



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 01:36 AM UTC

PDB ID : 5TOU / pdb_00005tou
Title : STRUCTURE OF C-PHYCOCYANIN FROM ARCTIC PSEUDAN-
ABAENA SP. LW0831
Authors : Wang, Q.M.; Li, C.Y.; Su, H.N.; Zhang, Y.Z.; Xie, B.B.
Deposited on : 2016-10-18
Resolution : 2.04 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

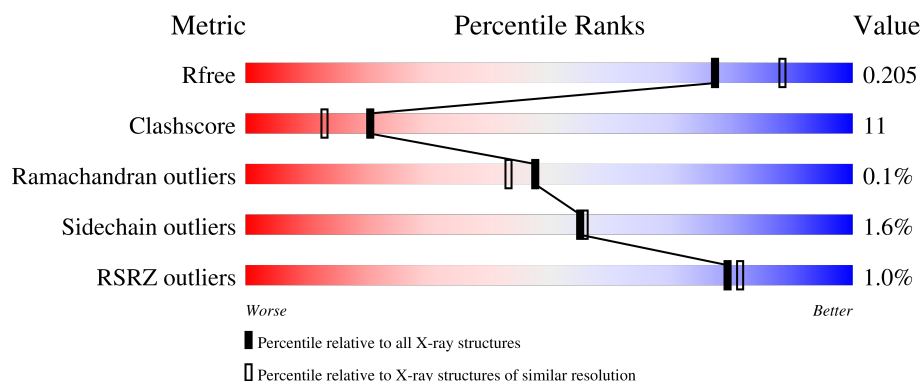
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	162	90% 10%
1	C	162	2% 87% 12% .
1	E	162	88% 11% .
1	G	162	93% 7%
1	I	162	2% 88% 11% .

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Mol	Chain	Length	Quality of chain
1	K	162	89% 11%
2	B	172	2% 95% 5%
2	D	172	4% 86% 12%
2	F	172	% 87% 12%
2	H	172	2% 91% 9%
2	J	172	% 88% 12%
2	L	172	% 92% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17226 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.

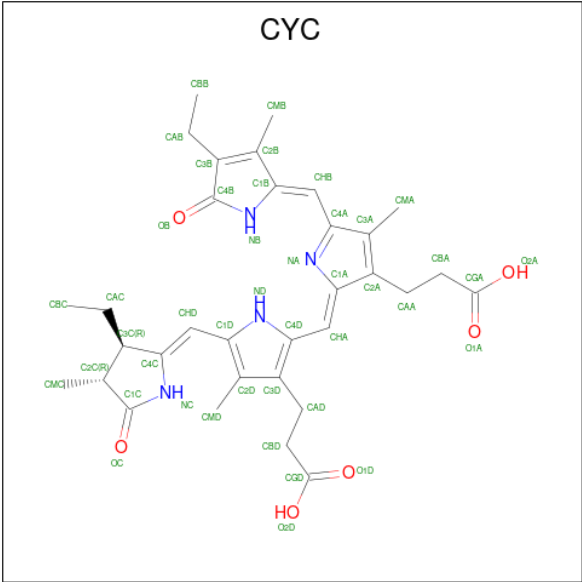
- Molecule 1 is a protein called Phycocyanin alpha-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	162	Total	C	N	O	S	0	1	0
			1215	760	202	246	7			
1	A	162	Total	C	N	O	S	0	1	0
			1215	760	202	246	7			
1	E	162	Total	C	N	O	S	0	0	0
			1209	757	201	244	7			
1	I	162	Total	C	N	O	S	0	0	0
			1209	757	201	244	7			
1	G	162	Total	C	N	O	S	0	2	0
			1222	764	203	248	7			
1	K	162	Total	C	N	O	S	0	0	0
			1209	757	201	244	7			

- Molecule 2 is a protein called Phycocyanin beta-1 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	172	Total	C	N	O	S	0	1	0
			1253	776	219	249	9			
2	B	172	Total	C	N	O	S	0	0	0
			1248	773	218	248	9			
2	F	172	Total	C	N	O	S	0	0	0
			1247	773	218	247	9			
2	J	172	Total	C	N	O	S	0	0	0
			1247	773	218	247	9			
2	H	172	Total	C	N	O	S	0	0	0
			1247	773	218	247	9			
2	L	172	Total	C	N	O	S	0	0	0
			1248	773	218	248	9			

- Molecule 3 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			43	33	4	6		
3	K	1	Total	C	N	O	0	0
			43	33	4	6		
3	L	1	Total	C	N	O	0	0
			43	33	4	6		
3	L	1	Total	C	N	O	0	0
			43	33	4	6		

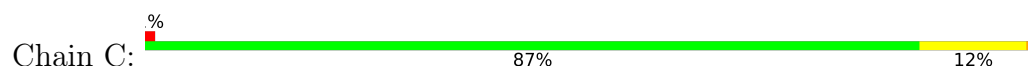
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	144	Total	O	0	0
			144	144		
4	D	171	Total	O	0	0
			171	171		
4	A	160	Total	O	0	0
			160	160		
4	B	138	Total	O	0	0
			138	138		
4	E	128	Total	O	0	0
			128	128		
4	F	113	Total	O	0	0
			113	113		
4	I	119	Total	O	0	0
			119	119		
4	J	123	Total	O	0	0
			123	123		
4	G	156	Total	O	0	0
			156	156		
4	H	150	Total	O	0	0
			150	150		
4	K	122	Total	O	0	0
			122	122		
4	L	159	Total	O	0	0
			159	159		

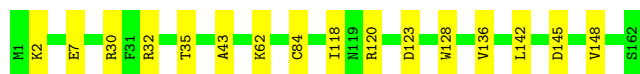
3 Residue-property plots [i](#)

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.

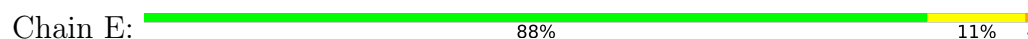
- Molecule 1: Phycocyanin alpha-1 subunit



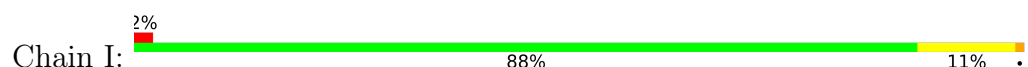
- Molecule 1: Phycocyanin alpha-1 subunit



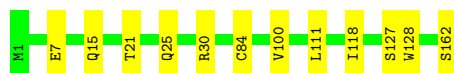
- Molecule 1: Phycocyanin alpha-1 subunit



- Molecule 1: Phycocyanin alpha-1 subunit



- Molecule 1: Phycocyanin alpha-1 subunit



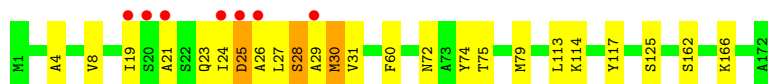
- Molecule 1: Phycocyanin alpha-1 subunit

Chain K:  89% 11%

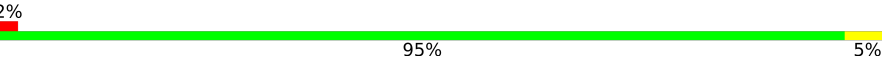


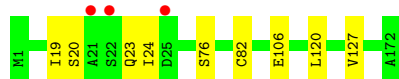
• Molecule 2: Phycocyanin beta-1 subunit

Chain D:  4% 86% 12%



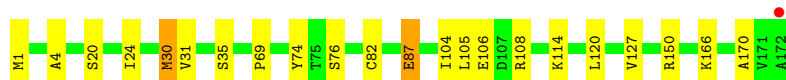
• Molecule 2: Phycocyanin beta-1 subunit

Chain B:  2% 95% 5%



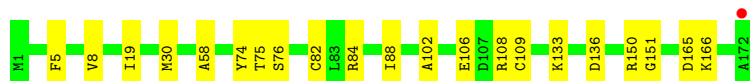
• Molecule 2: Phycocyanin beta-1 subunit

Chain F:  2% 87% 12%

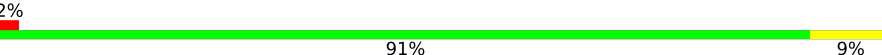


• Molecule 2: Phycocyanin beta-1 subunit

Chain J:  2% 88% 12%

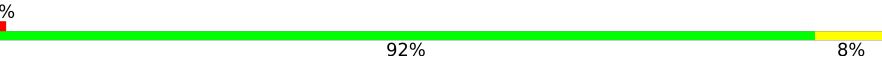


• Molecule 2: Phycocyanin beta-1 subunit

Chain H:  2% 91% 9%



• Molecule 2: Phycocyanin beta-1 subunit

Chain L:  2% 92% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.58Å 175.72Å 194.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.93 – 2.04 43.93 – 2.04	Depositor EDS
% Data completeness (in resolution range)	95.3 (43.93-2.04) 96.6 (43.93-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.52 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.6.4 _486	Depositor
R, R_{free}	0.172 , 0.207 0.171 , 0.205	Depositor DCC
R_{free} test set	7142 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17226	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.50	0/1237	0.74	0/1676
1	C	0.50	0/1237	0.71	0/1676
1	E	0.46	0/1231	0.69	0/1668
1	G	0.49	0/1244	0.73	0/1686
1	I	0.48	0/1231	0.75	0/1668
1	K	0.45	0/1231	0.73	0/1668
2	B	0.49	0/1252	0.73	0/1691
2	D	0.50	0/1257	0.72	0/1699
2	F	0.45	0/1251	0.73	0/1691
2	H	0.46	0/1251	0.72	0/1691
2	J	0.47	0/1251	0.74	0/1691
2	L	0.50	0/1252	0.73	0/1691
All	All	0.48	0/14925	0.73	0/20196

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1215	0	1180	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1215	0	1179	24	0
1	E	1209	0	1176	33	0
1	G	1222	0	1185	25	0
1	I	1209	0	1176	26	0
1	K	1209	0	1176	20	0
2	B	1248	0	1249	11	0
2	D	1253	0	1252	29	1
2	F	1247	0	1249	20	0
2	H	1247	0	1248	15	0
2	J	1247	0	1248	22	1
2	L	1248	0	1248	9	0
3	A	43	0	38	12	0
3	B	86	0	74	18	0
3	C	43	0	37	11	0
3	D	86	0	74	13	0
3	E	43	0	38	15	0
3	F	86	0	75	22	0
3	G	43	0	37	9	0
3	H	86	0	74	23	0
3	I	43	0	38	16	0
3	J	86	0	73	25	0
3	K	43	0	38	13	0
3	L	86	0	73	21	0
4	A	160	0	0	2	0
4	B	138	0	0	1	0
4	C	144	0	0	2	0
4	D	171	0	0	8	0
4	E	128	0	0	0	0
4	F	113	0	0	3	0
4	G	156	0	0	1	0
4	H	150	0	0	3	0
4	I	119	0	0	3	0
4	J	123	0	0	3	0
4	K	122	0	0	2	0
4	L	159	0	0	2	0
All	All	17226	0	15235	345	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (345) 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)
2:F:82:CYS:SG	3:F:201:CYC:HAC2	1.19	1.73
2:F:82:CYS:SG	3:F:201:CYC:CAC	2.10	1.40
2:B:82:CYS:SG	3:B:201:CYC:HAC2	1.66	1.34
1:K:84:CYS:SG	3:K:200:CYC:HAC2	1.68	1.32
1:I:84:CYS:SG	3:I:200:CYC:HAC2	1.76	1.26
1:A:84:CYS:SG	3:A:200:CYC:HAC2	1.77	1.24
1:E:84:CYS:SG	3:E:200:CYC:HAC2	1.78	1.23
3:H:202:CYC:HBD1	3:H:202:CYC:HHA	1.29	1.12
2:B:82:CYS:SG	3:B:201:CYC:CAC	2.53	0.96
1:K:84:CYS:SG	3:K:200:CYC:CAC	2.56	0.93
1:I:84:CYS:SG	3:I:200:CYC:CAC	2.60	0.89
1:A:84:CYS:SG	3:A:200:CYC:CAC	2.61	0.89
1:A:120:ARG:HD3	1:G:162:SER:O	1.73	0.88
1:E:84:CYS:SG	3:E:200:CYC:CAC	2.62	0.86
2:D:27:LEU:N	4:D:302:HOH:O	2.06	0.86
2:D:21:ALA:HA	2:D:24:ILE:HG22	1.58	0.85
3:F:202:CYC:HHA	3:F:202:CYC:HBD1	1.59	0.85
3:B:201:CYC:HB	3:B:201:CYC:CMA	1.90	0.84
1:E:153:TYR:OH	1:G:21[B]:THR:HG21	1.76	0.84
2:B:20:SER:H	2:B:23:GLN:HE21	1.24	0.84
2:F:82:CYS:SG	3:F:201:CYC:CB	2.69	0.80
2:D:125[A]:SER:OG	4:D:301:HOH:O	1.99	0.79
2:F:82:CYS:CB	3:F:201:CYC:HAC2	2.14	0.78
3:F:202:CYC:HB	3:F:202:CYC:CMA	1.98	0.77
3:J:201:CYC:HB	3:J:201:CYC:CMA	1.97	0.77
3:B:202:CYC:CMA	3:B:202:CYC:HB	1.97	0.76
3:L:202:CYC:CMA	3:L:202:CYC:HB	1.99	0.76
3:H:202:CYC:HB	3:H:202:CYC:CMA	1.99	0.76
1:C:100:VAL:HG21	2:D:19:ILE:HG13	1.67	0.75
2:L:8:VAL:HG12	2:L:19:ILE:HD12	1.69	0.74
3:I:200:CYC:HBD1	3:I:200:CYC:HHA	1.70	0.73
3:J:202:CYC:HBB2	3:J:202:CYC:HMB3	1.70	0.71
1:K:74:TYR:OH	4:K:301:HOH:O	2.05	0.71
1:I:128:TRP:CD2	3:I:200:CYC:HMC3	2.25	0.71
2:J:8:VAL:HG12	2:J:19:ILE:HD12	1.73	0.71
3:C:200:CYC:HB	3:C:200:CYC:CMA	2.04	0.71
3:G:200:CYC:CMA	3:G:200:CYC:HB	2.04	0.71
3:H:202:CYC:HBD1	3:H:202:CYC:CHA	2.12	0.70
2:J:109:CYS:HA	3:J:202:CYC:HBB3	1.74	0.70
3:L:201:CYC:HC	3:L:201:CYC:CMD	2.06	0.69
2:D:26:ALA:N	4:D:302:HOH:O	2.25	0.69
3:K:200:CYC:HB	3:K:200:CYC:CMA	2.05	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:201:CYC:HB	3:D:201:CYC:CMA	2.06	0.68
1:E:148:VAL:HG12	3:H:202:CYC:HBB2	1.76	0.68
3:I:200:CYC:CMA	3:I:200:CYC:HB	2.06	0.68
3:B:201:CYC:NB	3:B:201:CYC:HMA3	2.10	0.67
1:E:128:TRP:CD2	3:E:200:CYC:HMC3	2.29	0.67
1:I:32:ARG:NH2	4:I:301:HOH:O	2.14	0.66
3:D:202:CYC:HC	3:D:202:CYC:CMD	2.08	0.66
2:J:109:CYS:HA	3:J:202:CYC:CBB	2.24	0.66
3:H:201:CYC:HC	3:H:201:CYC:CMD	2.08	0.66
2:D:26:ALA:O	2:D:29:ALA:N	2.28	0.65
3:B:201:CYC:HB	3:B:201:CYC:HMA3	1.61	0.65
2:D:24:ILE:O	2:D:26:ALA:N	2.27	0.65
3:B:201:CYC:HB	3:B:201:CYC:HMA2	1.61	0.65
1:E:2:LYS:HE2	1:G:15:GLN:HE22	1.62	0.65
3:B:201:CYC:CMA	3:B:201:CYC:NB	2.61	0.64
3:F:201:CYC:CMD	3:F:201:CYC:HC	2.10	0.64
3:J:202:CYC:HC	3:J:202:CYC:CMD	2.10	0.64
2:D:24:ILE:C	4:D:302:HOH:O	2.41	0.64
2:F:4:ALA:HB3	2:F:30:MET:HE3	1.80	0.64
2:F:87:GLU:HG2	4:F:305:HOH:O	1.96	0.64
3:F:202:CYC:HBD1	3:F:202:CYC:CHA	2.27	0.64
2:B:106:GLU:OE1	4:B:302:HOH:O	2.14	0.64
1:E:153:TYR:CZ	1:G:21[B]:THR:HG21	2.32	0.64
1:E:2:LYS:HE2	1:G:15:GLN:NE2	2.13	0.63
2:J:106:GLU:HG2	2:J:166:LYS:HE3	1.79	0.63
3:H:202:CYC:HHA	3:H:202:CYC:CBD	2.19	0.63
3:A:200:CYC:HB	3:A:200:CYC:CMA	2.12	0.63
3:E:200:CYC:HB	3:E:200:CYC:CMA	2.13	0.62
1:E:84:CYS:SG	3:E:200:CYC:CBC	2.88	0.61
1:I:84:CYS:SG	3:I:200:CYC:CBC	2.89	0.61
1:A:120:ARG:NH2	4:A:301:HOH:O	2.33	0.61
3:D:202:CYC:HB	3:D:202:CYC:CMA	2.13	0.61
2:D:19:ILE:HG12	4:D:337:HOH:O	2.00	0.61
3:I:200:CYC:HB	3:I:200:CYC:HMA2	1.65	0.61
3:I:200:CYC:HC	3:I:200:CYC:CMD	2.13	0.61
1:E:25:GLN:HE21	1:G:30:ARG:HA	1.66	0.61
1:I:47:LYS:NZ	1:I:141:GLY:HA3	2.14	0.61
3:F:201:CYC:CMA	3:F:201:CYC:HB	2.13	0.61
2:D:24:ILE:HG13	2:D:25:ASP:H	1.66	0.61
2:B:20:SER:H	2:B:23:GLN:NE2	1.96	0.61
1:E:25:GLN:NE2	1:G:30:ARG:HD2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:201:CYC:CMA	3:H:201:CYC:HB	2.14	0.60
1:A:84:CYS:SG	3:A:200:CYC:CBC	2.88	0.60
3:J:202:CYC:HB	3:J:202:CYC:CMA	2.13	0.60
3:K:200:CYC:HB	3:K:200:CYC:HMA2	1.66	0.60
2:D:25:ASP:O	2:D:28:SER:HB2	2.01	0.60
1:I:128:TRP:CE3	3:I:200:CYC:HMC3	2.36	0.60
1:G:21[A]:THR:HG22	4:G:334:HOH:O	2.01	0.60
2:J:108:ARG:NE	4:J:303:HOH:O	2.34	0.59
3:G:200:CYC:CMD	3:G:200:CYC:HC	2.15	0.59
2:J:74:TYR:O	2:J:75:THR:OG1	2.17	0.59
1:E:153:TYR:CE1	1:G:21[B]:THR:HG21	2.38	0.59
3:J:201:CYC:HB	3:J:201:CYC:HMA1	1.66	0.59
3:L:201:CYC:HB	3:L:201:CYC:CMA	2.15	0.59
1:E:128:TRP:CE3	3:E:200:CYC:HMC3	2.37	0.59
1:E:128:TRP:HE3	3:E:200:CYC:H3C	1.68	0.59
1:I:84:CYS:HA	3:I:200:CYC:HHD	1.83	0.59
3:K:200:CYC:HC	3:K:200:CYC:CMD	2.16	0.59
1:G:128:TRP:CE3	3:G:200:CYC:HMC3	2.38	0.58
2:H:74:TYR:O	2:H:75:THR:OG1	2.18	0.58
3:C:200:CYC:HC	3:C:200:CYC:CMD	2.16	0.58
3:H:201:CYC:HB	3:H:201:CYC:HMA2	1.69	0.58
3:F:201:CYC:HB	3:F:201:CYC:HMA2	1.69	0.58
3:F:202:CYC:HB	3:F:202:CYC:HMA1	1.69	0.58
2:J:150:ARG:NH1	4:J:302:HOH:O	2.34	0.58
3:I:200:CYC:CMA	3:I:200:CYC:NB	2.67	0.58
2:D:21:ALA:HA	2:D:24:ILE:CG2	2.31	0.57
2:L:108:ARG:O	3:L:201:CYC:HBB1	2.04	0.57
2:J:88:ILE:HG21	3:J:202:CYC:HBB2	1.86	0.57
3:J:202:CYC:HB	3:J:202:CYC:HMA2	1.69	0.57
3:E:200:CYC:HC	3:E:200:CYC:CMD	2.17	0.57
2:F:30:MET:HG3	2:F:31:VAL:N	2.20	0.57
1:E:128:TRP:CE3	3:E:200:CYC:H3C	2.39	0.57
2:J:136:ASP:OD1	4:J:301:HOH:O	2.18	0.57
3:L:201:CYC:HC	3:L:201:CYC:HMD2	1.69	0.57
3:D:202:CYC:HB	3:D:202:CYC:HMA2	1.69	0.57
3:D:201:CYC:HB	3:D:201:CYC:HMA2	1.69	0.57
3:B:202:CYC:HB	3:B:202:CYC:HMA1	1.69	0.56
1:C:30:ARG:HD2	1:I:25:GLN:HE22	1.69	0.56
3:E:200:CYC:HB	3:E:200:CYC:HMA2	1.71	0.56
1:K:84:CYS:SG	3:K:200:CYC:CBC	2.93	0.56
1:E:107:MET:HE2	1:E:111:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:202:CYC:HC	3:D:202:CYC:HMD2	1.70	0.56
3:H:201:CYC:HC	3:H:201:CYC:HMD2	1.70	0.56
3:C:200:CYC:HB	3:C:200:CYC:HMA2	1.70	0.56
2:D:21:ALA:CA	2:D:24:ILE:HG22	2.33	0.56
3:J:201:CYC:HC	3:J:201:CYC:CMD	2.18	0.56
3:L:201:CYC:HB	3:L:201:CYC:HMA2	1.69	0.56
1:A:148:VAL:HG12	3:L:202:CYC:HBB2	1.88	0.55
3:I:200:CYC:HBD1	3:I:200:CYC:CHA	2.35	0.55
3:G:200:CYC:HB	3:G:200:CYC:HMA2	1.70	0.55
1:C:17:ARG:HH12	1:I:2:LYS:HD3	1.72	0.55
3:J:202:CYC:HC	3:J:202:CYC:HMD2	1.71	0.55
1:C:134:LYS:NZ	4:C:301:HOH:O	2.38	0.55
3:J:201:CYC:HMA1	3:J:201:CYC:NB	2.22	0.55
1:I:47:LYS:HZ3	1:I:141:GLY:HA3	1.72	0.55
1:C:30:ARG:HA	1:I:25:GLN:HE21	1.70	0.55
1:C:128:TRP:CE3	3:C:200:CYC:HMC3	2.41	0.55
3:D:201:CYC:HC	3:D:201:CYC:CMD	2.20	0.55
1:E:30:ARG:HH11	1:G:25:GLN:NE2	2.05	0.55
3:F:201:CYC:HC	3:F:201:CYC:HMD2	1.72	0.55
2:L:87:GLU:HG2	4:L:401:HOH:O	2.05	0.55
2:J:106:GLU:OE2	2:J:166:LYS:HE2	2.07	0.55
3:J:202:CYC:HMB3	3:J:202:CYC:CBB	2.37	0.54
2:H:77:ARG:NH1	3:H:201:CYC:O1D	2.31	0.54
1:E:25:GLN:NE2	1:G:30:ARG:HH11	2.05	0.54
1:K:137:LYS:HG3	1:K:154:ILE:HG21	1.89	0.54
3:K:200:CYC:CMA	3:K:200:CYC:NB	2.70	0.54
3:F:202:CYC:HMA1	3:F:202:CYC:NB	2.23	0.54
1:I:114:GLY:O	1:I:118:ILE:HD13	2.08	0.54
2:H:74:TYR:CD2	2:H:75:THR:HG23	2.43	0.54
1:C:63:PHE:O	1:C:66:THR:HB	2.08	0.53
3:H:202:CYC:HB	3:H:202:CYC:HMA1	1.74	0.53
3:L:202:CYC:CMD	3:L:202:CYC:HC	2.21	0.53
2:J:74:TYR:CD2	2:J:75:THR:HG23	2.44	0.53
3:L:202:CYC:HB	3:L:202:CYC:HMA2	1.74	0.53
3:H:202:CYC:HC	3:H:202:CYC:CMD	2.22	0.53
1:C:25:GLN:HE21	1:I:30:ARG:HA	1.74	0.53
3:J:201:CYC:HC	3:J:201:CYC:HMD2	1.74	0.53
2:F:106:GLU:HG2	2:F:166:LYS:NZ	2.24	0.53
1:K:128:TRP:CD2	3:K:200:CYC:HMC3	2.44	0.52
2:L:11:GLN:O	2:L:15:ARG:HD3	2.09	0.52
2:B:20:SER:N	2:B:23:GLN:HE21	2.01	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:CYS:SG	3:B:201:CYC:CBC	2.97	0.52
1:C:30:ARG:HD2	1:I:25:GLN:NE2	2.24	0.52
3:J:202:CYC:CMA	3:J:202:CYC:NB	2.73	0.52
1:K:84:CYS:HA	3:K:200:CYC:HHD	1.92	0.52
3:L:202:CYC:HB	3:L:202:CYC:HMA1	1.73	0.52
3:B:202:CYC:HMA1	3:B:202:CYC:NB	2.23	0.52
3:B:202:CYC:CMD	3:B:202:CYC:NC	2.73	0.52
2:J:106:GLU:HG2	2:J:166:LYS:CE	2.39	0.52
3:L:201:CYC:CMA	3:L:201:CYC:NB	2.73	0.52
3:C:200:CYC:CMD	3:C:200:CYC:NC	2.73	0.52
2:D:4:ALA:HB3	2:D:30:MET:CE	2.40	0.52
3:I:200:CYC:NB	3:I:200:CYC:HMA3	2.24	0.52
2:D:25:ASP:C	4:D:302:HOH:O	2.52	0.52
3:A:200:CYC:HBD1	3:A:200:CYC:HHA	1.92	0.52
2:B:19:ILE:CD1	2:B:24:ILE:HG12	2.40	0.52
3:B:202:CYC:CMD	3:B:202:CYC:HC	2.22	0.52
1:I:111:LEU:C	1:I:111:LEU:HD23	2.35	0.52
3:I:200:CYC:HC	3:I:200:CYC:HMD2	1.74	0.52
3:H:202:CYC:CMD	3:H:202:CYC:NC	2.73	0.52
2:J:88:ILE:CG2	3:J:202:CYC:HBB2	2.39	0.52
3:H:201:CYC:CMA	3:H:201:CYC:NB	2.73	0.52
3:C:200:CYC:CMA	3:C:200:CYC:NB	2.73	0.52
3:D:202:CYC:CMA	3:D:202:CYC:NB	2.73	0.52
3:L:202:CYC:CMD	3:L:202:CYC:NC	2.73	0.52
3:D:201:CYC:CMD	3:D:201:CYC:NC	2.73	0.52
1:E:30:ARG:HD2	1:G:25:GLN:NE2	2.24	0.52
3:E:200:CYC:CMA	3:E:200:CYC:NB	2.72	0.52
1:A:128:TRP:HE3	3:A:200:CYC:H3C	1.75	0.51
3:F:202:CYC:HC	3:F:202:CYC:CMD	2.22	0.51
3:G:200:CYC:CMA	3:G:200:CYC:NB	2.73	0.51
3:D:201:CYC:CMA	3:D:201:CYC:NB	2.73	0.51
3:F:202:CYC:CMD	3:F:202:CYC:NC	2.73	0.51
2:J:151:GLY:HA3	3:J:201:CYC:CMD	2.40	0.51
3:H:201:CYC:CMD	3:H:201:CYC:NC	2.73	0.51
3:B:202:CYC:CMA	3:B:202:CYC:NB	2.73	0.51
3:D:202:CYC:CMD	3:D:202:CYC:NC	2.73	0.51
2:J:5:PHE:CE2	2:J:30:MET:HE1	2.45	0.51
1:E:30:ARG:HH11	1:G:25:GLN:HE22	1.59	0.51
2:F:108:ARG:O	3:F:201:CYC:HBB1	2.11	0.51
3:J:201:CYC:CMD	3:J:201:CYC:NC	2.73	0.51
2:H:77:ARG:NH2	4:H:303:HOH:O	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:HA	1:K:25:GLN:HE21	1.76	0.51
3:G:200:CYC:CMD	3:G:200:CYC:NC	2.73	0.51
3:H:202:CYC:HMA1	3:H:202:CYC:NB	2.25	0.51
1:E:30:ARG:HA	1:G:25:GLN:HE21	1.75	0.51
3:F:201:CYC:CMD	3:F:201:CYC:NC	2.73	0.51
2:H:37:ARG:HA	2:H:156:LEU:HD21	1.92	0.51
3:K:200:CYC:HC	3:K:200:CYC:HMD2	1.76	0.51
3:L:202:CYC:HMA1	3:L:202:CYC:NB	2.25	0.51
2:F:106:GLU:HG2	2:F:166:LYS:HZ2	1.74	0.51
3:F:201:CYC:CMA	3:F:201:CYC:NB	2.73	0.51
3:H:202:CYC:HB	3:H:202:CYC:HMA2	1.74	0.51
3:L:202:CYC:HC	3:L:202:CYC:HMD2	1.76	0.51
3:D:201:CYC:HC	3:D:201:CYC:HMD2	1.76	0.50
1:E:148:VAL:CG1	3:H:202:CYC:HBB2	2.40	0.50
3:B:202:CYC:HB	3:B:202:CYC:HMA2	1.75	0.50
1:E:25:GLN:HE22	1:G:30:ARG:HD2	1.76	0.50
3:H:202:CYC:CHA	3:H:202:CYC:CBD	2.86	0.50
1:E:90:TYR:O	1:E:94:MET:HG2	2.12	0.50
3:B:202:CYC:HC	3:B:202:CYC:HMD2	1.77	0.50
3:K:200:CYC:NB	3:K:200:CYC:HMA3	2.27	0.50
3:J:202:CYC:CMD	3:J:202:CYC:NC	2.73	0.50
3:L:201:CYC:CMD	3:L:201:CYC:NC	2.73	0.50
3:C:200:CYC:HC	3:C:200:CYC:HMD2	1.76	0.50
3:G:200:CYC:HC	3:G:200:CYC:HMD2	1.76	0.50
1:K:63:PHE:HB3	1:K:65:TYR:CE1	2.47	0.50
3:A:200:CYC:HB	3:A:200:CYC:HMA2	1.77	0.49
1:C:90:TYR:O	1:C:94:MET:HG2	2.12	0.49
1:A:84:CYS:HA	3:A:200:CYC:HHD	1.94	0.49
2:D:21:ALA:O	2:D:24:ILE:O	2.30	0.49
3:H:202:CYC:CMA	3:H:202:CYC:NB	2.73	0.49
3:H:202:CYC:HC	3:H:202:CYC:HMD2	1.76	0.49
2:H:88:ILE:HG21	3:H:201:CYC:HAB1	1.94	0.49
2:D:113:LEU:HD11	2:D:117:TYR:CZ	2.47	0.49
1:A:128:TRP:CE3	3:A:200:CYC:H3C	2.48	0.49
1:E:84:CYS:HA	3:E:200:CYC:HHD	1.95	0.49
3:E:200:CYC:NB	3:E:200:CYC:HMA3	2.28	0.49
1:I:84:CYS:CB	3:I:200:CYC:HAC2	2.41	0.49
3:J:201:CYC:HB	3:J:201:CYC:HMA2	1.76	0.49
3:F:202:CYC:HB	3:F:202:CYC:HMA2	1.75	0.49
3:F:202:CYC:HC	3:F:202:CYC:HMD2	1.77	0.49
1:C:118:ILE:HD13	3:C:200:CYC:HMA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:VAL:HG21	2:H:19:ILE:HD12	1.93	0.48
2:F:1:MET:HE3	4:F:331:HOH:O	2.13	0.48
2:D:24:ILE:C	2:D:26:ALA:N	2.71	0.48
2:H:97:ILE:HG12	2:H:160:ILE:HG12	1.94	0.48
1:A:120:ARG:HD3	1:G:162:SER:C	2.35	0.48
1:C:127:SER:OG	1:K:123:ASP:OD1	2.31	0.48
1:E:25:GLN:HE22	1:G:30:ARG:HH11	1.62	0.48
1:K:144:GLY:O	1:K:148:VAL:HG23	2.13	0.47
1:K:140:HIS:CE1	1:K:142:LEU:HB2	2.49	0.47
1:C:2:LYS:HG3	1:C:7:GLU:OE2	2.15	0.47
2:J:58:ALA:HB3	2:J:133:LYS:HD3	1.95	0.47
2:J:84:ARG:NH1	3:J:202:CYC:O1A	2.47	0.47
2:H:151:GLY:HA3	3:H:202:CYC:CMD	2.45	0.47
1:A:145:ASP:OD1	3:L:202:CYC:HMA2	2.15	0.47
1:A:32:ARG:HH22	3:L:202:CYC:CMA	2.27	0.47
1:E:15:GLN:OE1	1:E:17:ARG:HD3	2.15	0.47
2:F:69:PRO:HA	2:F:74:TYR:CG	2.50	0.47
2:J:76:SER:HA	1:K:118:ILE:HD11	1.97	0.47
3:L:202:CYC:CMA	3:L:202:CYC:NB	2.73	0.47
3:F:202:CYC:CMA	3:F:202:CYC:NB	2.73	0.46
3:J:201:CYC:CMA	3:J:201:CYC:NB	2.73	0.46
3:J:202:CYC:CBB	3:J:202:CYC:CMB	2.94	0.46
1:C:30:ARG:HA	1:I:25:GLN:NE2	2.29	0.46
3:A:200:CYC:NB	3:A:200:CYC:HMA3	2.30	0.46
3:A:200:CYC:CMA	3:A:200:CYC:NB	2.78	0.46
1:C:111:LEU:HD23	1:C:111:LEU:C	2.41	0.46
2:H:135:LYS:HD2	4:H:332:HOH:O	2.16	0.46
1:C:2:LYS:HG3	1:C:7:GLU:CD	2.40	0.46
2:D:162:SER:O	2:D:166:LYS:HG3	2.15	0.45
1:E:55:ALA:HB3	1:E:88:ILE:HG21	1.97	0.45
3:E:200:CYC:HC	3:E:200:CYC:HMD2	1.81	0.45
1:C:25:GLN:NE2	1:I:30:ARG:HD2	2.32	0.45
1:K:84:CYS:CB	3:K:200:CYC:HAC2	2.41	0.45
1:A:123:ASP:OD1	1:G:127[A]:SER:OG	2.34	0.45
1:A:118:ILE:HD11	2:F:76:SER:HA	1.99	0.44
2:J:82:CYS:HA	3:J:202:CYC:CHD	2.47	0.44
1:G:100:VAL:HG21	2:H:19:ILE:CD1	2.47	0.44
1:A:32:ARG:NH2	3:L:202:CYC:CMA	2.80	0.44
1:A:43:ALA:HB3	1:A:142:LEU:HD21	1.99	0.44
3:C:200:CYC:NB	3:C:200:CYC:HMA3	2.32	0.44
2:B:120:LEU:HD11	3:B:201:CYC:HAA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:72:MEN:HB2	3:L:201:CYC:OC	2.18	0.44
1:A:35:THR:HB	4:A:338:HOH:O	2.17	0.44
2:B:127:VAL:HG22	3:B:201:CYC:H3C	1.99	0.44
3:G:200:CYC:NB	3:G:200:CYC:HMA3	2.32	0.44
1:C:128:TRP:CD2	3:C:200:CYC:HMC3	2.53	0.44
2:L:112:GLY:HA2	4:L:387:HOH:O	2.17	0.43
2:D:8:VAL:HG13	2:D:23:GLN:CD	2.43	0.43
1:K:128:TRP:CE3	3:K:200:CYC:H3C	2.54	0.43
2:D:26:ALA:O	2:D:29:ALA:HB3	2.19	0.43
2:D:30:MET:HG3	2:D:31:VAL:N	2.33	0.43
2:D:26:ALA:C	4:D:302:HOH:O	2.56	0.43
1:C:30:ARG:HH11	1:I:25:GLN:HE22	1.66	0.43
2:F:114:LYS:HB2	2:F:170:ALA:O	2.18	0.43
2:L:104:ILE:HG23	2:L:105:LEU:N	2.34	0.43
2:J:109:CYS:HA	3:J:202:CYC:HBB1	1.99	0.43
1:K:55:ALA:O	1:K:59:VAL:HG23	2.19	0.43
1:A:128:TRP:CD2	3:A:200:CYC:HMC3	2.54	0.43
1:I:84:CYS:CA	3:I:200:CYC:HHD	2.49	0.43
1:I:141:GLY:N	4:I:302:HOH:O	2.35	0.43
1:C:49:GLU:HG2	4:C:390:HOH:O	2.18	0.42
1:A:30:ARG:HD2	1:K:25:GLN:NE2	2.34	0.42
2:D:72:MEN:HB2	3:D:202:CYC:OC	2.19	0.42
1:G:84:CYS:HA	3:G:200:CYC:HAC1	1.60	0.42
1:G:118:ILE:HD11	2:L:76:SER:HA	2.01	0.42
2:D:8:VAL:HG12	2:D:19:ILE:HD12	2.02	0.42
2:F:106:GLU:OE2	2:F:166:LYS:HE3	2.19	0.42
1:G:111:LEU:C	1:G:111:LEU:HD23	2.45	0.42
1:C:84:CYS:HA	3:C:200:CYC:HAC1	1.71	0.42
1:A:30:ARG:HH11	1:K:25:GLN:HE22	1.68	0.42
1:I:87:ASP:O	1:I:90:TYR:HB2	2.20	0.42
2:H:77:ARG:NE	4:H:306:HOH:O	2.51	0.42
1:E:84:CYS:SG	3:E:200:CYC:H2C	2.60	0.42
2:D:114:LYS:HE2	4:D:305:HOH:O	2.19	0.42
2:D:60:PHE:CE2	2:D:79:MET:HE1	2.55	0.42
1:C:140:HIS:CE1	1:C:142:LEU:HB2	2.55	0.42
2:H:9:VAL:HG22	2:H:19:ILE:HD11	2.00	0.42
1:I:65:TYR:HB2	1:I:69:MET:HG3	2.02	0.41
1:E:135:TYR:CD1	1:E:135:TYR:C	2.98	0.41
2:F:150:ARG:HG3	4:F:315:HOH:O	2.19	0.41
2:L:151:GLY:HA3	3:L:202:CYC:CMD	2.51	0.41
2:F:104:ILE:HG23	2:F:105:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:332:HOH:O	2:J:108:ARG:HD3	2.20	0.41
2:F:4:ALA:HB3	2:F:30:MET:CE	2.50	0.41
1:E:30:ARG:HD2	1:G:25:GLN:HE22	1.86	0.41
1:C:118:ILE:HD11	2:B:76:SER:HA	2.02	0.41
1:K:123:ASP:HB2	4:K:398:HOH:O	2.20	0.40
1:E:63:PHE:HA	1:I:69:MET:HE1	2.03	0.40
2:F:127:VAL:HG22	3:F:201:CYC:H3C	2.02	0.40
1:C:25:GLN:NE2	1:I:30:ARG:HH11	2.19	0.40
2:D:4:ALA:HB3	2:D:30:MET:HE3	2.02	0.40
2:D:74:TYR:CD2	2:D:75:THR:HG23	2.57	0.40
1:E:55:ALA:O	1:E:59:VAL:HG23	2.21	0.40
2:F:20:SER:O	2:F:24:ILE:HG13	2.22	0.40
2:J:102:ALA:O	2:J:106:GLU:HG3	2.22	0.40
2:H:68:ALA:O	2:H:69:PRO:C	2.64	0.40
2:H:118:LEU:HD12	2:H:118:LEU:HA	1.88	0.40
1:K:90:TYR:O	1:K:94:MET:HG2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125[A]:SER:OG	2:J:165:ASP:OD2[1_455]	2.17	0.03

