:VAL:HA	2:F:31:PHE:CE2	2.26	0.71
5:J:132:GLN:HG3	2:R:15:GLN:HE22	1.56	0.71
2:F:51:ILE:O	2:F:55:THR:HG23	1.90	0.70
6:K:543:GLU:OE2	6:K:572:LYS:NZ	2.25	0.70
1:O:7:LEU:HD22	1:O:22:GLU:HB3	1.73	0.70
1:M:89:ILE:O	1:M:93:ILE:HG12	1.92	0.70
6:K:664:THR:HG21	6:K:666:ARG:HH21	1.56	0.70
1:E:139:SER:OG	1:E:142:ASP:OD2	2.10	0.69
2:H:21:ASP:HA	2:H:24:LEU:HD12	1.75	0.68
1:G:30:VAL:HG21	2:H:34:GLY:HA3	1.75	0.68
6:K:551:ARG:NH2	1:M:13:SER:O	2.27	0.68
2:B:74:THR:HG22	3:C:104:ILE:HG23	1.77	0.67
1:M:3:LEU:HD11	1:M:29:PHE:HB2	1.76	0.67
1:Q:127:MET:HE1	1:Q:130:LEU:HD12	1.77	0.67
1:E:46:ASN:O	1:E:50:ILE:HG12	1.95	0.67
6:K:253:ARG:HG2	6:K:253:ARG:HH11	1.57	0.66
1:M:73:ARG:HH12	1:M:74:LYS:HZ2	1.41	0.66
4:I:82:GLN:OE1	4:I:130:LEU:HD21	1.96	0.66
8:I:201:CYC:HC	8:I:201:CYC:HMD1	1.60	0.66
2:P:73:TYR:OH	1:Q:87:ARG:NH2	2.30	0.65
4:I:95:VAL:HG12	4:I:97:ASP:H	1.62	0.65
2:N:133:MET:O	2:N:137:VAL:HG12	1.96	0.65
2:B:96:MET:HG3	2:B:149:VAL:HG22	1.78	0.65
2:P:51:ILE:O	2:P:55:THR:OG1	2.15	0.65
2:R:96:MET:HE2	2:R:149:VAL:HG22	1.79	0.65
2:B:137:VAL:O	2:B:141:LEU:HB2	1.96	0.65
6:K:304:ARG:HH22	6:K:309:LEU:HD22	1.62	0.64
6:K:333:ARG:NH1	7:S:35:ASN:OD1	2.30	0.64
3:C:160:PRO:HD3	6:K:247:LYS:HD3	1.78	0.64
3:C:133:GLU:O	3:C:137:LEU:HB2	1.97	0.64
1:O:149:TYR:O	1:O:153:ILE:HG13	1.98	0.64
2:L:60:LEU:HB3	2:L:72:MET:HE1	1.80	0.64
2:B:134:LYS:HE2	2:B:154:ASP:OD1	1.98	0.63
3:C:104:ILE:HG21	2:D:13:ASP:OD1	1.97	0.63
6:K:58:GLN:HG3	2:L:24:LEU:HD22	1.79	0.63
1:A:146:VAL:HG12	1:A:150:PHE:CE1	2.34	0.63
2:D:19:LEU:HD23	2:D:23:SER:HB3	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:TYR:OH	1:E:87:ARG:NH2	2.31	0.63
6:K:281:MET:HB2	6:K:293:VAL:HG11	1.81	0.63
1:A:110:LYS:O	1:A:114:ASN:ND2	2.29	0.63
6:K:40:MET:HE3	6:K:40:MET:HA	1.80	0.63
1:M:2:SER:OG	2:N:3:ASP:OD2	2.14	0.63
6:K:268:SER:O	6:K:272:SER:OG	2.17	0.63
1:M:27:GLN:O	1:M:31:LYS:HG3	1.99	0.63
2:R:60:LEU:HB3	2:R:72:MET:HE1	1.80	0.63
1:M:73:ARG:HH12	1:M:74:LYS:NZ	1.97	0.62
1:E:30:VAL:HA	2:F:31:PHE:CD2	2.34	0.62
9:K:801:M1V:H20	9:K:801:M1V:CBB	2.22	0.62
4:I:44:ASN:HD21	5:J:19:LEU:HB2	1.64	0.62
2:L:137:VAL:O	2:L:141:LEU:HB2	1.99	0.62
1:M:109:ILE:HD11	1:M:113:TYR:CE2	2.35	0.62
1:O:5:THR:OG1	2:P:1:MET:HG3	2.00	0.62
1:M:87:ARG:NH2	2:N:13:ASP:OD1	2.33	0.62
1:Q:2:SER:HA	1:Q:95:ALA:HB1	1.82	0.62
4:I:116:LEU:HD22	8:I:201:CYC:HBD1	1.82	0.61
5:J:65:GLU:HA	5:J:68:ARG:HG3	1.82	0.61
1:A:4:VAL:HG13	1:A:26:PHE:CE2	2.35	0.61
3:C:123:ILE:O	3:C:127:LEU:HD12	2.01	0.61
3:C:50:ILE:HD11	3:C:138:LEU:HD21	1.83	0.61
6:K:67:ILE:HA	6:K:217:LYS:HD3	1.82	0.61
6:K:363:LEU:O	6:K:411:ARG:NH1	2.33	0.61
5:J:115:GLU:OE2	6:K:6:ASN:ND2	2.34	0.61
6:K:370:MET:HE1	6:K:443:VAL:HG23	1.82	0.61
9:K:801:M1V:H17	9:K:801:M1V:CHB	2.21	0.61
1:O:93:ILE:HD13	1:O:149:TYR:HE2	1.65	0.61
2:H:33:SER:OG	2:H:37:ARG:NH1	2.34	0.60
2:B:109:LEU:HG	2:B:159:GLY:HA3	1.83	0.60
1:A:101:LEU:HD11	1:A:153:ILE:HD11	1.83	0.60
1:G:112:MET:HE1	8:G:201:CYC:CHB	2.30	0.60
2:L:38:ALA:C	2:L:42:MET:HE3	2.26	0.60
1:O:10:SER:O	1:O:16:ARG:NH2	2.34	0.60
1:M:3:LEU:HD21	1:M:29:PHE:CD2	2.37	0.60
2:N:50:THR:HG22	2:N:54:LYS:NZ	2.17	0.60
1:G:14:GLU:HB2	1:G:16:ARG:HD3	1.83	0.60
1:Q:82:GLN:HB3	1:Q:130:LEU:HD11	1.84	0.60
1:O:61:ARG:NH2	1:O:129:CYS:SG	2.74	0.60
2:H:24:LEU:O	2:H:28:GLN:HG2	2.01	0.60
6:K:679:ILE:HA	2:R:71:MEN:HD2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:1:MET:HE1	7:S:33:TYR:N	2.17	0.60
2:L:76:ARG:NH2	8:L:201:CYC:O2D	2.34	0.60
1:A:91:TYR:OH	2:B:17:LYS:O	2.18	0.59
4:I:158:MET:N	4:I:159:PRO:HD2	2.17	0.59
1:M:49:ARG:HH12	1:M:50:ILE:HG13	1.68	0.59
1:O:57:LYS:HA	1:O:60:GLU:HG2	1.84	0.59
1:A:57:LYS:HZ1	1:A:61:ARG:HE	1.50	0.59
2:B:63:THR:HG23	2:B:65:ILE:HG22	1.85	0.59
2:L:36:LEU:HD22	2:L:144:GLU:OE1	2.03	0.59
6:K:265:PHE:HB2	6:K:417:ALA:HB2	1.84	0.59
5:J:84:ARG:HD3	6:K:266:PRO:HD3	1.85	0.59
5:J:123:PRO:HB2	5:J:126:PRO:HD2	1.85	0.59
1:A:127:MET:CE	1:A:154:ILE:HG12	2.32	0.59
4:I:127:MET:HG3	4:I:153:LEU:HD12	1.85	0.59
1:Q:87:ARG:NH2	2:R:13:ASP:OD1	2.35	0.59
2:P:3:ASP:HB3	2:P:98:ALA:HB1	1.84	0.59
1:O:11:ALA:HA	1:O:16:ARG:NH1	2.18	0.58
1:Q:27:GLN:HE21	2:R:38:ALA:HB3	1.68	0.58
3:C:55:THR:HG21	3:C:79:GLN:HE22	1.67	0.58
9:K:801:M1V:H10	9:K:801:M1V:H27	1.68	0.58
1:A:149:TYR:HA	1:A:152:LEU:HD23	1.86	0.58
4:I:4:ILE:HD12	4:I:26:ILE:CG2	2.33	0.58
3:C:20:PRO:HG3	2:D:42:MET:HE2	1.86	0.58
7:S:27:PHE:CD1	7:S:29:LYS:HE3	2.39	0.58
5:J:15:THR:HG21	5:J:17:ARG:NH1	2.19	0.58
1:A:129:CYS:O	1:A:133:GLU:HG2	2.04	0.57
2:B:65:ILE:HG23	2:B:72:MET:HE1	1.86	0.57
1:M:120:ILE:HG23	1:M:157:LEU:HD12	1.86	0.57
2:P:89:LEU:HD13	2:P:133:MET:HE3	1.86	0.57
2:D:144:GLU:H	2:D:144:GLU:CD	2.11	0.57
2:D:108:VAL:O	2:D:112:LEU:HB2	2.04	0.57
2:P:7:THR:O	2:P:11:THR:HG23	2.04	0.57
2:H:8:LEU:HD22	2:H:27:LEU:HD13	1.87	0.57
4:I:158:MET:N	4:I:159:PRO:CD	2.68	0.57
6:K:51:LEU:HA	2:L:32:ARG:HH22	1.70	0.57
4:I:23:LEU:HD23	4:I:26:ILE:HD11	1.85	0.56
6:K:4:ARG:NH1	6:K:449:TYR:OH	2.37	0.56
6:K:688:THR:HG22	6:K:691:GLU:HG2	1.85	0.56
1:A:39:ILE:HG21	1:A:93:ILE:HG12	1.87	0.56
4:I:157:LEU:C	4:I:159:PRO:HD2	2.30	0.56
6:K:32:ASP:OD1	2:L:90:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:152:ILE:HG21	6:K:157:TYR:CD1	2.40	0.56
1:E:62:CYS:HA	6:K:694:MET:HE3	1.87	0.56
1:E:151:ASP:HB2	2:H:42:MET:HE1	1.87	0.56
1:A:120:ILE:HG23	1:A:157:LEU:HD12	1.86	0.56
2:F:85:MET:HG3	2:F:133:MET:HE1	1.87	0.56
1:Q:127:MET:HA	1:Q:127:MET:HE2	1.87	0.56
2:B:89:LEU:HD12	2:B:133:MET:HE2	1.88	0.56
1:E:19:ALA:HB1	1:E:20:PRO:HD2	1.87	0.56
2:L:119:LEU:HD13	8:L:201:CYC:HBD1	1.88	0.56
2:N:61:LEU:HD22	8:O:201:CYC:HAA1	1.88	0.56
1:G:23:LEU:O	1:G:27:GLN:HG2	2.06	0.55
6:K:366:GLY:H	6:K:426:GLN:HE21	1.54	0.55
6:K:467:GLU:HB3	6:K:671:ARG:HH12	1.71	0.55
1:A:57:LYS:HE2	1:A:61:ARG:HB2	1.87	0.55
2:N:109:LEU:HD13	2:N:159:GLY:HA3	1.88	0.55
5:J:132:GLN:HG3	2:R:15:GLN:NE2	2.22	0.55
6:K:692:TYR:O	6:K:695:ARG:HA	2.07	0.55
1:E:23:LEU:HD23	2:F:42:MET:HE3	1.87	0.55
1:O:135:MET:HE1	1:O:147:ALA:HB2	1.88	0.55
1:A:89:ILE:HG23	1:A:149:TYR:HB2	1.88	0.55
1:M:6:GLU:OE1	1:M:99:ARG:HG3	2.07	0.55
1:A:74:LYS:HG2	8:A:201:CYC:HAD1	1.88	0.55
2:B:89:LEU:HB2	2:B:133:MET:HE1	1.89	0.55
4:I:88:LEU:HD11	8:I:201:CYC:HBB1	1.88	0.55
2:P:123:VAL:O	2:P:127:ILE:HD12	2.06	0.55
6:K:570:GLN:HA	6:K:575:LEU:HD12	1.88	0.55
2:N:77:ARG:HG2	8:N:201:CYC:HAD1	1.88	0.55
5:J:2:ARG:HG2	5:J:103:ASP:OD2	2.06	0.55
3:C:25:MET:HG3	4:I:3:VAL:HG21	1.88	0.55
2:F:126:THR:O	2:F:130:VAL:HG23	2.06	0.55
2:L:20:ASP:O	2:L:24:LEU:HD12	2.07	0.55
1:E:20:PRO:HG3	1:G:148:ALA:HB1	1.89	0.54
6:K:192:THR:HA	6:K:195:LEU:HD12	1.89	0.54
6:K:281:MET:HE3	6:K:321:LEU:HD11	1.89	0.54
2:H:74:THR:O	2:H:74:THR:OG1	2.24	0.54
5:J:126:PRO:HB2	8:J:201:CYC:HMC2	1.88	0.54
2:D:60:LEU:HB3	2:D:72:MET:HE1	1.89	0.54
2:B:44:ILE:HD11	2:B:137:VAL:HG13	1.87	0.54
1:O:131:LYS:HD2	1:O:150:PHE:HB3	1.88	0.54
1:A:99:ARG:NH2	6:K:289:GLU:OE2	2.40	0.54
6:K:27:GLY:CA	6:K:31:ARG:HH21	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:493:ARG:HG2	6:K:618:TYR:HB3	1.89	0.54
6:K:509:SER:HA	6:K:512:ILE:HG13	1.90	0.54
6:K:694:MET:HA	6:K:694:MET:CE	2.30	0.54
2:L:3:ASP:OD2	2:L:5:ILE:HG13	2.08	0.54
1:Q:34:GLU:OE2	1:Q:34:GLU:N	2.30	0.54
1:A:59:TRP:CE3	1:A:68:ASN:HB3	2.43	0.54
2:B:79:ALA:HA	2:B:82:ILE:HD12	1.89	0.54
1:G:112:MET:HG3	1:G:113:TYR:N	2.22	0.54
2:H:161:SER:OG	6:K:669:ALA:O	2.25	0.54
1:A:22:GLU:HA	1:A:25:ILE:HD12	1.90	0.54
1:A:147:ALA:HA	1:A:150:PHE:HD1	1.72	0.53
2:D:79:ALA:HB1	1:E:111:GLU:HG3	1.90	0.53
5:J:40:VAL:HG21	5:J:152:PHE:HZ	1.72	0.53
6:K:278:ARG:HH21	7:S:23:GLN:HB3	1.72	0.53
1:O:29:PHE:CE1	1:O:96:GLY:HA3	2.43	0.53
2:P:85:MET:HE3	8:P:201:CYC:HBC3	1.90	0.53
1:A:135:MET:HE1	1:A:147:ALA:HB2	1.90	0.53
1:G:123:ILE:HD13	8:G:201:CYC:H3C	1.89	0.53
1:M:51:VAL:O	1:M:55:SER:OG	2.26	0.53
1:G:58:PHE:HD1	1:G:125:GLU:OE1	1.91	0.53
6:K:552:GLN:HG2	6:K:658:PRO:HB2	1.90	0.53
2:L:90:ARG:NH1	2:L:94:TYR:OH	2.37	0.53
2:N:74:THR:HG22	1:O:104:ILE:HG23	1.91	0.53
3:C:155:GLN:NE2	5:J:46:ALA:O	2.42	0.53
5:J:40:VAL:CG2	5:J:152:PHE:CZ	2.89	0.53
6:K:596:TRP:O	2:P:107:ARG:NH1	2.41	0.53
2:P:8:LEU:HD22	2:P:23:SER:HB2	1.90	0.53
2:D:112:LEU:HD23	2:D:160:LEU:HD21	1.90	0.53
4:I:84:TRP:CD1	4:I:87:ARG:HH21	2.26	0.53
3:C:120:LEU:HB2	6:K:247:LYS:HE2	1.90	0.53
6:K:432:TYR:OH	2:L:108:VAL:O	2.23	0.53
1:A:53:ASN:HB3	1:A:133:GLU:OE2	2.08	0.53
8:E:201:CYC:HMA3	8:E:201:CYC:HB	1.74	0.53
2:H:55:THR:HG21	2:H:85:MET:HE1	1.90	0.53
2:L:137:VAL:HG11	2:L:149:VAL:HG11	1.90	0.53
6:K:365:ARG:NH1	6:K:366:GLY:O	2.40	0.53
2:P:108:VAL:HG13	8:P:201:CYC:HBB2	1.91	0.53
1:A:141:GLU:O	1:A:145:GLU:HG2	2.08	0.53
1:E:30:VAL:HA	2:F:31:PHE:HE2	1.74	0.53
2:B:83:ARG:HD3	7:S:22:LEU:HD22	1.91	0.53
1:G:16:ARG:O	2:H:94:TYR:OH	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:ASP:OD1	2:D:90:ARG:NH2	2.42	0.52
6:K:195:LEU:CD2	9:K:801:M1V:H31	2.39	0.52
1:Q:26:PHE:O	1:Q:30:VAL:HG12	2.09	0.52
7:S:1:MET:HE1	7:S:33:TYR:H	1.73	0.52
2:D:109:LEU:HD13	2:D:159:GLY:HA3	1.89	0.52
1:E:63:PRO:HA	1:E:68:ASN:HD21	1.74	0.52
6:K:157:TYR:CD2	6:K:162:MET:HE2	2.44	0.52
2:B:20:ASP:OD1	2:B:20:ASP:N	2.38	0.52
2:H:77:ARG:HG2	8:H:201:CYC:HAD1	1.91	0.52
2:N:78:TYR:OH	1:O:115:ASN:ND2	2.43	0.52
3:C:148:PRO:HG2	4:I:20:LYS:HE3	1.92	0.52
6:K:167:ARG:NH1	9:K:801:M1V:O1C	2.41	0.52
6:K:497:VAL:HG11	6:K:668:LEU:HD22	1.91	0.52
2:L:8:LEU:HD11	2:L:23:SER:HB3	1.91	0.52
2:P:106:GLU:HG2	2:P:107:ARG:HG2	1.92	0.52
2:B:71:MEN:HE22	8:B:201:CYC:HBD2	1.92	0.52
6:K:54:LEU:HD12	6:K:181:VAL:HG22	1.91	0.52
3:C:158:VAL:C	3:C:160:PRO:HD2	2.35	0.52
6:K:27:GLY:HA2	6:K:31:ARG:HH21	1.75	0.52
6:K:497:VAL:HG13	8:R:201:CYC:HAA1	1.92	0.52
1:E:145:GLU:OE1	1:G:24:ARG:NH1	2.43	0.52
1:A:46:ASN:O	1:A:50:ILE:HG13	2.10	0.51
1:G:7:LEU:HG	1:G:22:GLU:HB3	1.91	0.51
6:K:36:ASN:OD1	6:K:36:ASN:N	2.41	0.51
6:K:328:MET:HB2	6:K:405:GLU:HA	1.91	0.51
2:D:104:LEU:HD22	2:D:156:ILE:HD11	1.91	0.51
1:E:14:GLU:OE2	1:G:99:ARG:NH2	2.42	0.51
5:J:125:ALA:HB2	2:P:69:GLY:HA3	1.91	0.51
7:S:1:MET:HA	7:S:67:ALA:HA	1.91	0.51
6:K:195:LEU:HD21	9:K:801:M1V:H31	1.92	0.51
1:M:3:LEU:HD23	1:M:4:VAL:N	2.26	0.51
1:A:135:MET:HE2	1:A:143:ALA:HB1	1.91	0.51
6:K:248:PRO:HB2	6:K:267:GLU:HG2	1.91	0.51
1:O:23:LEU:O	1:O:27:GLN:HG2	2.11	0.51
2:F:127:ILE:O	2:F:131:GLN:HG2	2.11	0.51
5:J:12:TYR:CE2	5:J:23:ALA:HB2	2.45	0.51
2:F:55:THR:HG21	2:F:133:MET:HG3	1.93	0.51
2:F:111:GLY:O	2:F:115:THR:OG1	2.26	0.51
2:P:144:GLU:HA	2:P:147:LYS:HE3	1.93	0.51
5:J:152:PHE:H	5:J:152:PHE:HD2	1.59	0.51
2:N:24:LEU:O	2:N:28:GLN:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:87:ARG:NH1	2:R:16:GLY:O	2.44	0.51
2:L:77:ARG:HG2	8:L:201:CYC:HAD1	1.93	0.51
2:N:81:CYS:O	2:N:85:MET:HG2	2.11	0.50
1:M:73:ARG:CZ	1:M:74:LYS:HD2	2.42	0.50
1:O:57:LYS:O	1:O:60:GLU:HG2	2.10	0.50
2:B:29:GLU:O	2:B:33:SER:OG	2.29	0.50
5:J:149:ASP:O	5:J:152:PHE:HE2	1.95	0.50
2:N:83:ARG:NH1	8:N:201:CYC:O1A	2.44	0.50
1:G:107:VAL:HB	2:L:76:ARG:HB3	1.92	0.50
6:K:49:THR:O	6:K:53:ARG:HG3	2.11	0.50
6:K:395:SER:O	7:S:42:ARG:NH1	2.45	0.50
1:Q:27:GLN:HE21	2:R:38:ALA:CB	2.24	0.50
5:J:149:ASP:O	5:J:152:PHE:CE2	2.64	0.50
1:O:57:LYS:HD3	1:O:133:GLU:OE1	2.11	0.50
1:Q:101:LEU:HD11	1:Q:153:ILE:HD11	1.94	0.50
1:A:63:PRO:HA	1:A:68:ASN:HD21	1.76	0.50
4:I:138:LEU:HD13	4:I:142:ASP:HB3	1.93	0.50
9:C:201:M1V:H8	9:C:201:M1V:CHA	2.41	0.50
2:D:73:TYR:HH	1:E:87:ARG:NH2	2.10	0.50
4:I:39:ILE:HA	4:I:42:ILE:HD12	1.93	0.50
2:L:77:ARG:HG2	8:L:201:CYC:HMD1	1.94	0.50
2:P:85:MET:HG2	8:P:201:CYC:HBC1	1.93	0.50
1:G:37:VAL:HG11	2:H:28:GLN:NE2	2.27	0.50
1:G:85:TYR:HB3	1:G:127:MET:HE1	1.93	0.50
5:J:109:VAL:HG12	5:J:110:LEU:HD13	1.93	0.50
6:K:188:ILE:O	6:K:192:THR:HB	2.11	0.50
1:Q:78:CYS:O	1:Q:82:GLN:HG3	2.12	0.50
1:E:108:GLY:HA2	1:E:111:GLU:OE2	2.12	0.49
5:J:84:ARG:NH1	8:J:201:CYC:O2A	2.44	0.49
2:R:15:GLN:HB2	2:R:17:LYS:HG2	1.93	0.49
2:D:46:ALA:HB2	4:I:151:ASP:HB3	1.95	0.49
1:G:106:THR:HA	1:G:109:ILE:HB	1.94	0.49
6:K:43:LEU:HD13	2:L:97:LEU:HD22	1.94	0.49
2:L:55:THR:O	2:L:59:SER:OG	2.27	0.49
1:E:100:PRO:HA	7:S:64:THR:HG21	1.95	0.49
1:E:138:LEU:HB3	1:E:142:ASP:HB2	1.94	0.49
6:K:478:THR:HB	2:L:114:GLU:HA	1.95	0.49
6:K:496:LEU:HD13	6:K:616:PRO:HD2	1.95	0.49
1:M:27:GLN:HA	1:M:30:VAL:HG12	1.94	0.49
1:E:72:ASP:OD1	1:E:72:ASP:N	2.40	0.49
2:F:119:LEU:HB2	2:F:121:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:422:ASN:HB3	6:K:446:PHE:HZ	1.78	0.49
6:K:596:TRP:CE2	6:K:635:PHE:HB2	2.47	0.49
1:A:14:GLU:HG3	1:A:16:ARG:HG2	1.94	0.49
2:H:4:ALA:O	2:H:8:LEU:HB2	2.13	0.49
2:L:20:ASP:C	2:L:24:LEU:HD12	2.37	0.49
1:A:6:GLU:HA	1:A:9:LEU:HD12	1.94	0.49
5:J:92:TYR:HE1	5:J:108:ARG:HD3	1.78	0.49
6:K:600:TYR:HD2	6:K:603:LYS:HG3	1.78	0.49
2:R:96:MET:HE2	2:R:149:VAL:CG2	2.41	0.49
3:C:21:GLY:HA3	4:I:97:ASP:OD2	2.13	0.49
1:E:125:GLU:OE2	1:E:125:GLU:HA	2.13	0.49
1:Q:19:ALA:HB3	1:Q:22:GLU:OE2	2.13	0.49
1:A:59:TRP:CZ3	1:A:68:ASN:HB3	2.48	0.49
2:D:1:MET:HA	2:D:106:GLU:OE2	2.11	0.49
1:M:28:ASP:HA	1:M:31:LYS:NZ	2.27	0.49
1:Q:73:ARG:HH21	1:Q:74:LYS:HZ3	1.61	0.49
2:B:85:MET:HG2	8:B:201:CYC:HBC1	1.95	0.49
1:O:53:ASN:O	1:O:57:LYS:HG2	2.13	0.49
8:H:201:CYC:HB	8:H:201:CYC:HMA3	1.78	0.49
4:I:110:ARG:CD	4:I:159:PRO:HG2	2.41	0.49
6:K:224:VAL:HG22	6:K:229:ALA:HB1	1.95	0.49
2:R:24:LEU:O	2:R:28:GLN:HG2	2.13	0.49
1:A:112:MET:HG3	2:F:78:TYR:CG	2.48	0.48
2:B:89:LEU:HB2	2:B:133:MET:CE	2.43	0.48
2:H:107:ARG:NH1	6:K:347:GLU:O	2.36	0.48
1:G:28:ASP:HA	1:G:31:LYS:HE2	1.95	0.48
1:M:30:VAL:HG21	2:N:34:GLY:HA3	1.95	0.48
1:A:16:ARG:O	2:B:94:TYR:OH	2.25	0.48
1:E:65:THR:OG1	1:E:68:ASN:OD1	2.30	0.48
2:F:71:MEN:HE22	8:F:201:CYC:HBD2	1.94	0.48
6:K:694:MET:HA	6:K:694:MET:HE2	1.96	0.48
4:I:3:VAL:HG23	4:I:6:GLN:HE21	1.79	0.48
2:D:74:THR:O	2:D:74:THR:OG1	2.30	0.48
2:L:28:GLN:NE2	2:L:32:ARG:HH21	2.11	0.48
6:K:29:HIS:NE2	2:L:107:ARG:HD2	2.29	0.48
3:C:12:ASP:OD2	2:D:107:ARG:NH1	2.42	0.48
2:N:1:MET:HE3	2:N:1:MET:HB2	1.80	0.48
1:O:2:SER:O	1:O:5:THR:HG22	2.13	0.48
1:O:29:PHE:HE1	1:O:96:GLY:HA3	1.78	0.48
1:O:47:GLU:HG3	2:P:18:TYR:OH	2.13	0.48
2:H:110:ASN:ND2	6:K:438:LYS:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:615:ARG:NH2	6:K:647:ASP:OD2	2.43	0.48
1:M:3:LEU:HD23	1:M:4:VAL:H	1.79	0.48
1:M:27:GLN:HE22	2:N:38:ALA:HB3	1.79	0.48
3:C:110:LYS:HD2	3:C:120:LEU:HD13	1.96	0.47
4:I:40:VAL:HG21	4:I:94:ALA:HB2	1.96	0.47
6:K:328:MET:HE3	6:K:328:MET:O	2.14	0.47
1:O:43:LEU:HD21	1:O:138:LEU:HD11	1.96	0.47
2:R:117:ASN:N	2:R:117:ASN:HD22	2.12	0.47
2:B:96:MET:HE3	2:B:96:MET:HB3	1.74	0.47
3:C:26:ILE:HD12	2:D:97:LEU:HD11	1.95	0.47
6:K:598:ASN:HA	2:P:106:GLU:OE2	2.13	0.47
2:R:56:VAL:HG22	2:R:60:LEU:HD12	1.95	0.47
3:C:158:VAL:O	3:C:160:PRO:HD2	2.14	0.47
1:G:128:ARG:HG3	1:G:154:ILE:HD12	1.95	0.47
7:S:7:THR:HB	7:S:52:LYS:HB3	1.96	0.47
2:B:61:LEU:HD21	3:C:116:ILE:HD13	1.97	0.47
3:C:129:CYS:O	3:C:133:GLU:HG2	2.14	0.47
2:D:102:SER:O	2:D:106:GLU:HG3	2.14	0.47
1:E:95:ALA:HA	2:F:5:ILE:HG21	1.96	0.47
5:J:152:PHE:CD2	5:J:153:ILE:HG13	2.49	0.47
2:L:54:LYS:HG2	2:L:58:LYS:HE3	1.97	0.47
1:A:152:LEU:O	1:A:155:GLN:HG2	2.15	0.47
2:D:108:VAL:HA	8:D:201:CYC:HBB3	1.96	0.47
1:G:85:TYR:CB	1:G:127:MET:HE1	2.45	0.47
4:I:100:PRO:HG3	5:J:9:ILE:HG21	1.97	0.47
6:K:164:ARG:HD3	9:K:801:M1V:H16	1.95	0.47
2:L:33:SER:O	2:L:36:LEU:HG	2.15	0.47
2:L:39:LYS:O	2:L:43:THR:HG22	2.15	0.47
1:M:80:ARG:HH12	8:M:201:CYC:HBA2	1.79	0.47
7:S:2:ARG:HD3	7:S:66:LEU:HB2	1.96	0.47
3:C:53:ARG:HG3	3:C:56:ARG:HH21	1.78	0.47
4:I:101:LEU:O	4:I:106:VAL:HG23	2.14	0.47
2:L:28:GLN:NE2	2:L:32:ARG:HE	2.12	0.47
2:L:108:VAL:HB	2:L:109:LEU:HD22	1.97	0.47
7:S:39:GLU:O	7:S:43:ILE:HG23	2.14	0.47
6:K:622:GLU:HB3	6:K:626:TYR:CE2	2.49	0.47
2:N:116:TYR:HE2	2:N:126:THR:HG21	1.78	0.47
1:G:21:LYS:O	1:G:25:ILE:HG12	2.14	0.47
2:H:41:ALA:HB2	2:H:96:MET:HE1	1.96	0.47
4:I:63:PRO:HA	4:I:68:ASN:HD22	1.78	0.47
1:O:116:LEU:HB3	1:O:118:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:VAL:HG22	2:H:31:PHE:HA	1.96	0.47
6:K:321:LEU:HD22	6:K:331:PHE:CG	2.49	0.47
2:L:25:ASP:O	2:L:29:GLU:OE2	2.31	0.47
2:L:38:ALA:O	2:L:42:MET:HE3	2.15	0.47
1:O:46:ASN:O	1:O:50:ILE:HG13	2.15	0.47
2:P:54:LYS:O	2:P:58:LYS:HG2	2.15	0.46
2:B:115:THR:O	2:B:119:LEU:HD12	2.16	0.46
2:D:3:ASP:OD1	2:D:6:THR:OG1	2.28	0.46
2:F:47:ASN:HB2	2:F:140:MET:HE1	1.97	0.46
6:K:504:SER:O	6:K:508:ILE:HG12	2.14	0.46
1:Q:46:ASN:HB2	1:Q:49:ARG:CG	2.45	0.46
8:Q:201:CYC:HMA1	8:Q:201:CYC:HB	1.80	0.46
1:G:118:ILE:HG21	1:G:123:ILE:HD11	1.96	0.46
2:H:108:VAL:HG12	2:H:109:LEU:HD12	1.97	0.46
5:J:74:TYR:HH	6:K:174:ARG:HH22	1.57	0.46
2:L:119:LEU:HD11	8:L:201:CYC:HAA2	1.98	0.46
2:D:76:ARG:NH2	7:S:66:LEU:HD21	2.30	0.46
6:K:620:ARG:O	6:K:624:SER:CB	2.63	0.46
3:C:53:ARG:HH11	3:C:53:ARG:HB2	1.80	0.46
2:F:109:LEU:HD13	2:F:159:GLY:HA3	1.97	0.46
1:O:2:SER:HA	1:O:95:ALA:HB1	1.98	0.46
1:O:84:TRP:CD1	1:O:87:ARG:HH21	2.33	0.46
1:Q:80:ARG:NH2	8:Q:201:CYC:O1A	2.49	0.46
1:Q:82:GLN:NE2	1:Q:126:CYS:SG	2.89	0.46
2:F:43:THR:HB	2:F:141:LEU:HD21	1.95	0.46
4:I:16:ARG:NH1	4:I:22:GLU:OE1	2.47	0.46
8:P:201:CYC:HB	8:P:201:CYC:HMA3	1.80	0.46
1:E:129:CYS:O	1:E:133:GLU:HG2	2.16	0.46
6:K:336:GLY:HA3	6:K:389:VAL:HG11	1.97	0.46
1:Q:80:ARG:HG2	1:Q:80:ARG:HH11	1.81	0.46
1:Q:84:TRP:O	1:Q:88:LEU:HG	2.15	0.46
1:A:65:THR:OG1	1:A:68:ASN:OD1	2.32	0.46
2:F:65:ILE:HD11	2:F:122:PRO:HG3	1.97	0.46
1:G:54:GLY:HA3	1:G:130:LEU:HD22	1.97	0.46
5:J:2:ARG:N	5:J:103:ASP:OD2	2.49	0.46
5:J:152:PHE:CE2	5:J:153:ILE:HG13	2.51	0.46
2:L:2:GLN:NE2	2:L:7:THR:HB	2.30	0.46
2:L:58:LYS:HB3	2:L:58:LYS:HE2	1.60	0.46
1:M:71:VAL:HG21	1:M:74:LYS:HD3	1.98	0.46
1:Q:18:PRO:HD3	2:R:94:TYR:HE1	1.80	0.46
2:R:33:SER:O	2:R:37:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:MET:HE3	2:D:103:ILE:HD13	1.96	0.46
4:I:128:ARG:HD3	4:I:154:ILE:HD13	1.98	0.46
5:J:77:ARG:HH21	5:J:78:ARG:HD3	1.81	0.46
2:L:15:GLN:HG3	2:L:17:LYS:HE3	1.97	0.46
2:L:78:TYR:O	2:L:82:ILE:HG12	2.16	0.46
6:K:459:TYR:OH	8:P:201:CYC:O2A	2.25	0.46
1:E:27:GLN:OE1	1:E:31:LYS:NZ	2.47	0.45
6:K:620:ARG:O	6:K:624:SER:HB3	2.16	0.45
6:K:333:ARG:HH21	7:S:32:PRO:HG2	1.80	0.45
2:L:28:GLN:HE21	2:L:32:ARG:HE	1.64	0.45
2:L:116:TYR:HE2	2:L:126:THR:HG21	1.81	0.45
1:M:16:ARG:HH12	1:M:19:ALA:HB2	1.82	0.45
1:G:104:ILE:HG23	2:L:74:THR:HG22	1.98	0.45
4:I:158:MET:O	4:I:158:MET:SD	2.74	0.45
6:K:664:THR:HG21	6:K:666:ARG:NH2	2.27	0.45
1:M:112:MET:HE1	8:M:201:CYC:NB	2.31	0.45
1:Q:34:GLU:H	1:Q:34:GLU:CD	2.21	0.45
2:F:84:ASP:OD1	8:F:201:CYC:ND	2.47	0.45
6:K:678:ALA:HB3	2:R:77:ARG:HH12	1.82	0.45
1:A:4:VAL:HG13	1:A:26:PHE:HE2	1.78	0.45
4:I:110:ARG:HG2	4:I:120:LEU:HD13	1.98	0.45
6:K:255:GLY:HA2	6:K:260:ASP:OD1	2.17	0.45
6:K:546:ILE:HG23	6:K:581:PHE:CZ	2.52	0.45
2:R:128:ARG:HA	2:R:131:GLN:HE21	1.82	0.45
2:F:137:VAL:HG13	2:F:141:LEU:HD12	1.97	0.45
4:I:141:GLU:O	4:I:145:GLU:HG2	2.17	0.45
6:K:507:GLU:HG3	1:M:99:ARG:CZ	2.45	0.45
2:R:140:MET:O	2:R:141:LEU:HD23	2.17	0.45
3:C:63:PRO:HA	3:C:68:ASN:HD22	1.81	0.45
2:D:79:ALA:CB	1:E:111:GLU:HG3	2.47	0.45
2:F:50:THR:HG22	2:F:54:LYS:HZ2	1.82	0.45
5:J:15:THR:HG21	5:J:17:ARG:CZ	2.46	0.45
6:K:663:VAL:HG21	6:K:668:LEU:HD13	1.99	0.45
2:B:28:GLN:HB3	2:B:32:ARG:HH11	1.81	0.45
2:H:91:TYR:CZ	2:H:107:ARG:HG2	2.52	0.45
6:K:472:ALA:HB1	6:K:474:PHE:HE1	1.81	0.45
2:L:8:LEU:HD21	2:L:23:SER:HB3	1.99	0.45
2:N:73:TYR:OH	1:O:87:ARG:NH2	2.40	0.45
1:O:57:LYS:HB2	1:O:57:LYS:HE3	1.84	0.45
2:R:137:VAL:O	2:R:141:LEU:HB2	2.17	0.45
1:E:121:ARG:NH1	4:I:117:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:40:VAL:CG2	5:J:152:PHE:HZ	2.27	0.45
1:O:57:LYS:HA	1:O:60:GLU:CG	2.47	0.45
2:R:57:ALA:HA	2:R:61:LEU:HD12	1.99	0.45
2:R:77:ARG:HG2	8:R:201:CYC:HAD1	1.98	0.45
7:S:35:ASN:O	7:S:39:GLU:HG2	2.17	0.45
1:A:112:MET:HG3	2:F:78:TYR:CD2	2.52	0.45
3:C:162:PRO:HG2	5:J:53:ARG:HB2	1.99	0.45
6:K:363:LEU:HD22	6:K:397:GLU:HG2	1.98	0.45
1:A:57:LYS:HG2	1:A:132:GLU:OE1	2.17	0.44
8:B:201:CYC:HMA1	7:S:25:THR:HG23	2.00	0.44
6:K:440:PRO:HB2	6:K:443:VAL:HG12	1.99	0.44
1:E:82:GLN:HG3	8:E:201:CYC:HBC1	2.00	0.44
2:F:124:GLY:O	2:F:127:ILE:HG13	2.17	0.44
1:G:18:PRO:HD3	2:H:94:TYR:HE1	1.82	0.44
1:G:82:GLN:O	1:G:86:VAL:HG12	2.16	0.44
2:H:71:MEN:HE22	8:H:201:CYC:HBD2	1.99	0.44
6:K:67:ILE:HD13	6:K:217:LYS:HG2	1.99	0.44
6:K:251:ARG:HB2	6:K:265:PHE:HB3	2.00	0.44
6:K:360:ARG:HB2	6:K:429:LEU:HD21	2.00	0.44
6:K:609:HIS:O	6:K:613:LEU:HB2	2.17	0.44
1:M:16:ARG:O	2:N:94:TYR:OH	2.34	0.44
1:O:63:PRO:HA	1:O:68:ASN:HD21	1.82	0.44
2:D:1:MET:HG2	2:D:103:ILE:HA	1.97	0.44
2:D:74:THR:HG22	1:E:104:ILE:HG23	2.00	0.44
4:I:54:GLY:HA3	4:I:130:LEU:HD22	2.00	0.44
1:M:91:TYR:OH	2:N:17:LYS:O	2.29	0.44
1:O:18:PRO:HD3	2:P:94:TYR:HE1	1.82	0.44
2:F:41:ALA:HB2	2:F:96:MET:HE1	1.99	0.44
2:L:28:GLN:O	2:L:32:ARG:HD3	2.18	0.44
1:M:73:ARG:NH1	8:M:201:CYC:O2D	2.50	0.44
1:O:93:ILE:HD13	1:O:149:TYR:CE2	2.48	0.44
1:Q:127:MET:HA	1:Q:127:MET:CE	2.47	0.44
1:A:85:TYR:O	1:A:89:ILE:HG13	2.18	0.44
2:F:27:LEU:HD23	2:F:31:PHE:HD1	1.83	0.44
2:L:40:ALA:O	2:L:44:ILE:HB	2.17	0.44
4:I:22:GLU:O	4:I:26:ILE:HG12	2.17	0.44
4:I:102:GLU:HG3	4:I:152:TYR:HE2	1.83	0.44
6:K:31:ARG:HD2	6:K:33:ARG:HH21	1.81	0.44
6:K:635:PHE:HB3	1:O:13:SER:HB2	1.98	0.44
2:L:114:GLU:CD	2:L:114:GLU:H	2.25	0.44
1:O:101:LEU:HD11	1:O:153:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:23:LEU:HD12	2:R:42:MET:HE3	1.98	0.44
1:A:25:ILE:HD11	6:K:42:THR:OG1	2.18	0.44
2:B:115:THR:HG22	2:B:119:LEU:HD11	1.99	0.44
2:F:85:MET:HG3	2:F:133:MET:CE	2.47	0.44
2:L:51:ILE:HD11	2:L:140:MET:HE2	2.00	0.44
3:C:143:ALA:O	3:C:147:ILE:HG12	2.17	0.44
1:M:27:GLN:NE2	2:N:38:ALA:HB3	2.32	0.44
1:Q:109:ILE:HD12	1:Q:109:ILE:HA	1.82	0.44
1:G:123:ILE:HD13	8:G:201:CYC:HMC2	2.00	0.44
4:I:57:ARG:HD3	4:I:61:ARG:NH2	2.33	0.44
5:J:12:TYR:HE2	5:J:23:ALA:HB2	1.83	0.44
5:J:75:THR:HB	6:K:191:ASN:ND2	2.33	0.44
7:S:2:ARG:CZ	7:S:66:LEU:HD22	2.48	0.44
2:F:55:THR:OG1	2:F:133:MET:HE3	2.18	0.43
8:G:201:CYC:HAA1	2:L:61:LEU:HD22	1.99	0.43
5:J:108:ARG:HE	6:K:261:GLN:HB3	1.83	0.43
6:K:56:ILE:HD11	6:K:228:ALA:HB1	2.00	0.43
6:K:463:ASN:ND2	6:K:602:THR:OG1	2.51	0.43
1:O:139:SER:OG	1:O:142:ASP:OD2	2.34	0.43
5:J:53:ARG:O	5:J:57:LYS:HG2	2.18	0.43
5:J:58:LYS:HE3	5:J:133:ILE:HG23	2.01	0.43
5:J:88:TYR:OH	6:K:264:SER:N	2.44	0.43
6:K:543:GLU:HA	6:K:546:ILE:HD13	2.00	0.43
8:O:201:CYC:HB	8:O:201:CYC:HMA3	1.83	0.43
2:R:37:ARG:NH1	2:R:96:MET:O	2.50	0.43
3:C:89:ILE:HG12	3:C:149:TYR:HB3	2.00	0.43
6:K:193:ARG:HD2	6:K:245:VAL:HG21	2.00	0.43
2:L:96:MET:HA	2:L:152:TYR:CE2	2.53	0.43
2:N:96:MET:HE3	2:N:96:MET:HB3	1.95	0.43
2:B:75:CYS:SG	3:C:112:LEU:HD13	2.59	0.43
6:K:365:ARG:NE	6:K:397:GLU:OE2	2.51	0.43
2:N:109:LEU:HD11	2:N:156:ILE:HA	1.99	0.43
1:Q:27:GLN:NE2	2:R:38:ALA:HB3	2.33	0.43
1:O:123:ILE:H	1:O:123:ILE:HG13	1.54	0.43
1:Q:49:ARG:NH2	1:Q:53:ASN:HD22	2.16	0.43
2:D:1:MET:HE2	2:D:1:MET:HB2	1.89	0.43
2:D:46:ALA:HA	4:I:155:ALA:HB2	2.01	0.43
2:D:144:GLU:CD	2:D:145:ALA:H	2.26	0.43
1:E:112:MET:HE1	8:E:201:CYC:C1B	2.48	0.43
2:H:122:PRO:HB2	2:H:125:ALA:HB3	2.00	0.43
5:J:125:ALA:HA	5:J:128:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:104:LEU:HD11	2:P:152:TYR:HB3	2.01	0.43
2:B:76:ARG:NH2	7:S:12:SER:O	2.51	0.43
1:E:80:ARG:NH2	1:E:81:ASP:OD1	2.38	0.43
1:G:21:LYS:HE2	1:G:21:LYS:HB3	1.81	0.43
2:H:105:ASP:HA	2:H:109:LEU:HB2	2.01	0.43
1:A:37:VAL:HG22	2:B:24:LEU:HD22	1.99	0.43
2:B:28:GLN:OE1	2:B:32:ARG:NH1	2.51	0.43
1:E:61:ARG:O	6:K:694:MET:SD	2.76	0.43
2:H:134:LYS:O	2:H:138:ASN:HB2	2.18	0.43
1:M:28:ASP:HA	1:M:31:LYS:HZ2	1.84	0.43
1:M:140:ASP:N	1:M:140:ASP:OD1	2.52	0.43
2:P:85:MET:HE3	8:P:201:CYC:CBC	2.49	0.43
6:K:371:GLU:HA	6:K:374:GLN:HG3	2.01	0.43
2:L:3:ASP:HA	2:L:98:ALA:HB1	2.00	0.43
2:L:104:LEU:HD13	2:L:156:ILE:HG13	1.99	0.43
7:S:3:MET:H	7:S:57:THR:HB	1.84	0.43
1:A:91:TYR:HA	1:A:94:LEU:HD12	1.99	0.42
3:C:112:LEU:HD21	9:C:201:M1V:H31	2.01	0.42
5:J:72:MEN:HE23	5:J:122:VAL:HG22	2.00	0.42
1:M:3:LEU:HD21	1:M:29:PHE:CG	2.53	0.42
2:B:58:LYS:HE2	2:B:58:LYS:HB2	1.76	0.42
2:B:84:ASP:OD2	2:B:116:TYR:OH	2.25	0.42
3:C:160:PRO:HB3	6:K:247:LYS:HG2	2.01	0.42
6:K:169:LEU:HD23	6:K:169:LEU:HA	1.90	0.42
6:K:463:ASN:HA	6:K:603:LYS:HG2	2.01	0.42
1:O:89:ILE:HG21	1:O:146:VAL:HG13	2.00	0.42
2:B:7:THR:O	2:B:11:THR:HG23	2.19	0.42
3:C:22:GLU:CD	4:I:6:GLN:HE22	2.27	0.42
2:D:74:THR:HB	1:E:104:ILE:HA	2.01	0.42
1:E:7:LEU:HG	1:E:22:GLU:HG2	2.01	0.42
5:J:76:THR:HA	5:J:79:TYR:HB3	2.01	0.42
5:J:89:TYR:HB2	5:J:134:MET:HE1	2.00	0.42
6:K:251:ARG:N	6:K:265:PHE:O	2.52	0.42
6:K:313:GLU:O	6:K:315:THR:N	2.53	0.42
1:A:120:ILE:HA	1:A:123:ILE:HD12	2.00	0.42
3:C:162:PRO:HD2	5:J:53:ARG:HG2	2.02	0.42
1:E:142:ASP:OD2	1:E:142:ASP:N	2.44	0.42
5:J:21:ARG:HA	5:J:21:ARG:HD2	1.75	0.42
2:B:24:LEU:O	2:B:28:GLN:HG2	2.19	0.42
6:K:195:LEU:HD23	6:K:198:ILE:HB	2.01	0.42
6:K:661:ARG:HB2	6:K:662:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:80:ARG:HD3	1:O:84:TRP:CZ2	2.54	0.42
2:D:58:LYS:HB2	2:D:58:LYS:HE2	1.86	0.42
6:K:287:ASP:OD1	6:K:287:ASP:N	2.49	0.42
6:K:560:GLY:HA2	6:K:563:ARG:HG2	2.02	0.42
1:O:55:SER:OG	1:O:79:GLN:OE1	2.22	0.42
8:A:201:CYC:HAA1	2:F:61:LEU:HD22	2.02	0.42
3:C:81:ASP:OD2	3:C:113:TYR:OH	2.36	0.42
6:K:304:ARG:NH1	2:L:83:ARG:HD3	2.34	0.42
1:Q:16:ARG:O	2:R:94:TYR:OH	2.36	0.42
1:Q:53:ASN:O	1:Q:57:LYS:HG2	2.20	0.42
2:R:103:ILE:HD12	2:R:103:ILE:HA	1.84	0.42
1:A:111:GLU:H	1:A:111:GLU:HG2	1.71	0.42
2:B:3:ASP:OD1	2:B:6:THR:OG1	2.28	0.42
2:D:21:ASP:O	2:D:25:ASP:OD1	2.38	0.42
2:D:137:VAL:O	2:D:141:LEU:HB2	2.20	0.42
1:E:16:ARG:O	2:F:94:TYR:OH	2.30	0.42
5:J:66:LEU:HD11	5:J:126:PRO:HB3	2.00	0.42
6:K:313:GLU:H	6:K:313:GLU:HG3	1.64	0.42
2:P:8:LEU:HD23	2:P:8:LEU:HA	1.90	0.42
2:B:83:ARG:NH1	7:S:17:ARG:HB2	2.35	0.42
2:B:133:MET:O	2:B:137:VAL:HG23	2.20	0.42
2:D:37:ARG:HH21	2:D:148:GLU:CD	2.27	0.42
2:F:59:SER:O	2:F:128:ARG:NH2	2.53	0.42
1:G:38:ARG:HB3	1:G:38:ARG:NH1	2.35	0.42
5:J:85:ASP:OD2	5:J:117:TYR:OH	2.28	0.42
1:A:102:GLU:HA	1:A:106:THR:OG1	2.20	0.42
1:A:134:ALA:HA	1:A:137:VAL:HG22	2.02	0.42
2:D:160:LEU:HA	2:D:160:LEU:HD23	1.84	0.42
4:I:4:ILE:HD11	4:I:29:PHE:CD2	2.54	0.42
1:O:78:CYS:HA	8:O:201:CYC:HAC1	1.92	0.42
1:G:9:LEU:HB3	6:K:342:ARG:NH2	2.34	0.41
4:I:4:ILE:HD13	4:I:4:ILE:N	2.35	0.41
6:K:515:LEU:N	6:K:655:ASN:O	2.49	0.41
2:L:60:LEU:HD21	2:L:129:ALA:HB2	2.01	0.41
1:M:54:GLY:HA3	1:M:130:LEU:HD22	2.02	0.41
1:Q:98:GLU:H	1:Q:98:GLU:HG3	1.58	0.41
6:K:576:ILE:HB	6:K:580:GLU:HB2	2.02	0.41
2:L:141:LEU:HA	2:L:141:LEU:HD12	1.65	0.41
6:K:578:VAL:HB	6:K:655:ASN:HA	2.02	0.41
2:N:137:VAL:HG11	2:N:153:PHE:CE2	2.55	0.41
1:O:126:CYS:O	1:O:130:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:43:ILE:HD11	7:S:50:ILE:HG12	2.01	0.41
3:C:21:GLY:HA3	4:I:97:ASP:CG	2.46	0.41
3:C:87:ARG:HA	2:D:18:TYR:CE1	2.56	0.41
1:G:98:GLU:H	1:G:98:GLU:CD	2.29	0.41
1:M:141:GLU:O	1:M:145:GLU:HG2	2.21	0.41
2:N:82:ILE:HD12	2:N:82:ILE:HA	1.87	0.41
2:L:72:MET:HG2	2:L:78:TYR:HA	2.03	0.41
2:L:84:ASP:OD2	2:L:116:TYR:OH	2.27	0.41
1:M:49:ARG:NH1	1:M:137:VAL:HG11	2.35	0.41
1:M:131:LYS:HE2	1:M:135:MET:HE2	2.03	0.41
2:R:106:GLU:C	2:R:110:ASN:HD21	2.27	0.41
1:A:92:SER:OG	1:A:101:LEU:HB2	2.20	0.41
3:C:36:GLN:HA	3:C:39:LEU:HD23	2.02	0.41
1:G:94:LEU:HA	1:G:94:LEU:HD23	1.87	0.41
2:H:126:THR:HG23	8:H:201:CYC:HMC2	2.03	0.41
6:K:542:VAL:O	6:K:545:VAL:N	2.52	0.41
1:O:14:GLU:HB2	1:O:16:ARG:NE	2.22	0.41
1:Q:35:GLN:HG3	1:Q:38:ARG:HH21	1.85	0.41
3:C:98:ASP:CG	3:C:102:ARG:HE	2.27	0.41
1:G:42:ALA:O	1:G:46:ASN:OD1	2.39	0.41
2:P:77:ARG:HG2	8:P:201:CYC:HAD1	2.01	0.41
7:S:62:ALA:HB3	7:S:66:LEU:HD23	2.02	0.41
2:B:91:TYR:OH	2:B:107:ARG:HD2	2.20	0.41
1:E:94:LEU:HD22	2:F:27:LEU:HD11	2.01	0.41
2:F:137:VAL:CG1	2:F:141:LEU:HD12	2.50	0.41
1:M:9:LEU:HD12	1:M:99:ARG:HH12	1.86	0.41
2:P:54:LYS:HD3	2:P:136:VAL:HG13	2.02	0.41
1:Q:46:ASN:O	1:Q:49:ARG:HG3	2.21	0.41
2:B:12:SER:OG	2:B:17:LYS:O	2.39	0.41
2:B:13:ASP:OD1	2:F:73:TYR:OH	2.30	0.41
1:E:78:CYS:HA	8:E:201:CYC:HHD	2.02	0.41
1:G:112:MET:O	1:G:116:LEU:HG	2.21	0.41
6:K:40:MET:HA	6:K:40:MET:CE	2.48	0.41
6:K:51:LEU:HD22	2:L:32:ARG:NH1	2.36	0.41
6:K:693:MET:HE1	6:K:695:ARG:HH21	1.85	0.41
1:M:137:VAL:HG23	1:M:138:LEU:HG	2.02	0.41
1:O:106:THR:HA	1:O:109:ILE:CG1	2.50	0.41
2:P:73:TYR:O	2:P:77:ARG:HB2	2.20	0.41
2:R:12:SER:OG	2:R:17:LYS:O	2.39	0.41
7:S:1:MET:SD	7:S:2:ARG:N	2.94	0.41
2:B:87:PHE:HE1	2:B:108:VAL:HG22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:SER:O	2:H:128:ARG:NH2	2.54	0.40
6:K:34:TYR:OH	2:L:89:LEU:HD22	2.21	0.40
1:M:102:GLU:HA	1:M:106:THR:OG1	2.20	0.40
1:O:50:ILE:HD12	1:O:51:VAL:HG23	2.03	0.40
2:P:39:LYS:O	2:P:43:THR:OG1	2.39	0.40
1:A:67:SER:O	1:A:75:THR:OG1	2.35	0.40
4:I:13:ARG:HE	4:I:13:ARG:HB3	1.73	0.40
4:I:157:LEU:C	4:I:159:PRO:CD	2.94	0.40
6:K:278:ARG:NH2	7:S:23:GLN:OE1	2.54	0.40
1:Q:99:ARG:NH1	1:Q:102:GLU:OE1	2.54	0.40
2:N:131:GLN:O	2:N:135:GLU:HG2	2.21	0.40
1:O:50:ILE:HD12	1:O:51:VAL:N	2.36	0.40
7:S:9:CYS:HB2	7:S:26:TYR:HD1	1.86	0.40
3:C:61:ILE:HD12	3:C:61:ILE:HA	1.92	0.40
1:M:49:ARG:NH1	1:M:50:ILE:HG13	2.35	0.40
1:O:101:LEU:HD21	1:O:153:ILE:HG12	2.03	0.40
1:Q:34:GLU:N	1:Q:34:GLU:CD	2.79	0.40
2:R:119:LEU:HD13	8:R:201:CYC:HBD1	2.02	0.40
1:A:80:ARG:HE	1:A:80:ARG:HB3	1.65	0.40
2:D:104:LEU:HD11	2:D:152:TYR:HB3	2.03	0.40
1:E:135:MET:SD	1:E:143:ALA:HB1	2.61	0.40
6:K:592:ARG:O	6:K:597:GLU:HG2	2.20	0.40
2:L:154:ASP:O	2:L:158:SER:OG	2.38	0.40
7:S:23:GLN:H	7:S:23:GLN:HG2	1.76	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 PDB entries followed by that with respect to all EM entries.

