



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:43 AM UTC

PDB ID : 1EYX / pdb_00001eyx
Title : CRYSTAL STRUCTURE OF R-PHYCOERYTHRIN AT 2.2 ANGSTROMS
Authors : Contreras-Martel, C.; Legrand, P.; Piras, C.; Vernede, X.; Martinez-Oyanedel, J.; Bunster, M.; Fontecilla-Camps, J.C.
Deposited on : 2000-05-09
Resolution : 2.25 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

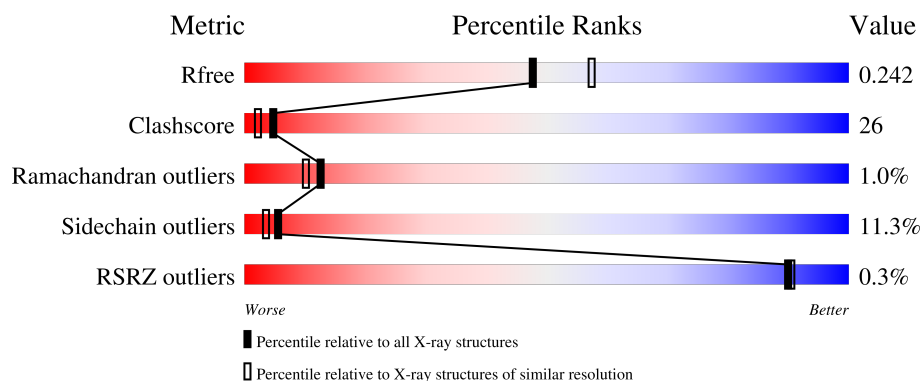
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



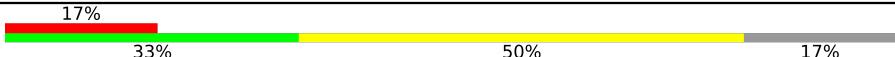
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	164	17% 57% 38% 5%
1	K	164	56% 37% 7%
2	B	177	50% 44% 6%
2	L	177	59% 34% 7%
3	G	6	17% 67% 33%

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Mol	Chain	Length	Quality of chain
3	H	6	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CYC	A	168	X	-	-	-
5	CYC	K	168	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5719 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 R-PHYCOERYTHRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1247	775	218	248	6			
1	K	164	Total	C	N	O	S	0	0	0
			1247	775	218	248	6			

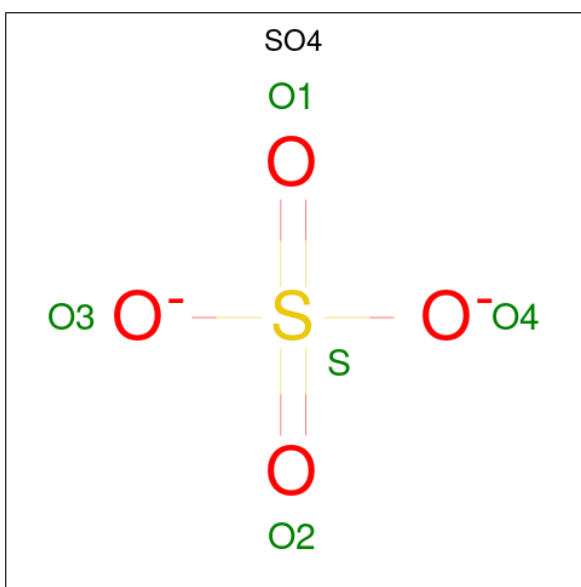
- Molecule 2 is a protein called R-PHYCOERYTHRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1298	800	227	260	11			
2	L	177	Total	C	N	O	S	0	0	0
			1298	800	227	260	11			

- Molecule 3 is a protein called R-PHYCOERYTHRIN.

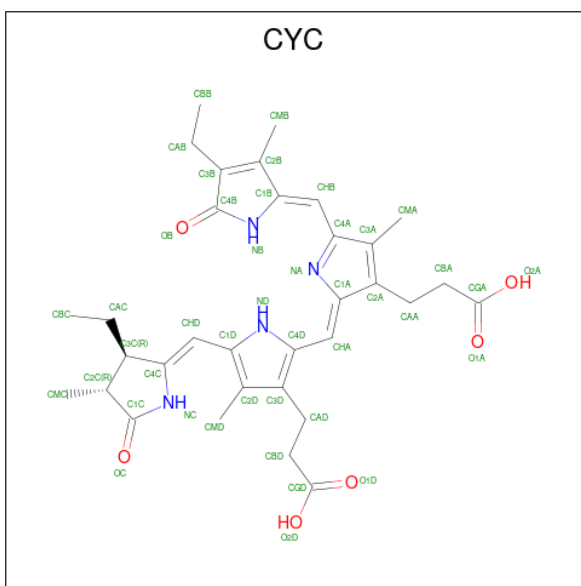
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	6	Total	C	N	O	0	0	0
			42	27	9	6			
3	H	5	Total	C	N	O	0	0	0
			37	24	8	5			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0

- Molecule 5 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $\text{C}_{33}\text{H}_{40}\text{N}_4\text{O}_6$).