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	161/162 (99%)	157 (98%)	4 (2%)	0	100	100
1	C	161/162 (99%)	159 (99%)	2 (1%)	0	100	100
1	E	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
1	G	162/162 (100%)	159 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	K	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
2	B	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
2	D	170/172 (99%)	164 (96%)	5 (3%)	1 (1%)	21	13
2	F	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	H	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	J	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	L	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
All	All	1979/2004 (99%)	1940 (98%)	38 (2%)	1 (0%)	48	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	25	ASP

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	126/125 (101%)	122 (97%)	4 (3%)	34	29
1	C	126/125 (101%)	123 (98%)	3 (2%)	43	40
1	E	125/125 (100%)	123 (98%)	2 (2%)	55	56
1	G	127/125 (102%)	126 (99%)	1 (1%)	73	77
1	I	125/125 (100%)	120 (96%)	5 (4%)	28	22
1	K	125/125 (100%)	125 (100%)	0	100	100
2	B	124/124 (100%)	124 (100%)	0	100	100
2	D	125/124 (101%)	123 (98%)	2 (2%)	55	56
2	F	124/124 (100%)	120 (97%)	4 (3%)	34	29
2	H	124/124 (100%)	122 (98%)	2 (2%)	55	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	124/124 (100%)	124 (100%)	0	100	100
2	L	124/124 (100%)	123 (99%)	1 (1%)	73	77
All	All	1499/1494 (100%)	1475 (98%)	24 (2%)	55	56

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	36	SER
1	C	66	THR
1	C	70	THR
2	D	28	SER
2	D	30	MET
1	A	2	LYS
1	A	7	GLU
1	A	62	LYS
1	A	136	VAL
1	E	10	SER
1	E	107	MET
2	F	30	MET
2	F	35	SER
2	F	87	GLU
2	F	120	LEU
1	I	19	LEU
1	I	49	GLU
1	I	53	SER
1	I	107	MET
1	I	118	ILE
1	G	7	GLU
2	H	118	LEU
2	H	146	ASN
2	L	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	25	GLN
1	C	78	GLN
1	C	159	ASN
2	D	146	ASN
1	A	15	GLN

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Mol	Chain	Res	Type
2	B	23	GLN
2	B	42	ASN
2	B	146	ASN
1	E	25	GLN
1	E	57	ASN
1	E	159	ASN
2	F	63	GLN
1	I	25	GLN
2	J	42	ASN
1	G	15	GLN
1	G	25	GLN
1	G	33	GLN
2	H	42	ASN
1	K	25	GLN
1	K	33	GLN
1	K	159	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	D	72	2	7,8,9	0.66	0	4,9,11	0.43	0
2	MEN	J	72	2	7,8,9	0.66	0	4,9,11	0.53	0
2	MEN	B	72	2	7,8,9	0.67	0	4,9,11	0.42	0
2	MEN	L	72	2	7,8,9	0.66	0	4,9,11	0.45	0
2	MEN	F	72	2	7,8,9	0.65	0	4,9,11	0.50	0
2	MEN	H	72	2	7,8,9	0.66	0	4,9,11	0.38	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	D	72	2	-	2/7/8/10	-
2	MEN	J	72	2	-	4/7/8/10	-
2	MEN	B	72	2	-	4/7/8/10	-
2	MEN	L	72	2	-	7/7/8/10	-
2	MEN	F	72	2	-	2/7/8/10	-
2	MEN	H	72	2	-	2/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	72	MEN	1	0
2	L	72	MEN	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
3	CYC	F	202	2	46,46,46	2.33	15 (32%)	63,67,67	2.82	25 (39%)
3	CYC	I	200	-	46,46,46	3.93	23 (50%)	63,67,67	3.34	27 (42%)
3	CYC	A	200	-	46,46,46	3.95	23 (50%)	63,67,67	3.13	24 (38%)
3	CYC	H	202	2	46,46,46	2.34	15 (32%)	63,67,67	2.79	24 (38%)
3	CYC	C	200	1	46,46,46	2.33	15 (32%)	63,67,67	2.79	24 (38%)
3	CYC	L	201	2	46,46,46	2.32	16 (34%)	63,67,67	2.84	25 (39%)
3	CYC	B	202	2	46,46,46	2.32	14 (30%)	63,67,67	2.81	25 (39%)
3	CYC	H	201	2	46,46,46	2.33	16 (34%)	63,67,67	2.84	25 (39%)
3	CYC	G	200	1	46,46,46	2.31	15 (32%)	63,67,67	2.83	24 (38%)
3	CYC	J	201	2	46,46,46	2.33	15 (32%)	63,67,67	2.82	25 (39%)
3	CYC	D	202	2	46,46,46	2.34	16 (34%)	63,67,67	2.82	24 (38%)
3	CYC	D	201	2	46,46,46	2.32	15 (32%)	63,67,67	2.82	25 (39%)
3	CYC	E	200	-	46,46,46	3.93	24 (52%)	63,67,67	3.38	28 (44%)
3	CYC	F	201	-	46,46,46	2.32	16 (34%)	63,67,67	2.86	25 (39%)
3	CYC	K	200	-	46,46,46	3.97	23 (50%)	63,67,67	3.36	29 (46%)
3	CYC	J	202	2	46,46,46	2.33	16 (34%)	63,67,67	2.82	25 (39%)
3	CYC	B	201	-	46,46,46	3.91	22 (47%)	63,67,67	3.33	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CYC	L	202	2	46,46,46	2.32	15 (32%)	63,67,67	2.84	25 (39%)

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
3	CYC	F	202	2	-	13/26/74/74	0/4/4/4
3	CYC	I	200	-	-	11/26/74/74	0/4/4/4
3	CYC	A	200	-	-	10/26/74/74	0/4/4/4
3	CYC	H	202	2	-	12/26/74/74	0/4/4/4
3	CYC	C	200	1	-	10/26/74/74	0/4/4/4
3	CYC	L	201	2	-	6/26/74/74	0/4/4/4
3	CYC	B	202	2	-	12/26/74/74	0/4/4/4
3	CYC	H	201	2	-	8/26/74/74	0/4/4/4
3	CYC	G	200	1	-	11/26/74/74	0/4/4/4
3	CYC	J	201	2	-	12/26/74/74	0/4/4/4
3	CYC	D	202	2	-	8/26/74/74	0/4/4/4
3	CYC	D	201	2	-	11/26/74/74	0/4/4/4
3	CYC	E	200	-	-	8/26/74/74	0/4/4/4
3	CYC	F	201	-	-	8/26/74/74	0/4/4/4
3	CYC	K	200	-	-	9/26/74/74	0/4/4/4
3	CYC	J	202	2	-	8/26/74/74	0/4/4/4
3	CYC	B	201	-	-	10/26/74/74	0/4/4/4
3	CYC	L	202	2	-	12/26/74/74	0/4/4/4