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	154/158 (98%)	152 (99%)	2 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	77/158 (49%)	76 (99%)	1 (1%)	0	100	100
1	G	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
1	M	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
1	O	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
1	Q	154/158 (98%)	149 (97%)	5 (3%)	0	100	100
2	B	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	47
2	D	110/161 (68%)	106 (96%)	3 (3%)	1 (1%)	14	37
2	F	157/161 (98%)	155 (99%)	2 (1%)	0	100	100
2	H	158/161 (98%)	155 (98%)	2 (1%)	1 (1%)	21	47
2	L	156/161 (97%)	153 (98%)	2 (1%)	1 (1%)	21	47
2	N	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	47
2	P	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
2	R	157/161 (98%)	154 (98%)	2 (1%)	1 (1%)	21	47
3	C	162/181 (90%)	155 (96%)	6 (4%)	1 (1%)	21	47
4	I	156/159 (98%)	152 (97%)	4 (3%)	0	100	100
5	J	164/169 (97%)	159 (97%)	5 (3%)	0	100	100
6	K	587/783 (75%)	554 (94%)	33 (6%)	0	100	100
7	S	65/67 (97%)	60 (92%)	5 (8%)	0	100	100
All	All	3193/3595 (89%)	3093 (97%)	93 (3%)	7 (0%)	44	70