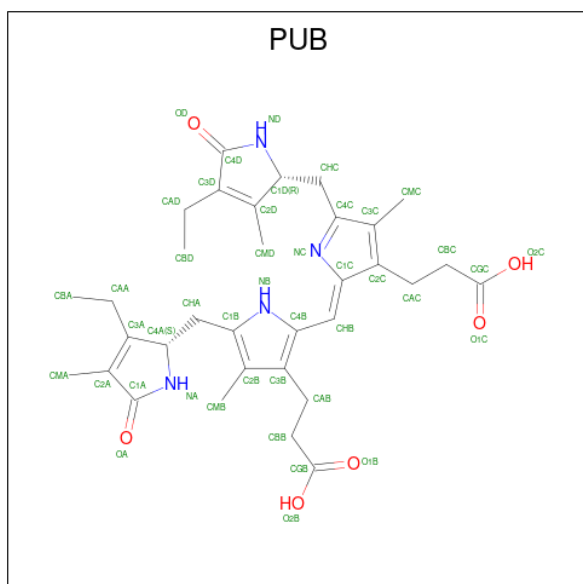
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 43	C 33	N 4	O 6	0	0
5	A	1	Total 43	C 33	N 4	O 6	0	0

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

- Molecule 6 is PHYCOUROBILIN (CCD ID: PUB) (formula: $C_{33}H_{42}N_4O_6$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	27	Total	O	0	0
			27	27		

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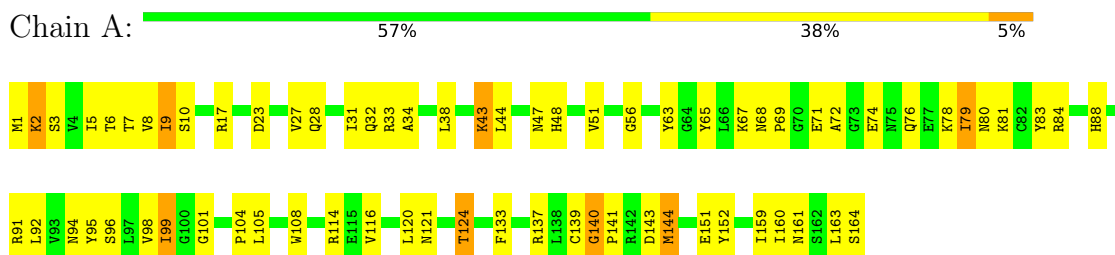
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	22	Total 22	O 22	0	0
7	K	31	Total 31	O 31	0	0
7	L	29	Total 29	O 29	0	0
7	H	1	Total 1	O 1	0	0

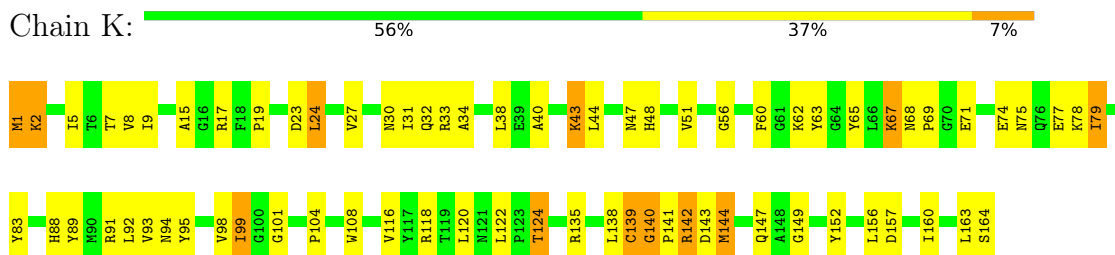
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