All (314) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	200	CYC	C3C-C4C	10.52	1.73	1.50
3	I	200	CYC	C3C-C4C	10.51	1.73	1.50
3	K	200	CYC	C3C-C4C	10.45	1.72	1.50
3	E	200	CYC	C3C-C4C	10.44	1.72	1.50
3	B	201	CYC	C3C-C4C	9.84	1.71	1.50
3	I	200	CYC	CAC-C3C	-9.02	1.36	1.54
3	A	200	CYC	CHD-C1D	9.01	1.60	1.40
3	B	201	CYC	OB-C4B	8.69	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	200	CYC	CAC-C3C	-8.68	1.37	1.54
3	E	200	CYC	CHD-C1D	8.67	1.60	1.40
3	K	200	CYC	CHD-C1D	8.65	1.60	1.40
3	A	200	CYC	CAC-C3C	-8.64	1.37	1.54
3	K	200	CYC	CAC-C3C	-8.61	1.37	1.54
3	B	201	CYC	CAC-C3C	-8.59	1.37	1.54
3	I	200	CYC	CHD-C1D	8.49	1.59	1.40
3	I	200	CYC	OB-C4B	8.33	1.39	1.23
3	K	200	CYC	OB-C4B	8.32	1.39	1.23
3	B	201	CYC	CHD-C1D	8.10	1.58	1.40
3	A	200	CYC	OB-C4B	8.05	1.38	1.23
3	E	200	CYC	OB-C4B	7.78	1.38	1.23
3	K	200	CYC	CHA-C1A	7.31	1.52	1.38
3	K	200	CYC	CHA-C4D	7.07	1.56	1.40
3	B	201	CYC	CHA-C1A	7.05	1.52	1.38
3	A	200	CYC	CHA-C4D	6.96	1.56	1.40
3	I	200	CYC	CHA-C4D	6.94	1.56	1.40
3	B	201	CYC	CHA-C4D	6.83	1.55	1.40
3	A	200	CYC	CHA-C1A	6.80	1.51	1.38
3	E	200	CYC	C4B-C3B	-6.48	1.36	1.48
3	A	200	CYC	C4B-C3B	-6.43	1.36	1.48
3	E	200	CYC	CHA-C4D	6.40	1.54	1.40
3	I	200	CYC	CHA-C1A	6.36	1.50	1.38
3	K	200	CYC	CHB-C1B	6.36	1.53	1.37
3	E	200	CYC	CHB-C1B	6.33	1.53	1.37
3	E	200	CYC	CHA-C1A	6.32	1.50	1.38
3	I	200	CYC	CHB-C1B	6.31	1.53	1.37
3	B	201	CYC	C4B-C3B	-6.30	1.36	1.48
3	E	200	CYC	C1A-C2A	-6.18	1.36	1.45
3	B	201	CYC	CHB-C1B	6.11	1.52	1.37
3	A	200	CYC	C1A-C2A	-5.98	1.36	1.45
3	A	200	CYC	CHB-C1B	5.95	1.52	1.37
3	K	200	CYC	C4B-C3B	-5.94	1.37	1.48
3	B	201	CYC	C1A-C2A	-5.92	1.36	1.45
3	I	200	CYC	C4B-C3B	-5.88	1.37	1.48
3	I	200	CYC	C1A-C2A	-5.84	1.36	1.45
3	E	200	CYC	C2C-C1C	-5.81	1.46	1.52
3	K	200	CYC	C2C-C1C	-5.80	1.46	1.52
3	I	200	CYC	C2C-C1C	-5.67	1.47	1.52
3	J	202	CYC	C3B-C2B	5.64	1.48	1.36
3	H	202	CYC	C3B-C2B	5.63	1.48	1.36
3	F	202	CYC	C3B-C2B	5.59	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	201	CYC	C3B-C2B	5.59	1.48	1.36
3	D	201	CYC	C3B-C2B	5.58	1.48	1.36
3	C	200	CYC	C3B-C2B	5.58	1.48	1.36
3	K	200	CYC	C1A-C2A	-5.57	1.37	1.45
3	B	202	CYC	C3B-C2B	5.57	1.48	1.36
3	D	202	CYC	C3B-C2B	5.54	1.48	1.36
3	F	201	CYC	C3B-C2B	5.53	1.48	1.36
3	H	201	CYC	C3B-C2B	5.53	1.48	1.36
3	D	202	CYC	CHA-C1A	5.52	1.49	1.38
3	L	202	CYC	C3B-C2B	5.52	1.48	1.36
3	L	201	CYC	C3B-C2B	5.52	1.48	1.36
3	H	202	CYC	CHA-C1A	5.52	1.49	1.38
3	G	200	CYC	C3B-C2B	5.51	1.48	1.36
3	H	201	CYC	CHA-C1A	5.50	1.49	1.38
3	L	201	CYC	CHA-C1A	5.45	1.49	1.38
3	J	202	CYC	CHA-C1A	5.43	1.48	1.38
3	C	200	CYC	CHA-C1A	5.41	1.48	1.38
3	F	202	CYC	CHA-C1A	5.40	1.48	1.38
3	F	201	CYC	CHA-C1A	5.38	1.48	1.38
3	L	201	CYC	C2A-C3A	5.38	1.48	1.36
3	F	201	CYC	C2A-C3A	5.37	1.48	1.36
3	G	200	CYC	C2A-C3A	5.36	1.48	1.36
3	J	201	CYC	C2A-C3A	5.36	1.48	1.36
3	H	201	CYC	C2A-C3A	5.36	1.48	1.36
3	D	201	CYC	CHA-C1A	5.35	1.48	1.38
3	J	201	CYC	CHA-C1A	5.35	1.48	1.38
3	D	202	CYC	C2A-C3A	5.35	1.48	1.36
3	L	202	CYC	C2A-C3A	5.35	1.48	1.36
3	A	200	CYC	C2C-C1C	-5.35	1.47	1.52
3	D	201	CYC	C2A-C3A	5.34	1.48	1.36
3	F	202	CYC	C2A-C3A	5.33	1.48	1.36
3	B	201	CYC	C2C-C1C	-5.33	1.47	1.52
3	L	202	CYC	CHA-C1A	5.33	1.48	1.38
3	G	200	CYC	CHA-C1A	5.31	1.48	1.38
3	B	202	CYC	CHA-C1A	5.30	1.48	1.38
3	C	200	CYC	C2A-C3A	5.30	1.48	1.36
3	J	202	CYC	C2A-C3A	5.29	1.48	1.36
3	H	202	CYC	C2A-C3A	5.29	1.48	1.36
3	B	202	CYC	C2A-C3A	5.28	1.48	1.36
3	K	200	CYC	CHB-C4A	5.20	1.52	1.40
3	A	200	CYC	CHB-C4A	5.10	1.52	1.40
3	I	200	CYC	CHB-C4A	5.05	1.52	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	200	CYC	CHB-C4A	5.01	1.52	1.40
3	H	202	CYC	CHB-C1B	4.88	1.49	1.37
3	F	202	CYC	CHB-C1B	4.82	1.49	1.37
3	B	202	CYC	CHB-C1B	4.81	1.49	1.37
3	J	201	CYC	CHB-C1B	4.81	1.49	1.37
3	B	201	CYC	CHB-C4A	4.80	1.51	1.40
3	C	200	CYC	CHB-C1B	4.80	1.49	1.37
3	K	200	CYC	C1B-C2B	-4.78	1.36	1.45
3	D	201	CYC	CHB-C1B	4.76	1.49	1.37
3	J	202	CYC	CHB-C1B	4.75	1.49	1.37
3	L	202	CYC	CHB-C1B	4.75	1.49	1.37
3	G	200	CYC	CHB-C1B	4.73	1.49	1.37
3	D	202	CYC	CHB-C1B	4.72	1.49	1.37
3	B	201	CYC	C1B-C2B	-4.72	1.36	1.45
3	L	201	CYC	CHB-C1B	4.69	1.49	1.37
3	H	201	CYC	CHB-C1B	4.69	1.49	1.37
3	I	200	CYC	C1B-C2B	-4.62	1.36	1.45
3	F	201	CYC	CHB-C1B	4.62	1.48	1.37
3	E	200	CYC	C1B-C2B	-4.54	1.37	1.45
3	A	200	CYC	C1B-C2B	-4.35	1.37	1.45
3	D	202	CYC	CHD-C1D	3.99	1.49	1.40
3	C	200	CYC	CHD-C1D	3.96	1.49	1.40
3	L	201	CYC	CHD-C1D	3.94	1.49	1.40
3	G	200	CYC	CHD-C1D	3.94	1.49	1.40
3	J	202	CYC	CHD-C1D	3.93	1.49	1.40
3	D	201	CYC	CHD-C1D	3.92	1.49	1.40
3	J	201	CYC	CHD-C1D	3.91	1.49	1.40
3	L	202	CYC	CHD-C1D	3.90	1.49	1.40
3	H	202	CYC	CHA-C4D	3.90	1.49	1.40
3	H	201	CYC	CHD-C1D	3.90	1.49	1.40
3	F	202	CYC	CHD-C1D	3.89	1.49	1.40
3	H	202	CYC	CHD-C1D	3.88	1.49	1.40
3	D	202	CYC	CHA-C4D	3.88	1.49	1.40
3	F	201	CYC	CHD-C1D	3.88	1.49	1.40
3	H	202	CYC	CHB-C4A	3.87	1.49	1.40
3	B	202	CYC	CHD-C1D	3.86	1.49	1.40
3	H	201	CYC	CHA-C4D	3.86	1.49	1.40
3	F	202	CYC	CHA-C4D	3.86	1.49	1.40
3	L	201	CYC	CHA-C4D	3.81	1.49	1.40
3	C	200	CYC	CHA-C4D	3.81	1.49	1.40
3	F	202	CYC	CHB-C4A	3.81	1.49	1.40
3	G	200	CYC	CHA-C4D	3.81	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	202	CYC	CHA-C4D	3.81	1.48	1.40
3	B	202	CYC	CHB-C4A	3.81	1.49	1.40
3	J	201	CYC	CHA-C4D	3.79	1.48	1.40
3	L	202	CYC	CHA-C4D	3.78	1.48	1.40
3	J	201	CYC	CHB-C4A	3.78	1.49	1.40
3	L	202	CYC	CHB-C4A	3.78	1.49	1.40
3	D	201	CYC	CHA-C4D	3.77	1.48	1.40
3	B	202	CYC	CHA-C4D	3.75	1.48	1.40
3	F	201	CYC	CHA-C4D	3.75	1.48	1.40
3	C	200	CYC	CHB-C4A	3.74	1.49	1.40
3	D	201	CYC	CHB-C4A	3.71	1.49	1.40
3	J	202	CYC	CHB-C4A	3.70	1.49	1.40
3	L	201	CYC	C3D-C2D	3.69	1.48	1.38
3	H	201	CYC	C3D-C2D	3.69	1.48	1.38
3	C	200	CYC	C3D-C2D	3.69	1.48	1.38
3	G	200	CYC	C3D-C2D	3.68	1.48	1.38
3	D	202	CYC	CHB-C4A	3.68	1.49	1.40
3	G	200	CYC	CHB-C4A	3.66	1.49	1.40
3	F	201	CYC	CHB-C4A	3.66	1.49	1.40
3	H	201	CYC	CHB-C4A	3.65	1.49	1.40
3	D	202	CYC	C3D-C2D	3.65	1.48	1.38
3	L	201	CYC	CHB-C4A	3.65	1.49	1.40
3	J	202	CYC	C3D-C2D	3.63	1.48	1.38
3	F	201	CYC	C3D-C2D	3.60	1.48	1.38
3	A	200	CYC	C4C-NC	3.56	1.44	1.37
3	B	201	CYC	C4A-C3A	-3.56	1.38	1.45
3	D	201	CYC	C3D-C2D	3.54	1.48	1.38
3	B	202	CYC	C3D-C2D	3.54	1.48	1.38
3	L	202	CYC	C3D-C2D	3.54	1.48	1.38
3	J	201	CYC	C3D-C2D	3.53	1.48	1.38
3	H	202	CYC	C3D-C2D	3.53	1.48	1.38
3	F	202	CYC	C3D-C2D	3.50	1.48	1.38
3	F	202	CYC	C1C-NC	-3.46	1.33	1.37
3	G	200	CYC	C1D-C2D	3.46	1.49	1.41
3	J	201	CYC	C1C-NC	-3.44	1.33	1.37
3	C	200	CYC	C1D-C2D	3.44	1.49	1.41
3	K	200	CYC	C4C-NC	3.44	1.44	1.37
3	E	200	CYC	C4C-NC	3.41	1.44	1.37
3	L	202	CYC	C1C-NC	-3.39	1.33	1.37
3	B	202	CYC	C1C-NC	-3.39	1.33	1.37
3	H	201	CYC	C1D-C2D	3.37	1.49	1.41
3	H	202	CYC	C1C-NC	-3.36	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	200	CYC	C4A-C3A	-3.36	1.38	1.45
3	L	201	CYC	C1D-C2D	3.36	1.49	1.41
3	B	201	CYC	C2C-C3C	-3.35	1.45	1.54
3	F	201	CYC	C1D-C2D	3.35	1.49	1.41
3	F	201	CYC	C1C-NC	-3.35	1.33	1.37
3	D	202	CYC	C1D-C2D	3.35	1.49	1.41
3	D	201	CYC	C1C-NC	-3.33	1.33	1.37
3	J	202	CYC	C1D-C2D	3.32	1.49	1.41
3	E	200	CYC	C2C-C3C	-3.32	1.45	1.54
3	F	202	CYC	C1D-C2D	3.32	1.49	1.41
3	J	201	CYC	C1D-C2D	3.31	1.49	1.41
3	L	202	CYC	C1D-C2D	3.30	1.49	1.41
3	D	201	CYC	C1D-C2D	3.28	1.49	1.41
3	B	202	CYC	C1D-C2D	3.27	1.49	1.41
3	H	201	CYC	C1C-NC	-3.25	1.33	1.37
3	D	202	CYC	C1C-NC	-3.23	1.33	1.37
3	J	202	CYC	C1C-NC	-3.22	1.33	1.37
3	H	202	CYC	C1D-C2D	3.22	1.49	1.41
3	I	200	CYC	C2C-C3C	-3.16	1.45	1.54
3	I	200	CYC	C4C-NC	3.15	1.43	1.37
3	K	200	CYC	C2C-C3C	-3.12	1.46	1.54
3	A	200	CYC	C2C-C3C	-3.12	1.46	1.54
3	G	200	CYC	C1C-NC	-3.10	1.33	1.37
3	L	201	CYC	C1C-NC	-3.09	1.33	1.37
3	K	200	CYC	C4A-C3A	-3.06	1.39	1.45
3	C	200	CYC	C1C-NC	-3.06	1.33	1.37
3	E	200	CYC	C4A-C3A	-3.01	1.39	1.45
3	I	200	CYC	C4D-C3D	-2.95	1.36	1.42
3	B	201	CYC	C4C-NC	2.92	1.43	1.37
3	A	200	CYC	C1D-ND	2.88	1.42	1.37
3	I	200	CYC	C4A-C3A	-2.86	1.39	1.45
3	H	202	CYC	C4D-C3D	2.86	1.49	1.42
3	J	201	CYC	OB-C4B	2.85	1.29	1.23
3	I	200	CYC	C3D-C2D	-2.84	1.31	1.38
3	B	201	CYC	C2A-C3A	-2.83	1.30	1.36
3	D	202	CYC	OB-C4B	2.83	1.28	1.23
3	E	200	CYC	C3B-C2B	-2.82	1.30	1.36
3	F	202	CYC	OB-C4B	2.82	1.28	1.23
3	L	202	CYC	OB-C4B	2.82	1.28	1.23
3	B	202	CYC	OB-C4B	2.81	1.28	1.23
3	G	200	CYC	OB-C4B	2.81	1.28	1.23
3	H	201	CYC	OB-C4B	2.81	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	200	CYC	OB-C4B	2.81	1.28	1.23
3	E	200	CYC	C2A-C3A	-2.80	1.30	1.36
3	D	202	CYC	C4D-C3D	2.80	1.49	1.42
3	E	200	CYC	C4D-C3D	-2.80	1.36	1.42
3	D	201	CYC	OB-C4B	2.79	1.28	1.23
3	F	202	CYC	C4D-C3D	2.77	1.48	1.42
3	K	200	CYC	C4D-C3D	-2.77	1.36	1.42
3	H	201	CYC	C4D-C3D	2.77	1.48	1.42
3	L	201	CYC	OB-C4B	2.76	1.28	1.23
3	H	202	CYC	OB-C4B	2.76	1.28	1.23
3	B	201	CYC	C4D-C3D	-2.75	1.36	1.42
3	J	202	CYC	C4D-C3D	2.75	1.48	1.42
3	J	202	CYC	OB-C4B	2.74	1.28	1.23
3	L	201	CYC	C4D-C3D	2.74	1.48	1.42
3	F	201	CYC	OB-C4B	2.74	1.28	1.23
3	K	200	CYC	C2A-C3A	-2.74	1.30	1.36
3	B	201	CYC	C1D-ND	2.74	1.42	1.37
3	B	201	CYC	C3B-C2B	-2.74	1.30	1.36
3	D	201	CYC	C4D-C3D	2.73	1.48	1.42
3	L	202	CYC	C4D-C3D	2.73	1.48	1.42
3	J	201	CYC	C4D-C3D	2.73	1.48	1.42
3	F	201	CYC	C4D-C3D	2.69	1.48	1.42
3	G	200	CYC	C4D-C3D	2.69	1.48	1.42
3	A	200	CYC	C3D-C2D	-2.68	1.31	1.38
3	B	202	CYC	C4D-C3D	2.68	1.48	1.42
3	C	200	CYC	C4D-C3D	2.67	1.48	1.42
3	J	202	CYC	C1B-C2B	2.66	1.49	1.45
3	H	202	CYC	C1B-C2B	2.65	1.49	1.45
3	I	200	CYC	C1D-ND	2.64	1.42	1.37
3	A	200	CYC	C3B-C2B	-2.63	1.31	1.36
3	K	200	CYC	C3D-C2D	-2.63	1.32	1.38
3	B	201	CYC	C3D-C2D	-2.63	1.32	1.38
3	K	200	CYC	CHD-C4C	-2.61	1.32	1.36
3	H	201	CYC	C1B-C2B	2.57	1.49	1.45
3	F	201	CYC	C1B-C2B	2.57	1.49	1.45
3	A	200	CYC	C2A-C3A	-2.57	1.31	1.36
3	D	202	CYC	C1B-C2B	2.57	1.49	1.45
3	L	201	CYC	C1B-C2B	2.56	1.49	1.45
3	C	200	CYC	C1B-C2B	2.56	1.49	1.45
3	D	201	CYC	C1B-C2B	2.54	1.49	1.45
3	F	202	CYC	C1B-C2B	2.54	1.49	1.45
3	L	202	CYC	C1B-C2B	2.53	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	201	CYC	C1B-C2B	2.52	1.49	1.45
3	G	200	CYC	C1B-C2B	2.50	1.49	1.45
3	K	200	CYC	C1D-ND	2.49	1.42	1.37
3	A	200	CYC	C4D-C3D	-2.49	1.37	1.42
3	B	201	CYC	CHD-C4C	-2.48	1.32	1.36
3	B	202	CYC	C1B-C2B	2.48	1.49	1.45
3	I	200	CYC	C3B-C2B	-2.44	1.31	1.36
3	I	200	CYC	C2A-C3A	-2.43	1.31	1.36
3	K	200	CYC	C3B-C2B	-2.40	1.31	1.36
3	E	200	CYC	C3D-C2D	-2.40	1.32	1.38
3	E	200	CYC	C1D-ND	2.39	1.41	1.37
3	K	200	CYC	C4D-ND	2.31	1.41	1.37
3	C	200	CYC	C2C-C1C	-2.30	1.50	1.52
3	E	200	CYC	CHD-C4C	-2.29	1.32	1.36
3	K	200	CYC	C4A-NA	2.26	1.41	1.36
3	H	201	CYC	C2C-C1C	-2.25	1.50	1.52
3	L	201	CYC	C2C-C1C	-2.23	1.50	1.52
3	F	201	CYC	C2C-C1C	-2.23	1.50	1.52
3	A	200	CYC	C4D-ND	2.21	1.41	1.37
3	F	202	CYC	C2C-C1C	-2.18	1.50	1.52
3	B	202	CYC	C4C-NC	-2.18	1.33	1.37
3	B	201	CYC	C4A-NA	2.18	1.41	1.36
3	J	202	CYC	C2C-C1C	-2.18	1.50	1.52
3	J	201	CYC	C4C-NC	-2.17	1.33	1.37
3	D	202	CYC	C1A-C2A	2.17	1.49	1.45
3	L	202	CYC	C4C-NC	-2.17	1.33	1.37
3	H	202	CYC	C4C-NC	-2.16	1.33	1.37
3	F	202	CYC	C4C-NC	-2.15	1.33	1.37
3	A	200	CYC	CHD-C4C	-2.15	1.33	1.36
3	E	200	CYC	C4A-NA	2.15	1.41	1.36
3	D	202	CYC	C2C-C1C	-2.14	1.50	1.52
3	I	200	CYC	C4D-ND	2.14	1.41	1.37
3	J	202	CYC	C4C-NC	-2.13	1.33	1.37
3	D	201	CYC	C4C-NC	-2.13	1.33	1.37
3	I	200	CYC	CHD-C4C	-2.12	1.33	1.36
3	D	202	CYC	C4C-NC	-2.12	1.33	1.37
3	L	201	CYC	C1A-C2A	2.11	1.49	1.45
3	H	201	CYC	C4C-NC	-2.11	1.33	1.37
3	L	201	CYC	C4C-NC	-2.11	1.33	1.37
3	F	201	CYC	C4C-NC	-2.11	1.33	1.37
3	A	200	CYC	C4A-NA	2.11	1.41	1.36
3	H	201	CYC	C1A-C2A	2.11	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	202	CYC	C1A-C2A	2.07	1.49	1.45
3	E	200	CYC	C1B-NB	2.06	1.41	1.37
3	C	200	CYC	C4C-NC	-2.06	1.33	1.37
3	G	200	CYC	C2C-C1C	-2.05	1.50	1.52
3	L	202	CYC	C2C-C1C	-2.04	1.50	1.52
3	F	201	CYC	C1A-C2A	2.03	1.48	1.45
3	H	202	CYC	C1A-C2A	2.03	1.48	1.45
3	I	200	CYC	C4A-NA	2.02	1.41	1.36
3	D	201	CYC	C1A-C2A	2.02	1.48	1.45
3	J	201	CYC	C2C-C1C	-2.01	1.50	1.52
3	G	200	CYC	C4C-NC	-2.01	1.33	1.37
3	E	200	CYC	C4D-ND	2.00	1.41	1.37