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	75	CYS
2	D	75	CYS
2	H	75	CYS
2	N	75	CYS
2	R	75	CYS
3	C	159	ARG
2	L	75	CYS

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

9 non-standard protein/DNA/RNA residues 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	MEN	N	71	2	7,8,9	0.92	0	4,9,11	1.18	1 (25%)
2	MEN	F	71	2	7,8,9	0.96	0	4,9,11	1.01	0
2	MEN	R	71	2	7,8,9	0.91	0	4,9,11	1.38	1 (25%)
2	MEN	L	71	2	7,8,9	0.97	0	4,9,11	0.49	0
2	MEN	P	71	2	7,8,9	0.93	0	4,9,11	0.93	0
2	MEN	D	71	2	7,8,9	0.91	0	4,9,11	1.24	1 (25%)
2	MEN	H	71	2	7,8,9	0.92	0	4,9,11	1.27	1 (25%)
5	MEN	J	72	5	7,8,9	0.93	0	4,9,11	1.09	1 (25%)
2	MEN	B	71	2	7,8,9	0.93	0	4,9,11	1.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	N	71	2	-	1/7/8/10	-
2	MEN	F	71	2	-	2/7/8/10	-
2	MEN	R	71	2	-	0/7/8/10	-
2	MEN	L	71	2	-	4/7/8/10	-
2	MEN	P	71	2	-	2/7/8/10	-
2	MEN	D	71	2	-	0/7/8/10	-
2	MEN	H	71	2	-	2/7/8/10	-
5	MEN	J	72	5	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	B	71	2	-	3/7/8/10	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	71	MEN	CB-CG-ND2	2.49	118.78	115.53
2	D	71	MEN	CB-CG-ND2	2.29	118.52	115.53
2	H	71	MEN	CB-CG-ND2	2.18	118.37	115.53
2	N	71	MEN	CB-CG-ND2	2.13	118.31	115.53
5	J	72	MEN	CB-CG-ND2	2.05	118.21	115.53

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	71	MEN	O-C-CA-CB
2	B	71	MEN	C-CA-CB-CG
5	J	72	MEN	C-CA-CB-CG
5	J	72	MEN	CB-CG-ND2-CE2
5	J	72	MEN	OD1-CG-ND2-CE2
2	P	71	MEN	C-CA-CB-CG
2	B	71	MEN	N-CA-CB-CG
5	J	72	MEN	N-CA-CB-CG
2	L	71	MEN	N-CA-CB-CG
2	P	71	MEN	N-CA-CB-CG
2	F	71	MEN	CA-CB-CG-OD1
2	F	71	MEN	CA-CB-CG-ND2
2	H	71	MEN	CA-CB-CG-OD1
2	H	71	MEN	CA-CB-CG-ND2
2	L	71	MEN	CA-CB-CG-ND2
2	N	71	MEN	N-CA-CB-CG
2	L	71	MEN	C-CA-CB-CG
2	L	71	MEN	CA-CB-CG-OD1

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	71	MEN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	71	MEN	1	0
2	H	71	MEN	1	0
5	J	72	MEN	1	0
2	B	71	MEN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	CYC	H	201	2	46,46,46	0.34	0	63,67,67	1.16	3 (4%)
8	CYC	O	201	1	46,46,46	0.35	0	63,67,67	1.13	2 (3%)
8	CYC	B	201	2	46,46,46	0.38	0	63,67,67	1.06	2 (3%)
8	CYC	N	201	2	46,46,46	0.36	0	63,67,67	1.30	3 (4%)
9	MIV	C	201	-	46,46,46	0.80	1 (2%)	66,67,67	1.10	3 (4%)
9	MIV	K	801	-	46,46,46	0.79	1 (2%)	66,67,67	1.00	2 (3%)
8	CYC	A	201	1	46,46,46	0.36	0	63,67,67	1.35	3 (4%)
8	CYC	F	201	2	46,46,46	0.27	0	63,67,67	0.96	2 (3%)
8	CYC	D	201	2	46,46,46	0.34	0	63,67,67	1.18	3 (4%)
8	CYC	J	201	5	46,46,46	0.38	0	63,67,67	1.20	3 (4%)
8	CYC	Q	201	1	46,46,46	0.37	0	63,67,67	1.29	3 (4%)
8	CYC	R	201	2	46,46,46	0.34	0	63,67,67	0.94	3 (4%)
8	CYC	E	201	1	46,46,46	0.36	0	63,67,67	1.20	3 (4%)
8	CYC	L	201	2	46,46,46	0.28	0	63,67,67	0.82	2 (3%)
8	CYC	M	201	1	46,46,46	0.36	0	63,67,67	1.22	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	CYC	P	201	2	46,46,46	0.41	0	63,67,67	1.20	3 (4%)
8	CYC	I	201	4	46,46,46	0.35	0	63,67,67	1.41	3 (4%)
8	CYC	G	201	1	46,46,46	0.35	0	63,67,67	1.25	3 (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
8	CYC	H	201	2	-	8/26/74/74	0/4/4/4
8	CYC	O	201	1	-	9/26/74/74	0/4/4/4
8	CYC	B	201	2	-	7/26/74/74	0/4/4/4
8	CYC	N	201	2	-	7/26/74/74	0/4/4/4
9	M1V	C	201	-	-	17/26/74/74	0/4/4/4
9	M1V	K	801	-	-	14/26/74/74	0/4/4/4
8	CYC	A	201	1	-	9/26/74/74	0/4/4/4
8	CYC	F	201	2	-	10/26/74/74	0/4/4/4
8	CYC	D	201	2	-	7/26/74/74	0/4/4/4
8	CYC	J	201	5	-	11/26/74/74	0/4/4/4
8	CYC	Q	201	1	-	11/26/74/74	0/4/4/4
8	CYC	R	201	2	-	7/26/74/74	0/4/4/4
8	CYC	E	201	1	-	10/26/74/74	0/4/4/4
8	CYC	L	201	2	-	10/26/74/74	0/4/4/4
8	CYC	M	201	1	-	8/26/74/74	0/4/4/4
8	CYC	P	201	2	-	9/26/74/74	0/4/4/4
8	CYC	I	201	4	-	9/26/74/74	0/4/4/4
8	CYC	G	201	1	-	6/26/74/74	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	201	M1V	C4A-C3A	2.65	1.49	1.44
9	K	801	M1V	C4A-C3A	2.56	1.49	1.44

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	201	CYC	C1D-CHD-C4C	8.16	141.69	127.76
8	I	201	CYC	C1D-CHD-C4C	8.08	141.56	127.76
8	N	201	CYC	C1D-CHD-C4C	7.22	140.08	127.76
8	G	201	CYC	C1D-CHD-C4C	6.60	139.04	127.76
8	E	201	CYC	C1B-CHB-C4A	6.42	143.81	128.06
8	Q	201	CYC	C1B-CHB-C4A	6.41	143.80	128.06
8	F	201	CYC	C1D-CHD-C4C	6.38	138.65	127.76
8	M	201	CYC	C1D-CHD-C4C	6.34	138.60	127.76
8	Q	201	CYC	C1D-CHD-C4C	6.19	138.33	127.76
8	H	201	CYC	C1B-CHB-C4A	6.01	142.81	128.06
8	P	201	CYC	C1B-CHB-C4A	5.94	142.63	128.06
8	D	201	CYC	C1B-CHB-C4A	5.87	142.48	128.06
8	J	201	CYC	C1D-CHD-C4C	5.83	137.72	127.76
8	D	201	CYC	C1D-CHD-C4C	5.81	137.68	127.76
8	O	201	CYC	C1B-CHB-C4A	5.71	142.08	128.06
8	P	201	CYC	C1D-CHD-C4C	5.71	137.51	127.76
8	M	201	CYC	C1B-CHB-C4A	5.70	142.05	128.06
8	N	201	CYC	C1B-CHB-C4A	5.64	141.91	128.06
8	I	201	CYC	C1B-CHB-C4A	5.62	141.86	128.06
8	G	201	CYC	C1B-CHB-C4A	5.45	141.44	128.06
8	J	201	CYC	C1B-CHB-C4A	5.45	141.43	128.06
8	R	201	CYC	C1D-CHD-C4C	5.34	136.88	127.76
8	O	201	CYC	C1D-CHD-C4C	5.30	136.81	127.76
8	B	201	CYC	C1D-CHD-C4C	5.18	136.61	127.76
8	H	201	CYC	C1D-CHD-C4C	5.15	136.56	127.76
8	B	201	CYC	C1B-CHB-C4A	5.14	140.68	128.06
8	A	201	CYC	C1B-CHB-C4A	5.04	140.42	128.06
8	E	201	CYC	C1D-CHD-C4C	4.90	136.13	127.76
8	L	201	CYC	C1D-CHD-C4C	4.48	135.41	127.76
9	C	201	M1V	C4B-CHB-C1C	3.44	135.74	128.22
8	R	201	CYC	C1B-CHB-C4A	3.43	136.47	128.06
9	K	801	M1V	C4B-CHB-C1C	3.31	135.45	128.22
8	J	201	CYC	C2C-C3C-C4C	2.98	105.81	101.34
9	C	201	M1V	CAC-C2C-C3C	2.75	133.01	127.87
8	Q	201	CYC	C2C-C3C-C4C	2.70	105.38	101.34
8	N	201	CYC	C2C-C3C-C4C	2.68	105.36	101.34
8	G	201	CYC	C2C-C3C-C4C	2.59	105.22	101.34
8	F	201	CYC	C2C-C3C-C4C	2.50	105.08	101.34
8	A	201	CYC	C2C-C3C-C4C	2.48	105.06	101.34
8	L	201	CYC	C2C-C3C-C4C	2.44	104.99	101.34
8	P	201	CYC	C2C-C3C-C4C	2.43	104.98	101.34
8	I	201	CYC	C2C-C3C-C4C	2.39	104.92	101.34
9	C	201	M1V	C1C-C2C-C3C	-2.39	104.14	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	201	CYC	CAC-C3C-C4C	-2.38	106.56	112.67
8	M	201	CYC	C2C-C3C-C4C	2.28	104.76	101.34
8	H	201	CYC	C2C-C3C-C4C	2.16	104.58	101.34
9	K	801	M1V	CAA-C3A-C4A	2.08	127.10	124.39
8	R	201	CYC	C2C-C3C-C4C	2.06	104.43	101.34
8	D	201	CYC	C2C-C3C-C4C	2.02	104.36	101.34

There are no chirality outliers.