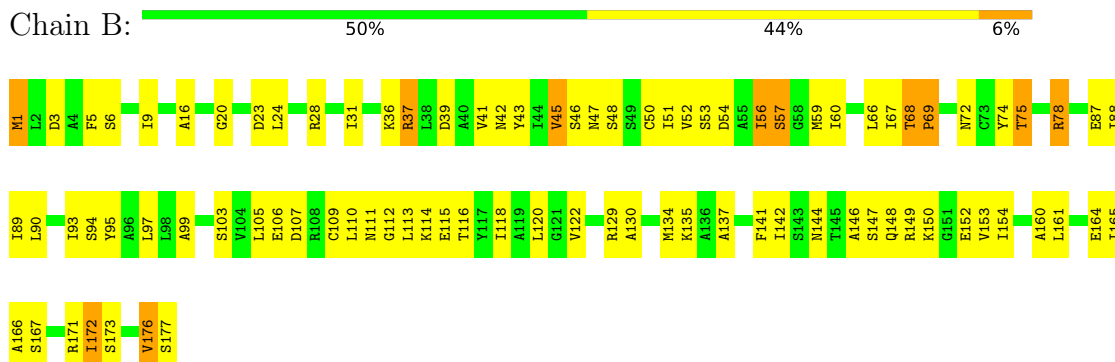
• Molecule 1: R-PHYCOERYTHRIN



• Molecule 1: R-PHYCOERYTHRIN

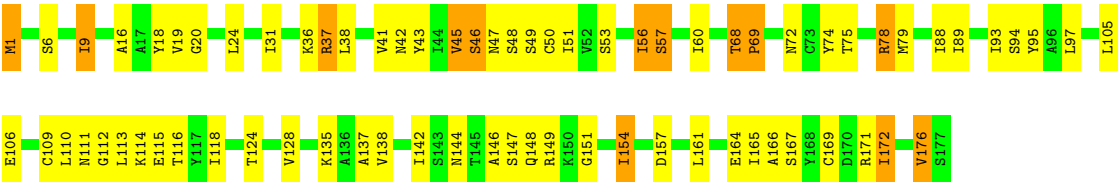


• Molecule 2: R-PHYCOERYTHRIN



• Molecule 2: R-PHYCOERYTHRIN

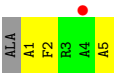




• Molecule 3: R-PHYCOERYTHRIN



• Molecule 3: R-PHYCOERYTHRIN



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	187.27Å 187.27Å 59.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	999.00 – 2.25 93.63 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.6 (999.00-2.25) 97.7 (93.63-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.26Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.180 , 0.279 0.153 , 0.242	Depositor DCC
R_{free} test set	1859 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.460 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5719	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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, SO4, CYC, PUB

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	0.34	0/1268	0.94	0/1713
1	K	0.36	0/1268	0.97	2/1713 (0.1%)
2	B	0.36	0/1300	0.94	0/1755
2	L	0.36	0/1300	0.93	0/1755
3	G	0.32	0/42	0.76	0/55
3	H	0.32	0/37	0.63	0/48
All	All	0.36	0/5215	0.94	2/7039 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	139	CYS	CA-C-N	5.55	130.59	121.87
1	K	139	CYS	C-N-CA	5.55	130.59	121.87