All (456) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	CYC	C2C-C1C-NC	11.78	118.09	108.29
3	J	202	CYC	C3B-C4B-NB	11.31	115.78	106.77
3	H	201	CYC	C3B-C4B-NB	11.29	115.77	106.77
3	D	202	CYC	C3B-C4B-NB	11.27	115.76	106.77
3	L	201	CYC	C3B-C4B-NB	11.27	115.75	106.77
3	K	200	CYC	C2C-C1C-NC	11.26	117.66	108.29
3	E	200	CYC	C2C-C1C-NC	11.25	117.65	108.29
3	G	200	CYC	C3B-C4B-NB	11.25	115.74	106.77
3	F	201	CYC	C3B-C4B-NB	11.23	115.72	106.77
3	D	201	CYC	C3B-C4B-NB	11.15	115.66	106.77
3	I	200	CYC	C2C-C1C-NC	11.12	117.54	108.29
3	H	202	CYC	C3B-C4B-NB	11.12	115.63	106.77
3	L	202	CYC	C3B-C4B-NB	11.08	115.60	106.77
3	F	202	CYC	C3B-C4B-NB	11.08	115.60	106.77
3	C	200	CYC	C3B-C4B-NB	11.04	115.57	106.77
3	J	201	CYC	C3B-C4B-NB	11.03	115.56	106.77
3	K	200	CYC	CHD-C4C-NC	-10.91	112.01	125.63
3	B	202	CYC	C3B-C4B-NB	10.87	115.44	106.77
3	I	200	CYC	CHD-C4C-NC	-10.75	112.21	125.63
3	E	200	CYC	CHD-C4C-NC	-10.55	112.46	125.63
3	B	201	CYC	C1C-NC-C4C	-10.08	100.76	113.41
3	A	200	CYC	CHD-C4C-NC	-9.68	113.54	125.63
3	I	200	CYC	C1D-CHD-C4C	-9.23	112.01	127.76
3	A	200	CYC	C2C-C1C-NC	9.12	115.88	108.29
3	K	200	CYC	C1D-CHD-C4C	-8.83	112.68	127.76
3	E	200	CYC	C1D-CHD-C4C	-8.43	113.37	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	200	CYC	C1B-NB-C4B	-8.26	100.53	110.66
3	A	200	CYC	C1B-NB-C4B	-8.07	100.76	110.66
3	A	200	CYC	C1D-CHD-C4C	-8.03	114.06	127.76
3	K	200	CYC	C1B-NB-C4B	-7.90	100.97	110.66
3	I	200	CYC	C1B-NB-C4B	-7.82	101.06	110.66
3	B	201	CYC	C1B-NB-C4B	-7.63	101.29	110.66
3	A	200	CYC	C3B-C4B-NB	6.85	112.23	106.77
3	B	201	CYC	OC-C1C-C2C	-6.54	120.97	126.17
3	E	200	CYC	OC-C1C-C2C	-6.47	121.03	126.17
3	E	200	CYC	C3B-C4B-NB	6.33	111.81	106.77
3	B	201	CYC	C3C-C4C-NC	-6.32	99.81	107.94
3	L	201	CYC	OB-C4B-C3B	-6.00	121.73	128.03
3	J	202	CYC	OB-C4B-C3B	-5.97	121.76	128.03
3	K	200	CYC	C3B-C4B-NB	5.91	111.48	106.77
3	H	201	CYC	OB-C4B-C3B	-5.89	121.84	128.03
3	I	200	CYC	C3B-C4B-NB	5.88	111.46	106.77
3	D	202	CYC	OB-C4B-C3B	-5.88	121.86	128.03
3	B	201	CYC	CHD-C4C-NC	-5.81	118.38	125.63
3	F	201	CYC	OB-C4B-C3B	-5.76	121.97	128.03
3	G	200	CYC	OB-C4B-C3B	-5.75	121.99	128.03
3	C	200	CYC	OB-C4B-C3B	-5.73	122.01	128.03
3	J	201	CYC	OB-C4B-C3B	-5.72	122.02	128.03
3	H	202	CYC	OB-C4B-C3B	-5.64	122.10	128.03
3	F	202	CYC	OB-C4B-C3B	-5.64	122.11	128.03
3	D	201	CYC	OB-C4B-C3B	-5.63	122.11	128.03
3	L	202	CYC	OB-C4B-C3B	-5.52	122.23	128.03
3	B	202	CYC	OB-C4B-C3B	-5.50	122.25	128.03
3	B	202	CYC	C3D-C4D-ND	5.38	114.32	107.57
3	L	202	CYC	C3D-C4D-ND	5.37	114.31	107.57
3	L	202	CYC	CAB-C3B-C4B	5.34	129.63	121.37
3	J	201	CYC	C3D-C4D-ND	5.34	114.26	107.57
3	G	200	CYC	CAB-C3B-C4B	5.33	129.62	121.37
3	D	201	CYC	C3D-C4D-ND	5.32	114.24	107.57
3	J	201	CYC	CAB-C3B-C4B	5.32	129.60	121.37
3	H	202	CYC	CAB-C3B-C4B	5.26	129.51	121.37
3	E	200	CYC	C1C-NC-C4C	-5.26	106.81	113.41
3	F	202	CYC	C3D-C4D-ND	5.22	114.11	107.57
3	G	200	CYC	C3D-C4D-ND	5.22	114.11	107.57
3	F	202	CYC	CAB-C3B-C4B	5.21	129.43	121.37
3	C	200	CYC	C3D-C4D-ND	5.20	114.09	107.57
3	F	201	CYC	C3D-C4D-ND	5.17	114.05	107.57
3	L	201	CYC	C3D-C4D-ND	5.15	114.03	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	CYC	C3B-C4B-NB	5.15	110.87	106.77
3	J	202	CYC	C3D-C4D-ND	5.14	114.02	107.57
3	B	202	CYC	CAB-C3B-C4B	5.14	129.31	121.37
3	H	202	CYC	C3D-C4D-ND	5.11	113.98	107.57
3	B	201	CYC	C4D-CHA-C1A	-5.09	117.10	128.22
3	I	200	CYC	C4D-CHA-C1A	-5.09	117.11	128.22
3	D	202	CYC	C3D-C4D-ND	5.09	113.94	107.57
3	H	201	CYC	C3D-C4D-ND	5.08	113.94	107.57
3	C	200	CYC	CAB-C3B-C4B	5.06	129.19	121.37
3	K	200	CYC	C1C-NC-C4C	-5.05	107.08	113.41
3	L	202	CYC	C2D-C1D-ND	5.05	114.31	107.43
3	D	202	CYC	CAB-C3B-C4B	5.05	129.17	121.37
3	H	201	CYC	CAB-C3B-C4B	5.02	129.14	121.37
3	B	202	CYC	C2D-C1D-ND	5.01	114.27	107.43
3	F	202	CYC	C2D-C1D-ND	4.97	114.21	107.43
3	F	201	CYC	CAB-C3B-C4B	4.97	129.06	121.37
3	D	201	CYC	CAB-C3B-C4B	4.94	129.01	121.37
3	J	201	CYC	C2D-C1D-ND	4.92	114.14	107.43
3	H	202	CYC	C2D-C1D-ND	4.92	114.13	107.43
3	D	201	CYC	C2D-C1D-ND	4.91	114.13	107.43
3	F	201	CYC	C2B-C1B-NB	4.87	114.07	106.97
3	L	201	CYC	CAB-C3B-C4B	4.87	128.90	121.37
3	L	201	CYC	C2B-C1B-NB	4.85	114.04	106.97
3	D	202	CYC	C2B-C1B-NB	4.84	114.03	106.97
3	H	201	CYC	C2B-C1B-NB	4.83	114.01	106.97
3	F	201	CYC	C2D-C1D-ND	4.82	114.01	107.43
3	J	202	CYC	C2B-C1B-NB	4.81	113.97	106.97
3	G	200	CYC	C2B-C1B-NB	4.79	113.95	106.97
3	D	201	CYC	C2B-C1B-NB	4.78	113.94	106.97
3	H	201	CYC	C2D-C1D-ND	4.75	113.91	107.43
3	J	202	CYC	C2D-C1D-ND	4.73	113.89	107.43
3	D	202	CYC	C2D-C1D-ND	4.72	113.86	107.43
3	B	201	CYC	CBC-CAC-C3C	4.70	123.39	113.41
3	G	200	CYC	C2D-C1D-ND	4.70	113.84	107.43
3	E	200	CYC	C4D-CHA-C1A	-4.70	117.97	128.22
3	L	201	CYC	C2D-C1D-ND	4.69	113.83	107.43
3	L	202	CYC	C2B-C1B-NB	4.66	113.77	106.97
3	C	200	CYC	C2D-C1D-ND	4.66	113.79	107.43
3	H	201	CYC	C1B-NB-C4B	-4.62	104.99	110.66
3	F	201	CYC	C1B-NB-C4B	-4.62	105.00	110.66
3	L	201	CYC	C1B-NB-C4B	-4.62	105.00	110.66
3	D	202	CYC	C1B-NB-C4B	-4.61	105.00	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	200	CYC	C2B-C1B-NB	4.61	113.69	106.97
3	J	201	CYC	C2B-C1B-NB	4.61	113.69	106.97
3	F	202	CYC	C2B-C1B-NB	4.58	113.65	106.97
3	B	202	CYC	C2B-C1B-NB	4.58	113.65	106.97
3	G	200	CYC	C1B-NB-C4B	-4.57	105.06	110.66
3	A	200	CYC	C1C-NC-C4C	-4.56	107.68	113.41
3	K	200	CYC	OC-C1C-C2C	-4.56	122.55	126.17
3	H	202	CYC	C2B-C1B-NB	4.53	113.57	106.97
3	J	202	CYC	C1B-NB-C4B	-4.52	105.11	110.66
3	I	200	CYC	OC-C1C-NC	-4.50	119.62	124.93
3	J	202	CYC	CAB-C3B-C4B	4.49	128.32	121.37
3	L	201	CYC	OC-C1C-C2C	-4.45	122.64	126.17
3	F	201	CYC	OC-C1C-C2C	-4.43	122.65	126.17
3	D	201	CYC	C1B-NB-C4B	-4.42	105.24	110.66
3	K	200	CYC	C4D-ND-C1D	-4.42	102.03	109.78
3	A	200	CYC	C4D-ND-C1D	-4.39	102.08	109.78
3	K	200	CYC	OC-C1C-NC	-4.38	119.76	124.93
3	L	201	CYC	C1B-C2B-C3B	-4.38	103.36	107.86
3	J	202	CYC	C1B-C2B-C3B	-4.38	103.36	107.86
3	L	202	CYC	C1B-NB-C4B	-4.38	105.29	110.66
3	E	200	CYC	C4D-ND-C1D	-4.37	102.10	109.78
3	I	200	CYC	C4D-ND-C1D	-4.37	102.10	109.78
3	G	200	CYC	OC-C1C-C2C	-4.37	122.70	126.17
3	I	200	CYC	C1C-NC-C4C	-4.37	107.93	113.41
3	F	201	CYC	C1B-C2B-C3B	-4.36	103.38	107.86
3	C	200	CYC	OC-C1C-C2C	-4.36	122.71	126.17
3	H	201	CYC	OC-C1C-C2C	-4.33	122.73	126.17
3	H	201	CYC	C1B-C2B-C3B	-4.33	103.41	107.86
3	J	201	CYC	C1B-NB-C4B	-4.31	105.37	110.66
3	B	201	CYC	C4D-ND-C1D	-4.31	102.22	109.78
3	D	201	CYC	C1B-C2B-C3B	-4.30	103.44	107.86
3	C	200	CYC	C1B-NB-C4B	-4.30	105.38	110.66
3	F	202	CYC	C1B-NB-C4B	-4.30	105.39	110.66
3	I	200	CYC	OC-C1C-C2C	-4.29	122.76	126.17
3	D	202	CYC	C1B-C2B-C3B	-4.28	103.46	107.86
3	J	202	CYC	OC-C1C-C2C	-4.27	122.77	126.17
3	D	202	CYC	OC-C1C-C2C	-4.25	122.79	126.17
3	H	202	CYC	C1B-NB-C4B	-4.25	105.45	110.66
3	K	200	CYC	C4D-CHA-C1A	-4.22	119.00	128.22
3	B	202	CYC	C1B-NB-C4B	-4.20	105.50	110.66
3	A	200	CYC	OC-C1C-C2C	-4.20	122.83	126.17
3	G	200	CYC	C1B-C2B-C3B	-4.11	103.64	107.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	202	CYC	C1B-C2B-C3B	-4.11	103.64	107.86
3	C	200	CYC	C1B-C2B-C3B	-4.09	103.66	107.86
3	L	202	CYC	C1D-CHD-C4C	-4.09	120.79	127.76
3	B	202	CYC	C1B-C2B-C3B	-4.07	103.68	107.86
3	F	202	CYC	C1B-C2B-C3B	-4.06	103.69	107.86
3	F	201	CYC	C1D-C2D-C3D	-4.06	102.68	107.76
3	J	201	CYC	C1B-C2B-C3B	-4.05	103.70	107.86
3	H	202	CYC	C1B-C2B-C3B	-4.04	103.71	107.86
3	F	202	CYC	C1D-CHD-C4C	-4.01	120.91	127.76
3	C	200	CYC	C1D-C2D-C3D	-4.01	102.75	107.76
3	H	201	CYC	C1D-C2D-C3D	-4.01	102.75	107.76
3	I	200	CYC	CHB-C4A-NA	-4.00	116.31	124.95
3	E	200	CYC	OB-C4B-C3B	-4.00	123.83	128.03
3	B	202	CYC	C1D-C2D-C3D	-3.98	102.78	107.76
3	A	200	CYC	C4D-CHA-C1A	-3.98	119.53	128.22
3	B	202	CYC	CMA-C3A-C4A	3.98	131.28	125.10
3	F	202	CYC	C1D-C2D-C3D	-3.98	102.79	107.76
3	L	202	CYC	C1D-C2D-C3D	-3.97	102.79	107.76
3	G	200	CYC	C1D-C2D-C3D	-3.97	102.80	107.76
3	D	201	CYC	OC-C1C-C2C	-3.95	123.03	126.17
3	J	201	CYC	C1D-C2D-C3D	-3.92	102.85	107.76
3	L	201	CYC	C1D-C2D-C3D	-3.92	102.86	107.76
3	A	200	CYC	CHB-C4A-NA	-3.91	116.52	124.95
3	J	202	CYC	C1D-C2D-C3D	-3.90	102.88	107.76
3	D	202	CYC	C1D-C2D-C3D	-3.89	102.90	107.76
3	D	201	CYC	C1D-C2D-C3D	-3.88	102.91	107.76
3	F	202	CYC	OC-C1C-C2C	-3.86	123.11	126.17
3	F	202	CYC	CMA-C3A-C4A	3.83	131.05	125.10
3	H	202	CYC	C1D-C2D-C3D	-3.83	102.97	107.76
3	K	200	CYC	CHB-C4A-NA	-3.82	116.70	124.95
3	J	201	CYC	C1D-CHD-C4C	-3.81	121.26	127.76
3	B	202	CYC	CHB-C4A-NA	-3.78	116.79	124.95
3	J	201	CYC	OC-C1C-C2C	-3.78	123.17	126.17
3	A	200	CYC	CHA-C4D-C3D	-3.77	119.13	127.22
3	J	201	CYC	CHB-C4A-NA	-3.76	116.83	124.95
3	L	202	CYC	CHB-C4A-NA	-3.75	116.84	124.95
3	D	201	CYC	C4D-C3D-C2D	-3.75	103.25	107.62
3	J	201	CYC	CMA-C3A-C4A	3.75	130.92	125.10
3	B	202	CYC	C1D-CHD-C4C	-3.75	121.37	127.76
3	L	202	CYC	CMA-C3A-C4A	3.74	130.91	125.10
3	H	202	CYC	OC-C1C-C2C	-3.73	123.20	126.17
3	F	201	CYC	C2C-C1C-NC	3.72	111.39	108.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	201	CYC	C4D-C3D-C2D	-3.72	103.29	107.62
3	H	202	CYC	C1D-CHD-C4C	-3.71	121.43	127.76
3	J	201	CYC	C4D-C3D-C2D	-3.71	103.30	107.62
3	E	200	CYC	CHA-C4D-C3D	-3.71	119.25	127.22
3	B	202	CYC	OC-C1C-C2C	-3.70	123.23	126.17
3	L	202	CYC	C4D-C3D-C2D	-3.70	103.32	107.62
3	F	202	CYC	CHB-C4A-NA	-3.69	116.98	124.95
3	H	202	CYC	C4D-C3D-C2D	-3.69	103.32	107.62
3	B	202	CYC	C4D-C3D-C2D	-3.69	103.32	107.62
3	H	202	CYC	CMA-C3A-C4A	3.69	130.83	125.10
3	J	202	CYC	C4D-C3D-C2D	-3.68	103.34	107.62
3	D	202	CYC	C4D-C3D-C2D	-3.67	103.35	107.62
3	G	200	CYC	C4D-C3D-C2D	-3.66	103.36	107.62
3	C	200	CYC	C4D-C3D-C2D	-3.64	103.38	107.62
3	H	201	CYC	C4D-C3D-C2D	-3.64	103.38	107.62
3	H	201	CYC	C2C-C1C-NC	3.63	111.31	108.29
3	L	202	CYC	OC-C1C-C2C	-3.63	123.29	126.17
3	L	201	CYC	CMB-C2B-C1B	3.60	128.54	124.16
3	A	200	CYC	OB-C4B-C3B	-3.60	124.25	128.03
3	D	201	CYC	C1D-CHD-C4C	-3.60	121.62	127.76
3	F	201	CYC	C4D-C3D-C2D	-3.60	103.43	107.62
3	I	200	CYC	C1B-CHB-C4A	-3.59	119.24	128.06
3	L	201	CYC	C2C-C1C-NC	3.59	111.27	108.29
3	F	202	CYC	C4D-C3D-C2D	-3.58	103.45	107.62
3	H	201	CYC	CMB-C2B-C1B	3.56	128.49	124.16
3	A	200	CYC	CHB-C4A-C3A	3.55	134.00	124.87
3	F	201	CYC	CMB-C2B-C1B	3.54	128.47	124.16
3	D	202	CYC	C2C-C1C-NC	3.52	111.22	108.29
3	F	202	CYC	C2C-C1C-NC	3.49	111.19	108.29
3	J	202	CYC	C2C-C1C-NC	3.47	111.18	108.29
3	D	202	CYC	CMB-C2B-C1B	3.47	128.38	124.16
3	K	200	CYC	CMA-C3A-C4A	3.46	130.48	125.10
3	H	202	CYC	CMB-C2B-C1B	3.46	128.37	124.16
3	J	202	CYC	CMB-C2B-C1B	3.45	128.35	124.16
3	K	200	CYC	CHA-C4D-C3D	-3.45	119.80	127.22
3	C	200	CYC	CMA-C3A-C4A	3.44	130.45	125.10
3	B	201	CYC	CHB-C4A-NA	-3.44	117.52	124.95
3	D	201	CYC	CMB-C2B-C1B	3.44	128.34	124.16
3	H	202	CYC	CHB-C4A-NA	-3.44	117.53	124.95
3	I	200	CYC	CHA-C4D-C3D	-3.43	119.85	127.22
3	B	201	CYC	OC-C1C-NC	-3.40	120.92	124.93
3	I	200	CYC	CAB-C3B-C4B	3.40	126.63	121.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	201	CYC	C2C-C1C-NC	3.40	111.11	108.29
3	A	200	CYC	CBC-CAC-C3C	3.37	120.56	113.41
3	B	201	CYC	CMA-C3A-C4A	3.37	130.33	125.10
3	B	202	CYC	C2C-C1C-NC	3.36	111.08	108.29
3	G	200	CYC	CHB-C4A-NA	-3.35	117.72	124.95
3	K	200	CYC	CAB-C3B-C4B	3.34	126.54	121.37
3	D	201	CYC	C2C-C1C-NC	3.34	111.07	108.29
3	K	200	CYC	CHB-C4A-C3A	3.34	133.45	124.87
3	L	201	CYC	CHB-C1B-NB	-3.34	118.94	126.06
3	K	200	CYC	C1B-CHB-C4A	-3.34	119.86	128.06
3	E	200	CYC	CHB-C4A-NA	-3.34	117.75	124.95
3	K	200	CYC	CBC-CAC-C3C	3.34	120.49	113.41
3	L	202	CYC	C2C-C1C-NC	3.32	111.05	108.29
3	C	200	CYC	C2C-C1C-NC	3.32	111.05	108.29
3	C	200	CYC	CHD-C1D-ND	-3.32	117.79	125.29
3	J	202	CYC	CHB-C1B-NB	-3.31	118.99	126.06
3	D	201	CYC	CHB-C4A-NA	-3.31	117.80	124.95
3	I	200	CYC	CHB-C4A-C3A	3.31	133.38	124.87
3	J	201	CYC	CMB-C2B-C1B	3.31	128.18	124.16
3	A	200	CYC	OC-C1C-NC	-3.30	121.04	124.93
3	D	201	CYC	CMA-C3A-C4A	3.29	130.22	125.10
3	L	202	CYC	CMB-C2B-C1B	3.29	128.16	124.16
3	G	200	CYC	C2C-C1C-NC	3.29	111.03	108.29
3	H	202	CYC	C2C-C1C-NC	3.29	111.02	108.29
3	I	200	CYC	C3C-C4C-NC	-3.28	103.72	107.94
3	G	200	CYC	CHD-C1D-ND	-3.27	117.90	125.29
3	B	201	CYC	C1D-CHD-C4C	-3.26	122.20	127.76
3	F	202	CYC	CMB-C2B-C1B	3.25	128.12	124.16
3	F	201	CYC	CHB-C1B-NB	-3.23	119.16	126.06
3	F	201	CYC	CHD-C1D-ND	-3.23	118.00	125.29
3	G	200	CYC	CMB-C2B-C1B	3.23	128.08	124.16
3	C	200	CYC	CMB-C2B-C1B	3.22	128.08	124.16
3	H	201	CYC	CHB-C1B-NB	-3.21	119.21	126.06
3	G	200	CYC	CMA-C3A-C4A	3.21	130.08	125.10
3	C	200	CYC	CHB-C4A-NA	-3.20	118.04	124.95
3	L	201	CYC	CHD-C1D-ND	-3.20	118.07	125.29
3	H	201	CYC	CHD-C1D-ND	-3.18	118.10	125.29
3	I	200	CYC	OB-C4B-C3B	-3.17	124.70	128.03
3	B	202	CYC	CMB-C2B-C1B	3.16	128.01	124.16
3	E	200	CYC	CAB-C3B-C4B	3.15	126.24	121.37
3	E	200	CYC	OC-C1C-NC	-3.14	121.22	124.93
3	B	202	CYC	C4A-C3A-C2A	-3.12	102.93	106.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	200	CYC	CMA-C3A-C4A	3.11	129.93	125.10
3	F	201	CYC	C4A-C3A-C2A	-3.10	102.95	106.48
3	D	201	CYC	C4A-C3A-C2A	-3.10	102.96	106.48
3	A	200	CYC	CAB-C3B-C4B	3.10	126.16	121.37
3	G	200	CYC	C4A-C3A-C2A	-3.09	102.97	106.48
3	D	202	CYC	C4A-C3A-C2A	-3.09	102.97	106.48
3	D	202	CYC	CHD-C1D-ND	-3.09	118.31	125.29
3	L	202	CYC	C4A-C3A-C2A	-3.08	102.98	106.48
3	D	202	CYC	CHB-C1B-NB	-3.07	119.50	126.06
3	F	201	CYC	C1A-C2A-C3A	-3.07	103.40	106.73
3	A	200	CYC	CMA-C3A-C4A	3.07	129.86	125.10
3	J	202	CYC	CMA-C3A-C4A	3.06	129.85	125.10
3	J	201	CYC	C4A-C3A-C2A	-3.05	103.01	106.48
3	H	201	CYC	C4A-C3A-C2A	-3.05	103.02	106.48
3	F	202	CYC	C4A-C3A-C2A	-3.04	103.02	106.48
3	L	201	CYC	C1A-C2A-C3A	-3.04	103.44	106.73
3	C	200	CYC	C4A-C3A-C2A	-3.03	103.04	106.48
3	D	201	CYC	CHB-C1B-NB	-3.02	119.61	126.06
3	B	201	CYC	OB-C4B-C3B	-3.01	124.87	128.03
3	L	201	CYC	C4A-C3A-C2A	-3.01	103.06	106.48
3	J	202	CYC	CHD-C1D-ND	-2.99	118.52	125.29
3	B	201	CYC	C1B-CHB-C4A	-2.99	120.72	128.06
3	H	201	CYC	C1A-C2A-C3A	-2.99	103.50	106.73
3	J	202	CYC	C4A-C3A-C2A	-2.97	103.10	106.48
3	G	200	CYC	C1A-C2A-C3A	-2.96	103.53	106.73
3	H	202	CYC	C4A-C3A-C2A	-2.95	103.13	106.48
3	E	200	CYC	CHB-C4A-C3A	2.95	132.44	124.87
3	J	202	CYC	C1A-C2A-C3A	-2.94	103.55	106.73
3	C	200	CYC	CMD-C2D-C1D	2.94	129.89	125.62
3	D	201	CYC	C1A-C2A-C3A	-2.93	103.55	106.73
3	F	201	CYC	CHB-C4A-NA	-2.93	118.62	124.95
3	F	201	CYC	C2A-C1A-NA	2.93	114.19	110.04
3	B	201	CYC	CHD-C1D-ND	-2.92	118.69	125.29
3	E	200	CYC	C1B-CHB-C4A	-2.92	120.89	128.06
3	C	200	CYC	C1A-C2A-C3A	-2.91	103.58	106.73
3	D	202	CYC	C1A-C2A-C3A	-2.89	103.60	106.73
3	L	202	CYC	C1A-C2A-C3A	-2.88	103.61	106.73
3	G	200	CYC	C2A-C1A-NA	2.88	114.12	110.04
3	J	201	CYC	C1A-C2A-C3A	-2.86	103.63	106.73
3	C	200	CYC	C2A-C1A-NA	2.86	114.10	110.04
3	B	201	CYC	CAB-C3B-C4B	2.86	125.80	121.37
3	F	201	CYC	CMD-C2D-C1D	2.86	129.78	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	201	CYC	CMA-C3A-C4A	2.85	129.52	125.10
3	D	201	CYC	C2A-C1A-NA	2.84	114.07	110.04
3	L	202	CYC	C2A-C1A-NA	2.83	114.05	110.04
3	A	200	CYC	C3C-C4C-NC	-2.83	104.30	107.94
3	L	201	CYC	C2A-C1A-NA	2.82	114.04	110.04
3	J	201	CYC	C2A-C1A-NA	2.82	114.04	110.04
3	B	202	CYC	C2A-C1A-NA	2.82	114.04	110.04
3	K	200	CYC	C2B-C1B-NB	2.82	111.08	106.97
3	E	200	CYC	CAD-CBD-CGD	2.80	121.10	113.67
3	H	201	CYC	C2A-C1A-NA	2.80	114.01	110.04
3	H	201	CYC	CMD-C2D-C1D	2.80	129.69	125.62
3	J	202	CYC	C2A-C1A-NA	2.78	113.98	110.04
3	D	202	CYC	CMA-C3A-C4A	2.78	129.41	125.10
3	E	200	CYC	C3C-C4C-NC	-2.77	104.37	107.94
3	G	200	CYC	CMD-C2D-C1D	2.76	129.63	125.62
3	B	202	CYC	C1A-C2A-C3A	-2.76	103.74	106.73
3	C	200	CYC	C1D-CHD-C4C	-2.76	123.06	127.76
3	F	202	CYC	C1A-C2A-C3A	-2.75	103.75	106.73
3	D	202	CYC	CMD-C2D-C1D	2.75	129.62	125.62
3	B	201	CYC	C1A-C2A-C3A	2.75	109.70	106.73
3	K	200	CYC	C3C-C4C-NC	-2.74	104.41	107.94
3	B	201	CYC	CHB-C4A-C3A	2.74	131.92	124.87
3	J	202	CYC	CHB-C4A-NA	-2.73	119.05	124.95
3	E	200	CYC	C3D-C4D-ND	2.73	110.99	107.57
3	E	200	CYC	C1A-NA-C4A	-2.73	101.50	106.52
3	H	201	CYC	CHB-C4A-NA	-2.73	119.07	124.95
3	H	202	CYC	C1A-C2A-C3A	-2.73	103.78	106.73
3	J	202	CYC	CMD-C2D-C1D	2.72	129.58	125.62
3	D	202	CYC	CHB-C4A-NA	-2.71	119.09	124.95
3	D	202	CYC	C2A-C1A-NA	2.70	113.87	110.04
3	F	202	CYC	C2A-C1A-NA	2.70	113.86	110.04
3	B	201	CYC	C1A-NA-C4A	-2.69	101.58	106.52
3	H	201	CYC	CMA-C3A-C4A	2.69	129.28	125.10
3	L	201	CYC	CMD-C2D-C1D	2.68	129.51	125.62
3	A	200	CYC	C2B-C1B-NB	2.67	110.86	106.97
3	B	201	CYC	C2B-C1B-NB	2.67	110.86	106.97
3	B	201	CYC	CHA-C4D-C3D	-2.66	121.50	127.22
3	E	200	CYC	C2B-C1B-NB	2.66	110.85	106.97
3	B	202	CYC	C3C-C4C-NC	2.66	111.37	107.94
3	I	200	CYC	C2B-C1B-NB	2.66	110.84	106.97
3	L	201	CYC	CMA-C3A-C4A	2.65	129.22	125.10
3	K	200	CYC	C1A-C2A-C3A	2.65	109.59	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	201	CYC	CHB-C4A-NA	-2.65	119.23	124.95
3	C	200	CYC	CHB-C1B-NB	-2.64	120.42	126.06
3	E	200	CYC	CMA-C3A-C4A	2.62	129.18	125.10
3	K	200	CYC	CAD-C3D-C4D	-2.62	121.61	125.77
3	L	202	CYC	C3C-C4C-NC	2.62	111.31	107.94
3	B	202	CYC	CHB-C1B-NB	-2.61	120.48	126.06
3	K	200	CYC	CBB-CAB-C3B	2.61	119.48	112.42
3	J	201	CYC	C3C-C4C-NC	2.60	111.29	107.94
3	H	202	CYC	C2A-C1A-NA	2.60	113.72	110.04
3	I	200	CYC	C1A-NA-C4A	-2.59	101.77	106.52
3	H	202	CYC	CHB-C1B-NB	-2.59	120.55	126.06
3	F	202	CYC	CMD-C2D-C1D	2.58	129.37	125.62
3	A	200	CYC	C3D-C4D-ND	2.58	110.80	107.57
3	L	202	CYC	C4D-ND-C1D	-2.57	105.27	109.78
3	G	200	CYC	CHB-C1B-NB	-2.57	120.58	126.06
3	F	201	CYC	C1D-CHD-C4C	-2.55	123.41	127.76
3	B	202	CYC	C4D-ND-C1D	-2.55	105.30	109.78
3	L	202	CYC	CHB-C1B-NB	-2.55	120.62	126.06
3	D	201	CYC	C3C-C4C-NC	2.55	111.22	107.94
3	E	200	CYC	CHB-C1B-C2B	-2.54	121.89	126.97
3	H	201	CYC	C3C-C4C-NC	2.53	111.19	107.94
3	F	202	CYC	CHB-C1B-NB	-2.52	120.68	126.06
3	B	202	CYC	CMD-C2D-C1D	2.52	129.28	125.62
3	F	201	CYC	C3C-C4C-NC	2.52	111.19	107.94
3	H	202	CYC	C3C-C4C-NC	2.51	111.18	107.94
3	L	202	CYC	CMD-C2D-C1D	2.51	129.26	125.62
3	I	200	CYC	CBC-CAC-C3C	2.50	118.73	113.41
3	F	202	CYC	C3C-C4C-NC	2.50	111.16	107.94
3	L	201	CYC	C3C-C4C-NC	2.49	111.15	107.94
3	B	202	CYC	CHA-C4D-C3D	-2.48	121.89	127.22
3	F	202	CYC	C4D-ND-C1D	-2.48	105.43	109.78
3	D	201	CYC	CMD-C2D-C1D	2.48	129.22	125.62
3	J	201	CYC	C4D-ND-C1D	-2.48	105.43	109.78
3	D	201	CYC	C4D-ND-C1D	-2.46	105.46	109.78
3	I	200	CYC	CBB-CAB-C3B	2.46	119.08	112.42
3	J	201	CYC	CMD-C2D-C1D	2.45	129.18	125.62
3	J	202	CYC	C3C-C4C-NC	2.44	111.09	107.94
3	J	202	CYC	C1D-CHD-C4C	-2.44	123.60	127.76
3	D	202	CYC	C1D-CHD-C4C	-2.44	123.60	127.76
3	G	200	CYC	C1D-CHD-C4C	-2.43	123.61	127.76
3	D	202	CYC	C3C-C4C-NC	2.43	111.07	107.94
3	A	200	CYC	C1A-C2A-C3A	2.43	109.35	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	201	CYC	CHB-C1B-NB	-2.42	120.89	126.06
3	H	201	CYC	C1D-CHD-C4C	-2.42	123.63	127.76
3	L	202	CYC	CHA-C4D-C3D	-2.42	122.02	127.22
3	H	202	CYC	C4D-ND-C1D	-2.39	105.58	109.78
3	H	202	CYC	CMD-C2D-C1D	2.38	129.08	125.62
3	D	201	CYC	CHD-C1D-ND	-2.35	119.98	125.29
3	J	201	CYC	CHA-C4D-C3D	-2.35	122.17	127.22
3	B	201	CYC	C3D-C4D-ND	2.35	110.51	107.57
3	K	200	CYC	C1A-NA-C4A	-2.31	102.28	106.52
3	A	200	CYC	C1B-CHB-C4A	-2.31	122.39	128.06
3	D	201	CYC	CHA-C4D-C3D	-2.30	122.28	127.22
3	B	201	CYC	CHB-C1B-C2B	-2.29	122.41	126.97
3	K	200	CYC	CHB-C1B-C2B	-2.28	122.42	126.97
3	B	202	CYC	CHD-C1D-ND	-2.27	120.17	125.29
3	E	200	CYC	CBC-CAC-C3C	2.26	118.20	113.41
3	F	201	CYC	C4D-ND-C1D	-2.26	105.82	109.78
3	I	200	CYC	CHB-C1B-C2B	-2.25	122.49	126.97
3	I	200	CYC	C3D-C4D-ND	2.24	110.38	107.57
3	L	201	CYC	C1B-CHB-C4A	-2.24	122.55	128.06
3	F	202	CYC	CHA-C4D-C3D	-2.23	122.42	127.22
3	J	202	CYC	C4D-ND-C1D	-2.22	105.88	109.78
3	L	201	CYC	C1D-CHD-C4C	-2.22	123.98	127.76
3	I	200	CYC	C2C-C3C-C4C	2.22	104.66	101.34
3	J	201	CYC	CHD-C1D-ND	-2.22	120.28	125.29
3	G	200	CYC	C4D-ND-C1D	-2.21	105.90	109.78
3	D	202	CYC	C4D-ND-C1D	-2.19	105.94	109.78
3	J	202	CYC	C1B-CHB-C4A	-2.18	122.69	128.06
3	B	201	CYC	CMD-C2D-C1D	2.17	128.78	125.62
3	F	201	CYC	C1B-CHB-C4A	-2.16	122.74	128.06
3	H	201	CYC	C1B-CHB-C4A	-2.16	122.74	128.06
3	C	200	CYC	C4D-ND-C1D	-2.16	105.99	109.78
3	L	201	CYC	C4D-ND-C1D	-2.16	105.99	109.78
3	H	201	CYC	C4D-ND-C1D	-2.14	106.02	109.78
3	E	200	CYC	CAD-C3D-C4D	-2.13	122.39	125.77
3	C	200	CYC	CBC-CAC-C3C	-2.12	108.92	113.41
3	K	200	CYC	C3D-C4D-ND	2.12	110.22	107.57
3	A	200	CYC	CHA-C4D-ND	2.12	130.07	125.29
3	I	200	CYC	C1A-C2A-C3A	2.11	109.01	106.73
3	E	200	CYC	O2A-CGA-CBA	2.10	120.64	114.00
3	A	200	CYC	C1A-NA-C4A	-2.10	102.66	106.52
3	F	202	CYC	CHD-C1D-ND	-2.09	120.56	125.29
3	H	202	CYC	CAD-C3D-C4D	2.09	129.08	125.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	202	CYC	CHD-C1D-ND	-2.08	120.58	125.29
3	K	200	CYC	CHA-C4D-ND	2.07	129.97	125.29
3	B	201	CYC	O2A-CGA-CBA	2.04	120.45	114.00
3	I	200	CYC	O2A-CGA-CBA	2.02	120.39	114.00
3	K	200	CYC	C2D-C1D-ND	2.02	110.18	107.43
3	E	200	CYC	C2C-C3C-C4C	2.01	104.36	101.34
3	K	200	CYC	OB-C4B-C3B	-2.01	125.92	128.03
3	E	200	CYC	O2D-CGD-CBD	2.00	120.33	114.00
3	G	200	CYC	CAA-CBA-CGA	-2.00	108.36	113.67
3	K	200	CYC	O2A-CGA-CBA	2.00	120.32	114.00

There are no chirality outliers.