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	201	CYC	NA-C4A-CHB-C1B
8	A	201	CYC	C3A-C4A-CHB-C1B
8	D	201	CYC	C3A-C4A-CHB-C1B
8	D	201	CYC	C4B-C3B-CAB-CBB
8	E	201	CYC	NA-C4A-CHB-C1B
8	E	201	CYC	C3A-C4A-CHB-C1B
8	E	201	CYC	NC-C4C-CHD-C1D
8	E	201	CYC	C3C-C4C-CHD-C1D
8	F	201	CYC	NA-C4A-CHB-C1B
8	F	201	CYC	C3A-C4A-CHB-C1B
8	H	201	CYC	C4B-C3B-CAB-CBB
8	I	201	CYC	NC-C4C-CHD-C1D
8	J	201	CYC	C2C-C3C-CAC-CBC
8	J	201	CYC	C4C-C3C-CAC-CBC
8	L	201	CYC	NA-C4A-CHB-C1B
8	L	201	CYC	C3A-C4A-CHB-C1B
8	M	201	CYC	NC-C4C-CHD-C1D
8	N	201	CYC	NA-C4A-CHB-C1B
8	O	201	CYC	C4B-C3B-CAB-CBB
8	Q	201	CYC	NC-C4C-CHD-C1D
8	Q	201	CYC	C3C-C4C-CHD-C1D
8	R	201	CYC	NA-C4A-CHB-C1B
8	R	201	CYC	C3A-C4A-CHB-C1B
9	C	201	M1V	C1C-C2C-CAC-CBC
9	C	201	M1V	C3C-C4C-CHC-C1D
9	C	201	M1V	NC-C4C-CHC-C1D
9	K	801	M1V	C3C-C4C-CHC-C1D
9	K	801	M1V	NC-C4C-CHC-C1D
9	K	801	M1V	C2D-C1D-CHC-C4C
9	K	801	M1V	ND-C1D-CHC-C4C
9	C	201	M1V	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	C	201	M1V	C4A-C3A-CAA-CBA
8	G	201	CYC	ND-C1D-CHD-C4C
8	J	201	CYC	ND-C1D-CHD-C4C
8	L	201	CYC	ND-C1D-CHD-C4C
8	M	201	CYC	ND-C1D-CHD-C4C
8	P	201	CYC	ND-C1D-CHD-C4C
8	R	201	CYC	ND-C1D-CHD-C4C
9	C	201	M1V	NB-C1B-CHA-C4A
8	B	201	CYC	C2D-C1D-CHD-C4C
8	D	201	CYC	C2D-C1D-CHD-C4C
8	F	201	CYC	C2D-C1D-CHD-C4C
8	H	201	CYC	C2D-C1D-CHD-C4C
8	J	201	CYC	C2D-C1D-CHD-C4C
8	L	201	CYC	C2D-C1D-CHD-C4C
8	M	201	CYC	C2D-C1D-CHD-C4C
8	O	201	CYC	C2D-C1D-CHD-C4C
8	P	201	CYC	C2D-C1D-CHD-C4C
8	R	201	CYC	C2D-C1D-CHD-C4C
9	C	201	M1V	C2B-C1B-CHA-C4A
9	C	201	M1V	C4B-C3B-CAB-CBB
9	K	801	M1V	C4B-C3B-CAB-CBB
9	C	201	M1V	C3C-C2C-CAC-CBC
8	A	201	CYC	C2A-CAA-CBA-CGA
9	K	801	M1V	C2B-C3B-CAB-CBB
8	A	201	CYC	ND-C1D-CHD-C4C
8	B	201	CYC	ND-C1D-CHD-C4C
8	D	201	CYC	ND-C1D-CHD-C4C
8	E	201	CYC	ND-C1D-CHD-C4C
8	F	201	CYC	ND-C1D-CHD-C4C
8	H	201	CYC	ND-C1D-CHD-C4C
8	N	201	CYC	ND-C1D-CHD-C4C
8	O	201	CYC	ND-C1D-CHD-C4C
8	Q	201	CYC	ND-C1D-CHD-C4C
8	A	201	CYC	C2D-C1D-CHD-C4C
8	E	201	CYC	C2D-C1D-CHD-C4C
8	G	201	CYC	C2D-C1D-CHD-C4C
8	I	201	CYC	C2D-C1D-CHD-C4C
8	N	201	CYC	C2D-C1D-CHD-C4C
8	Q	201	CYC	C2D-C1D-CHD-C4C
9	C	201	M1V	C2B-C3B-CAB-CBB
8	I	201	CYC	ND-C1D-CHD-C4C
8	F	201	CYC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
8	L	201	CYC	C2A-CAA-CBA-CGA
8	L	201	CYC	C2B-C3B-CAB-CBB
8	B	201	CYC	NA-C4A-CHB-C1B
8	D	201	CYC	NA-C4A-CHB-C1B
8	G	201	CYC	NA-C4A-CHB-C1B
8	H	201	CYC	NA-C4A-CHB-C1B
8	I	201	CYC	NA-C4A-CHB-C1B
8	J	201	CYC	NA-C4A-CHB-C1B
8	M	201	CYC	NA-C4A-CHB-C1B
8	O	201	CYC	NA-C4A-CHB-C1B
8	P	201	CYC	NA-C4A-CHB-C1B
8	Q	201	CYC	NA-C4A-CHB-C1B
9	C	201	M1V	ND-C1D-CHC-C4C
9	K	801	M1V	NA-C4A-CHA-C1B
8	I	201	CYC	C2B-C3B-CAB-CBB
8	B	201	CYC	C3A-C4A-CHB-C1B
8	G	201	CYC	C3A-C4A-CHB-C1B
8	H	201	CYC	C3A-C4A-CHB-C1B
8	I	201	CYC	C3A-C4A-CHB-C1B
8	J	201	CYC	C3A-C4A-CHB-C1B
8	M	201	CYC	C3A-C4A-CHB-C1B
8	N	201	CYC	C3A-C4A-CHB-C1B
8	O	201	CYC	C3A-C4A-CHB-C1B
8	P	201	CYC	C3A-C4A-CHB-C1B
8	Q	201	CYC	C3A-C4A-CHB-C1B
8	R	201	CYC	C4B-C3B-CAB-CBB
8	B	201	CYC	C2A-CAA-CBA-CGA
9	C	201	M1V	C3B-CAB-CBB-CGB
9	K	801	M1V	C3A-C4A-CHA-C1B
8	M	201	CYC	C2A-CAA-CBA-CGA
9	C	201	M1V	C2D-C1D-CHC-C4C
9	K	801	M1V	NB-C1B-CHA-C4A
8	N	201	CYC	C4B-C3B-CAB-CBB
9	K	801	M1V	C2B-C1B-CHA-C4A
8	P	201	CYC	C2B-C1B-CHB-C4A
8	D	201	CYC	NC-C4C-CHD-C1D
9	C	201	M1V	NA-C4A-CHA-C1B
8	E	201	CYC	CAA-CBA-CGA-O1A
8	E	201	CYC	CAA-CBA-CGA-O2A
8	R	201	CYC	CAA-CBA-CGA-O1A
8	M	201	CYC	CAA-CBA-CGA-O1A
8	J	201	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
8	Q	201	CYC	CAA-CBA-CGA-O1A
8	L	201	CYC	CAD-CBD-CGD-O1D
8	O	201	CYC	CAD-CBD-CGD-O1D
8	A	201	CYC	CAD-CBD-CGD-O2D
8	O	201	CYC	CAA-CBA-CGA-O1A
8	Q	201	CYC	CAD-CBD-CGD-O1D
8	R	201	CYC	CAA-CBA-CGA-O2A
8	I	201	CYC	CAA-CBA-CGA-O2A
8	Q	201	CYC	C2A-CAA-CBA-CGA
8	H	201	CYC	CAA-CBA-CGA-O1A
8	J	201	CYC	CAD-CBD-CGD-O1D
8	O	201	CYC	CAA-CBA-CGA-O2A
8	A	201	CYC	CAA-CBA-CGA-O1A
8	B	201	CYC	CAA-CBA-CGA-O1A
8	E	201	CYC	CAD-CBD-CGD-O1D
8	N	201	CYC	CAA-CBA-CGA-O1A
8	P	201	CYC	CAA-CBA-CGA-O1A
8	A	201	CYC	CAD-CBD-CGD-O1D
8	M	201	CYC	CAA-CBA-CGA-O2A
8	O	201	CYC	CAD-CBD-CGD-O2D
8	I	201	CYC	CAA-CBA-CGA-O1A
8	N	201	CYC	CAA-CBA-CGA-O2A
8	Q	201	CYC	CAA-CBA-CGA-O2A
8	A	201	CYC	CAA-CBA-CGA-O2A
8	E	201	CYC	CAD-CBD-CGD-O2D
8	L	201	CYC	CAA-CBA-CGA-O2A
9	K	801	M1V	CAC-CBC-CGC-O1C
8	B	201	CYC	CAA-CBA-CGA-O2A
8	P	201	CYC	CAA-CBA-CGA-O2A
8	Q	201	CYC	CAD-CBD-CGD-O2D
9	K	801	M1V	CAB-CBB-CGB-O2B
8	H	201	CYC	CAA-CBA-CGA-O2A
8	L	201	CYC	CAD-CBD-CGD-O2D
9	C	201	M1V	C3A-C4A-CHA-C1B
8	F	201	CYC	CAA-CBA-CGA-O1A
9	C	201	M1V	CAB-CBB-CGB-O2B
9	K	801	M1V	CAC-CBC-CGC-O2C
8	F	201	CYC	CAA-CBA-CGA-O2A
8	H	201	CYC	C2B-C1B-CHB-C4A
8	G	201	CYC	CAA-CBA-CGA-O1A
8	G	201	CYC	CAA-CBA-CGA-O2A
8	J	201	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
9	K	801	M1V	CAB-CBB-CGB-O1B
8	L	201	CYC	CAA-CBA-CGA-O1A
9	C	201	M1V	CAB-CBB-CGB-O1B
8	J	201	CYC	CAA-CBA-CGA-O1A
8	F	201	CYC	CAD-CBD-CGD-O2D
8	P	201	CYC	CAD-CBD-CGD-O1D
8	P	201	CYC	CAD-CBD-CGD-O2D
8	F	201	CYC	CAD-CBD-CGD-O1D
8	D	201	CYC	CAA-CBA-CGA-O2A
8	F	201	CYC	C2A-CAA-CBA-CGA
8	I	201	CYC	CAD-CBD-CGD-O2D
8	J	201	CYC	C4B-C3B-CAB-CBB

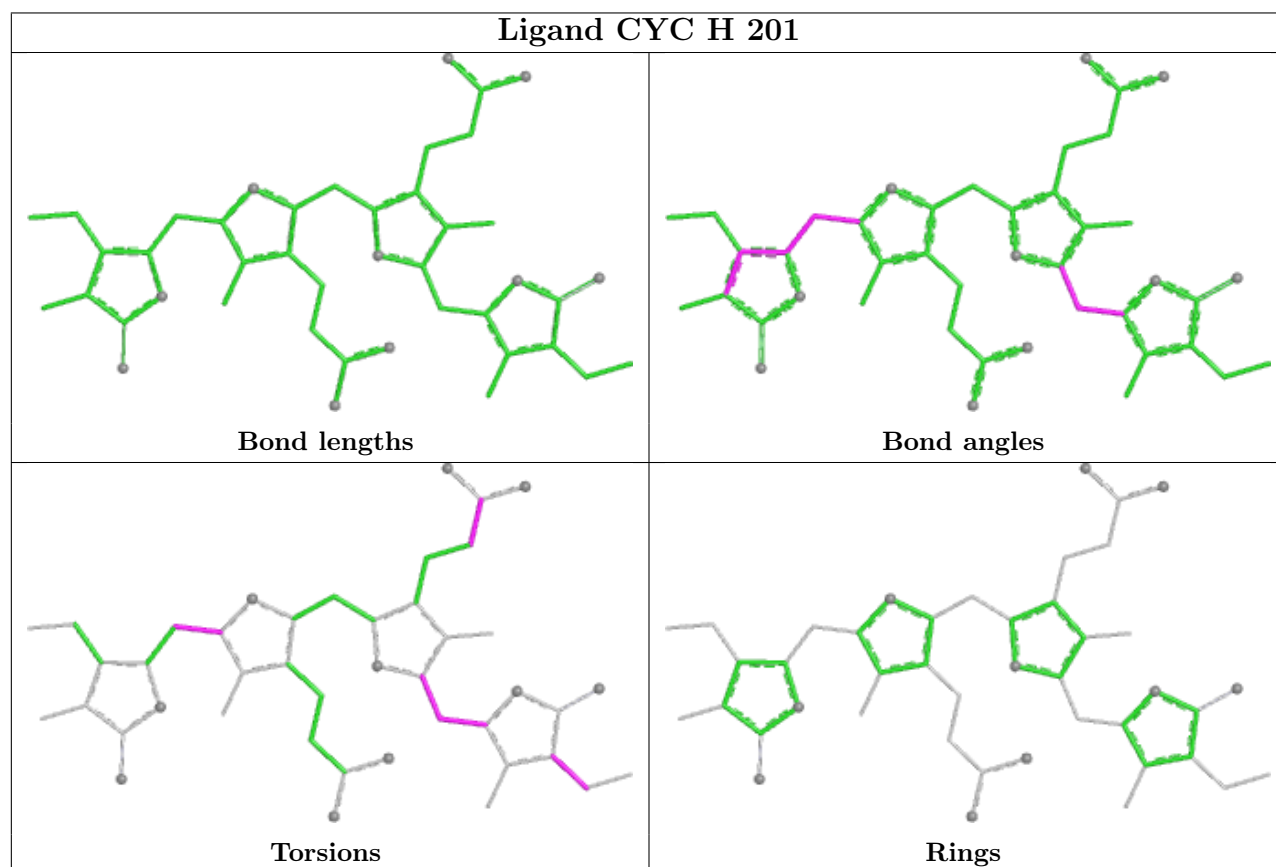
There are no ring outliers.

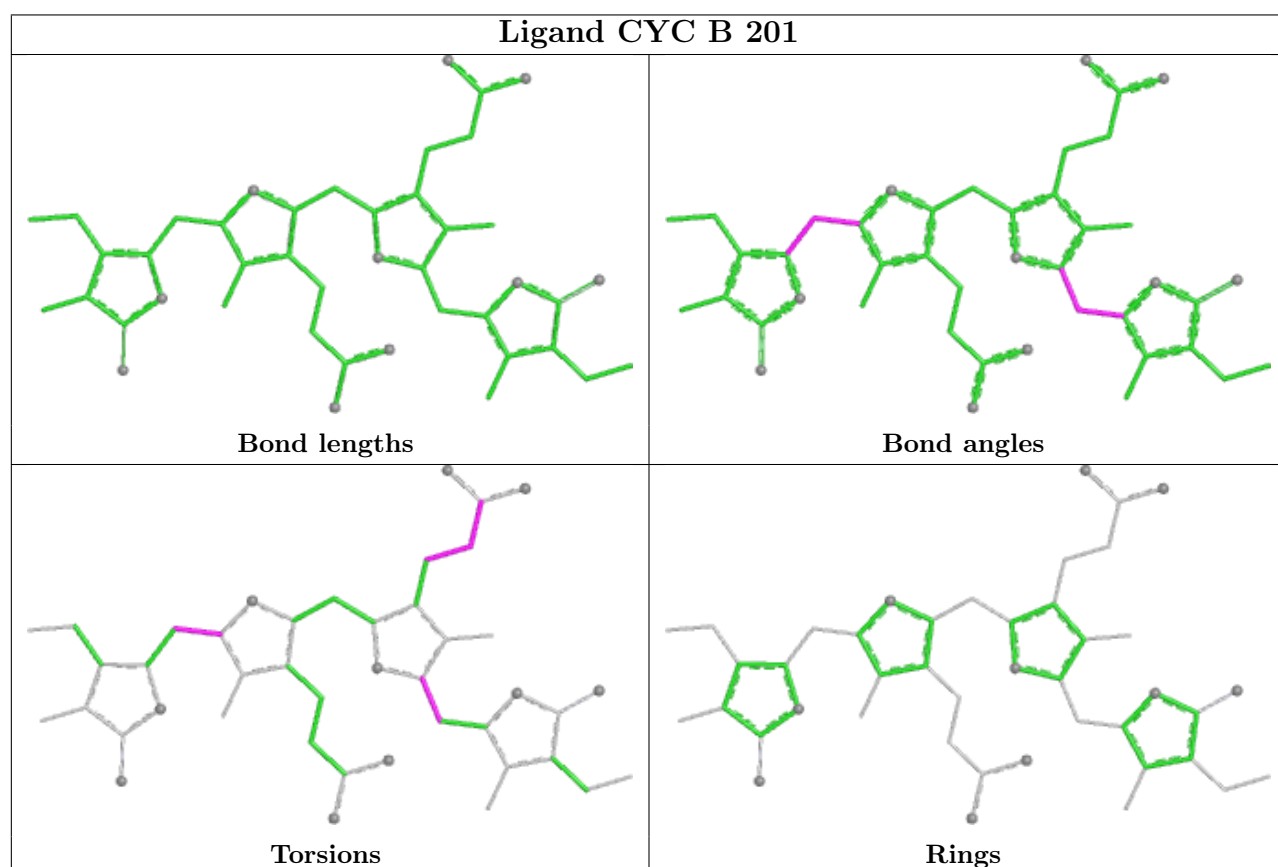
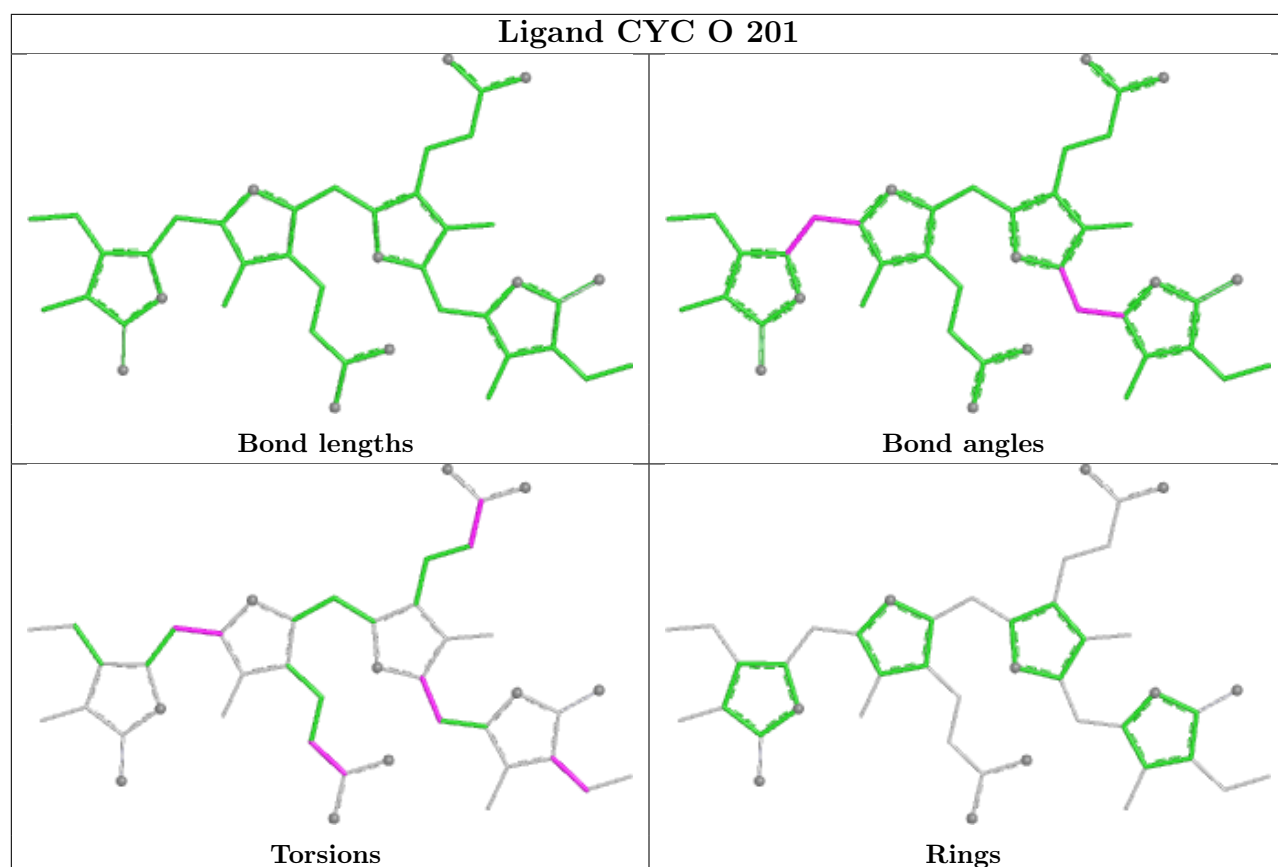
18 monomers are involved in 65 short contacts:

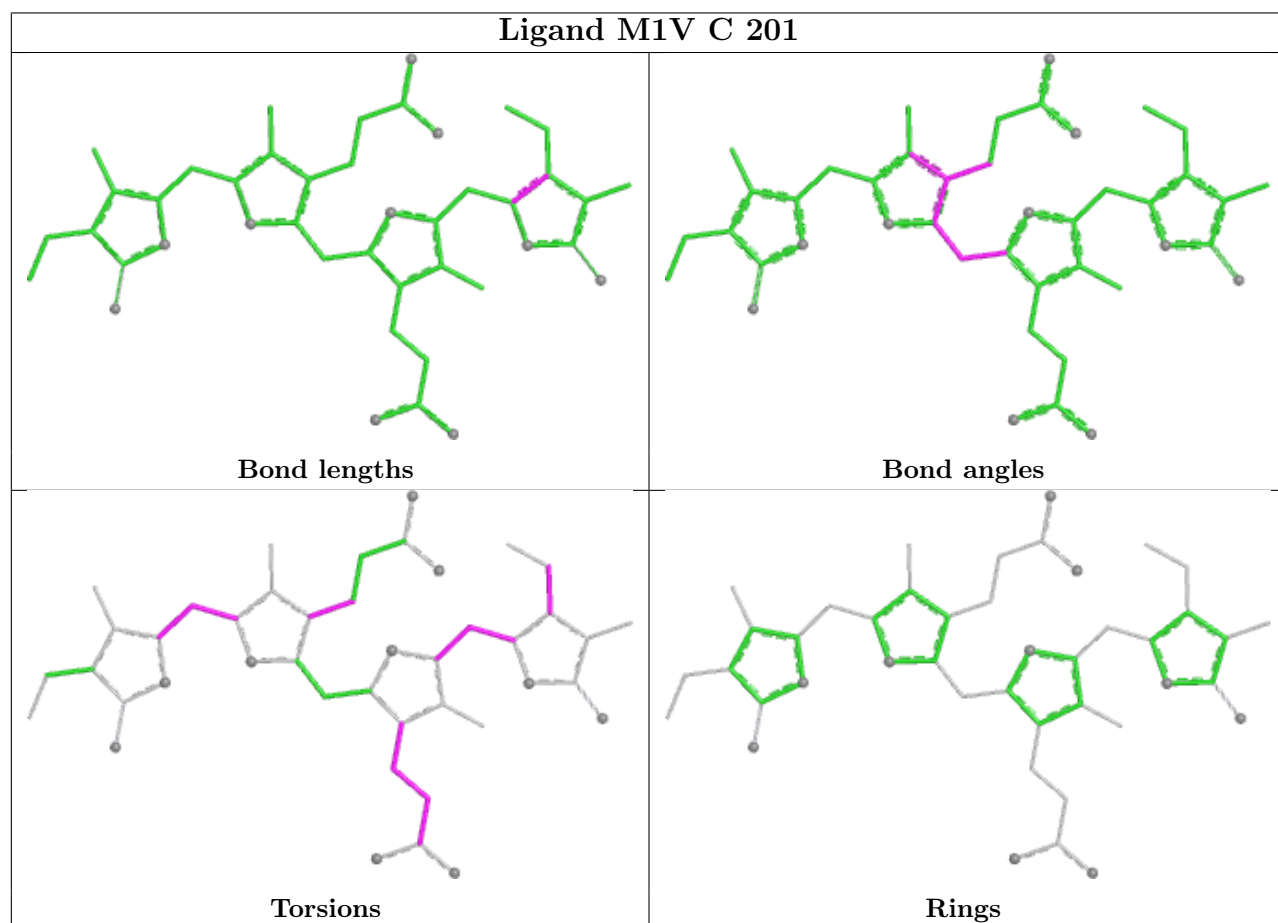
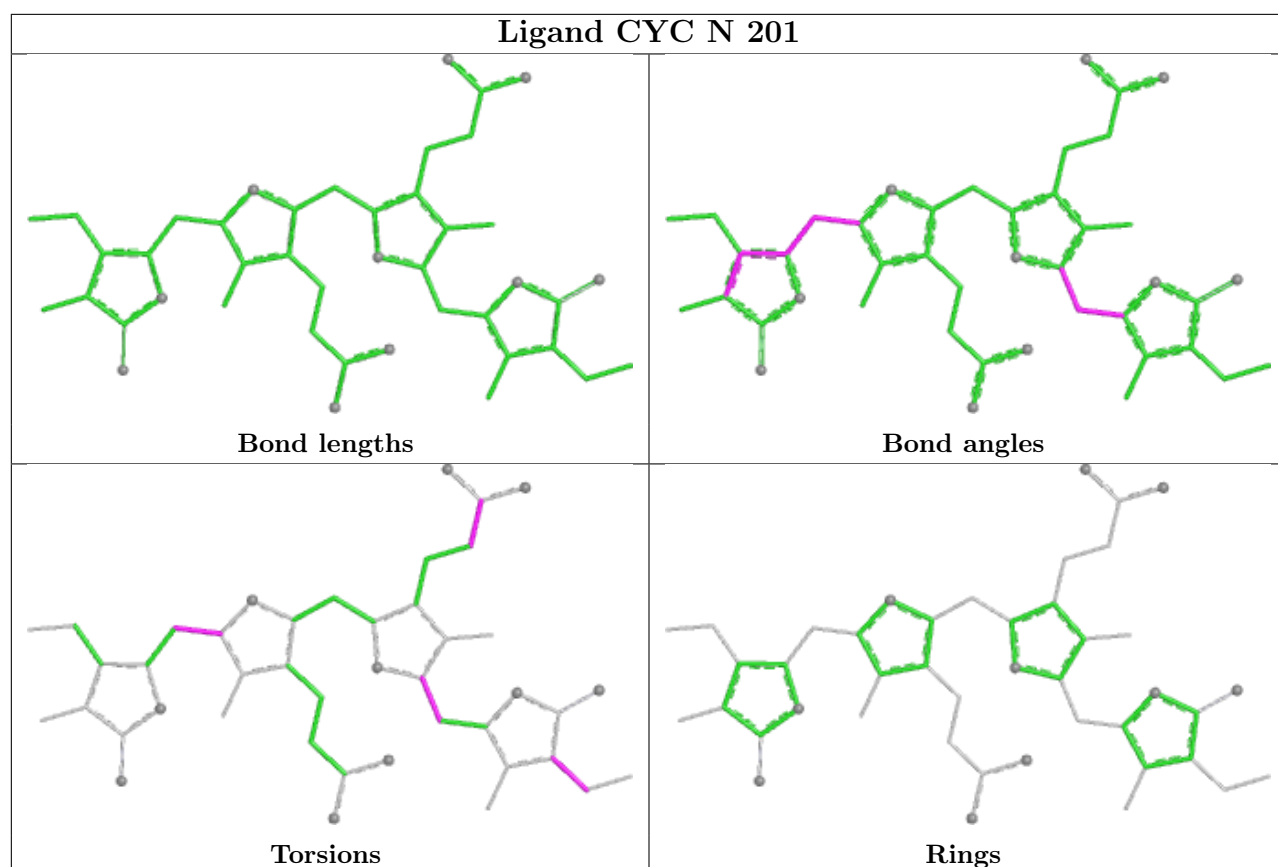
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	201	CYC	4	0
8	O	201	CYC	3	0
8	B	201	CYC	3	0
8	N	201	CYC	2	0
9	C	201	M1V	6	0
9	K	801	M1V	9	0
8	A	201	CYC	2	0
8	F	201	CYC	2	0
8	D	201	CYC	1	0
8	J	201	CYC	2	0
8	Q	201	CYC	2	0
8	R	201	CYC	3	0
8	E	201	CYC	4	0
8	L	201	CYC	5	0
8	M	201	CYC	3	0
8	P	201	CYC	7	0
8	I	201	CYC	3	0
8	G	201	CYC	4	0

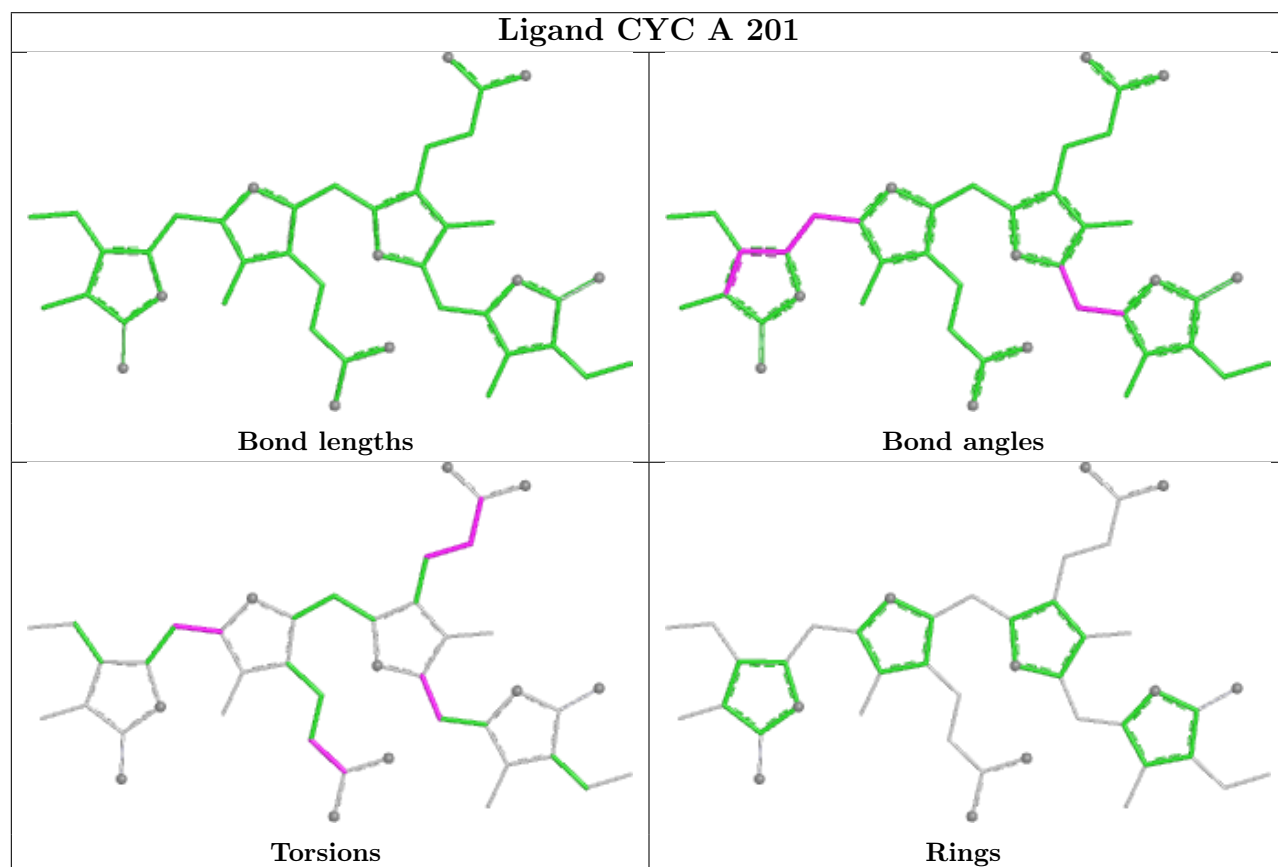
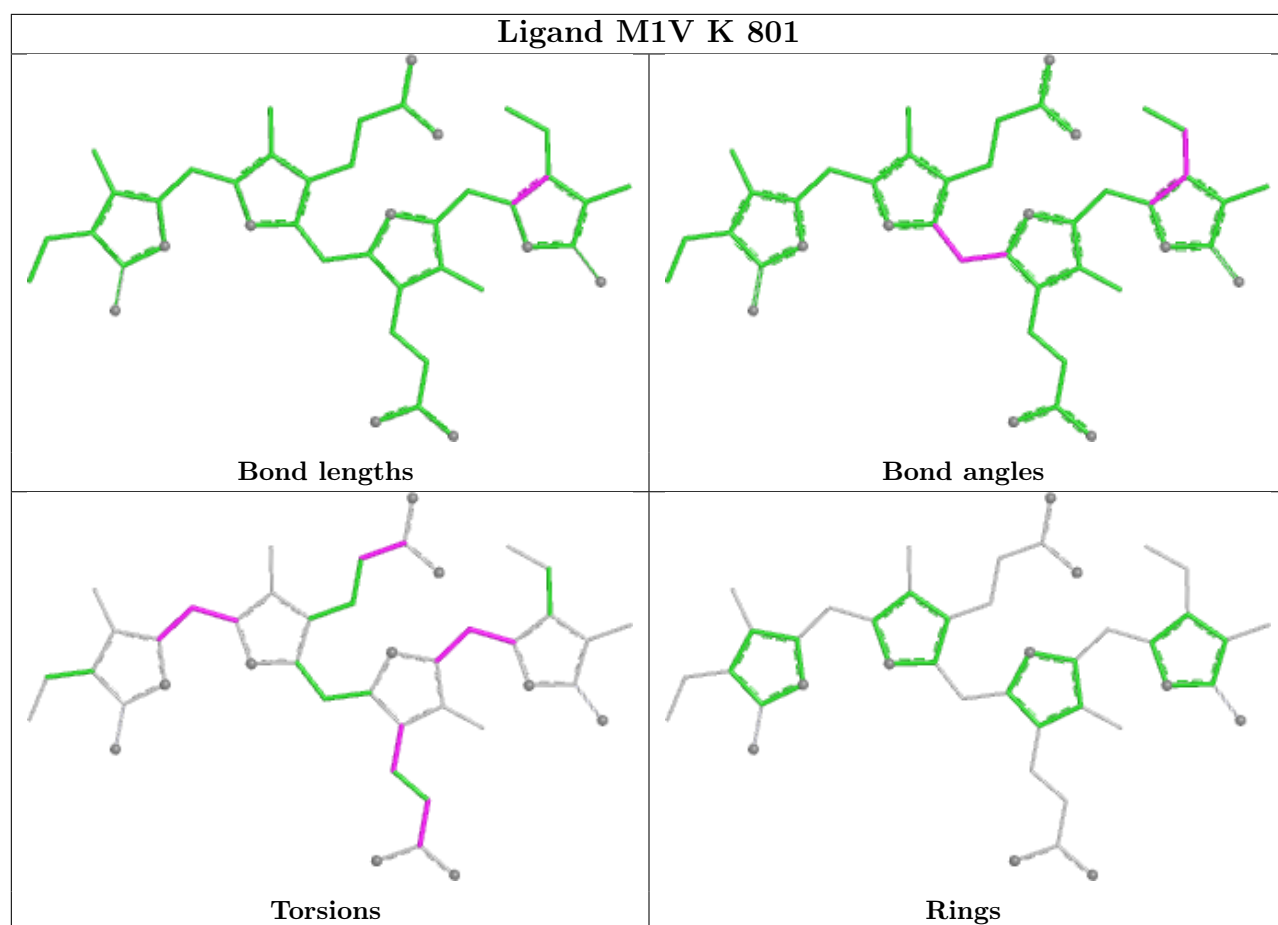
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

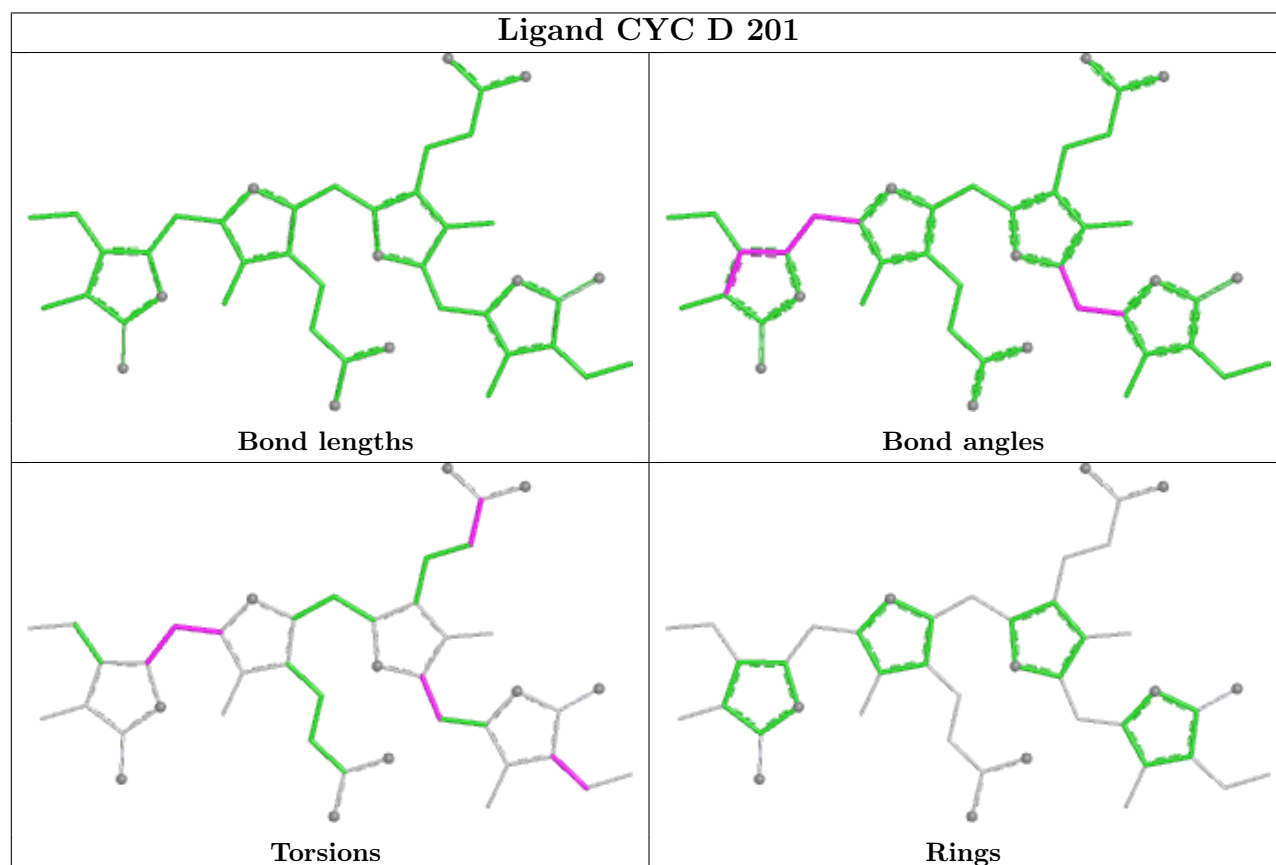
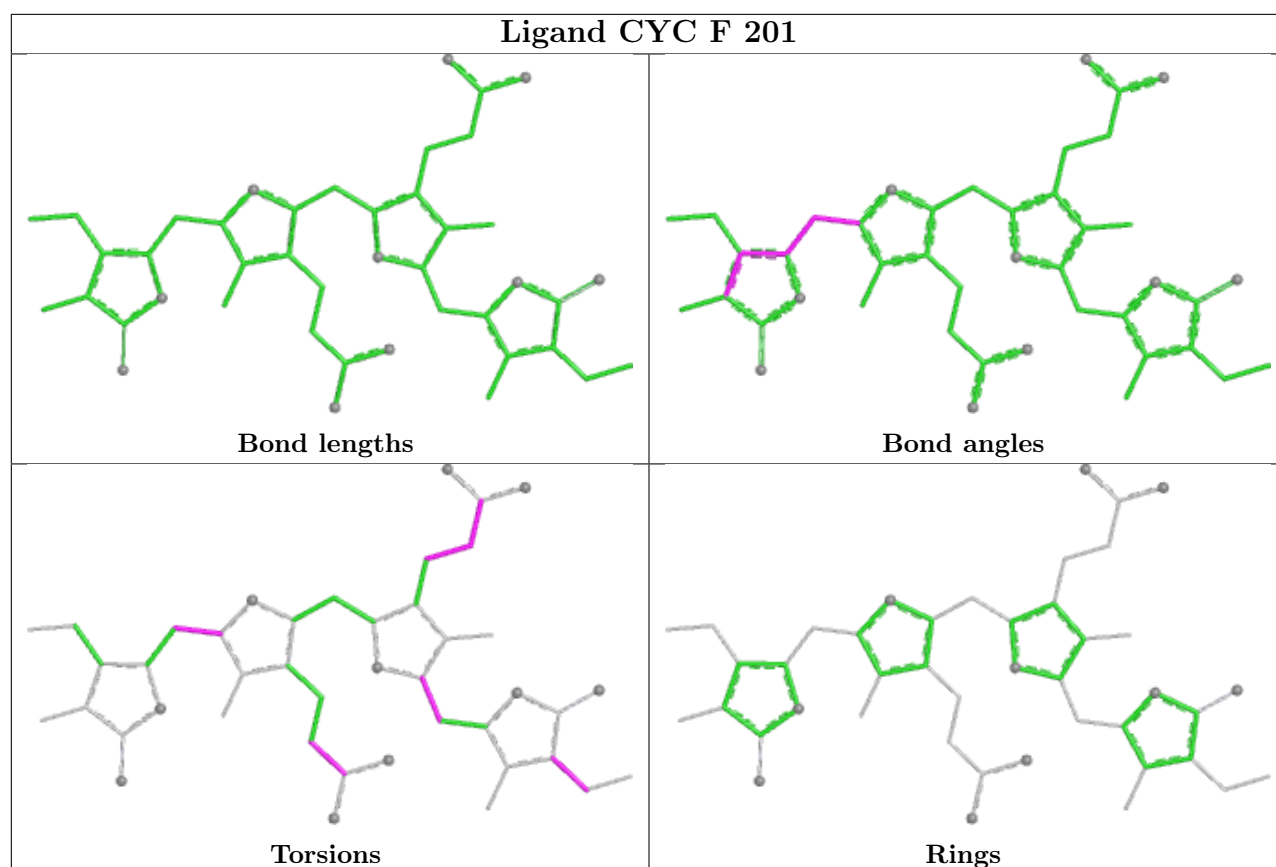
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