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	1247	0	1215	61	0
1	K	1247	0	1215	67	0
2	B	1298	0	1300	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1298	0	1300	82	0
3	G	42	0	44	3	0
3	H	37	0	39	5	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	86	0	74	10	0
5	B	86	0	74	15	0
5	K	86	0	74	6	0
5	L	86	0	74	18	0
6	B	43	0	33	3	0
6	L	43	0	33	2	0
7	A	27	0	0	0	0
7	B	22	0	0	0	0
7	H	1	0	0	0	0
7	K	31	0	0	1	0
7	L	29	0	0	0	0
All	All	5719	0	5475	283	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (283) 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:B:106:GLU:HG2	2:B:110:LEU:HD12	1.50	0.93
2:B:36:LYS:HD3	5:B:183:CYC:HMD3	1.52	0.91
2:L:114:LYS:HB2	2:L:176:VAL:HA	1.54	0.89
1:K:44:LEU:HD12	5:K:168:CYC:HBB1	1.53	0.89
1:A:32:GLN:HG3	1:K:32:GLN:HG3	1.55	0.87
1:A:44:LEU:HD12	5:A:168:CYC:HBB1	1.60	0.83
2:B:59:MET:HE3	2:B:66:LEU:HD13	1.61	0.81
2:B:89:ILE:HG23	2:B:172:ILE:HD12	1.64	0.80
2:L:88:ILE:HG21	5:L:181:CYC:HAB1	1.64	0.80
2:L:53:SER:O	2:L:57:SER:HB2	1.82	0.79
2:B:47:ASN:O	2:B:51:ILE:HG13	1.84	0.76
2:B:20:GLY:O	2:B:24:LEU:HB2	1.86	0.76
1:K:75:ASN:OD1	1:K:78:LYS:HG3	1.86	0.75
1:K:94:ASN:O	1:K:98:VAL:HG23	1.86	0.75
2:L:20:GLY:O	2:L:24:LEU:HB2	1.85	0.75
1:K:68:ASN:O	1:K:71:GLU:HB2	1.87	0.74
1:K:27:VAL:O	1:K:30:ASN:HB2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASN:O	1:A:71:GLU:HB2	1.88	0.74
2:B:154:ILE:HD11	5:B:183:CYC:HAD2	1.71	0.73
1:K:5:ILE:O	1:K:9:ILE:HG13	1.89	0.73
1:A:76:GLN:HG3	1:A:80:ASN:ND2	2.04	0.73
2:L:89:ILE:HG23	2:L:172:ILE:HD12	1.71	0.72
2:B:148:GLN:HB2	6:B:179:PUB:OA	1.89	0.72
3:G:3:PHE:HB3	3:G:4:ARG:NH1	2.05	0.72
2:B:43:TYR:HD2	2:B:142:ILE:HA	1.53	0.71
2:B:37:ARG:O	2:B:41:VAL:HG23	1.91	0.71
2:B:88:ILE:HG21	5:B:181:CYC:HAB1	1.71	0.70
1:A:33:ARG:NE	5:L:183:CYC:HAB1	2.05	0.70
2:L:146:ALA:HB3	2:L:149:ARG:O	1.92	0.70
1:A:99:ILE:HD12	1:A:104:PRO:HD3	1.74	0.70
2:B:75:THR:HG1	2:B:78:ARG:HG3	1.55	0.70
1:K:108:TRP:O	5:K:166:CYC:HAB2	1.91	0.70
1:K:99:ILE:HD13	2:L:6:SER:HB3	1.74	0.69
2:L:36:LYS:HD3	5:L:183:CYC:HMD3	1.75	0.69
1:K:89:TYR:O	1:K:93:VAL:HG23	1.94	0.68
3:G:3:PHE:HB3	3:G:4:ARG:HH11	1.59	0.68
2:B:146:ALA:HB3	2:B:149:ARG:O	1.94	0.68
2:L:148:GLN:HB2	6:L:179:PUB:OA	1.93	0.67
5:B:183:CYC:HAB1	1:K:33:ARG:NE	2.09	0.67
2:L:19:VAL:HG12	2:L:24:LEU:HD13	1.75	0.67
2:B:75:THR:OG1	2:B:78:ARG:HG3	1.95	0.67
1:A:47:ASN:O	1:A:51:VAL:HG23	1.94	0.66
1:K:104:PRO:O	1:K:108:TRP:HB2	1.94	0.66