All (179) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	200	CYC	NA-C4A-CHB-C1B
3	C	200	CYC	C2C-C3C-CAC-CBC
3	C	200	CYC	C4C-C3C-CAC-CBC
3	D	201	CYC	NA-C4A-CHB-C1B
3	D	201	CYC	C3A-C4A-CHB-C1B
3	D	201	CYC	C2C-C3C-CAC-CBC
3	D	201	CYC	C4C-C3C-CAC-CBC
3	D	202	CYC	NA-C4A-CHB-C1B
3	D	202	CYC	C3A-C4A-CHB-C1B
3	A	200	CYC	NC-C4C-CHD-C1D
3	B	201	CYC	NC-C4C-CHD-C1D
3	B	202	CYC	C4C-C3C-CAC-CBC
3	E	200	CYC	NC-C4C-CHD-C1D
3	F	201	CYC	NA-C4A-CHB-C1B
3	F	201	CYC	C3A-C4A-CHB-C1B
3	F	202	CYC	C2C-C3C-CAC-CBC
3	F	202	CYC	C4C-C3C-CAC-CBC
3	F	202	CYC	C4D-C3D-CAD-CBD
3	I	200	CYC	C2A-CAA-CBA-CGA
3	I	200	CYC	NC-C4C-CHD-C1D
3	J	201	CYC	C2B-C3B-CAB-CBB
3	J	201	CYC	C4B-C3B-CAB-CBB
3	J	201	CYC	C2C-C3C-CAC-CBC
3	J	201	CYC	C4C-C3C-CAC-CBC
3	J	202	CYC	NA-C4A-CHB-C1B
3	J	202	CYC	C3A-C4A-CHB-C1B
3	G	200	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
3	G	200	CYC	C2C-C3C-CAC-CBC
3	G	200	CYC	C4C-C3C-CAC-CBC
3	H	201	CYC	NA-C4A-CHB-C1B
3	H	201	CYC	C3A-C4A-CHB-C1B
3	H	202	CYC	C2C-C3C-CAC-CBC
3	H	202	CYC	C4C-C3C-CAC-CBC
3	K	200	CYC	NC-C4C-CHD-C1D
3	L	201	CYC	NA-C4A-CHB-C1B
3	L	201	CYC	C3A-C4A-CHB-C1B
3	L	202	CYC	C4C-C3C-CAC-CBC
3	D	202	CYC	C2B-C3B-CAB-CBB
3	H	201	CYC	C2B-C3B-CAB-CBB
3	B	202	CYC	C2B-C3B-CAB-CBB
3	F	202	CYC	C2B-C3B-CAB-CBB
3	L	202	CYC	C2B-C3B-CAB-CBB
3	J	202	CYC	C2B-C3B-CAB-CBB
3	C	200	CYC	ND-C1D-CHD-C4C
3	D	202	CYC	ND-C1D-CHD-C4C
3	B	201	CYC	ND-C1D-CHD-C4C
3	F	201	CYC	ND-C1D-CHD-C4C
3	J	202	CYC	ND-C1D-CHD-C4C
3	G	200	CYC	ND-C1D-CHD-C4C
3	H	201	CYC	ND-C1D-CHD-C4C
3	L	201	CYC	ND-C1D-CHD-C4C
3	D	201	CYC	C2D-C1D-CHD-C4C
3	B	201	CYC	C2D-C1D-CHD-C4C
3	B	202	CYC	C2D-C1D-CHD-C4C
3	F	202	CYC	C2D-C1D-CHD-C4C
3	J	201	CYC	C2D-C1D-CHD-C4C
3	H	202	CYC	C2D-C1D-CHD-C4C
3	L	202	CYC	C2D-C1D-CHD-C4C
3	B	201	CYC	C2B-C3B-CAB-CBB
3	H	202	CYC	C4D-C3D-CAD-CBD
3	F	201	CYC	C2B-C3B-CAB-CBB
3	C	200	CYC	C3A-C4A-CHB-C1B
3	G	200	CYC	C3A-C4A-CHB-C1B
3	D	201	CYC	ND-C1D-CHD-C4C
3	A	200	CYC	ND-C1D-CHD-C4C
3	B	202	CYC	ND-C1D-CHD-C4C
3	E	200	CYC	ND-C1D-CHD-C4C
3	F	202	CYC	ND-C1D-CHD-C4C
3	I	200	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
3	J	201	CYC	ND-C1D-CHD-C4C
3	H	202	CYC	ND-C1D-CHD-C4C
3	K	200	CYC	ND-C1D-CHD-C4C
3	L	202	CYC	ND-C1D-CHD-C4C
3	C	200	CYC	C2D-C1D-CHD-C4C
3	D	202	CYC	C2D-C1D-CHD-C4C
3	A	200	CYC	C2D-C1D-CHD-C4C
3	E	200	CYC	C2D-C1D-CHD-C4C
3	F	201	CYC	C2D-C1D-CHD-C4C
3	I	200	CYC	C2D-C1D-CHD-C4C
3	J	202	CYC	C2D-C1D-CHD-C4C
3	G	200	CYC	C2D-C1D-CHD-C4C
3	H	201	CYC	C2D-C1D-CHD-C4C
3	K	200	CYC	C2D-C1D-CHD-C4C
3	L	201	CYC	C2D-C1D-CHD-C4C
3	H	202	CYC	C2B-C3B-CAB-CBB
3	F	202	CYC	C2D-C3D-CAD-CBD
3	H	202	CYC	C2D-C3D-CAD-CBD
3	D	202	CYC	C4B-C3B-CAB-CBB
3	B	202	CYC	C4B-C3B-CAB-CBB
3	F	202	CYC	C4B-C3B-CAB-CBB
3	L	202	CYC	C4B-C3B-CAB-CBB
3	A	200	CYC	NA-C4A-CHB-C1B
3	B	201	CYC	NA-C4A-CHB-C1B
3	B	202	CYC	NA-C4A-CHB-C1B
3	E	200	CYC	NA-C4A-CHB-C1B
3	F	202	CYC	NA-C4A-CHB-C1B
3	I	200	CYC	NA-C4A-CHB-C1B
3	J	201	CYC	NA-C4A-CHB-C1B
3	H	202	CYC	NA-C4A-CHB-C1B
3	K	200	CYC	NA-C4A-CHB-C1B
3	L	202	CYC	NA-C4A-CHB-C1B
3	G	200	CYC	C2B-C3B-CAB-CBB
3	A	200	CYC	C3A-C4A-CHB-C1B
3	B	201	CYC	C3A-C4A-CHB-C1B
3	B	202	CYC	C3A-C4A-CHB-C1B
3	E	200	CYC	C3A-C4A-CHB-C1B
3	F	202	CYC	C3A-C4A-CHB-C1B
3	I	200	CYC	C3A-C4A-CHB-C1B
3	J	201	CYC	C3A-C4A-CHB-C1B
3	H	202	CYC	C3A-C4A-CHB-C1B
3	K	200	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
3	L	202	CYC	C3A-C4A-CHB-C1B
3	H	201	CYC	C4B-C3B-CAB-CBB
3	B	201	CYC	C2A-CAA-CBA-CGA
3	K	200	CYC	C2A-CAA-CBA-CGA
3	D	201	CYC	C2B-C3B-CAB-CBB
3	B	201	CYC	C4B-C3B-CAB-CBB
3	J	202	CYC	C4B-C3B-CAB-CBB
3	B	202	CYC	C2C-C3C-CAC-CBC
3	L	202	CYC	C2C-C3C-CAC-CBC
3	I	200	CYC	C4D-C3D-CAD-CBD
3	F	201	CYC	C4B-C3B-CAB-CBB
3	H	202	CYC	C4B-C3B-CAB-CBB
3	C	200	CYC	C2B-C3B-CAB-CBB
3	E	200	CYC	C2A-CAA-CBA-CGA
3	G	200	CYC	C3A-C2A-CAA-CBA
3	F	202	CYC	CAA-CBA-CGA-O2A
3	G	200	CYC	C1A-C2A-CAA-CBA
3	B	202	CYC	CAA-CBA-CGA-O2A
3	L	202	CYC	CAA-CBA-CGA-O2A
3	E	200	CYC	CAA-CBA-CGA-O2A
3	F	202	CYC	CAA-CBA-CGA-O1A
3	J	202	CYC	CAA-CBA-CGA-O1A
3	D	202	CYC	CAA-CBA-CGA-O1A
3	A	200	CYC	CAA-CBA-CGA-O2A
3	B	202	CYC	CAA-CBA-CGA-O1A
3	J	201	CYC	CAA-CBA-CGA-O2A
3	J	202	CYC	CAA-CBA-CGA-O2A
3	L	202	CYC	CAA-CBA-CGA-O1A
3	B	201	CYC	CAA-CBA-CGA-O2A
3	F	201	CYC	CAA-CBA-CGA-O1A
3	H	201	CYC	CAA-CBA-CGA-O1A
3	K	200	CYC	CAA-CBA-CGA-O2A
3	D	201	CYC	CAA-CBA-CGA-O2A
3	B	201	CYC	CAA-CBA-CGA-O1A
3	G	200	CYC	CAA-CBA-CGA-O2A
3	H	202	CYC	CAA-CBA-CGA-O2A
3	J	201	CYC	CAA-CBA-CGA-O1A
3	D	201	CYC	CAA-CBA-CGA-O1A
3	A	200	CYC	CAA-CBA-CGA-O1A
3	G	200	CYC	CAA-CBA-CGA-O1A
3	E	200	CYC	CAA-CBA-CGA-O1A
3	K	200	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	B	202	CYC	CAD-CBD-CGD-O2D
3	C	200	CYC	CAA-CBA-CGA-O2A
3	H	202	CYC	CAA-CBA-CGA-O1A
3	D	202	CYC	CAA-CBA-CGA-O2A
3	F	201	CYC	CAA-CBA-CGA-O2A
3	H	201	CYC	CAA-CBA-CGA-O2A
3	C	200	CYC	CAA-CBA-CGA-O1A
3	C	200	CYC	C3A-C2A-CAA-CBA
3	B	202	CYC	CAD-CBD-CGD-O1D
3	I	200	CYC	CAA-CBA-CGA-O2A
3	D	201	CYC	CAD-CBD-CGD-O2D
3	I	200	CYC	CAA-CBA-CGA-O1A
3	J	201	CYC	CAD-CBD-CGD-O2D
3	L	202	CYC	CAD-CBD-CGD-O2D
3	L	201	CYC	CAA-CBA-CGA-O1A
3	I	200	CYC	C2D-C3D-CAD-CBD
3	L	201	CYC	CAA-CBA-CGA-O2A
3	D	201	CYC	CAD-CBD-CGD-O1D
3	J	201	CYC	CAD-CBD-CGD-O1D
3	L	202	CYC	CAD-CBD-CGD-O1D
3	A	200	CYC	CAD-CBD-CGD-O2D
3	I	200	CYC	CAD-CBD-CGD-O1D
3	K	200	CYC	CAD-CBD-CGD-O2D
3	A	200	CYC	C3C-C4C-CHD-C1D
3	A	200	CYC	C2A-CAA-CBA-CGA
3	F	202	CYC	CAD-CBD-CGD-O2D

There are no ring outliers.

18 monomers are involved in 198 short contacts:

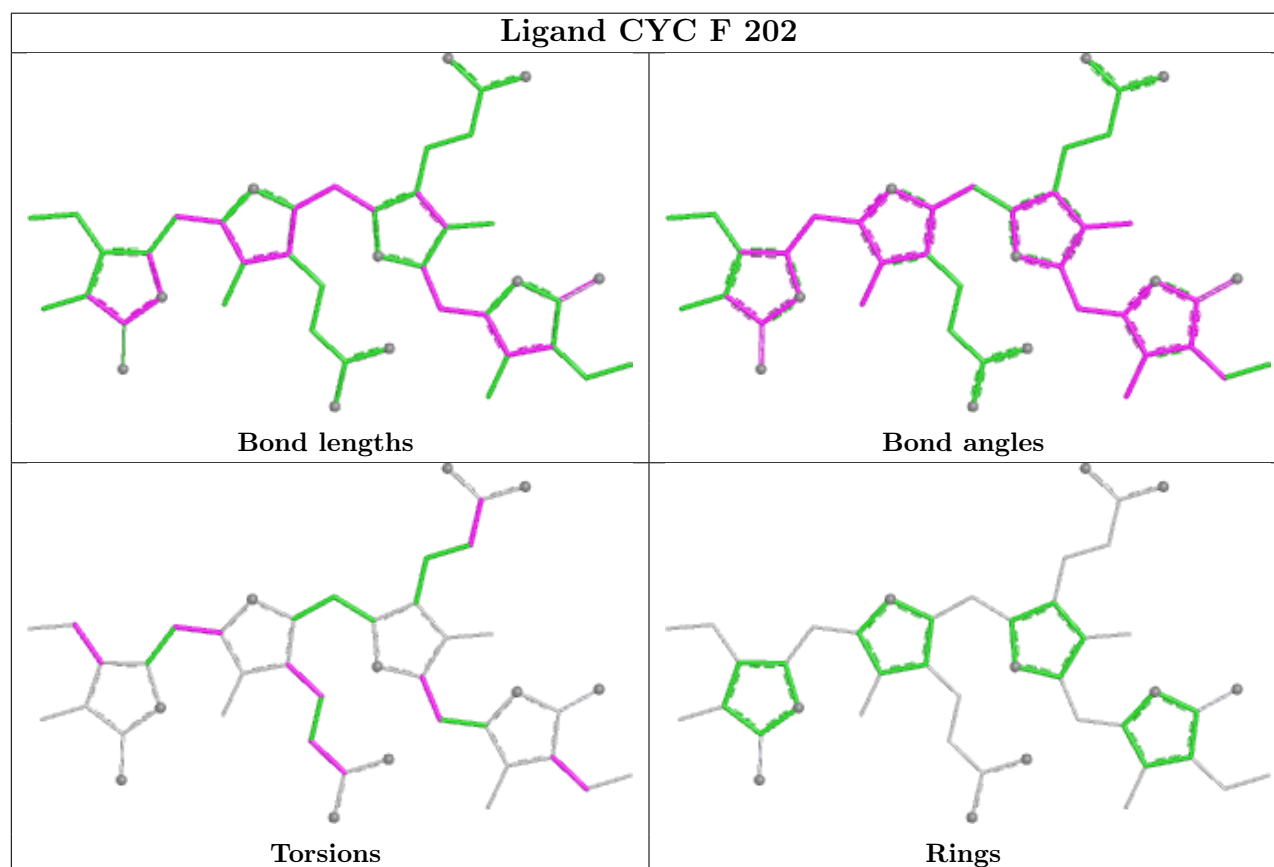
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	202	CYC	10	0
3	I	200	CYC	16	0
3	A	200	CYC	12	0
3	H	202	CYC	15	0
3	C	200	CYC	11	0
3	L	201	CYC	8	0
3	B	202	CYC	8	0
3	H	201	CYC	8	0
3	G	200	CYC	9	0
3	J	201	CYC	9	0
3	D	202	CYC	7	0

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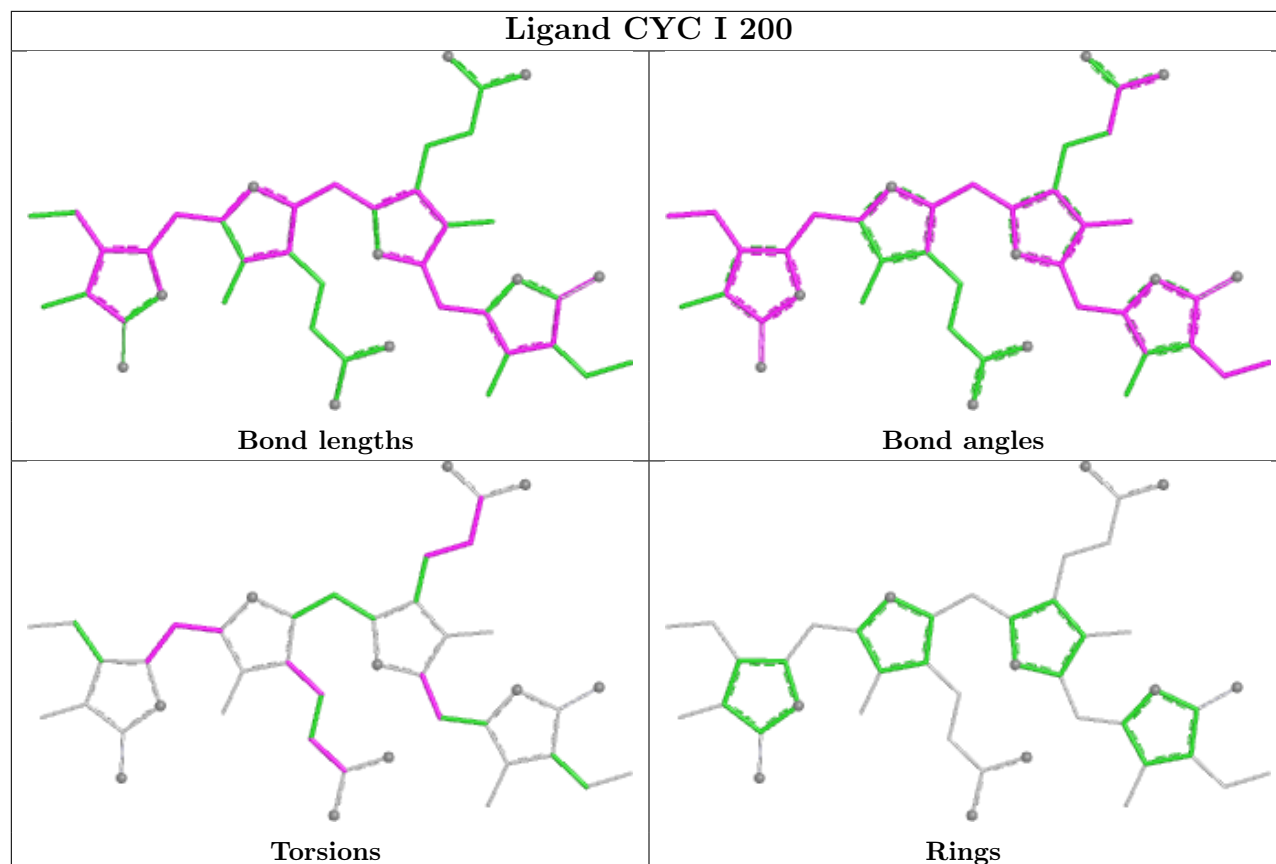
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	201	CYC	6	0
3	E	200	CYC	15	0
3	F	201	CYC	12	0
3	K	200	CYC	13	0
3	J	202	CYC	16	0
3	B	201	CYC	10	0
3	L	202	CYC	13	0

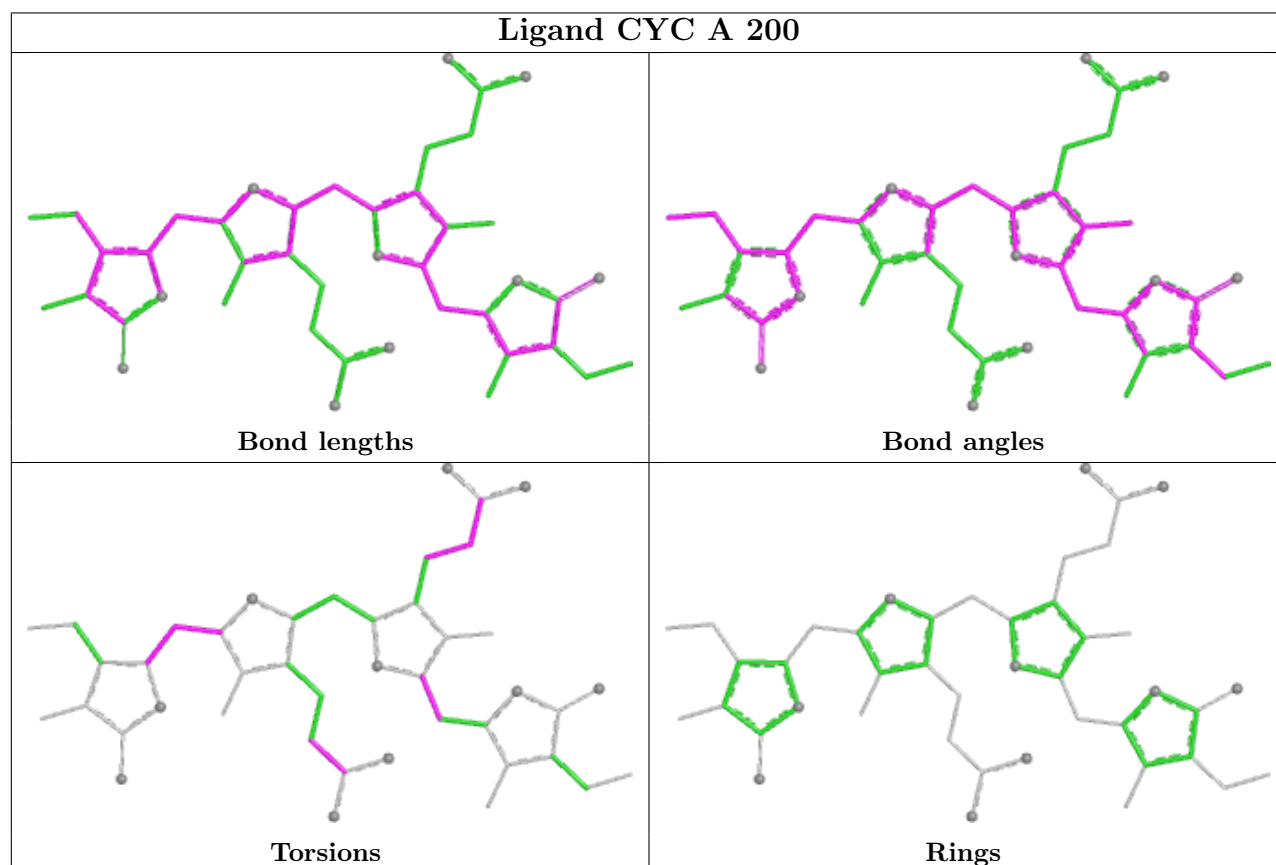
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

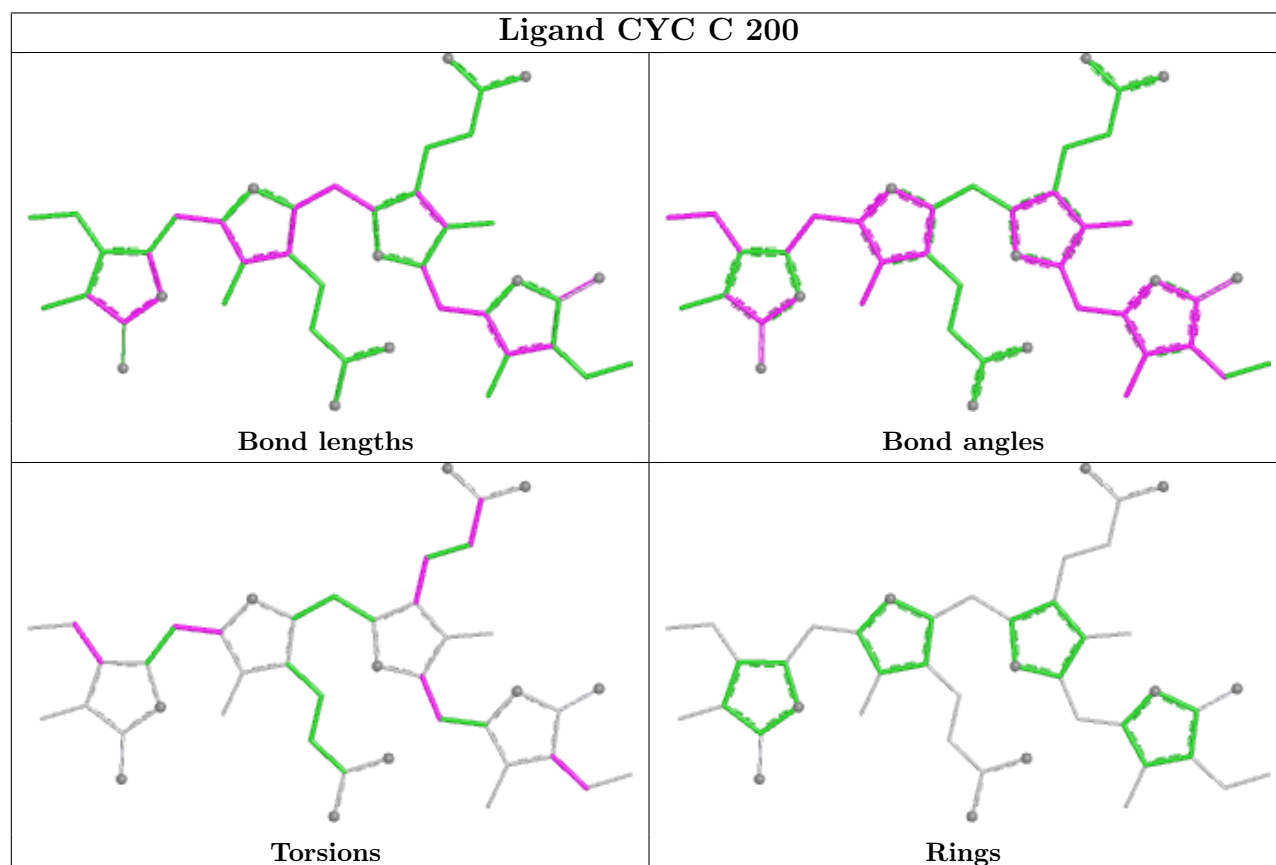
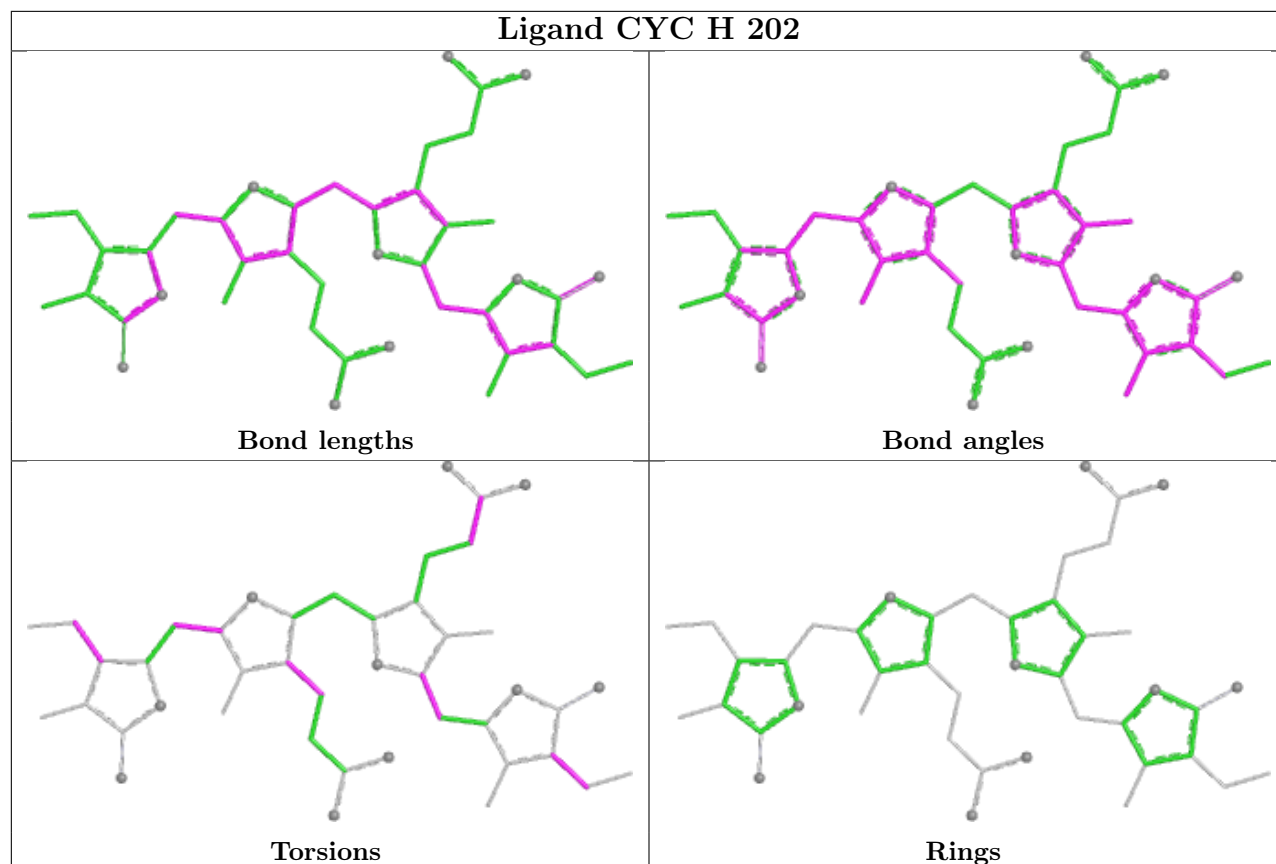