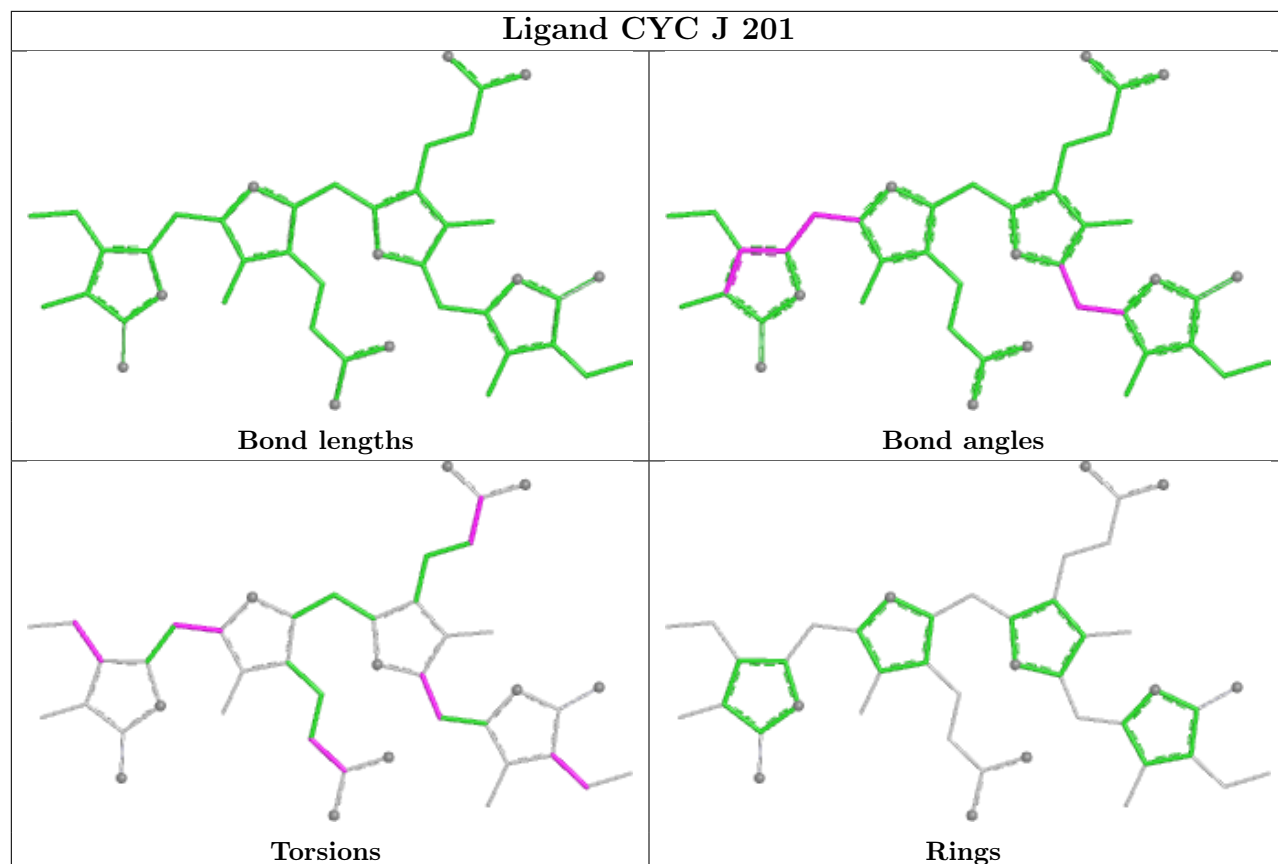




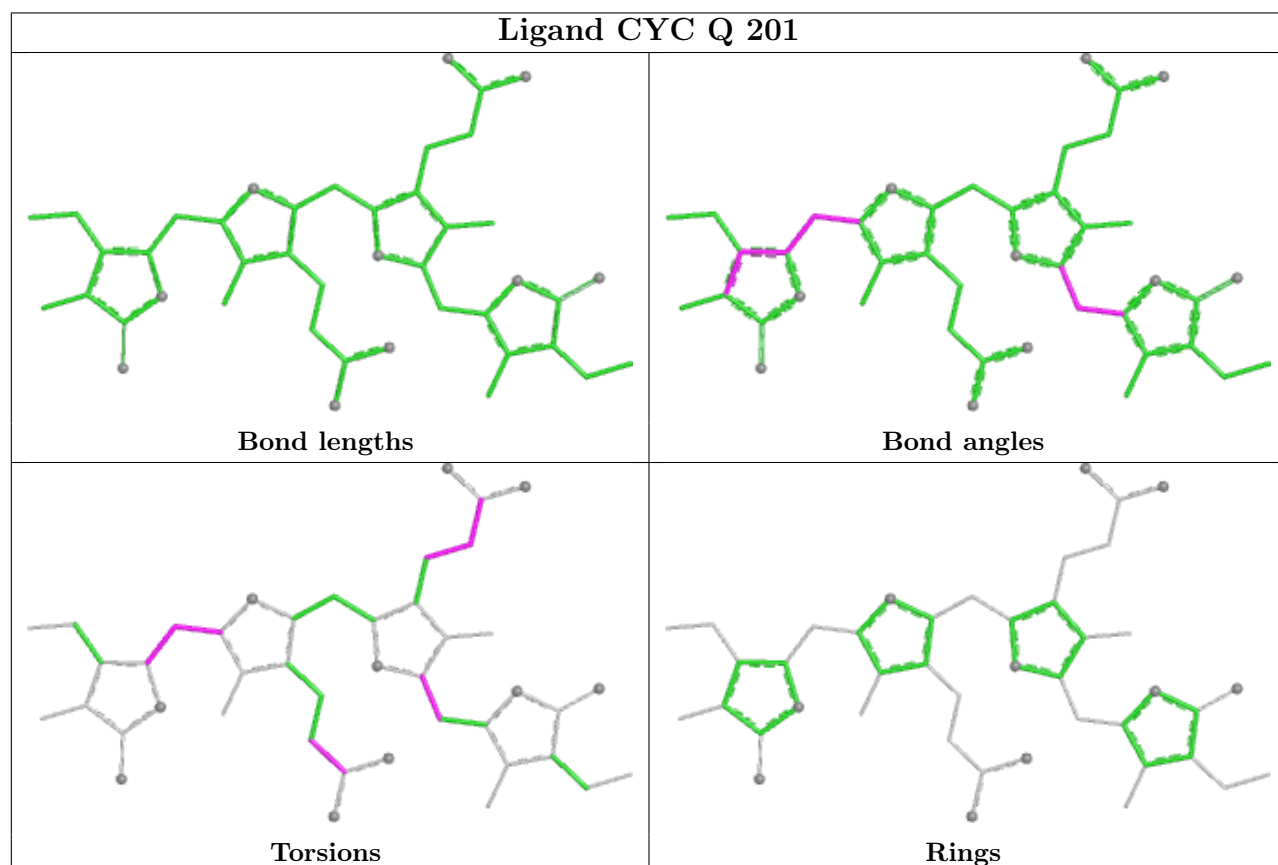


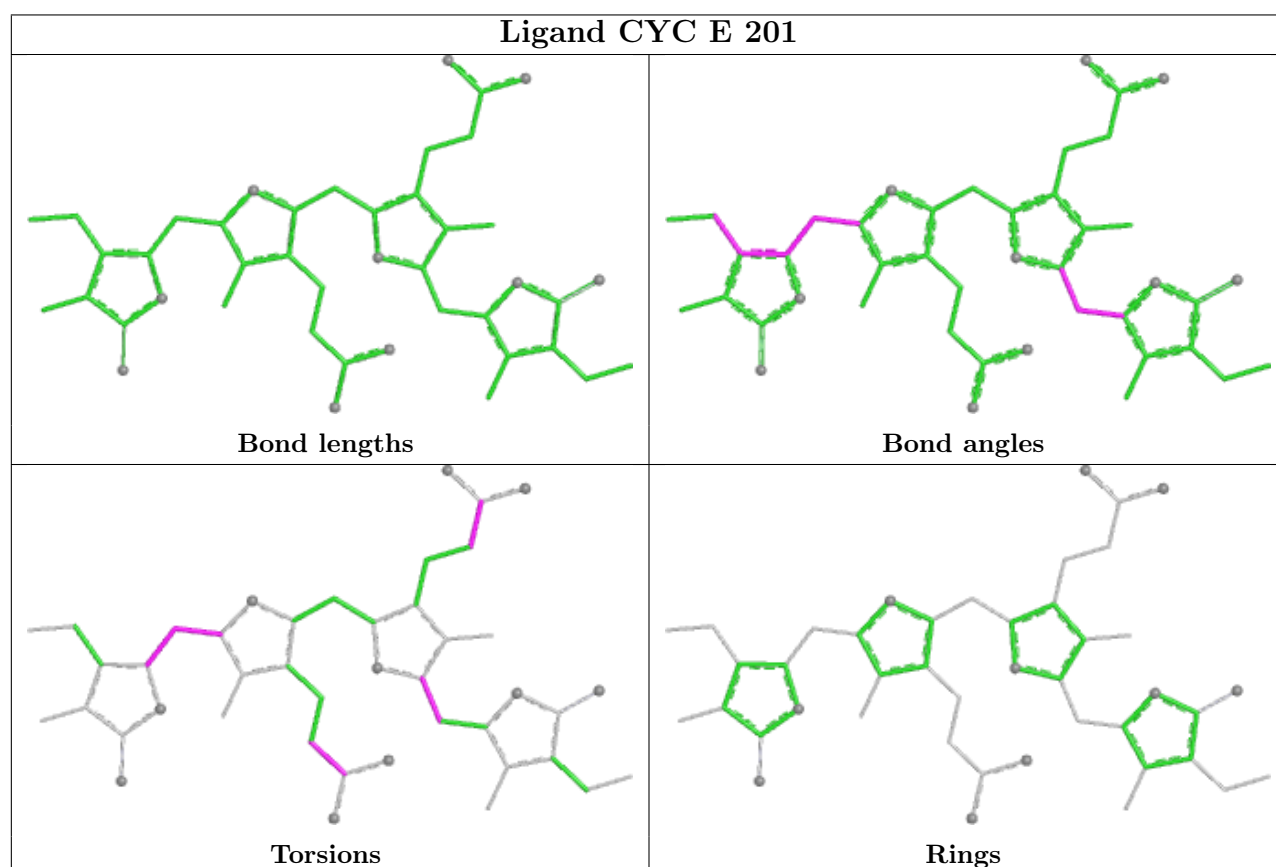
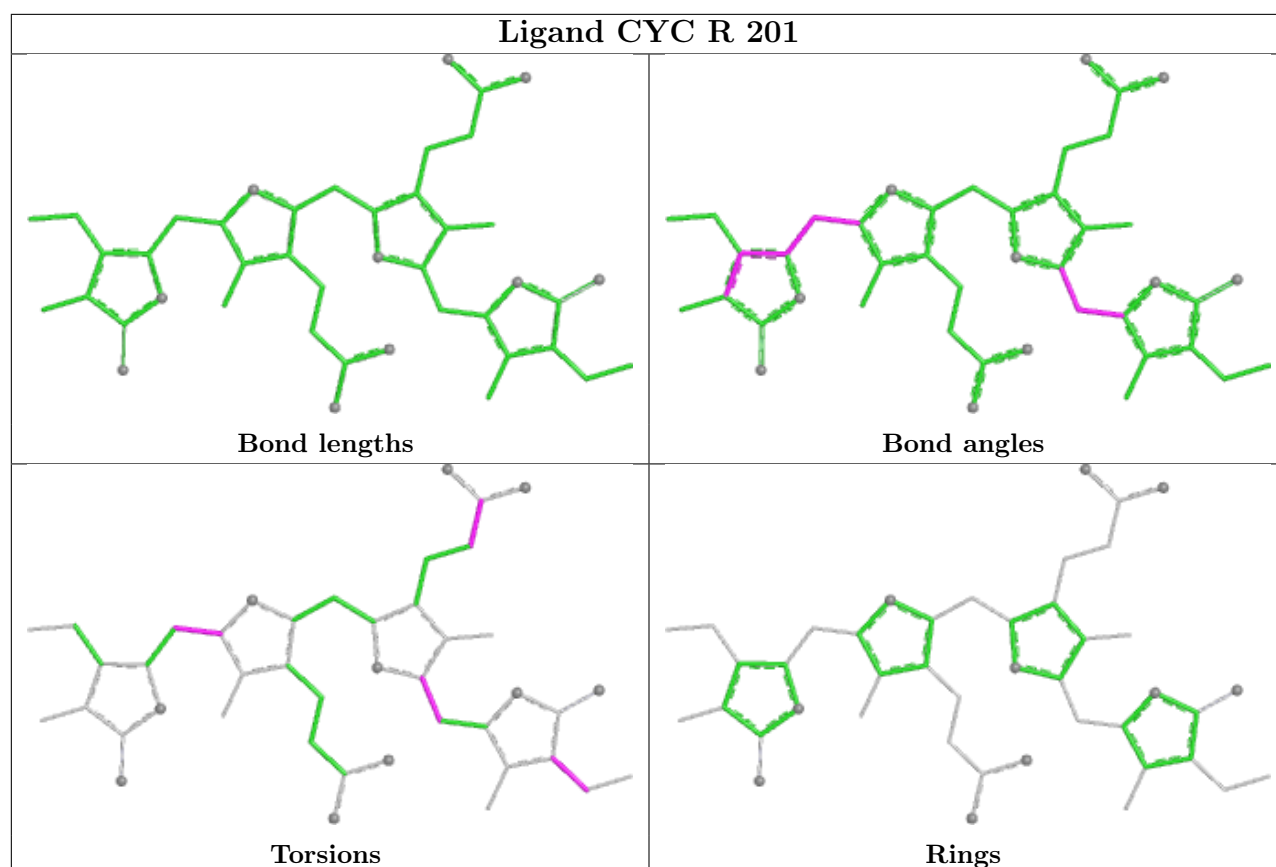