1:K:88:HIS:O	1:K:92:LEU:HG	1.95	0.66
1:A:9:ILE:HB	2:B:1:MET:HE1	1.78	0.65
1:K:47:ASN:O	1:K:51:VAL:HG23	1.96	0.65
2:L:41:VAL:HG22	2:L:97:LEU:HD23	1.77	0.65
2:L:113:LEU:HD11	5:L:181:CYC:HMB3	1.79	0.64
2:B:113:LEU:HA	3:G:3:PHE:HE1	1.61	0.64
2:B:43:TYR:OH	2:B:153:VAL:HG11	1.96	0.64
1:K:44:LEU:HD11	1:K:152:TYR:HE1	1.62	0.63
1:A:76:GLN:HG3	1:A:80:ASN:HD21	1.62	0.63
2:B:144:ASN:HB2	5:B:183:CYC:HMC3	1.81	0.63
5:K:166:CYC:HMD1	5:K:166:CYC:HBD2	1.81	0.62
1:A:99:ILE:HD13	2:B:6:SER:HB3	1.80	0.62
2:L:47:ASN:O	2:L:51:ILE:HG13	1.99	0.62
2:B:142:ILE:O	5:B:183:CYC:HMC1	1.99	0.61
3:H:1:ALA:O	3:H:5:ALA:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:HE2	1:A:84:ARG:NH1	2.16	0.61
2:B:53:SER:O	2:B:57:SER:HB2	2.01	0.61
1:A:51:VAL:HG21	5:A:168:CYC:HBB3	1.82	0.61
1:A:34:ALA:O	1:A:38:LEU:HG	2.00	0.60
2:B:167:SER:O	2:B:171:ARG:HG2	2.01	0.60
2:B:105:LEU:HD11	2:B:172:ILE:HD11	1.84	0.60
1:K:23:ASP:O	1:K:27:VAL:HG23	2.00	0.60
2:L:106:GLU:HG2	2:L:110:LEU:HD12	1.84	0.60
1:A:124:THR:HG21	1:A:163:LEU:O	2.01	0.59
2:L:97:LEU:HD13	2:L:165:ILE:HD13	1.83	0.59
1:A:44:LEU:O	1:A:48:HIS:HB3	2.03	0.59
2:B:110:LEU:HD21	2:B:172:ILE:HD13	1.85	0.59
2:L:113:LEU:HA	3:H:2:PHE:HE1	1.67	0.59
1:K:68:ASN:O	1:K:74:GLU:HB3	2.04	0.58
1:K:44:LEU:HD11	1:K:152:TYR:CE1	2.39	0.58
1:A:9:ILE:CB	2:B:1:MET:HE1	2.34	0.57
2:B:105:LEU:O	2:B:109:CYS:HB3	2.04	0.57
1:K:9:ILE:CG2	2:L:1:MET:HE1	2.34	0.57
2:B:148:GLN:HB2	6:B:179:PUB:C1A	2.33	0.57
2:L:43:TYR:HD2	2:L:142:ILE:HA	1.69	0.57
2:L:142:ILE:O	5:L:183:CYC:HMC1	2.04	0.57
1:A:108:TRP:O	5:A:166:CYC:HAB2	2.05	0.56
1:K:19:PRO:HD3	2:L:95:TYR:CE1	2.40	0.56
1:A:44:LEU:HD11	1:A:152:TYR:HE2	1.70	0.56
2:B:154:ILE:HD11	5:B:183:CYC:CAD	2.35	0.56
1:K:124:THR:HG21	1:K:163:LEU:O	2.04	0.56
2:L:105:LEU:O	2:L:109:CYS:HB3	2.06	0.56
2:L:112:GLY:HA2	2:L:115:GLU:OE1	2.05	0.56
1:A:44:LEU:HD11	1:A:152:TYR:CE2	2.41	0.56
1:A:94:ASN:O	1:A:98:VAL:HG23	2.05	0.56
1:A:78:LYS:O	5:A:166:CYC:HMD3	2.05	0.56
1:A:43:LYS:HG2	1:A:144:MET:HG2	1.88	0.55
1:A:161:ASN:OD1	2:L:49:SER:HB2	2.06	0.55
2:B:142:ILE:CD1	2:B:165:ILE:HG21	2.37	0.55
1:K:9:ILE:HB	2:L:1:MET:HE1	1.89	0.55
5:L:183:CYC:HMD1	5:L:183:CYC:HBD2	1.87	0.55
1:K:67:LYS:HE3	1:K:79:ILE:HD11	1.89	0.55
1:A:81:LYS:HE2	1:A:84:ARG:HH12	1.72	0.55
1:K:95:TYR:O	1:K:99:ILE:HG13	2.07	0.55
1:A:51:VAL:HG21	5:A:168:CYC:CBB	2.37	0.54