Ligand CYC I 200

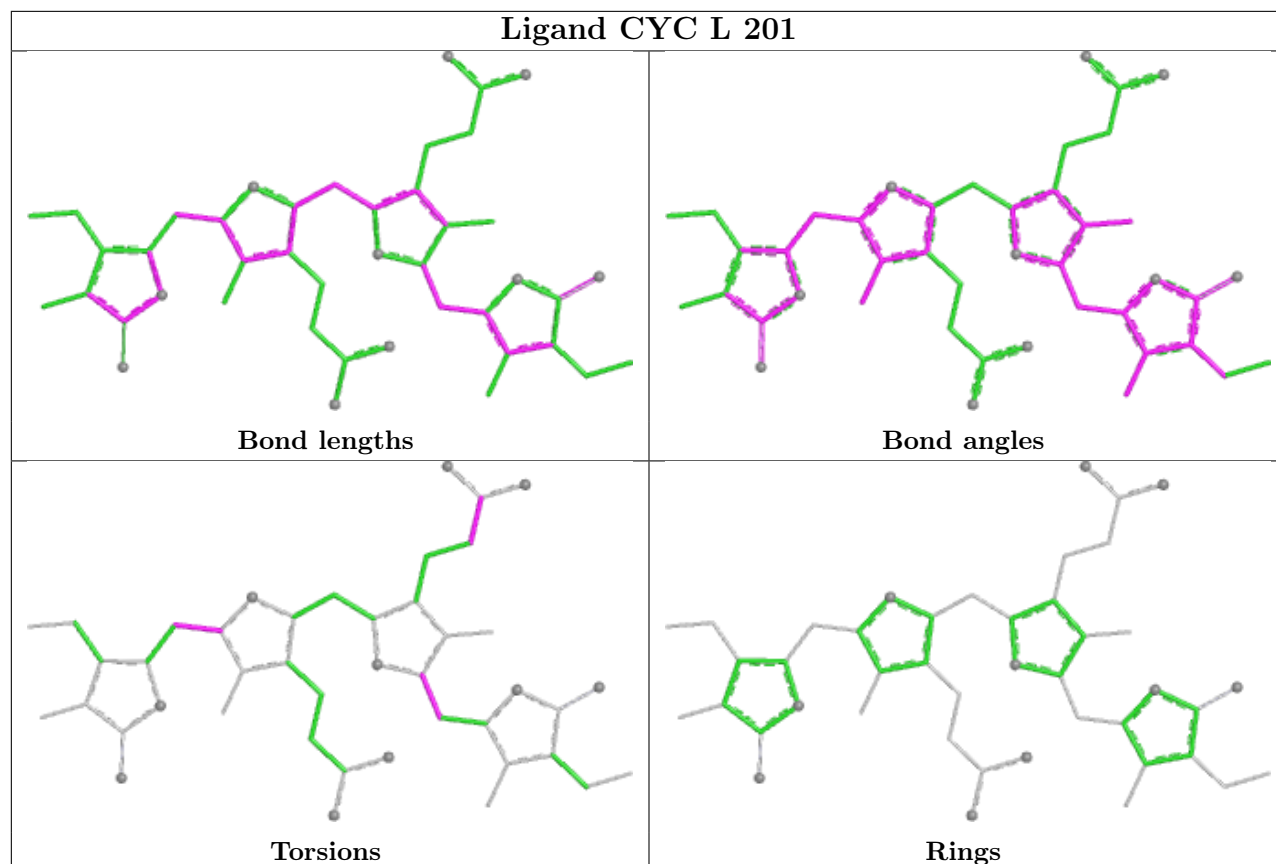


Ligand CYC A 200

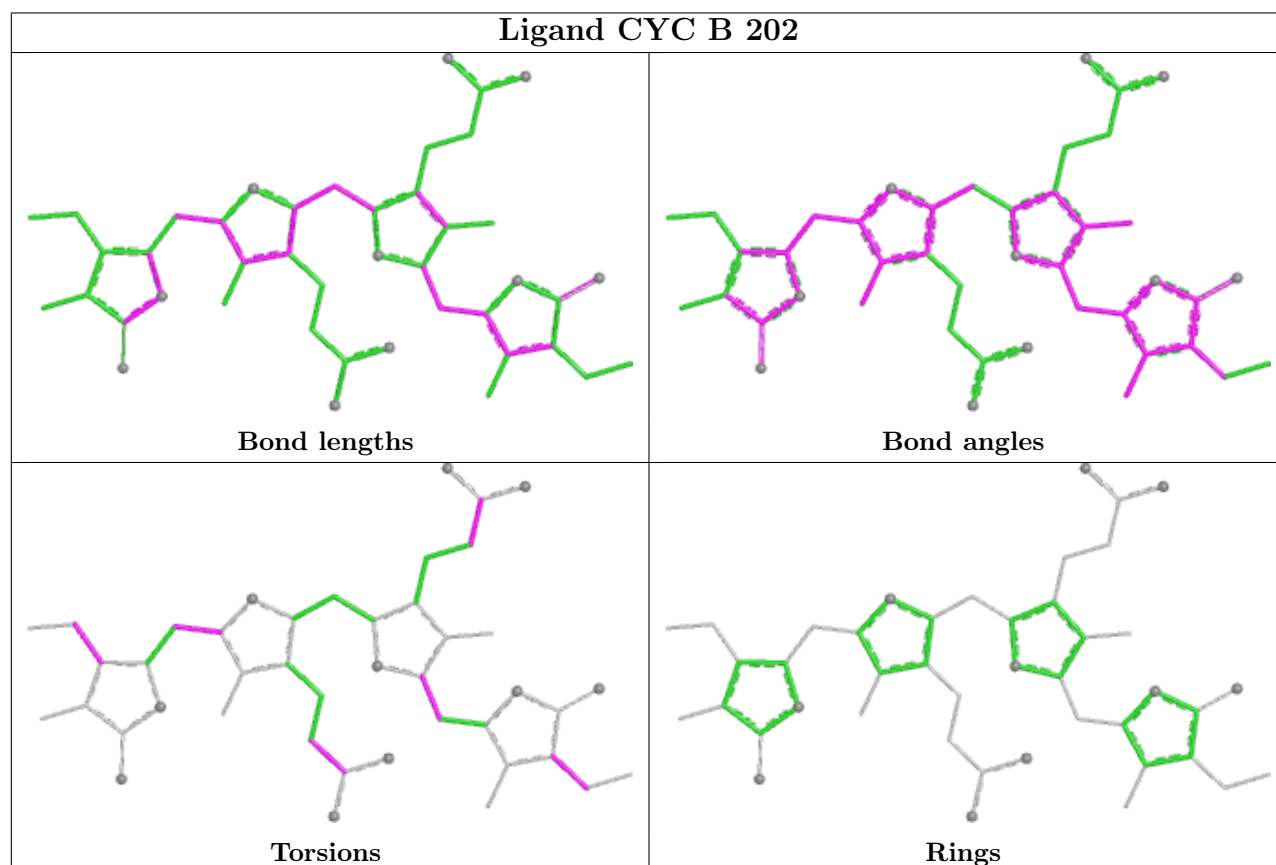


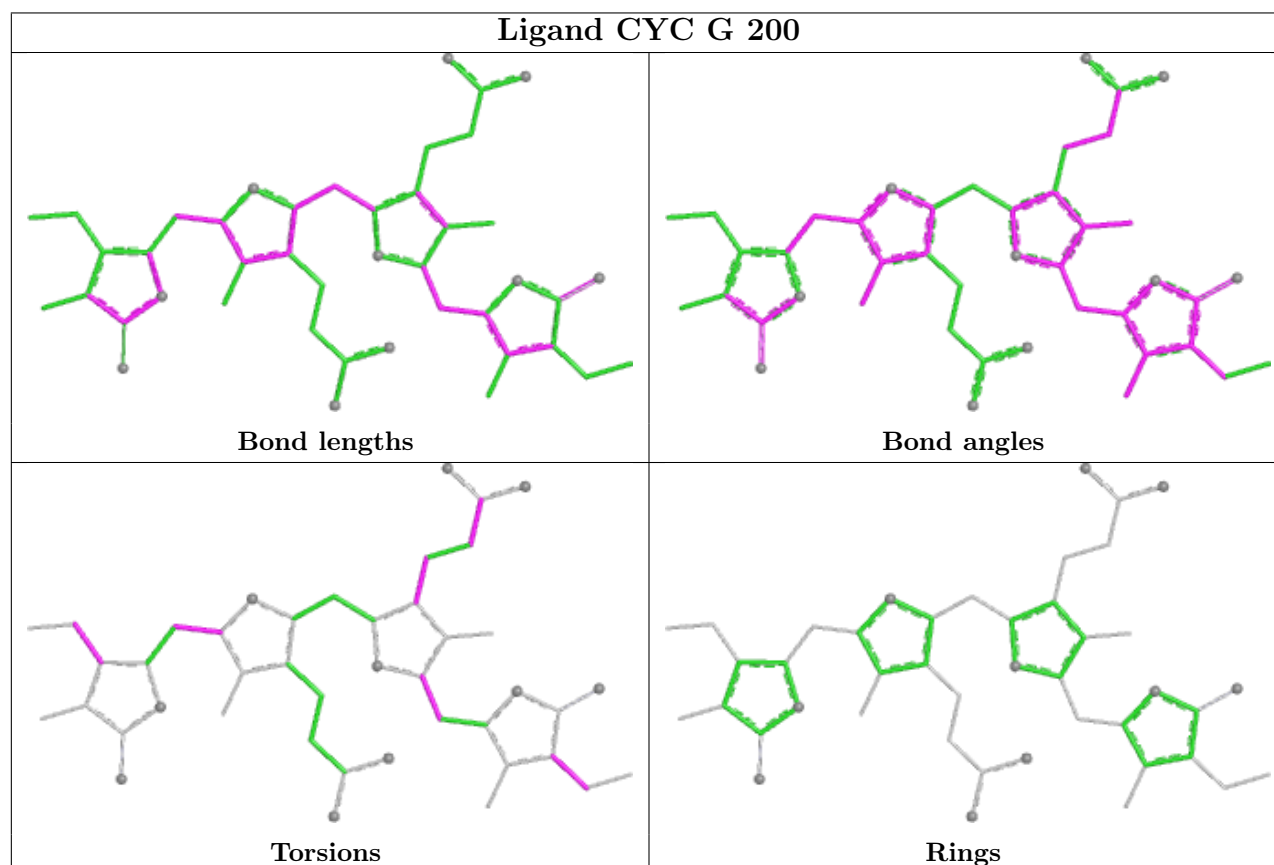
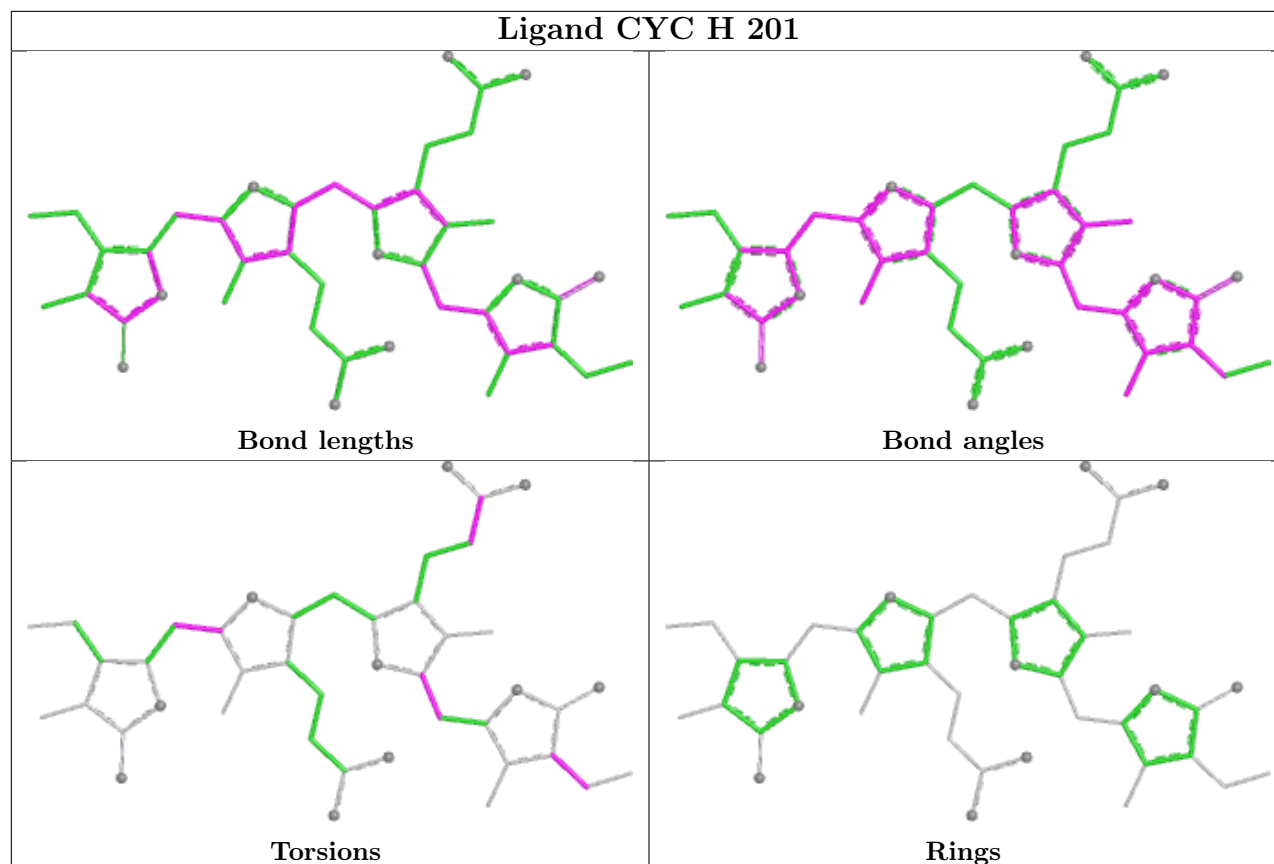


Ligand CYC L 201

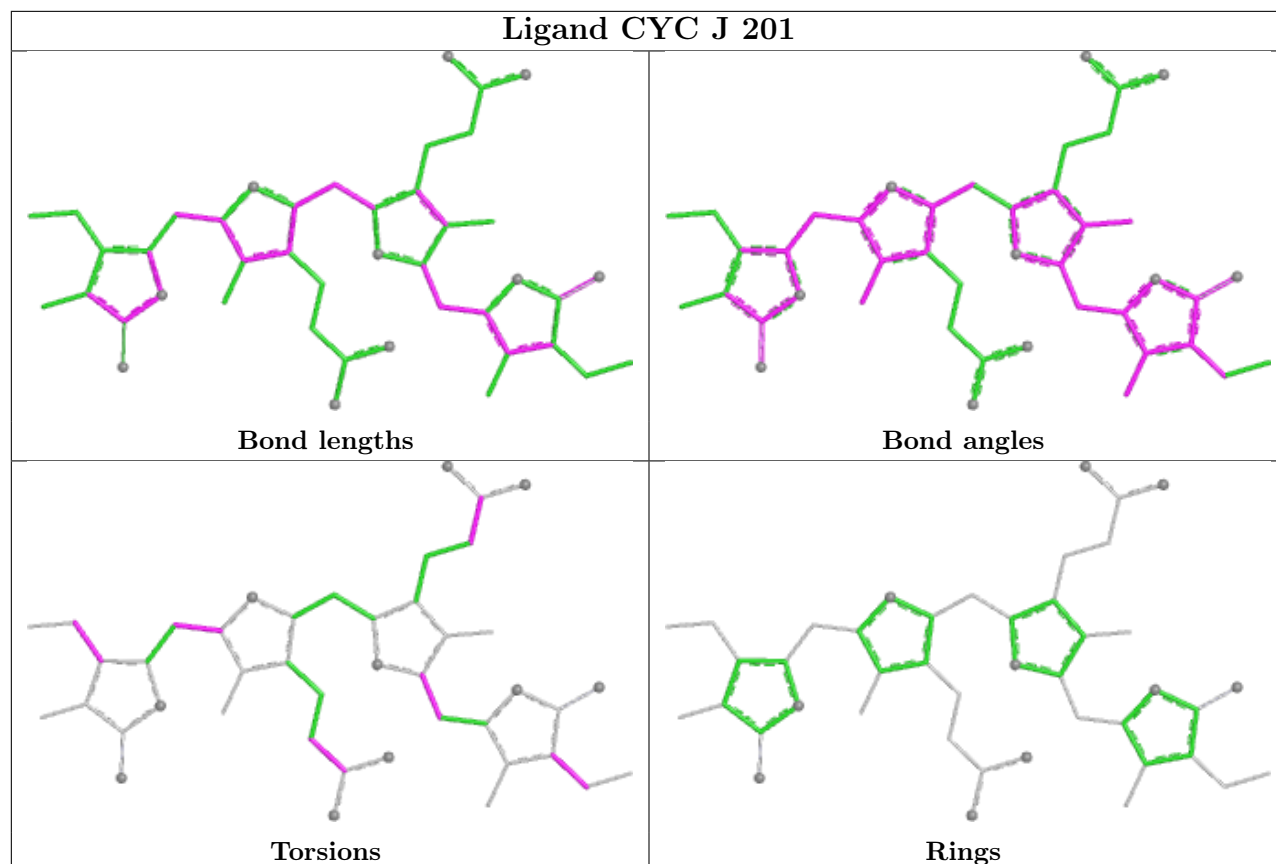


Ligand CYC B 202

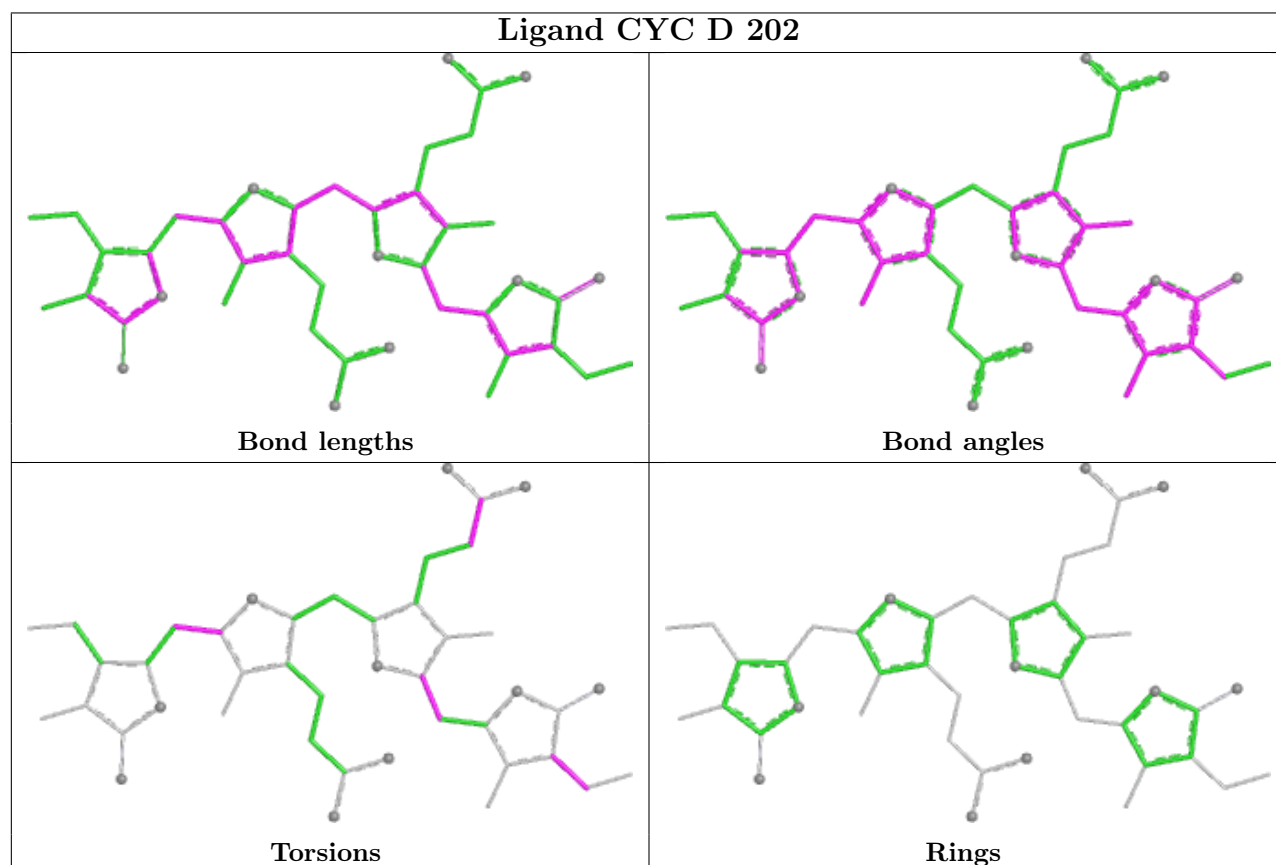


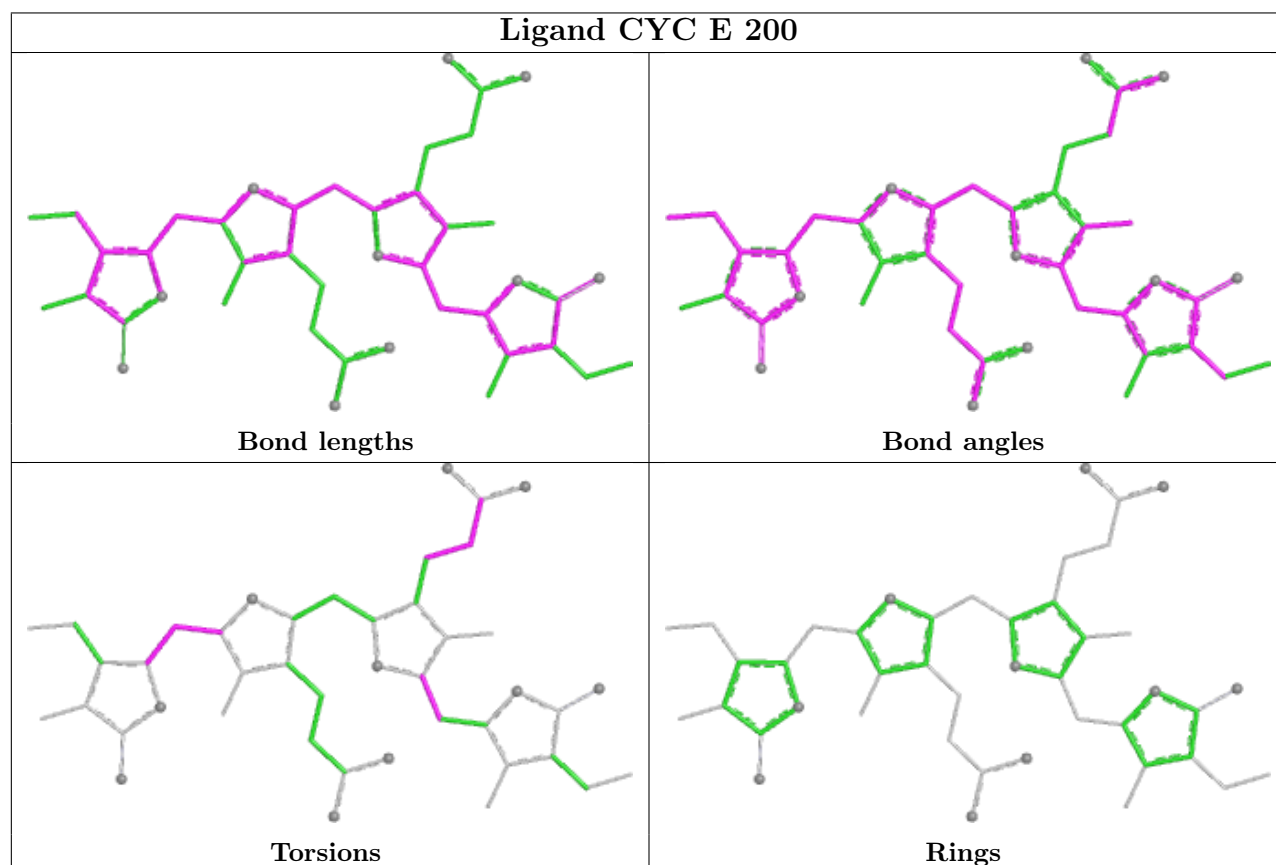
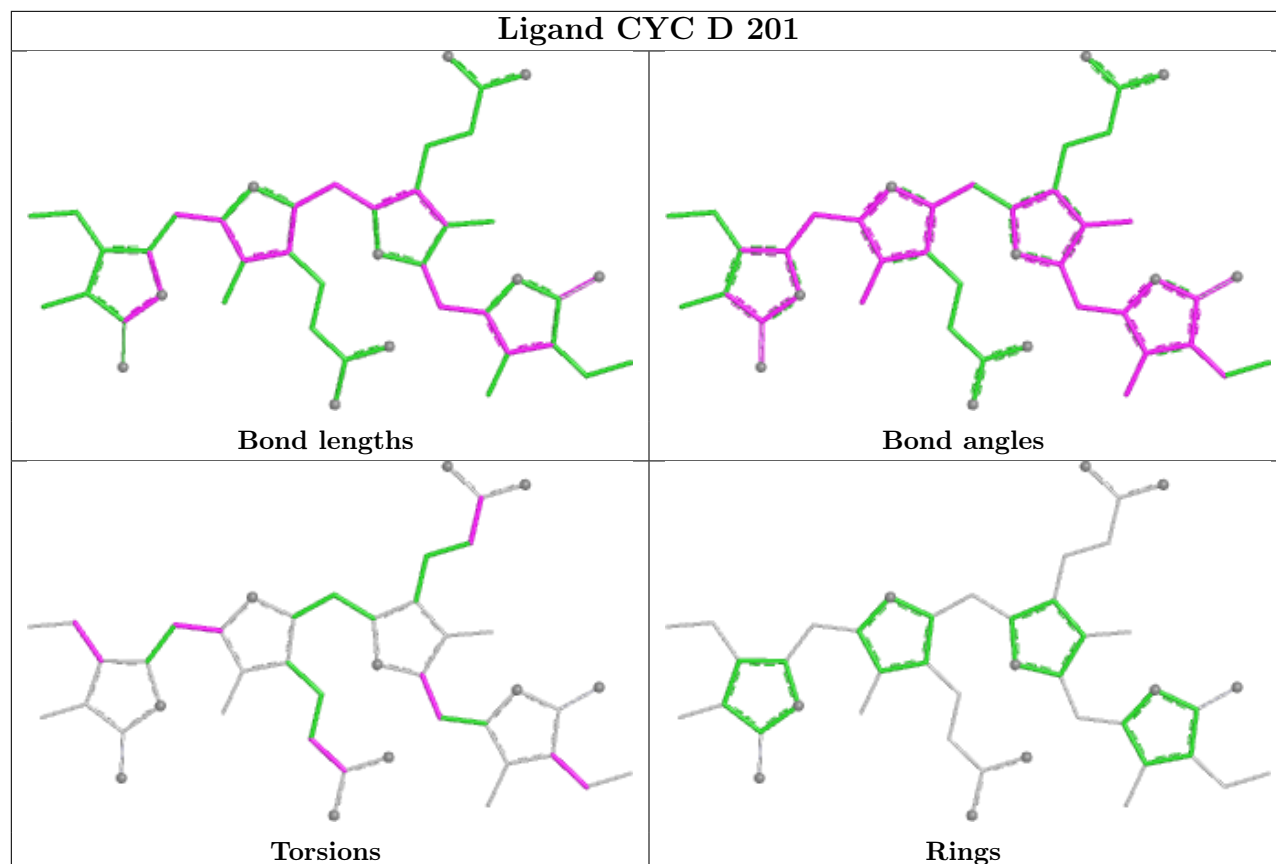