Ligand CYC J 201

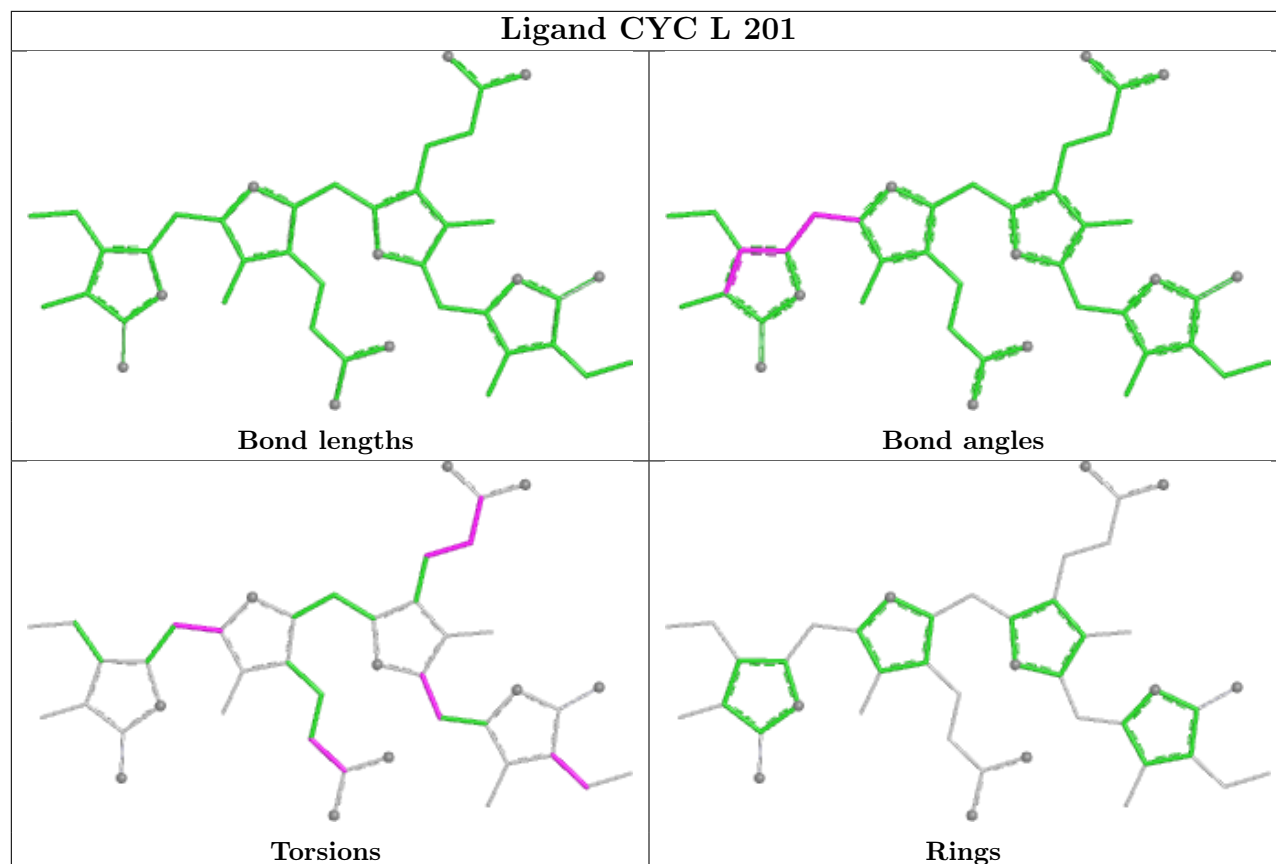


Ligand CYC Q 201

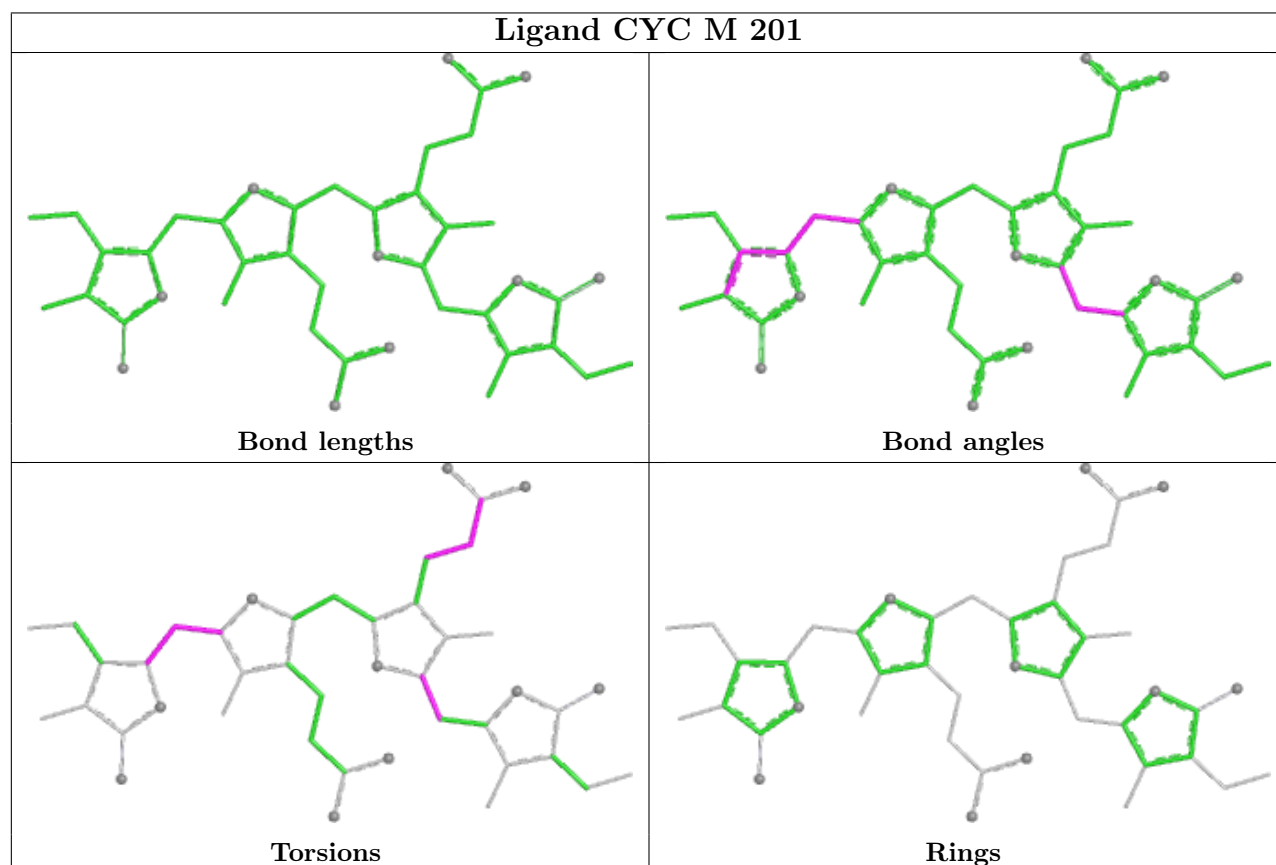


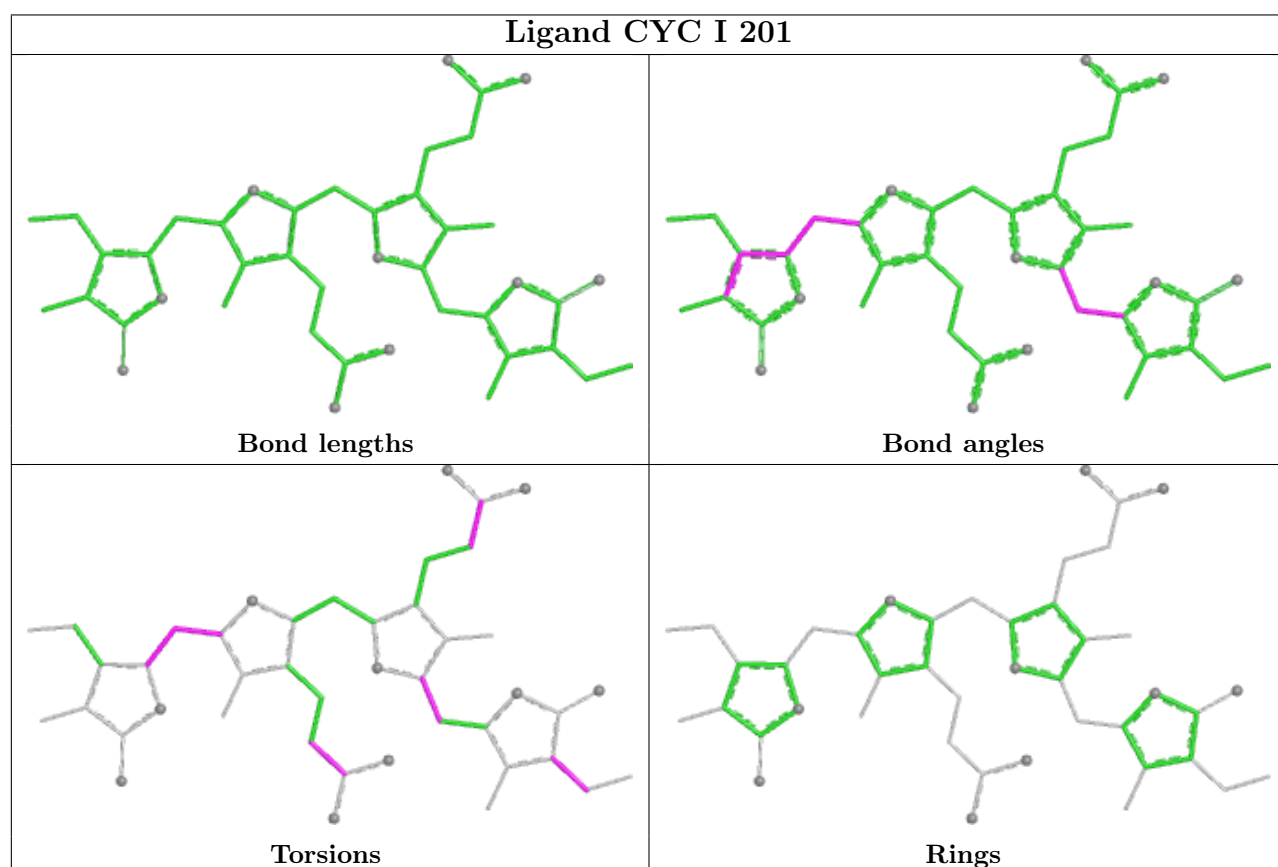
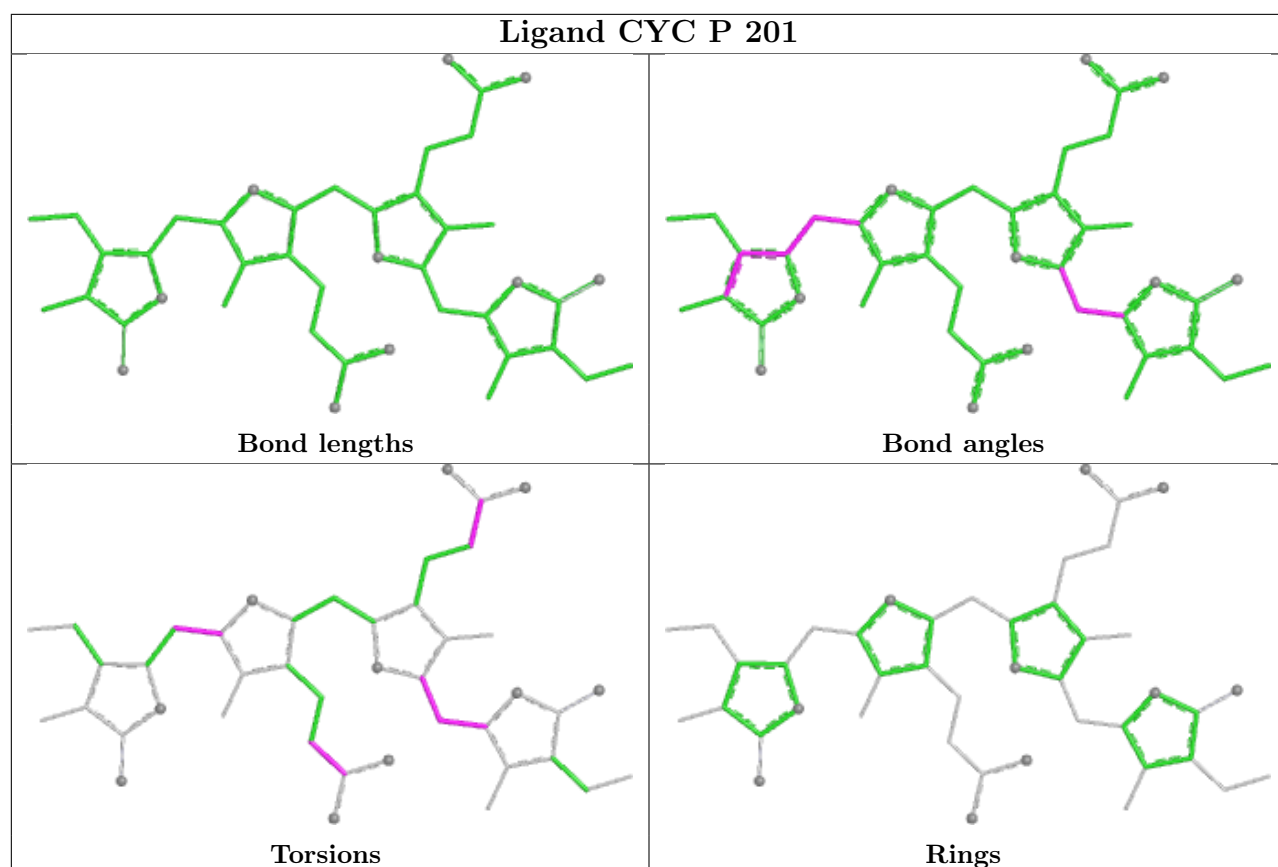


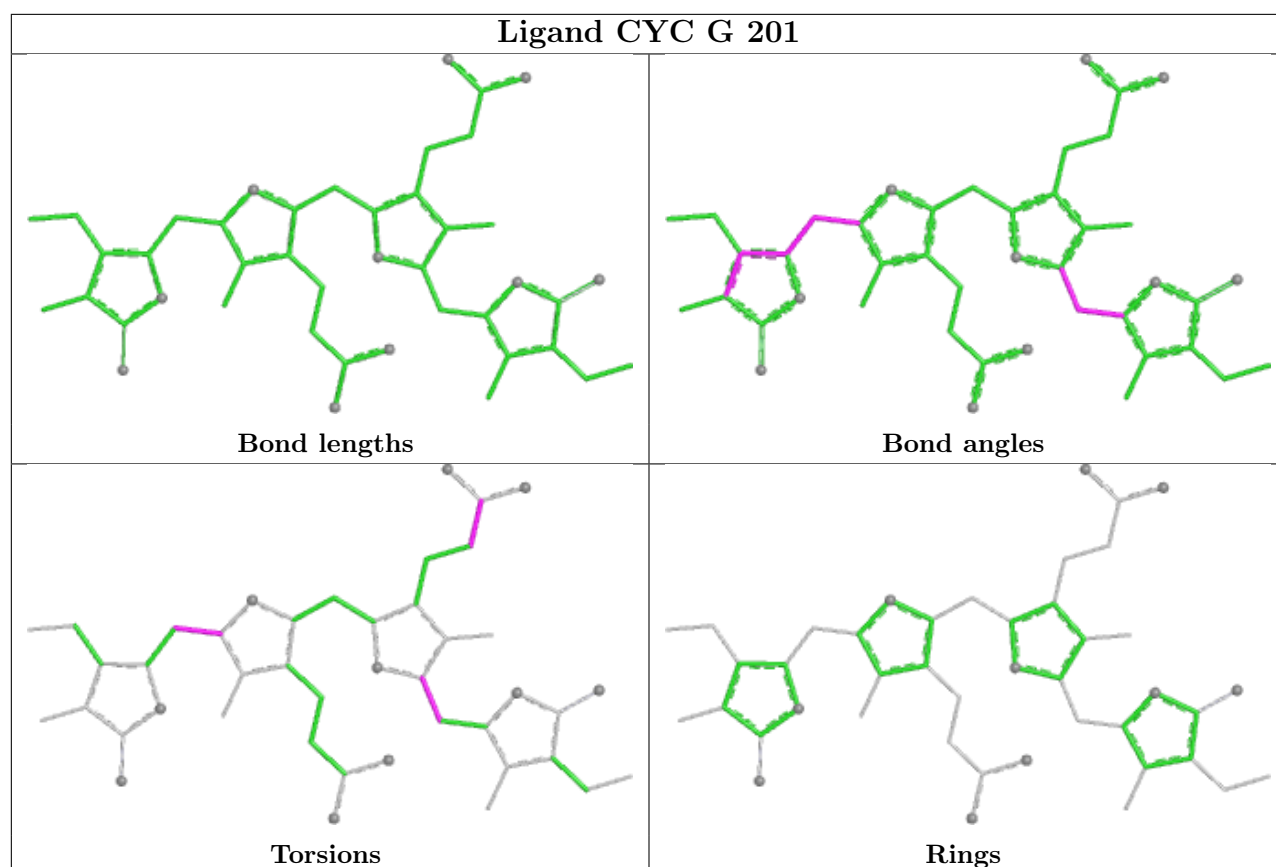
Ligand CYC L 201



Ligand CYC M 201







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.

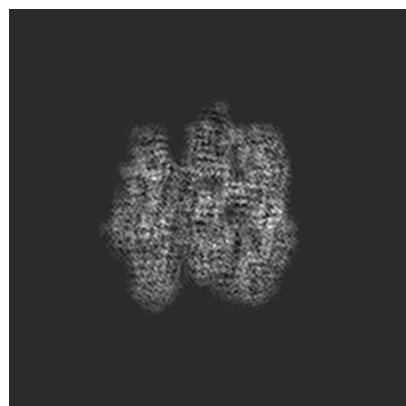
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42278. These allow visual inspection of the internal detail of the map and identification of artifacts.

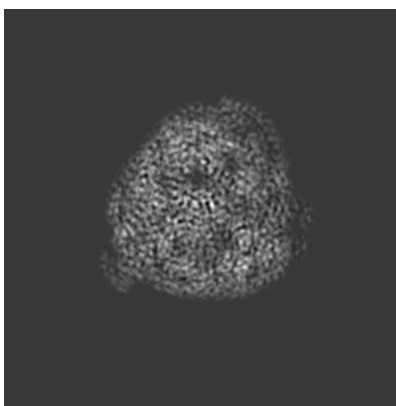
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

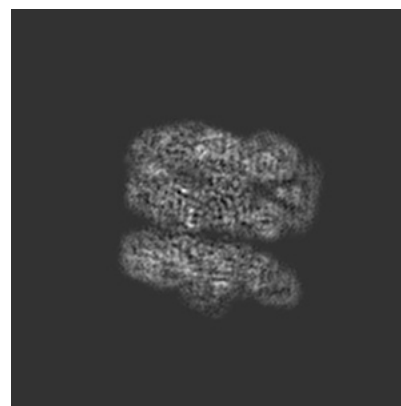
6.1.1 Primary map



X

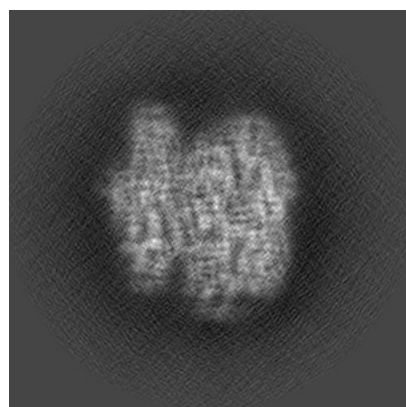


Y

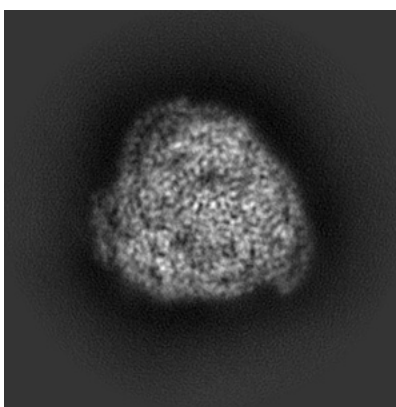


Z

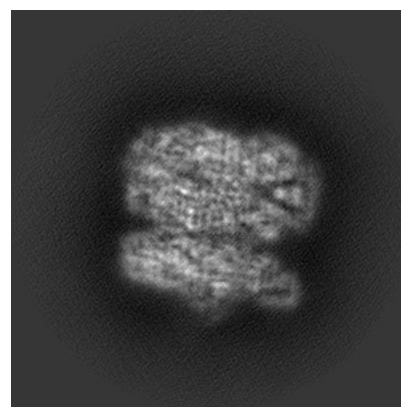
6.1.2 Raw map



X



Y

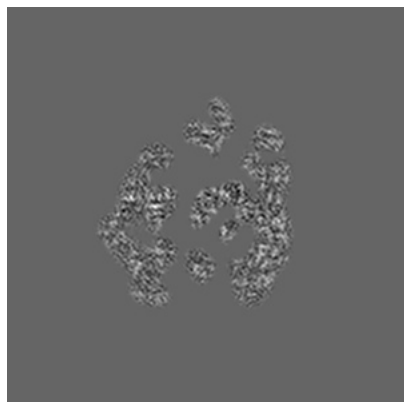


Z

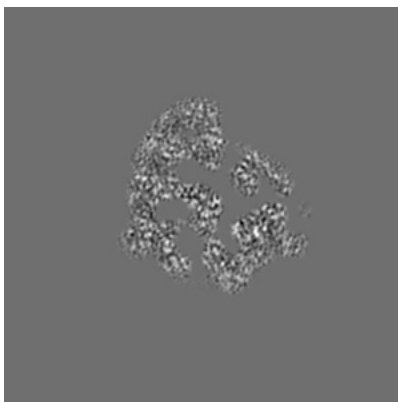
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

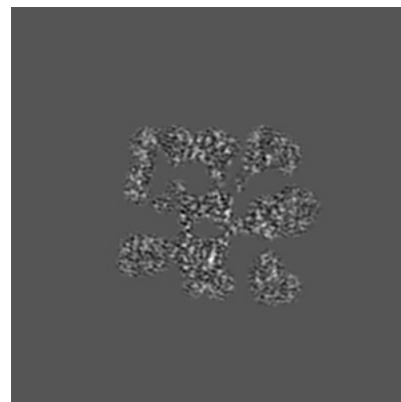
6.2.1 Primary map



X Index: 128

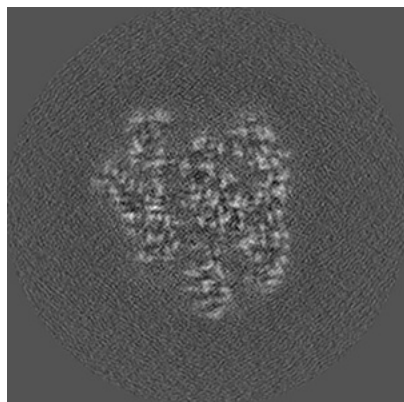


Y Index: 128

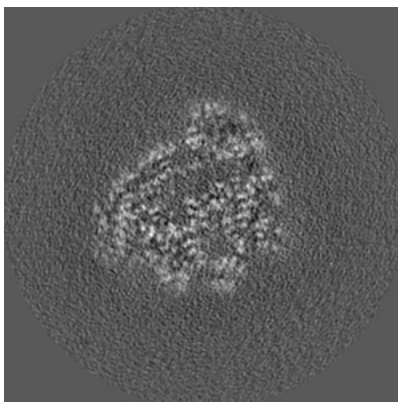


Z Index: 128

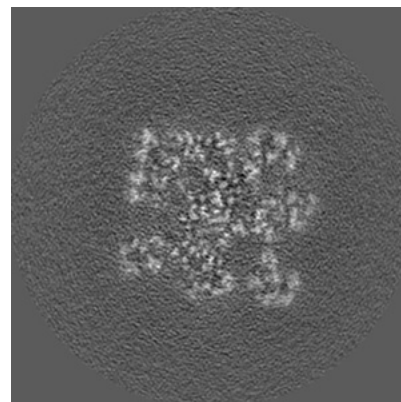
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

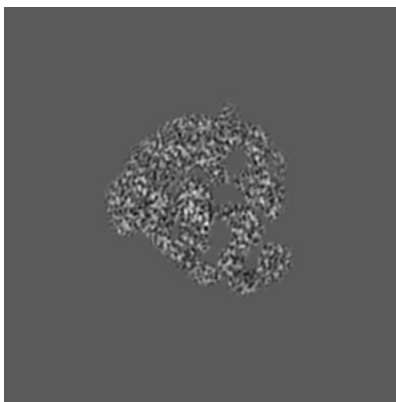
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

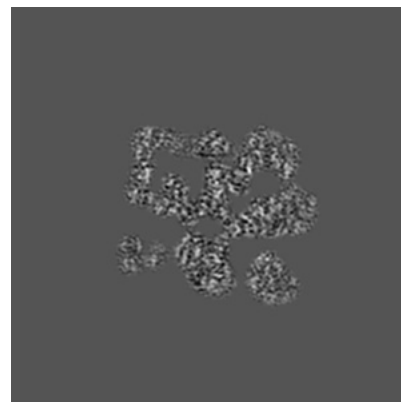
6.3.1 Primary map



X Index: 130

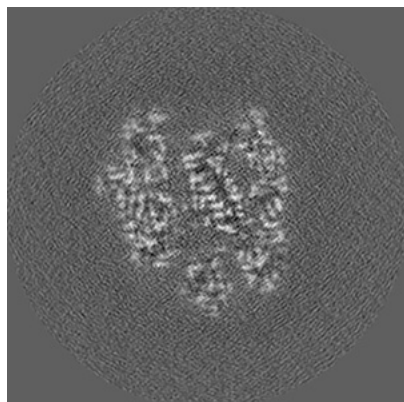


Y Index: 161

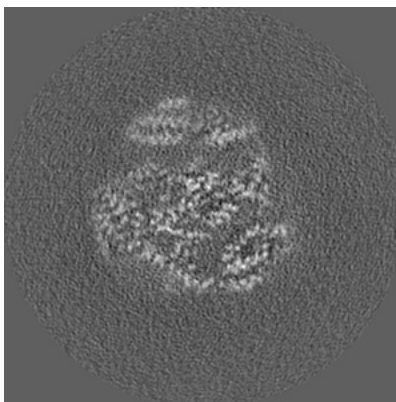


Z Index: 132

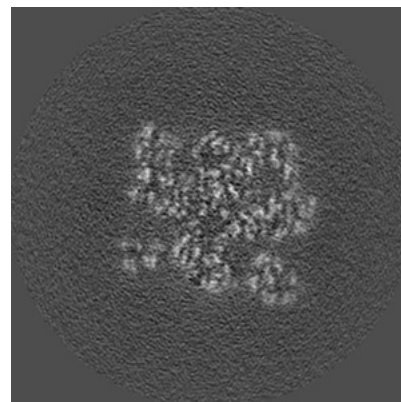
6.3.2 Raw map



X Index: 132



Y Index: 138

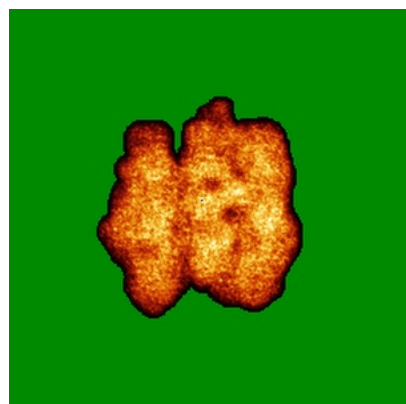


Z Index: 123

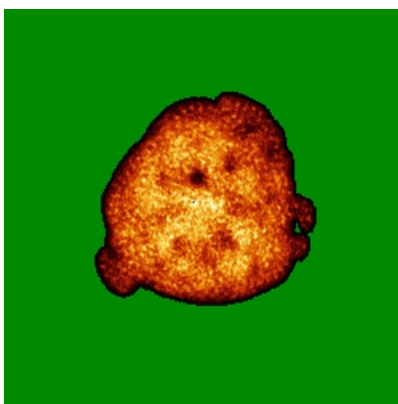
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

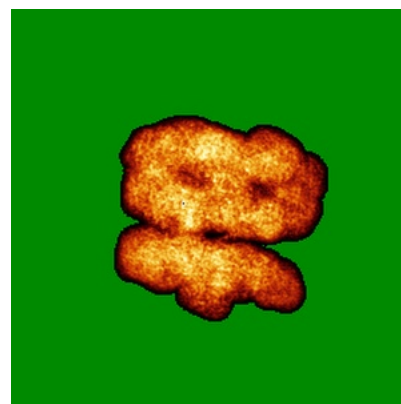
6.4.1 Primary map



X

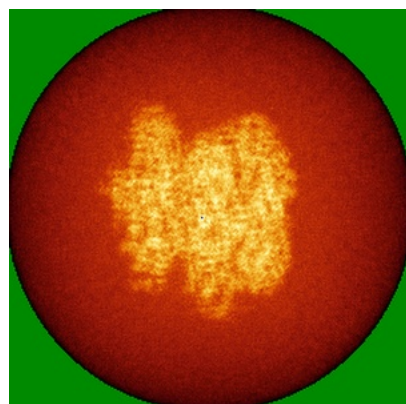


Y

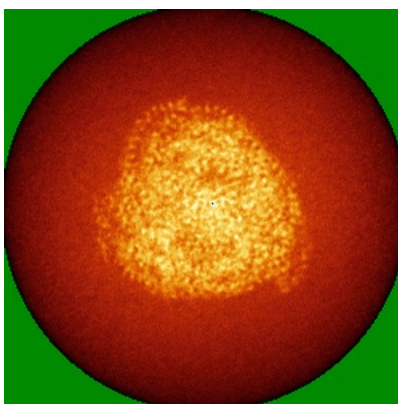


Z

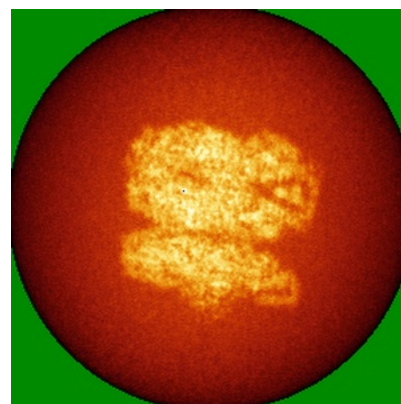
6.4.2 Raw map



X



Y

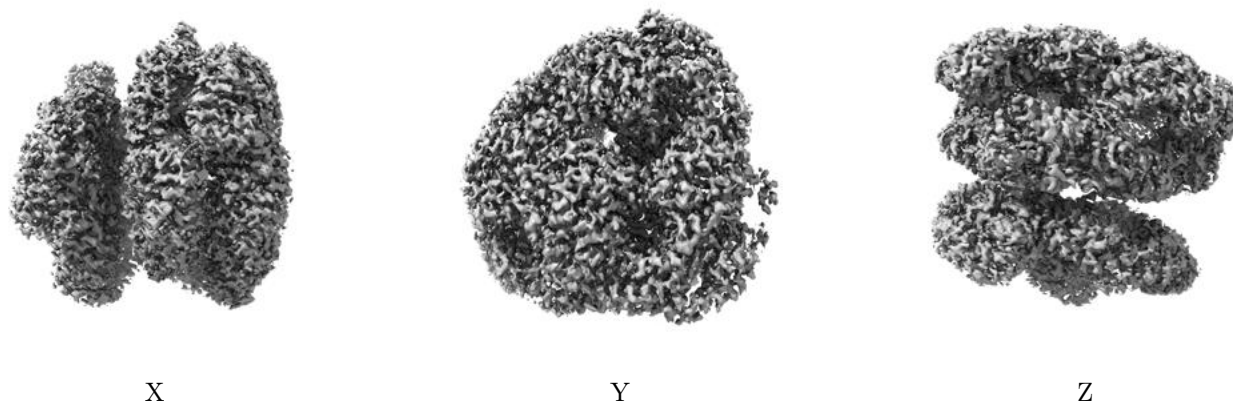


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

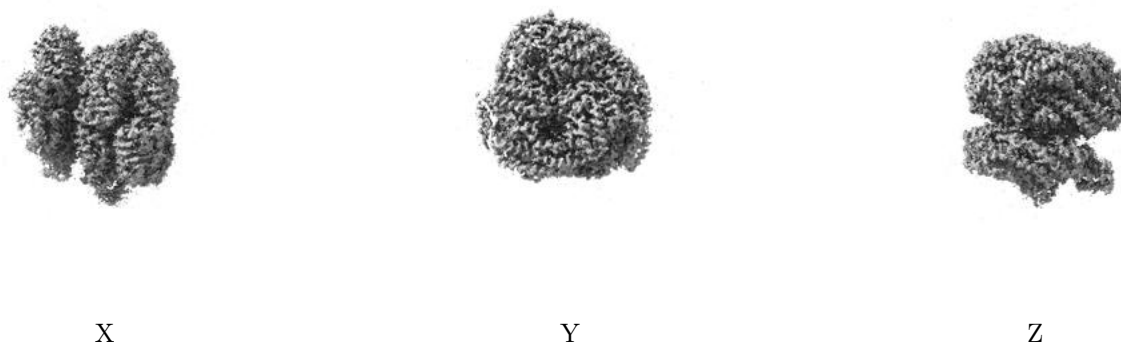
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0198. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