2:B:74:TYR:O	2:B:78:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:56:ILE:O	2:L:60:ILE:HG13	2.06	0.54
1:K:9:ILE:HG21	2:L:1:MET:HE1	1.88	0.54
1:K:34:ALA:O	1:K:38:LEU:HG	2.07	0.54
2:L:36:LYS:HD3	5:L:183:CYC:CMD	2.37	0.54
2:L:51:ILE:HG23	2:L:137:ALA:HB3	1.88	0.54
2:L:154:ILE:HD11	5:L:183:CYC:HAD2	1.90	0.54
1:A:88:HIS:O	1:A:92:LEU:HG	2.08	0.54
2:L:105:LEU:HD11	2:L:172:ILE:CD1	2.38	0.54
2:L:113:LEU:CD1	5:L:181:CYC:HMB3	2.38	0.54
2:B:68:THR:HG23	2:B:69:PRO:HD2	1.88	0.53
2:B:130:ALA:O	2:B:134:MET:HG3	2.08	0.53
2:L:72:MEN:HE22	5:L:181:CYC:HBD2	1.90	0.53
1:A:143:ASP:O	1:A:144:MET:HG3	2.09	0.53
1:K:9:ILE:CB	2:L:1:MET:HE1	2.38	0.53
2:L:37:ARG:HB2	2:L:37:ARG:HH11	1.74	0.53
2:B:41:VAL:O	2:B:45:VAL:HG13	2.09	0.53
2:B:105:LEU:HD11	2:B:172:ILE:CD1	2.39	0.53
1:K:40:ALA:O	1:K:44:LEU:HD13	2.08	0.53
2:B:60:ILE:HG21	2:B:67:ILE:HD13	1.91	0.53
2:L:113:LEU:O	2:L:116:THR:HB	2.08	0.53
1:A:28:GLN:O	1:A:32:GLN:HG2	2.09	0.53
5:B:183:CYC:HMD1	5:B:183:CYC:HBD2	1.90	0.53
2:L:93:ILE:HG22	2:L:165:ILE:HD11	1.90	0.53
2:L:68:THR:HG23	2:L:69:PRO:HD2	1.92	0.52
1:K:1:MET:HE3	1:K:104:PRO:HA	1.91	0.52
2:L:41:VAL:O	2:L:45:VAL:HG13	2.09	0.52
1:A:9:ILE:HD12	2:B:1:MET:HE1	1.92	0.52
1:A:44:LEU:CD1	5:A:168:CYC:HBB1	2.37	0.52
1:A:2:LYS:HE2	1:A:7:THR:OG1	2.09	0.52
1:A:31:ILE:HA	2:B:31:ILE:HG23	1.91	0.51
1:A:63:TYR:HB3	1:A:65:TYR:CE1	2.44	0.51
1:K:88:HIS:CD2	1:K:91:ARG:HH21	2.28	0.51
1:K:140:GLY:O	1:K:144:MET:O	2.29	0.51
2:L:135:LYS:HE3	2:L:166:ALA:HB1	1.91	0.51
1:K:43:LYS:HG2	1:K:144:MET:HG2	1.93	0.51
2:B:93:ILE:HG22	2:B:165:ILE:HD11	1.92	0.51
1:K:56:GLY:HA3	1:K:83:TYR:CE2	2.46	0.50
1:A:95:TYR:O	1:A:99:ILE:HG13	2.12	0.50
2:B:3:ASP:HB3	2:B:99:ALA:HB1	1.93	0.50
2:B:106:GLU:O	2:B:111:ASN:HB2	2.11	0.50
2:L:144:ASN:HB2	5:L:183:CYC:HMC3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:NH1	2:B:16:ALA:HA	2.27	0.50
2:L:105:LEU:HD11	2:L:172:ILE:HD11	1.93	0.50
1:A:9:ILE:HG23	2:B:95:TYR:CD1	2.47	0.49
1:A:140:GLY:O	1:A:144:MET:O	2.30	0.49
5:B:183:CYC:HMA2	1:K:147:GLN:HG3	1.94	0.49
1:K:60:PHE:HB3	1:K:67:LYS:NZ	2.28	0.49
1:K:116:VAL:O	1:K:120:LEU:HB2	2.13	0.49
1:A:137:ARG:HH22	5:A:168:CYC:CGD	2.26	0.49
2:B:56:ILE:O	2:B:60:ILE:HG13	2.13	0.49
1:K:62:LYS:HB2	7:K:383:HOH:O	2.13	0.48
2:B:135:LYS:HE2	2:B:166:ALA:HB1	1.96	0.48
5:L:181:CYC:HBB2	3:H:2:PHE:CE2	2.48	0.48
1:K:143:ASP:O	1:K:144:MET:HG3	2.13	0.48
1:A:96:SER:HB3	1:A:101:GLY:O	2.13	0.48
1:K:44:LEU:O	1:K:48:HIS:HB3	2.14	0.48