Ligand CYC J 201

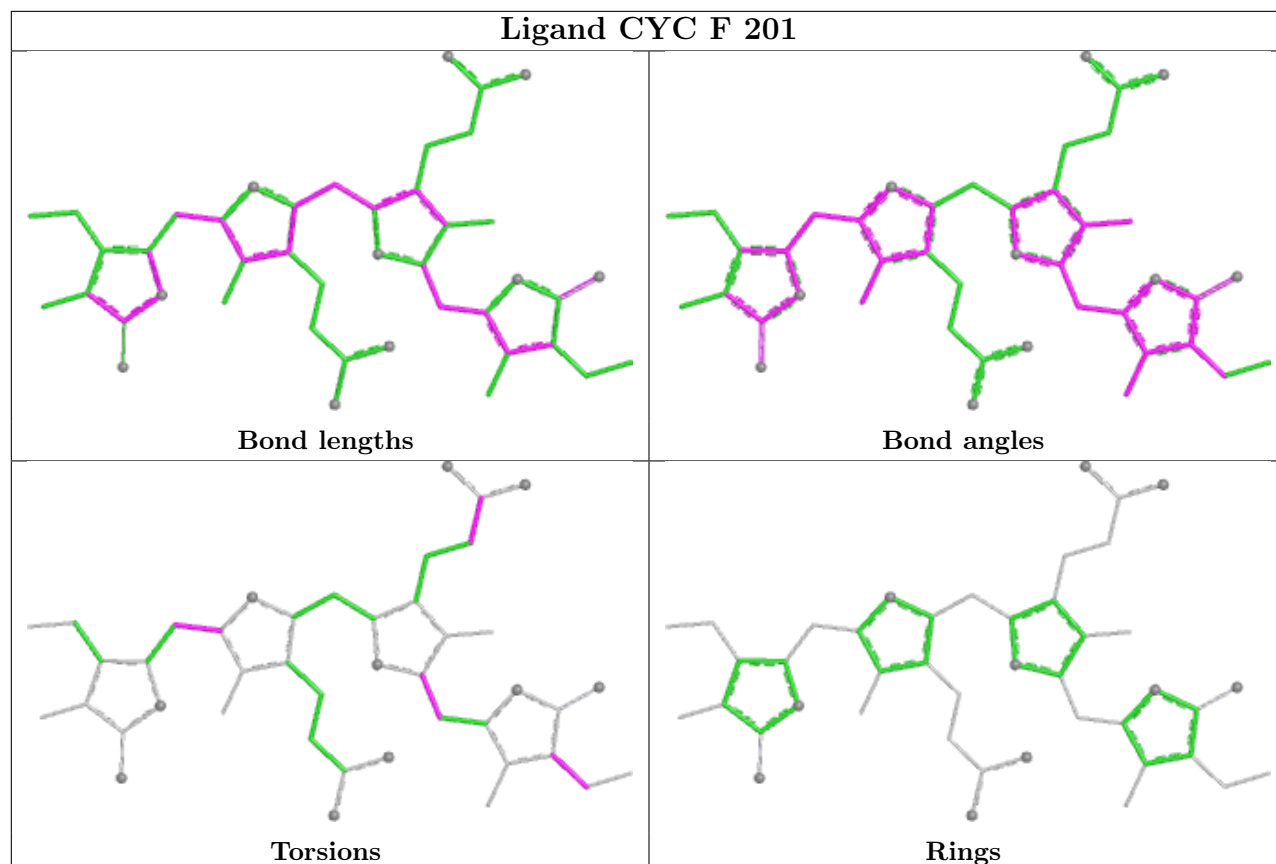


Ligand CYC D 202

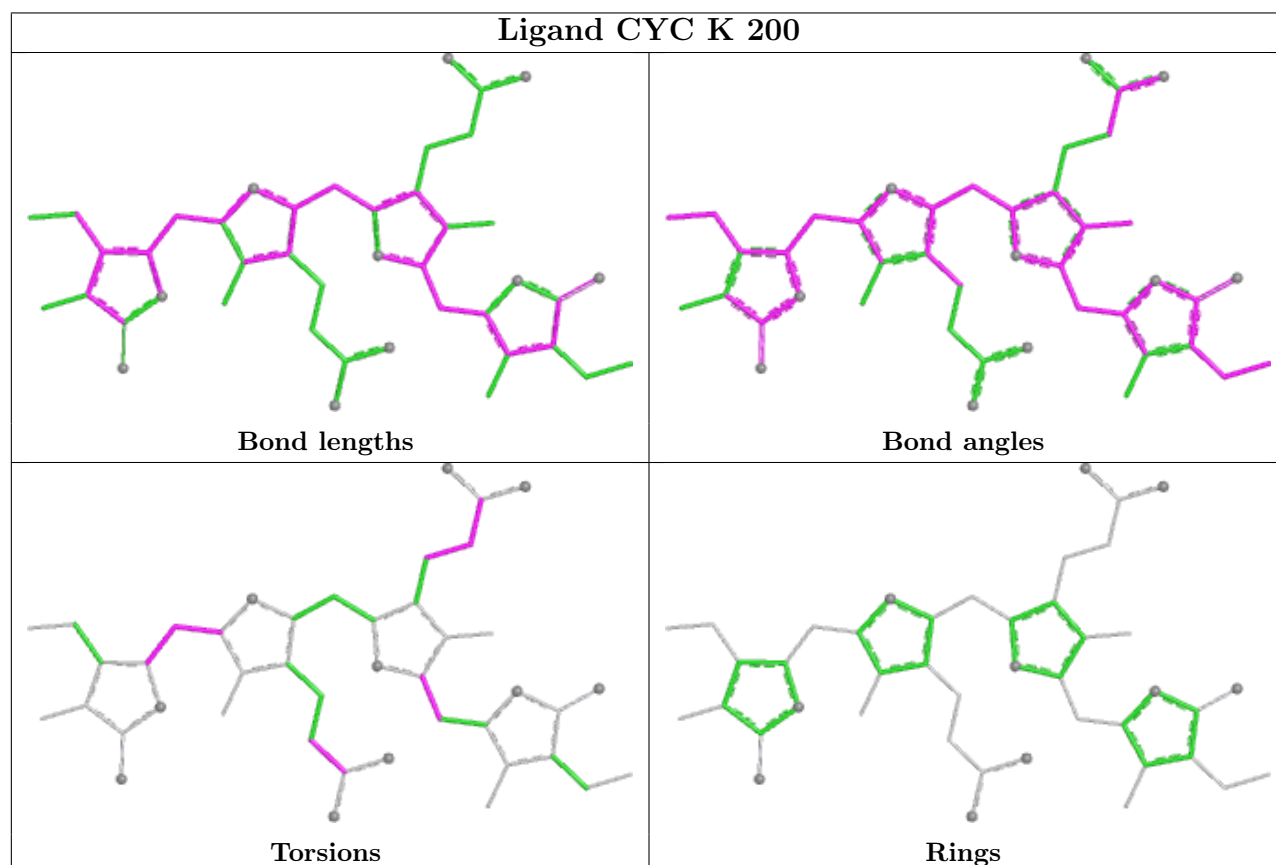




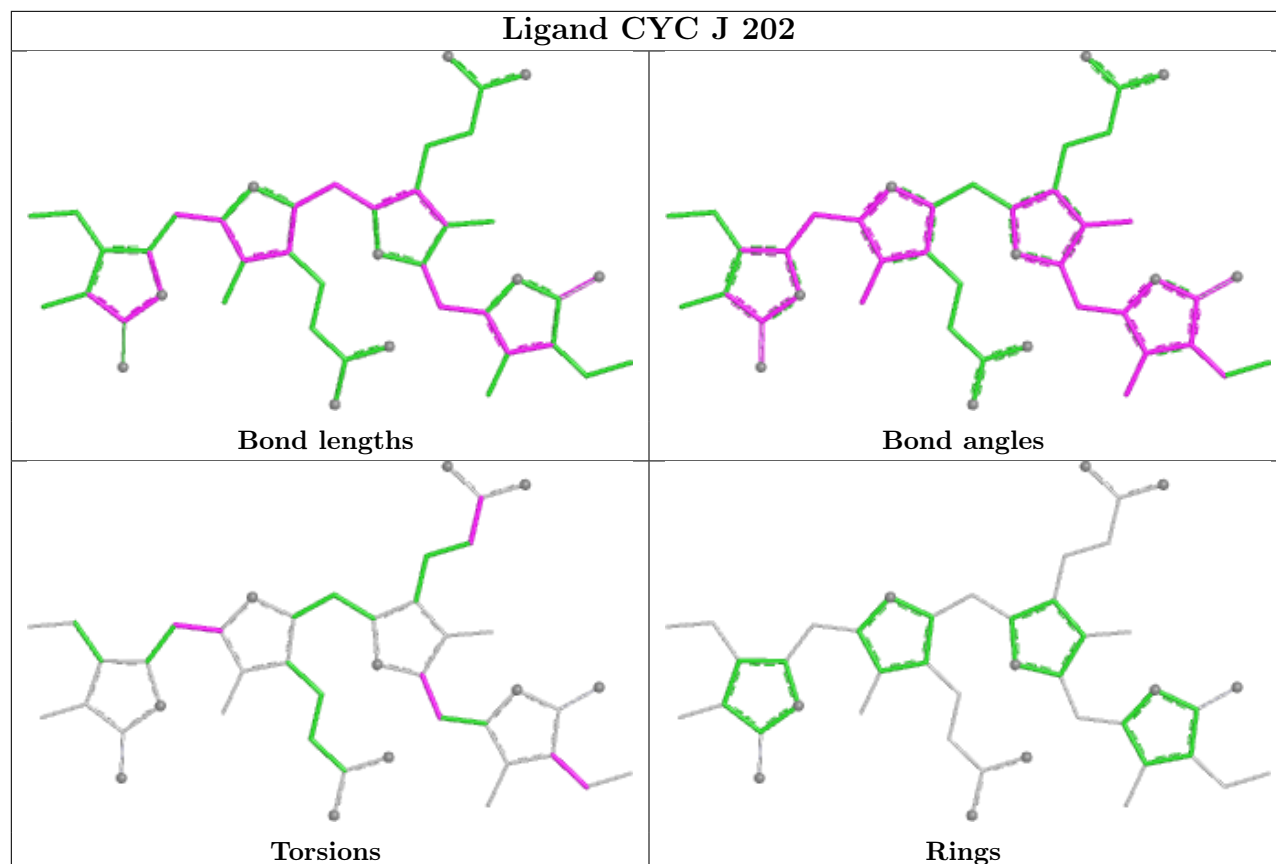
Ligand CYC F 201



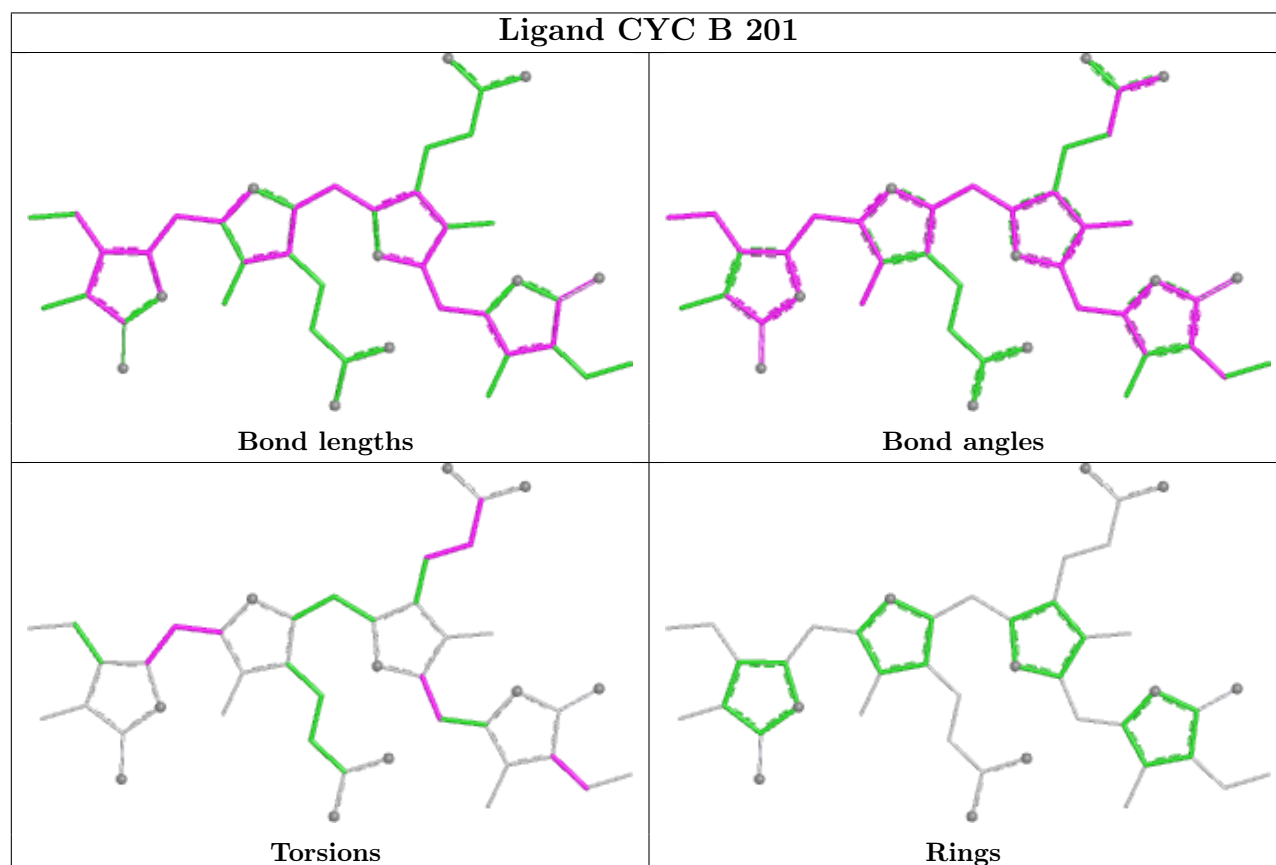
Ligand CYC K 200

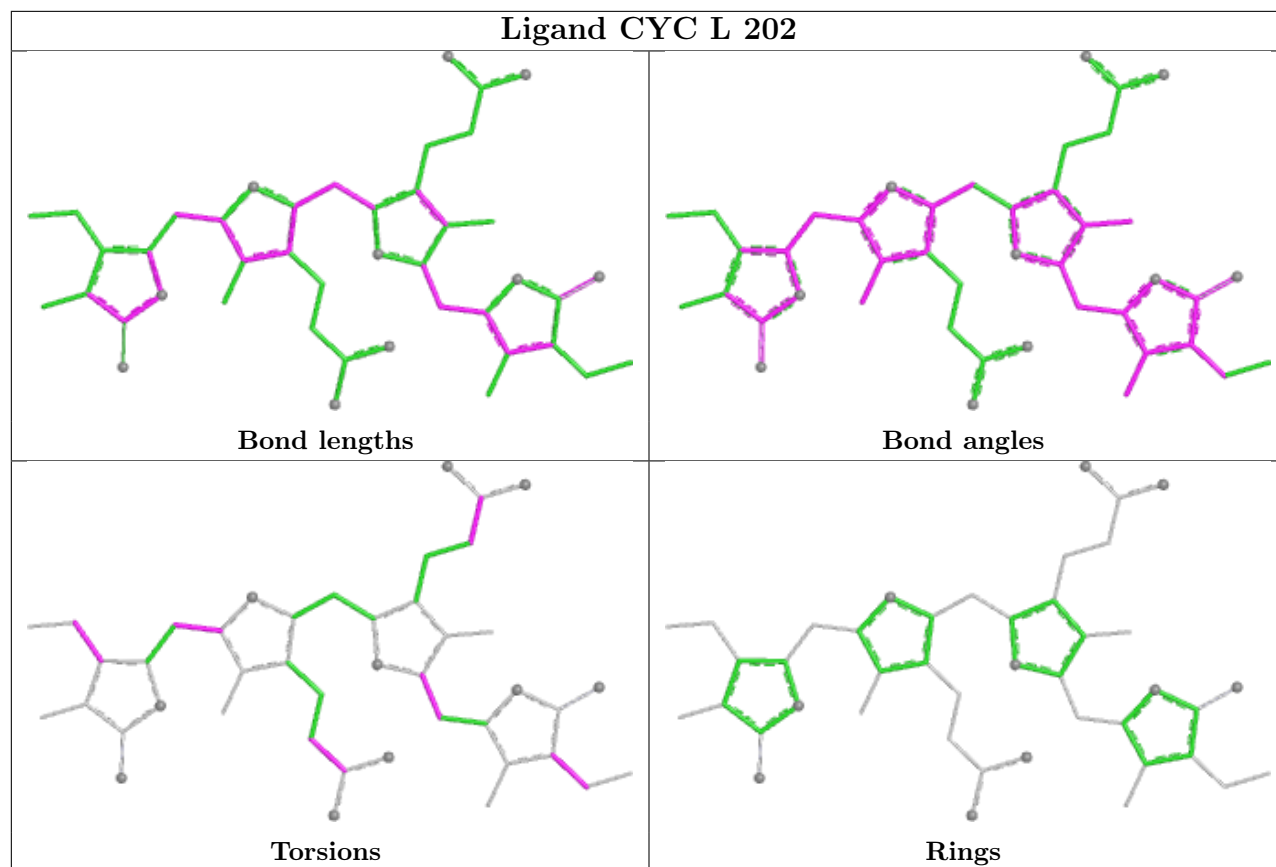


Ligand CYC J 202



Ligand CYC B 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 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	162/162 (100%)	-0.48	0 100 100	12, 22, 35, 41	1 (0%)
1	C	162/162 (100%)	-0.31	1 (0%) 85 87	13, 24, 39, 48	1 (0%)
1	E	162/162 (100%)	-0.39	0 100 100	18, 24, 38, 47	0
1	G	162/162 (100%)	-0.46	0 100 100	9, 23, 35, 52	2 (1%)
1	I	162/162 (100%)	-0.21	3 (1%) 66 68	20, 27, 44, 54	0
1	K	162/162 (100%)	-0.33	0 100 100	20, 26, 37, 53	0
2	B	171/172 (99%)	-0.27	3 (1%) 67 69	17, 25, 40, 81	0
2	D	171/172 (99%)	-0.29	7 (4%) 41 41	11, 23, 41, 66	1 (0%)
2	F	171/172 (99%)	-0.22	1 (0%) 85 87	18, 28, 41, 56	0
2	H	171/172 (99%)	-0.24	3 (1%) 67 69	17, 26, 39, 54	0
2	J	171/172 (99%)	-0.25	1 (0%) 85 87	18, 26, 43, 57	0
2	L	171/172 (99%)	-0.33	1 (0%) 85 87	18, 25, 42, 60	0
All	All	1998/2004 (99%)	-0.31	20 (1%) 79 81	9, 25, 40, 81	5 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	24	ILE	5.6
2	B	21	ALA	5.2
2	D	21	ALA	4.8
2	D	20	SER	3.3
2	H	21	ALA	3.3
2	D	26	ALA	2.8
2	D	25	ASP	2.7
2	B	22	SER	2.6
1	C	49	GLU	2.4
2	H	22	SER	2.3
2	D	19	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	32	ARG	2.3
1	I	143	SER	2.2
2	B	25	ASP	2.2
2	H	172	ALA	2.2
2	L	21	ALA	2.1
1	I	14	SER	2.1
2	D	29	ALA	2.1
2	F	172	ALA	2.1
2	J	172	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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	MEN	J	72	9/10	0.90	0.10	26,30,33,35	0
2	MEN	B	72	9/10	0.93	0.07	21,24,27,29	0
2	MEN	F	72	9/10	0.93	0.07	24,28,31,33	0
2	MEN	D	72	9/10	0.93	0.08	21,25,28,30	0
2	MEN	H	72	9/10	0.94	0.07	28,31,35,36	0
2	MEN	L	72	9/10	0.95	0.07	21,24,28,30	0

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
3	CYC	I	200	43/43	0.85	0.12	22,27,31,37	0
3	CYC	K	200	43/43	0.86	0.12	19,24,31,34	0
3	CYC	B	201	43/43	0.88	0.11	19,29,45,55	0

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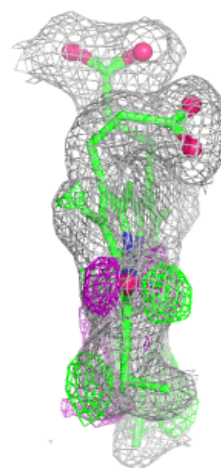
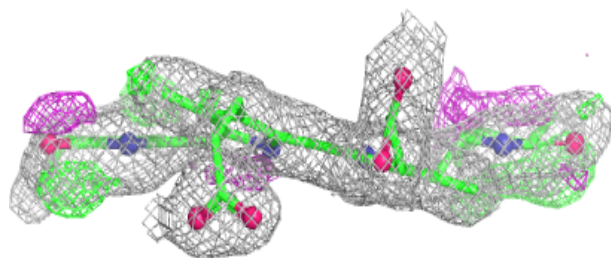
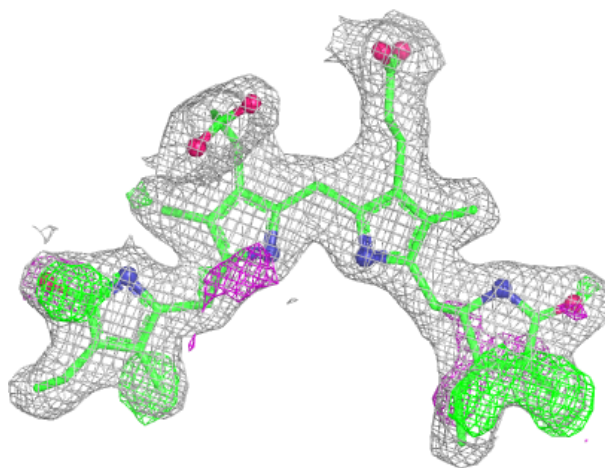
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CYC	D	202	43/43	0.88	0.11	22,29,43,55	0
3	CYC	J	202	43/43	0.88	0.11	26,33,43,55	0
3	CYC	A	200	43/43	0.88	0.10	17,22,27,33	0
3	CYC	F	201	43/43	0.89	0.12	23,31,45,60	0
3	CYC	H	201	43/43	0.89	0.10	23,31,42,56	0
3	CYC	E	200	43/43	0.89	0.10	17,24,32,33	0
3	CYC	F	202	43/43	0.90	0.10	23,33,44,53	0
3	CYC	C	200	43/43	0.90	0.10	16,24,31,41	0
3	CYC	H	202	43/43	0.90	0.10	20,24,36,39	0
3	CYC	J	201	43/43	0.90	0.09	20,30,38,45	0
3	CYC	L	201	43/43	0.90	0.11	20,27,43,58	0
3	CYC	L	202	43/43	0.90	0.09	20,27,34,40	0
3	CYC	G	200	43/43	0.91	0.09	15,21,27,35	0
3	CYC	D	201	43/43	0.91	0.10	21,27,44,55	0
3	CYC	B	202	43/43	0.91	0.10	23,30,36,44	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.

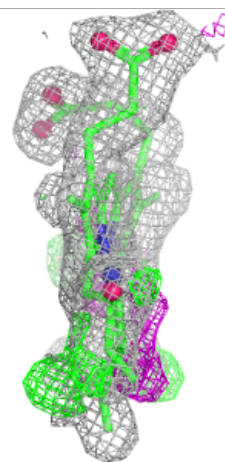
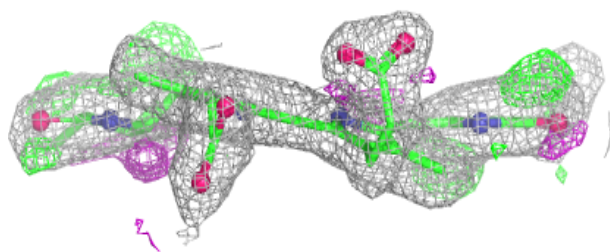
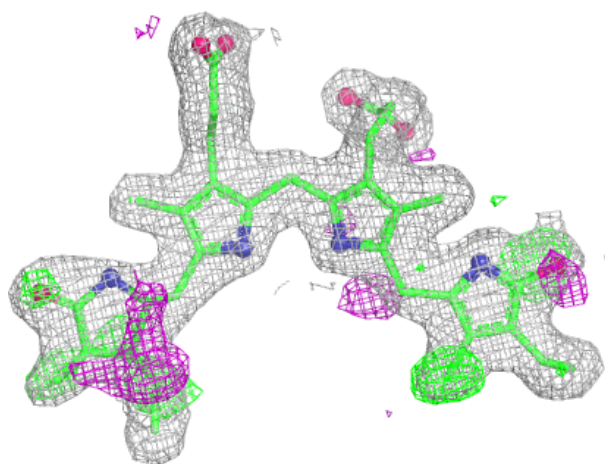
Electron density around CYC I 200:

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



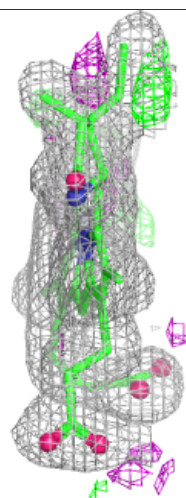
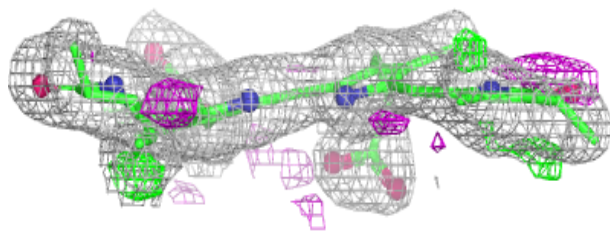
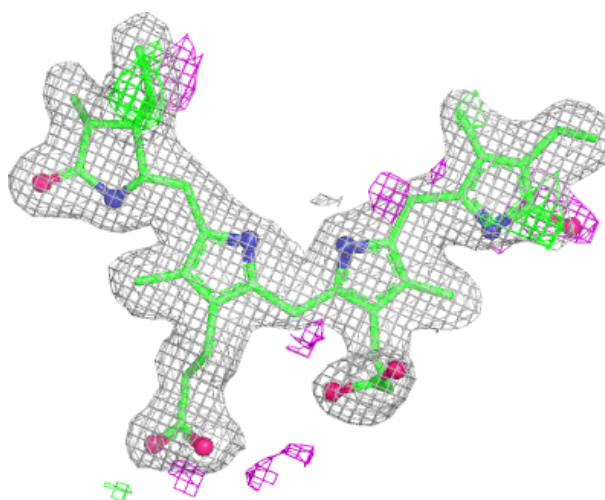
Electron density around CYC K 200:

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



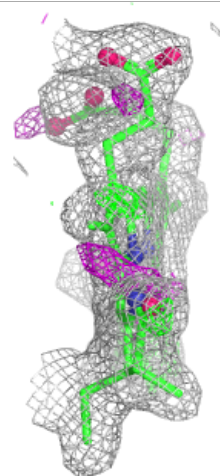
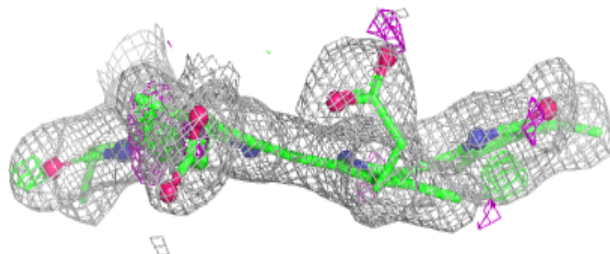
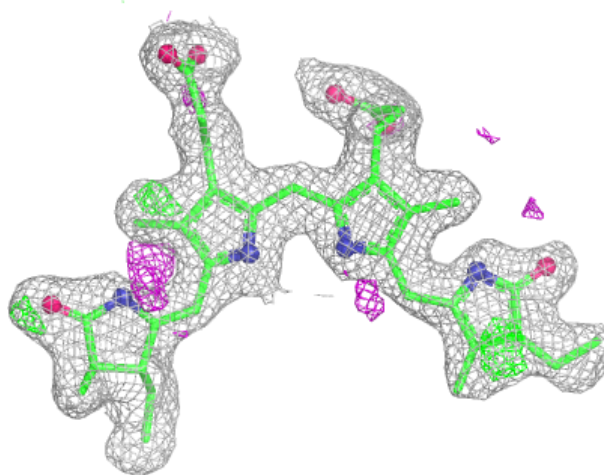
Electron density around CYC B 201:

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



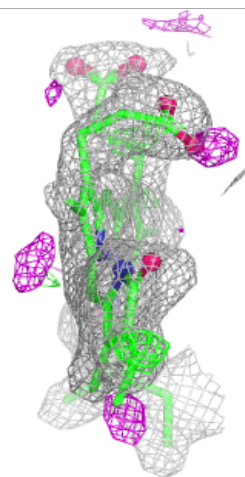
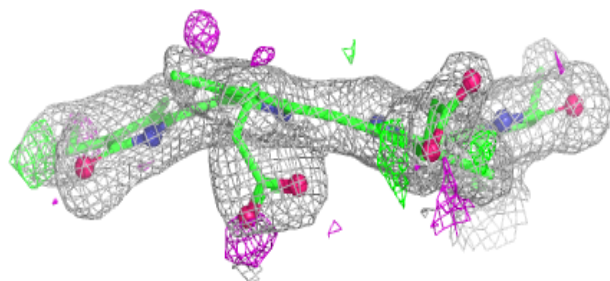
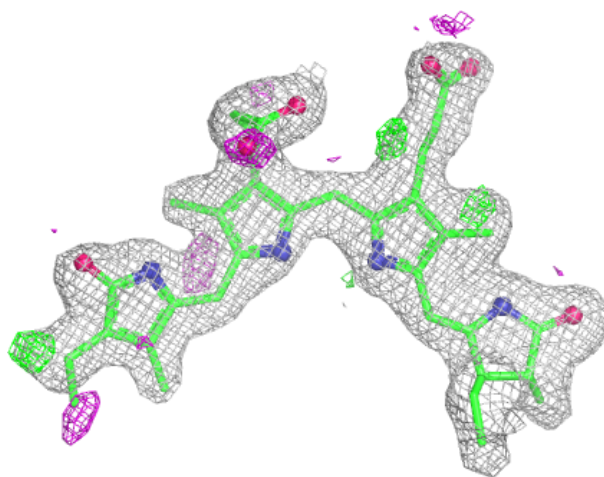
Electron density around CYC D 202:

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



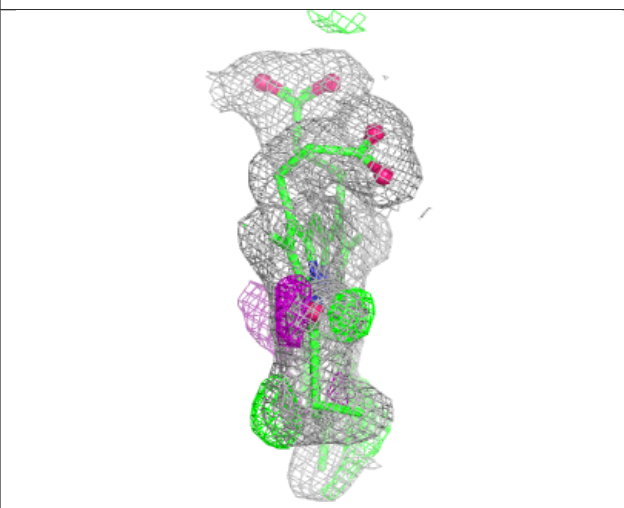
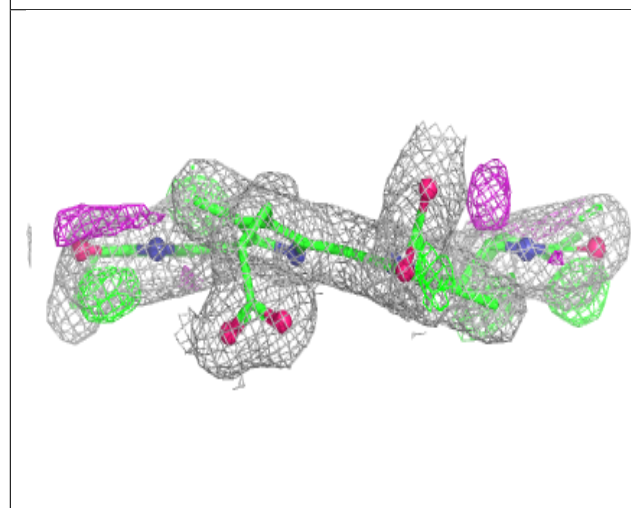
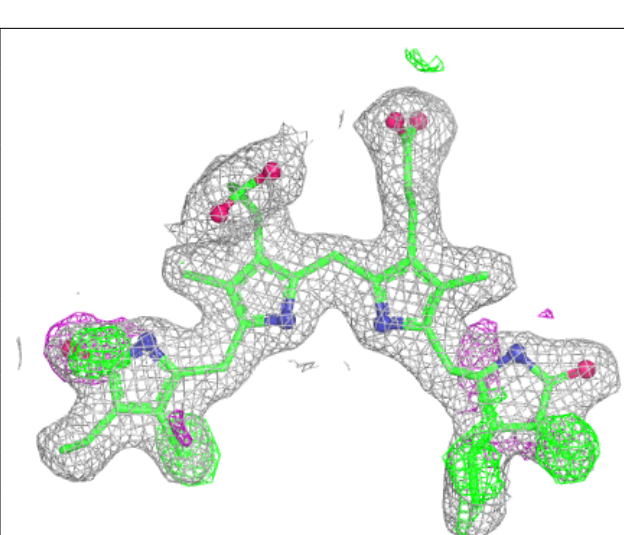
Electron density around CYC J 202:

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



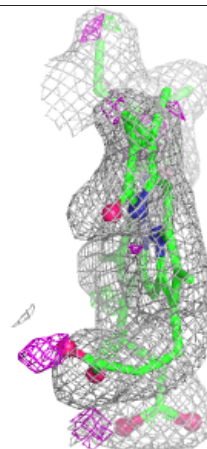
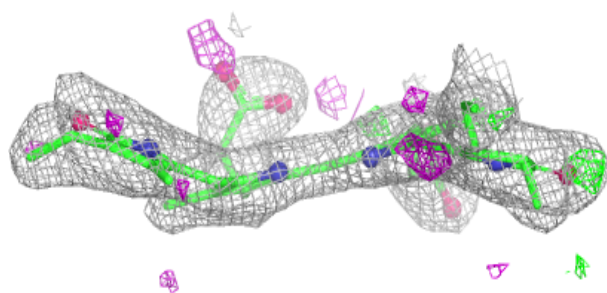
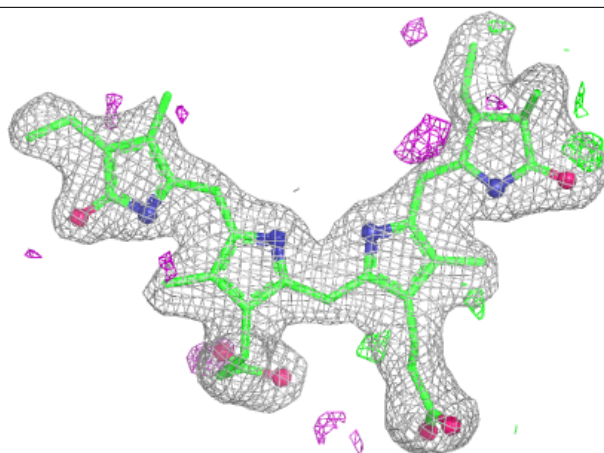
Electron density around CYC A 200:

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



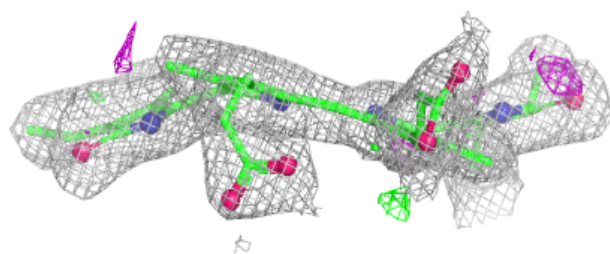
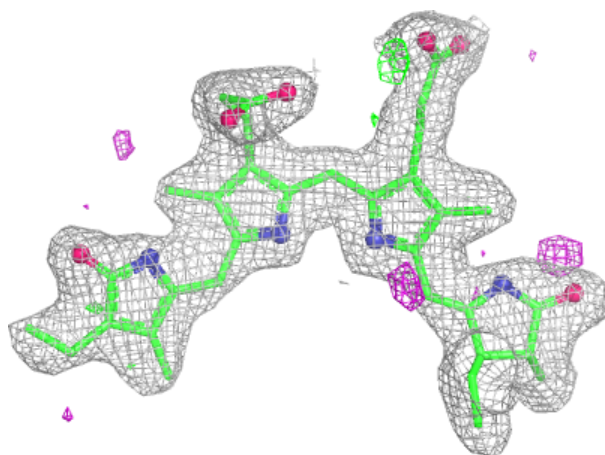
Electron density around CYC F 201:

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



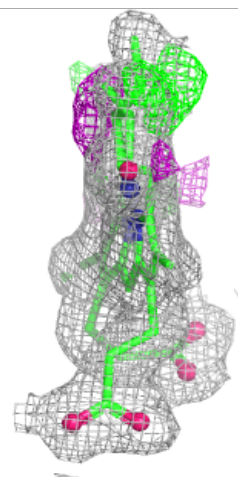
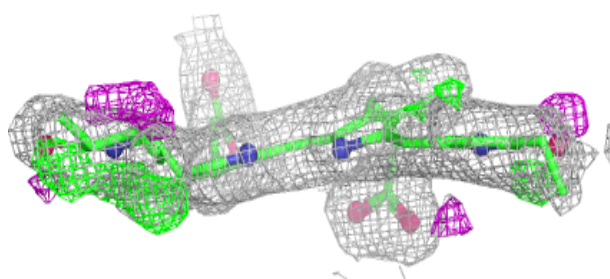
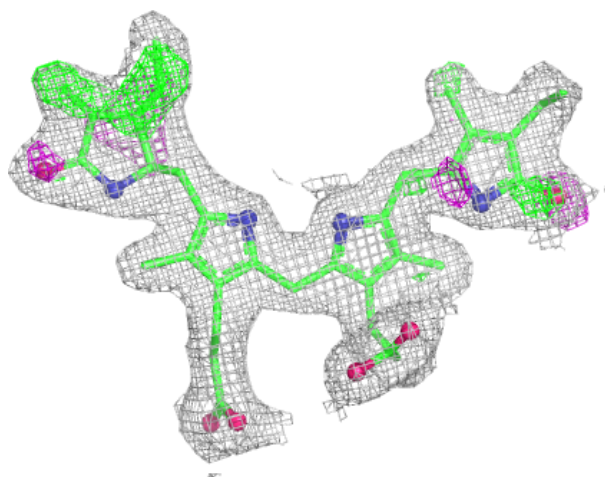
Electron density around CYC H 201:

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



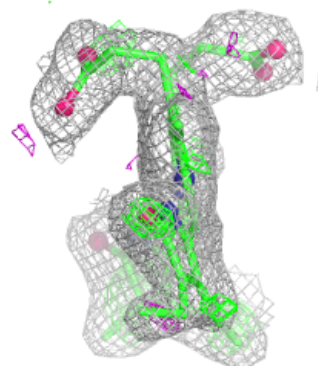
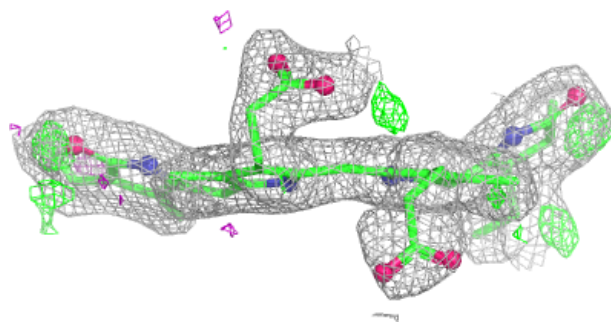
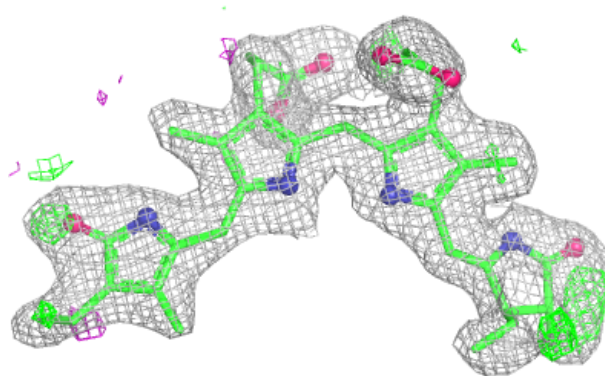
Electron density around CYC E 200:

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



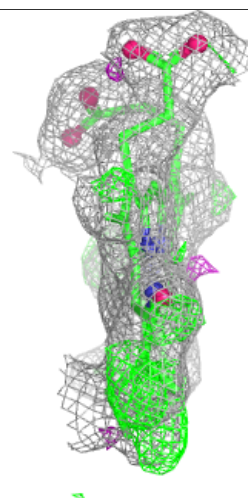
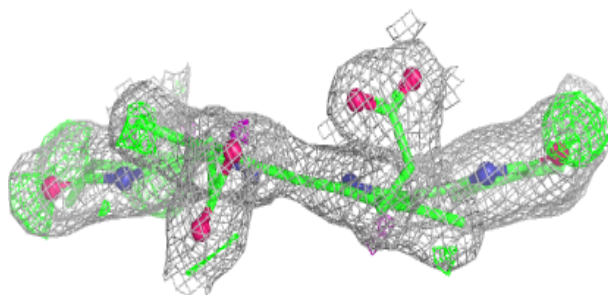
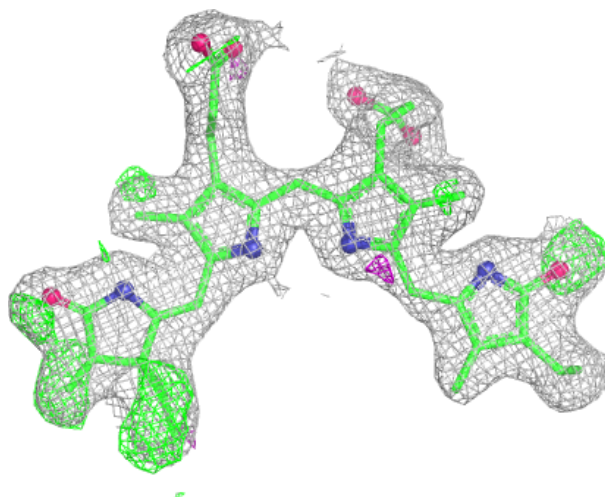
Electron density around CYC F 202:

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



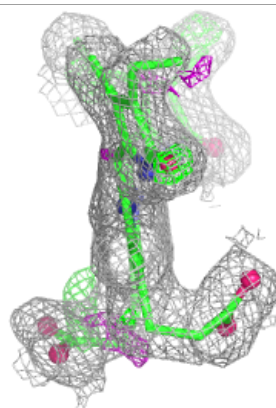
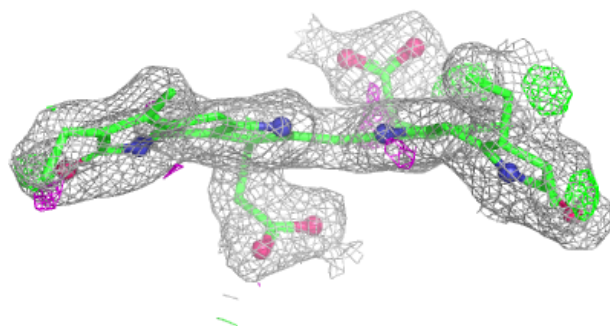
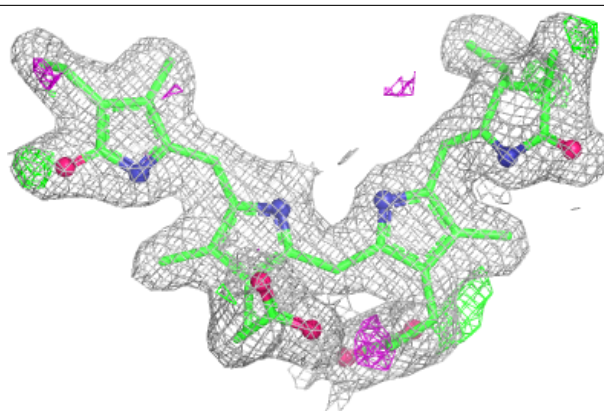
Electron density around CYC C 200:

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

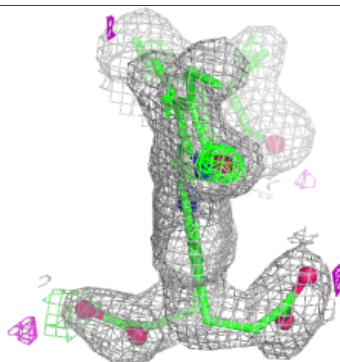
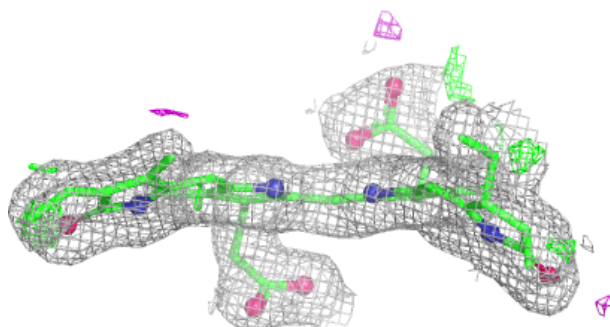
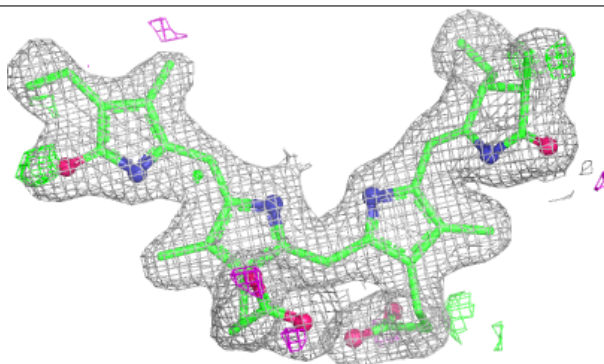


Electron density around CYC H 202:

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

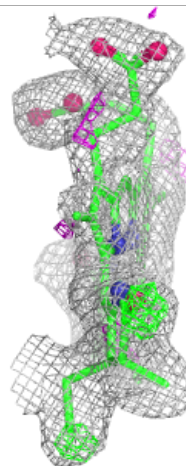
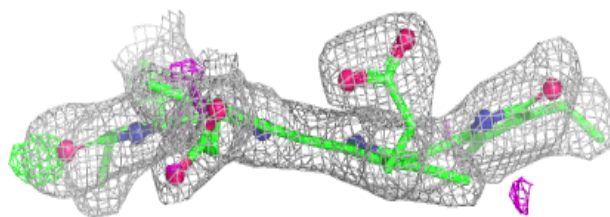
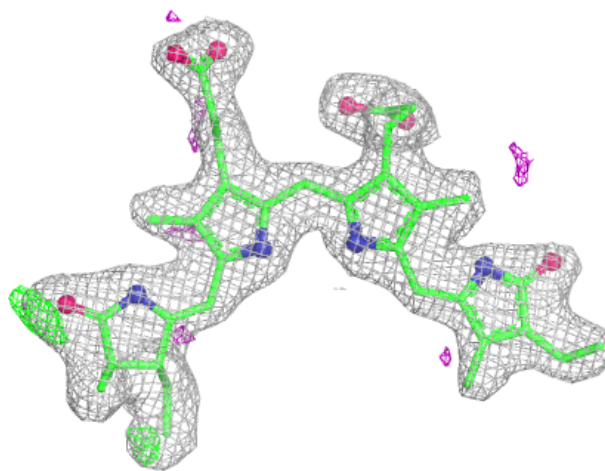
**Electron density around CYC J 201:**

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



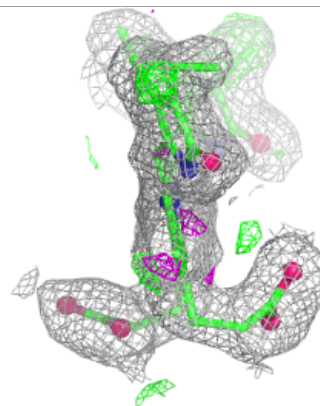
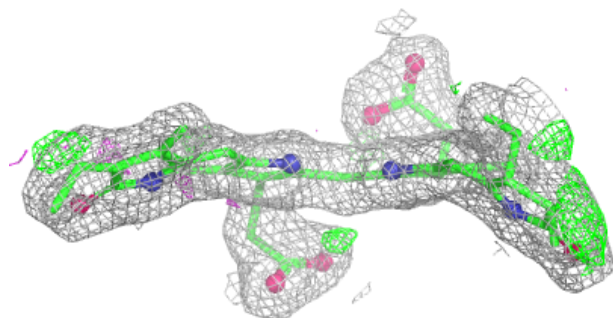
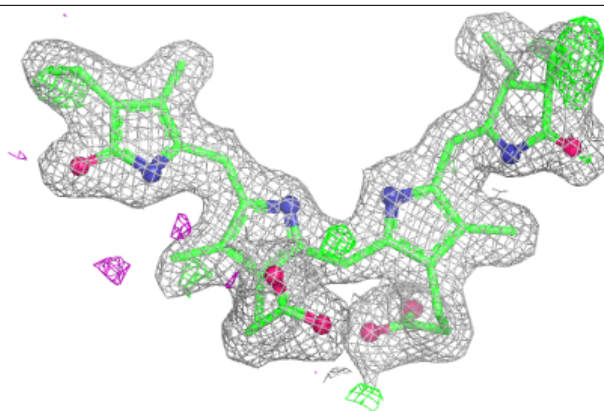
Electron density around CYC L 201:

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



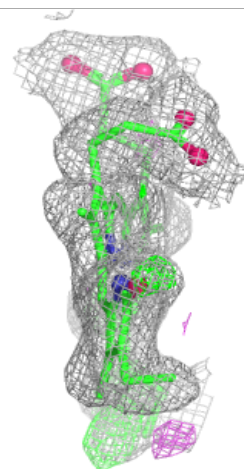
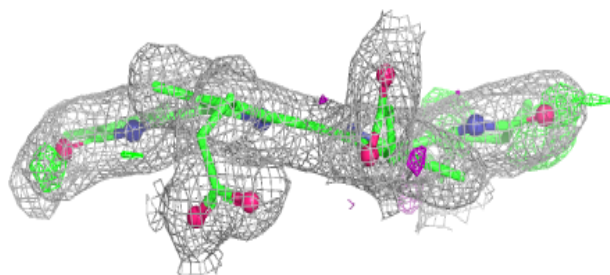
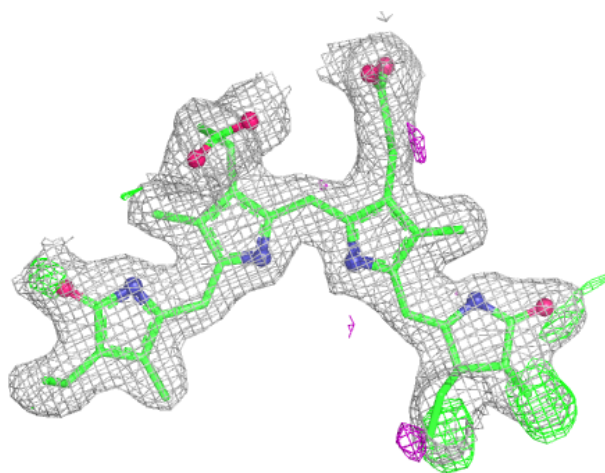
Electron density around CYC L 202:

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



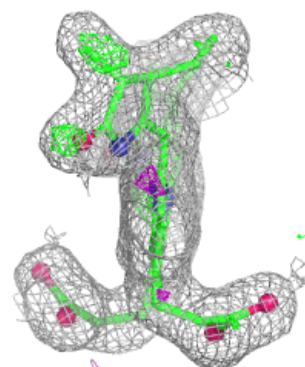
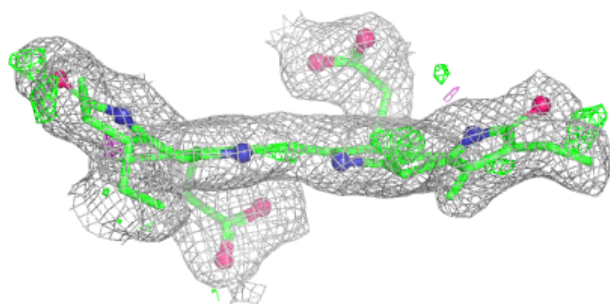
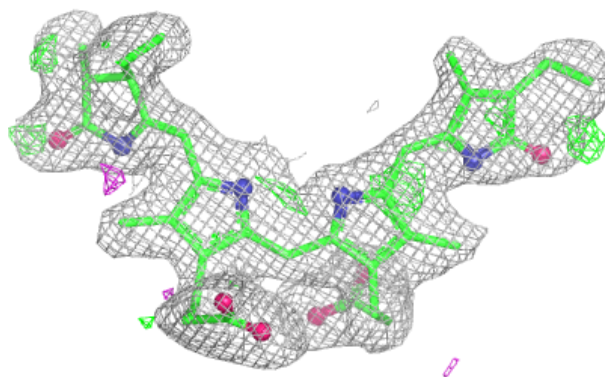
Electron density around CYC G 200:

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

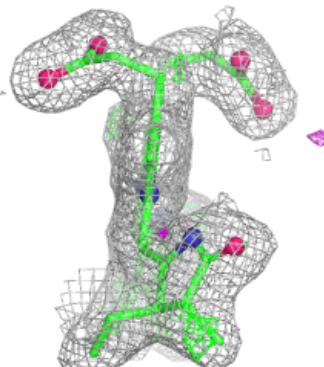
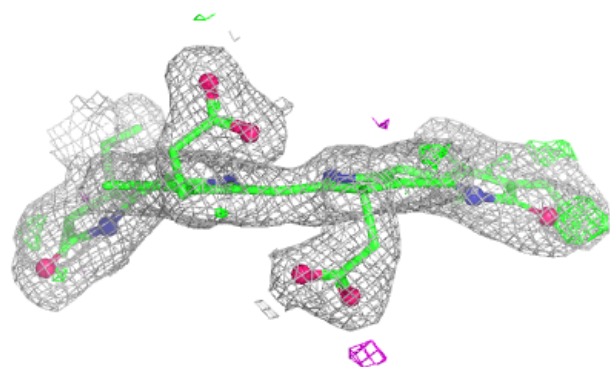
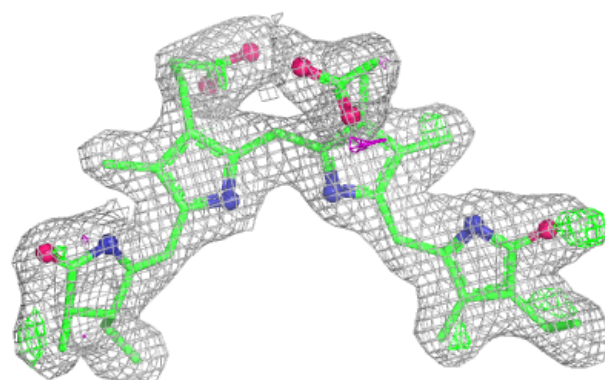


Electron density around CYC D 201:

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

**Electron density around CYC B 202:**

$2mF_o-DF_c$ (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.