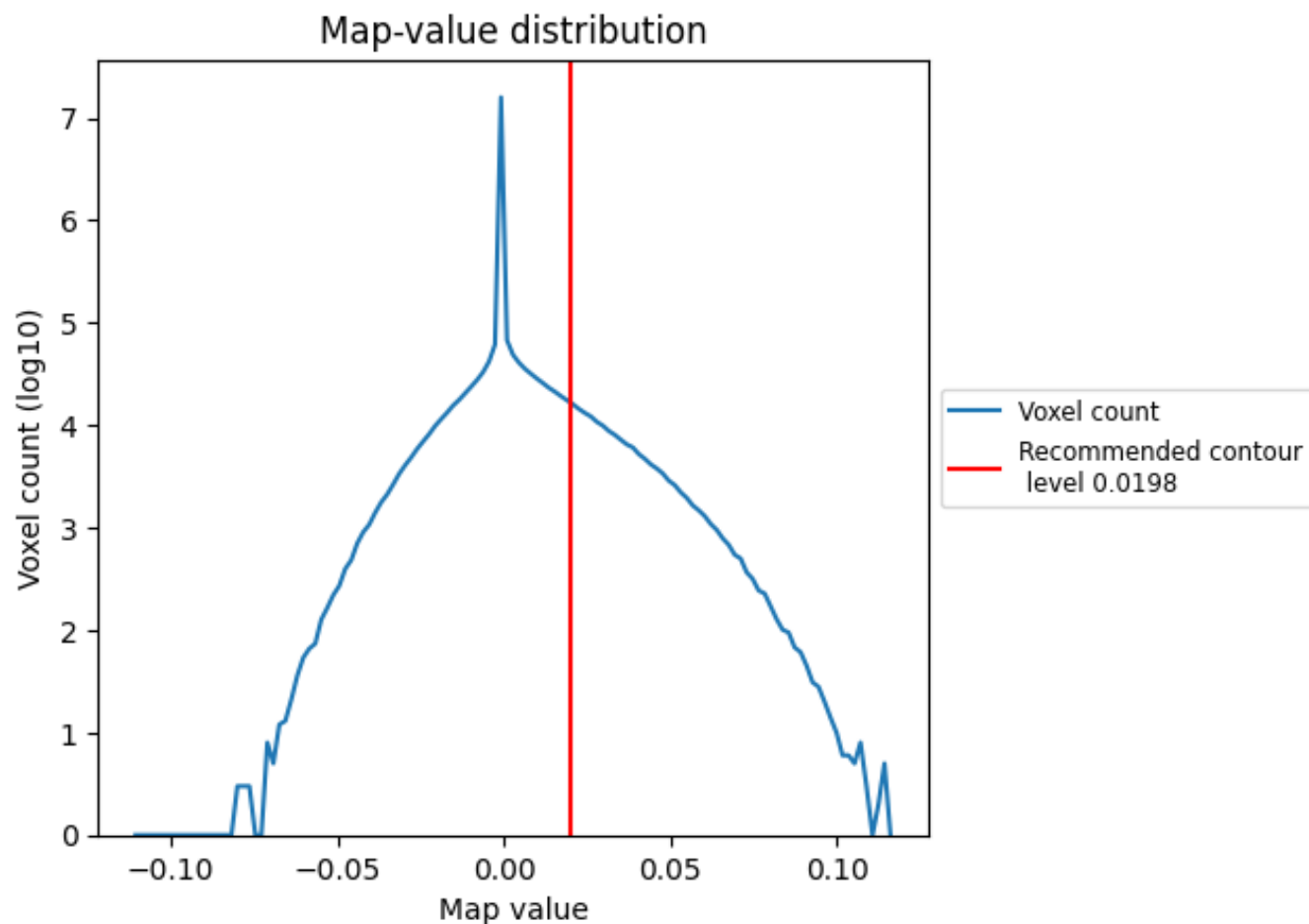
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

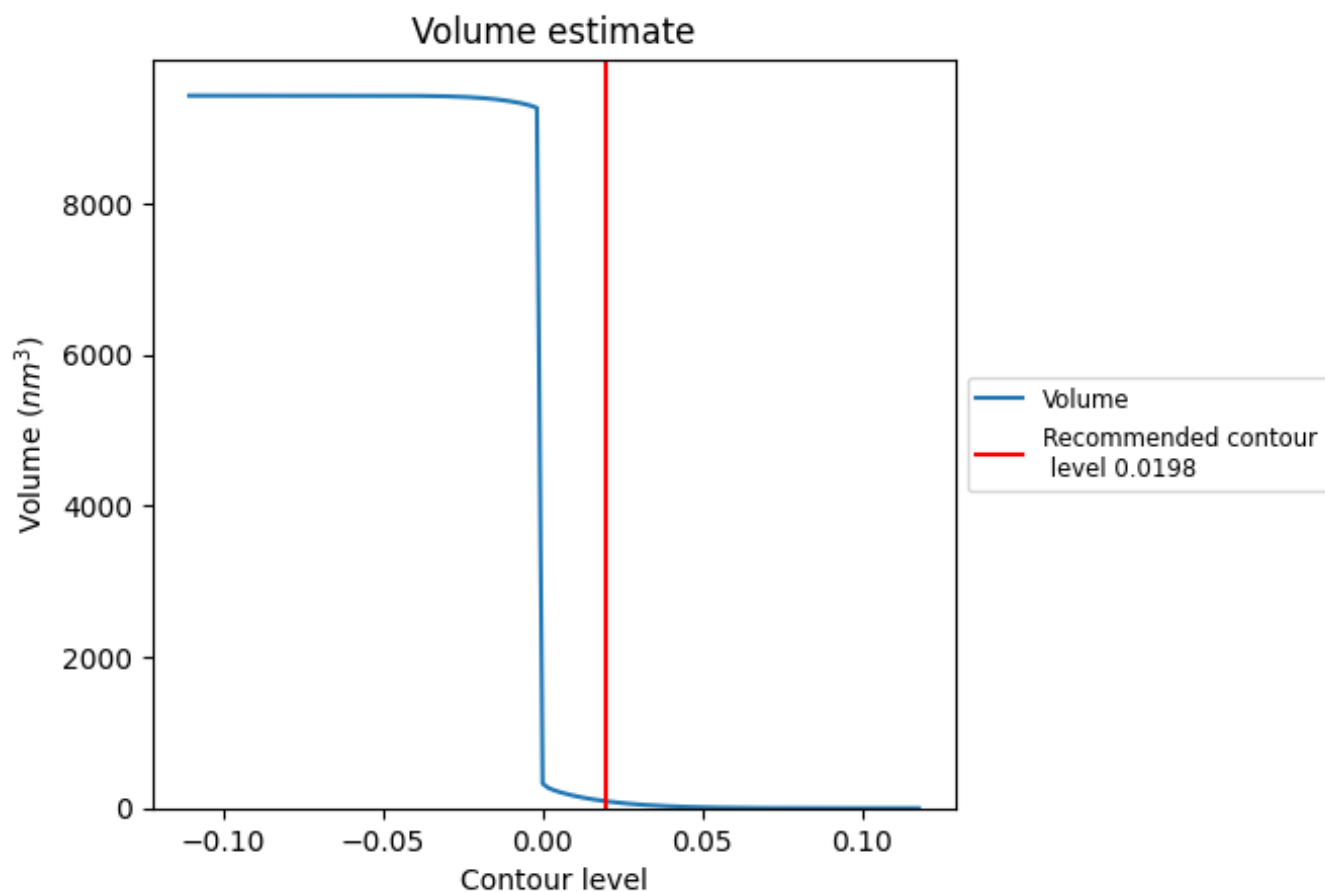
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

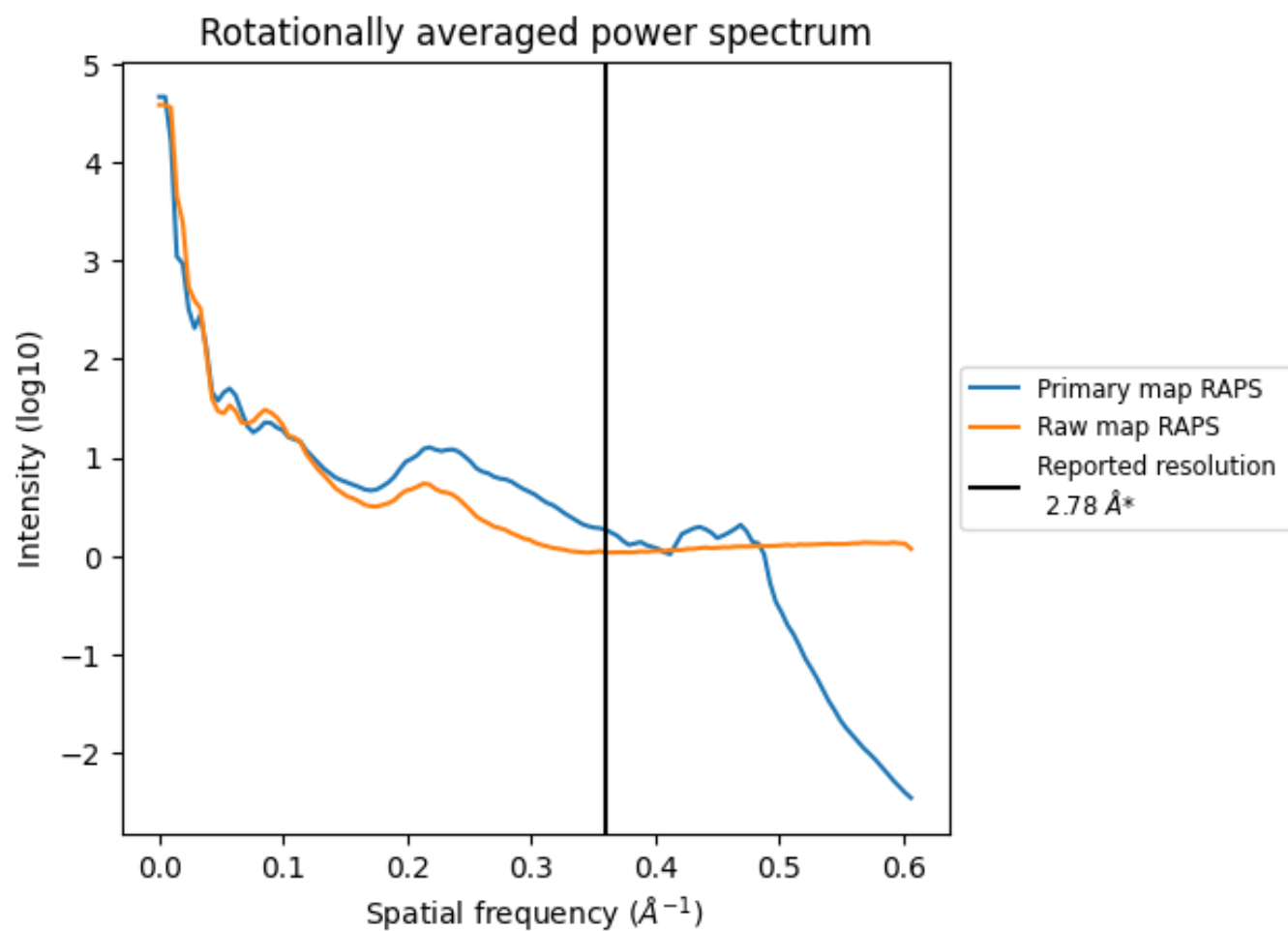
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 92 nm³; this corresponds to an approximate mass of 83 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

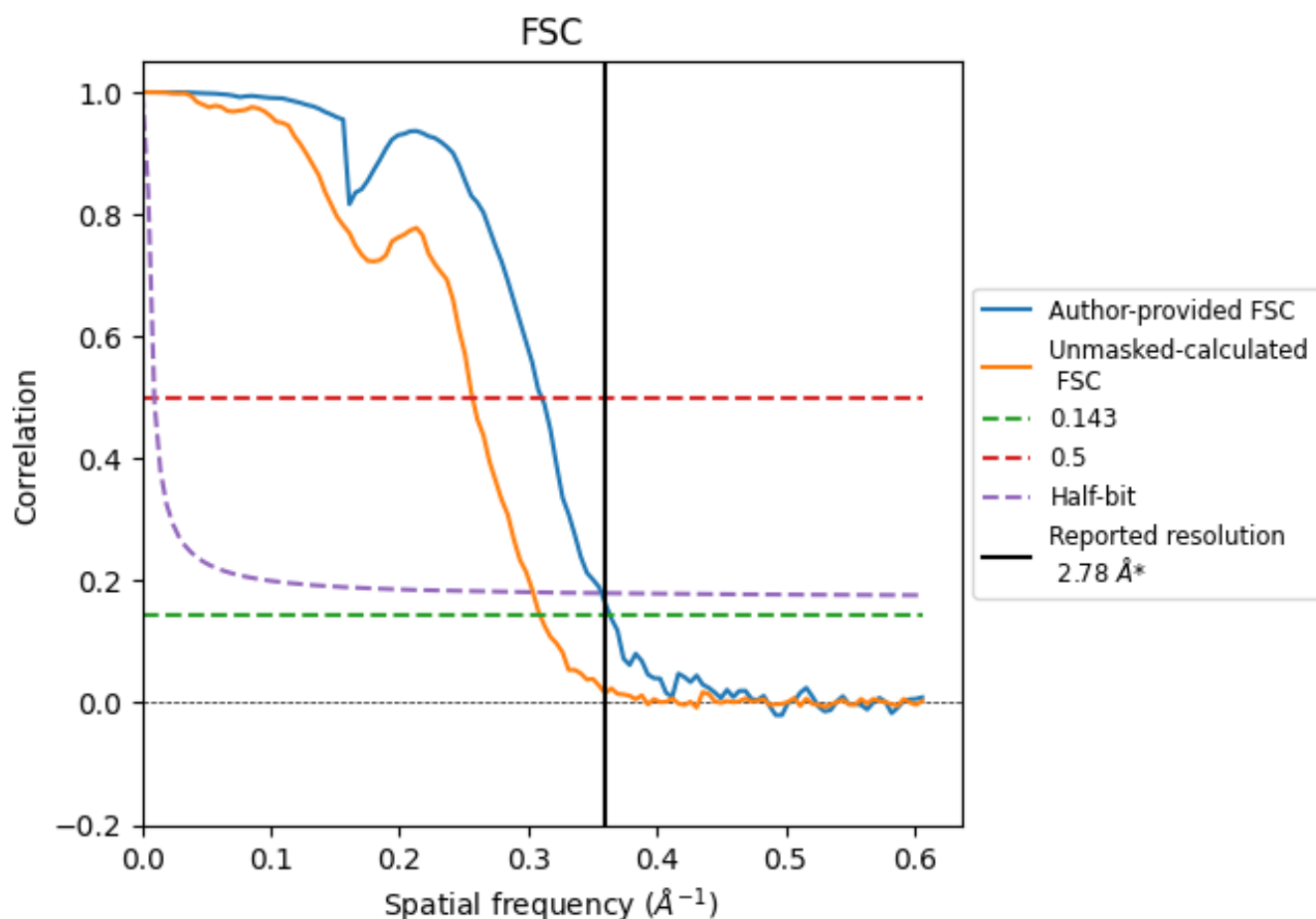


*Reported resolution corresponds to spatial frequency of 0.360 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.360 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.75	3.22	2.80
Unmasked-calculated*	3.23	3.90	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.23 differs from the reported value 2.78 by more than 10 %

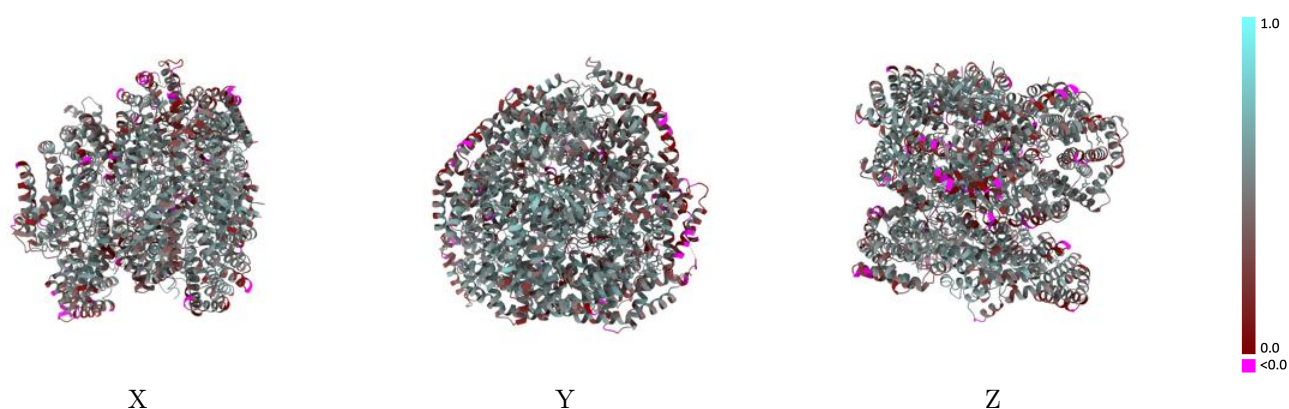
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42278 and PDB model 8UHE. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)

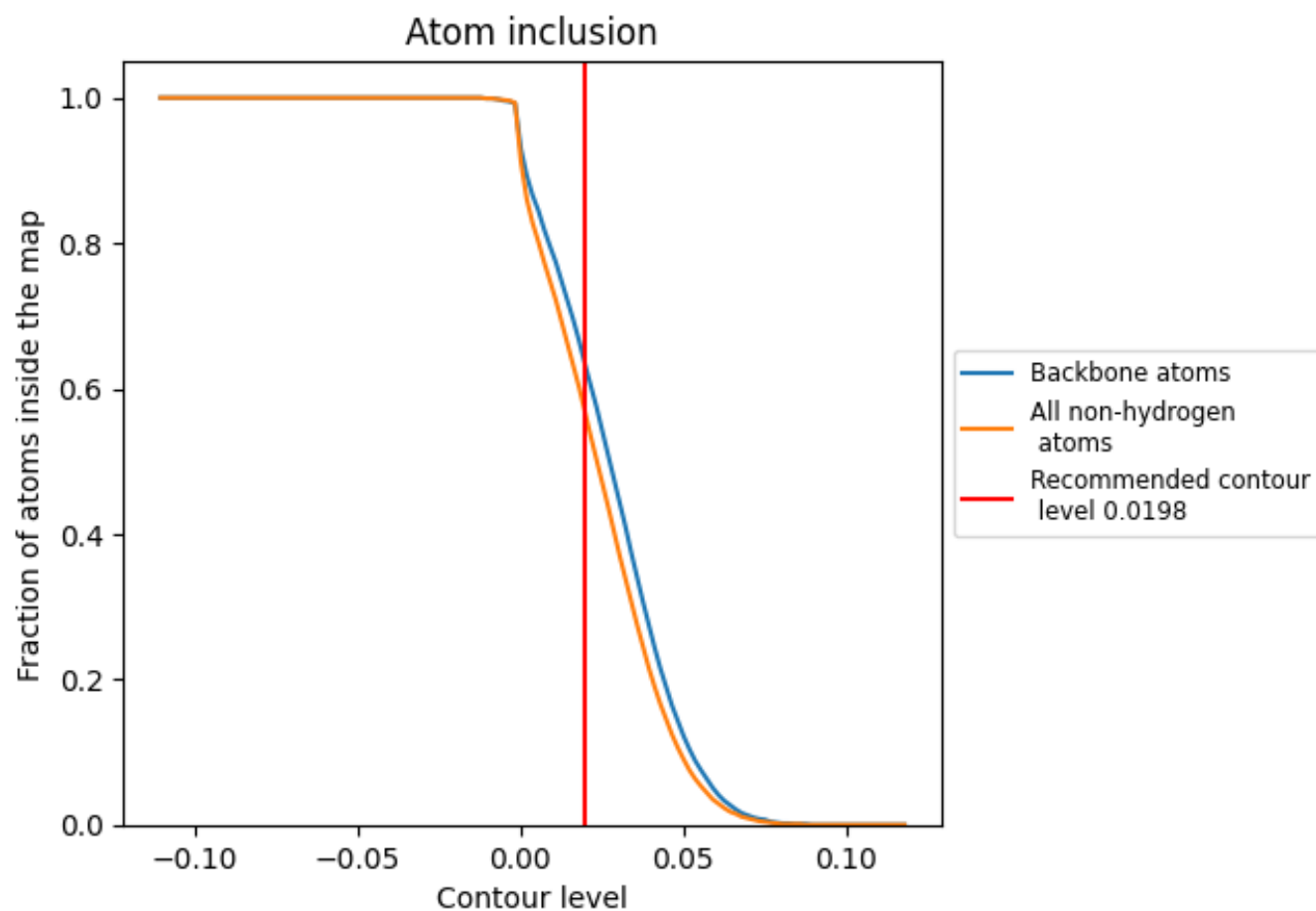


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0198) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5670	 0.4570
A	 0.4740	 0.4100
B	 0.5420	 0.4410
C	 0.5600	 0.4750
D	 0.7220	 0.5320
E	 0.6530	 0.4900
F	 0.6220	 0.4640
G	 0.6220	 0.4770
H	 0.5840	 0.4620
I	 0.6280	 0.5020
J	 0.6170	 0.4890
K	 0.5160	 0.4390
L	 0.5500	 0.4550
M	 0.4360	 0.3610
N	 0.6000	 0.4690
O	 0.5090	 0.4350
P	 0.5570	 0.4490
Q	 0.5430	 0.4360
R	 0.5790	 0.4630
S	 0.6530	 0.4890