2:B:144:ASN:HB2	5:B:183:CYC:CMC	2.44	0.48
1:K:15:ALA:CB	1:K:17:ARG:HD3	2.44	0.48
1:K:91:ARG:NH1	2:L:16:ALA:HA	2.29	0.48
2:L:109:CYS:O	3:H:2:PHE:HZ	1.97	0.48
2:B:89:ILE:CG2	2:B:172:ILE:HD12	2.41	0.47
2:B:103:SER:O	2:B:107:ASP:HB2	2.15	0.47
1:K:91:ARG:HA	2:L:18:TYR:CE2	2.49	0.47
2:L:138:VAL:HG11	2:L:165:ILE:HG12	1.97	0.47
1:A:17:ARG:O	2:B:95:TYR:OH	2.30	0.47
2:B:36:LYS:HD3	5:B:183:CYC:CMD	2.36	0.47
2:L:89:ILE:CG2	2:L:172:ILE:HD12	2.42	0.47
1:K:9:ILE:HD12	2:L:1:MET:CE	2.45	0.47
2:L:74:TYR:O	2:L:75:THR:OG1	2.29	0.47
2:L:89:ILE:HG23	2:L:172:ILE:CD1	2.43	0.47
2:L:154:ILE:HD11	5:L:183:CYC:CAD	2.45	0.47
1:K:19:PRO:HD3	2:L:95:TYR:HE1	1.80	0.47
2:B:176:VAL:HG23	2:B:176:VAL:O	2.15	0.47
1:A:133:PHE:O	1:A:137:ARG:N	2.48	0.46
2:L:37:ARG:NH2	2:L:164:GLU:OE1	2.48	0.46
2:L:106:GLU:O	2:L:111:ASN:HB2	2.14	0.46
2:B:3:ASP:CB	2:B:99:ALA:HB1	2.46	0.46
2:B:39:ASP:OD2	2:B:153:VAL:HG21	2.16	0.46
1:K:88:HIS:HD2	1:K:91:ARG:HH21	1.62	0.46
1:K:122:LEU:CD2	5:K:166:CYC:HMD2	2.44	0.46
1:A:68:ASN:HB3	1:A:69:PRO:HD2	1.96	0.46
2:B:173:SER:O	2:B:177:SER:OG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:43:LYS:HD2	1:K:43:LYS:HA	1.75	0.46
2:L:114:LYS:CB	2:L:176:VAL:HA	2.36	0.46
1:K:135:ARG:NH1	1:K:160:ILE:HD13	2.30	0.46
1:K:19:PRO:HG2	2:L:45:VAL:HG11	1.97	0.46
1:K:24:LEU:N	1:K:24:LEU:HD23	2.31	0.46
2:L:9:ILE:CD1	2:L:19:VAL:HG21	2.46	0.46
1:A:116:VAL:HG13	1:A:120:LEU:HD13	1.98	0.46
2:L:36:LYS:NZ	2:L:157:ASP:O	2.47	0.46
1:A:91:ARG:NH1	1:A:95:TYR:OH	2.48	0.46
2:B:74:TYR:O	2:B:75:THR:OG1	2.28	0.46
2:B:3:ASP:HB2	2:B:99:ALA:O	2.16	0.46
2:B:161:LEU:N	2:B:161:LEU:HD12	2.31	0.46
2:L:38:LEU:HD12	5:L:183:CYC:C4B	2.45	0.46
1:A:5:ILE:O	1:A:9:ILE:HG13	2.16	0.45
2:B:60:ILE:CG2	2:B:67:ILE:HD13	2.46	0.45
2:B:160:ALA:O	2:B:164:GLU:HB2	2.16	0.45
2:B:161:LEU:HD12	2:B:161:LEU:H	1.81	0.45
1:K:2:LYS:O	1:K:101:GLY:HA3	2.15	0.45
1:K:144:MET:HE1	1:K:149:GLY:HA2	1.97	0.45
2:L:88:ILE:CG2	5:L:181:CYC:HAB1	2.42	0.45
2:B:24:LEU:O	2:B:28:ARG:HG3	2.17	0.45
5:B:183:CYC:O1A	1:K:147:GLN:NE2	2.50	0.45
1:A:144:MET:HB2	1:A:144:MET:HE2	1.66	0.45
2:L:147:SER:HB3	6:L:179:PUB:O1B	2.17	0.45
2:B:144:ASN:O	2:B:144:ASN:ND2	2.50	0.45
1:A:98:VAL:O	2:B:5:PHE:HD1	2.00	0.45
1:K:63:TYR:HB3	1:K:65:TYR:CE1	2.52	0.45
1:A:121:ASN:O	1:A:121:ASN:ND2	2.49	0.45
1:A:139:CYS:HA	5:A:168:CYC:HBC3	1.98	0.45
2:B:89:ILE:HG23	2:B:172:ILE:CD1	2.41	0.45
2:L:149:ARG:HG3	2:L:149:ARG:HH11	1.81	0.45
1:A:9:ILE:HD12	2:B:1:MET:CE	2.46	0.44
1:A:72:ALA:O	1:A:78:LYS:HB3	2.16	0.44
2:B:43:TYR:CD2	2:B:142:ILE:HA	2.44	0.44
2:B:147:SER:O	2:B:150:LYS:HE2	2.17	0.44
1:A:23:ASP:O	1:A:27:VAL:HG23	2.18	0.44
2:B:149:ARG:NH2	1:K:157:ASP:OD2	2.49	0.44
2:B:51:ILE:HG23	2:B:137:ALA:HB3	1.99	0.44
1:K:31:ILE:HA	2:L:31:ILE:HG23	1.99	0.44
2:B:90:LEU:HA	2:B:93:ILE:HD12	2.00	0.44
2:L:72:MEN:OD1	5:L:181:CYC:HMD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:161:LEU:HD12	2:L:161:LEU:N	2.33	0.44
2:B:37:ARG:HH11	2:B:37:ARG:HB2	1.82	0.44
1:K:135:ARG:HA	1:K:156:LEU:HD13	2.00	0.43
2:L:115:GLU:CD	2:L:115:GLU:H	2.26	0.43
1:K:1:MET:HG3	1:K:99:ILE:CD1	2.49	0.43
2:L:124:THR:O	2:L:128:VAL:HG23	2.19	0.43
2:B:42:ASN:O	2:B:46:SER:HB2	2.19	0.43
2:B:59:MET:O	2:B:59:MET:HG2	2.18	0.43
1:K:2:LYS:HE2	1:K:7:THR:OG1	2.19	0.43
2:L:135:LYS:HD2	2:L:169:CYS:HB2	2.01	0.43
2:L:41:VAL:HA	2:L:97:LEU:HD23	2.01	0.43
2:L:144:ASN:HD21	2:L:151:GLY:H	1.67	0.43
1:K:31:ILE:O	1:K:31:ILE:HG22	2.19	0.43
1:A:68:ASN:O	1:A:74:GLU:HB3	2.18	0.42
2:L:24:LEU:HD12	2:L:24:LEU:HA	1.86	0.42
2:L:110:LEU:HD21	2:L:172:ILE:HG23	2.01	0.42
2:L:167:SER:O	2:L:171:ARG:HG3	2.19	0.42
2:L:106:GLU:HA	2:L:110:LEU:HB2	2.02	0.42
2:L:144:ASN:HB2	5:L:183:CYC:CMC	2.48	0.42
1:K:1:MET:HG2	2:L:6:SER:HB2	2.00	0.42
1:K:139:CYS:SG	1:K:142:ARG:HB3	2.59	0.42
1:A:5:ILE:HG21	2:B:99:ALA:HA	2.01	0.42
1:A:79:ILE:HG22	1:A:80:ASN:N	2.35	0.42
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.20	0.42
1:A:3:SER:H	1:A:6:THR:HB	1.85	0.42
2:B:72:MEN:HE21	2:B:78:ARG:NH2	2.35	0.42
1:K:1:MET:HE3	1:K:104:PRO:CA	2.49	0.42
2:L:154:ILE:O	2:L:154:ILE:HG13	2.19	0.42
2:B:41:VAL:HA	2:B:97:LEU:HD23	2.02	0.42
2:B:116:THR:HG22	2:B:120:LEU:CD1	2.49	0.42
1:A:56:GLY:HA3	1:A:83:TYR:CE2	2.55	0.41
2:B:97:LEU:HD13	2:B:165:ILE:HD13	2.02	0.41
1:K:68:ASN:HB3	1:K:69:PRO:HD2	2.02	0.41
2:B:52:VAL:HG21	2:B:87:GLU:HA	2.02	0.41
2:B:122:VAL:HG13	5:B:181:CYC:NC	2.35	0.41
2:L:60:ILE:CD1	2:L:79:MET:HE1	2.50	0.41
2:B:120:LEU:CD2	5:B:181:CYC:HAA2	2.50	0.41
1:A:78:LYS:HB3	5:A:166:CYC:CMD	2.50	0.41
2:B:72:MEN:O	2:B:78:ARG:HD3	2.20	0.41
2:B:112:GLY:HA2	2:B:115:GLU:OE1	2.20	0.41
2:B:149:ARG:HG3	2:B:149:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:MEN:O	2:B:78:ARG:HB3	2.21	0.41
2:L:42:ASN:O	2:L:46:SER:HB2	2.19	0.41
5:A:168:CYC:HC	5:A:168:CYC:HMD2	1.86	0.41
2:B:43:TYR:HB3	2:B:141:PHE:O	2.21	0.41
1:K:78:LYS:HE2	5:K:166:CYC:CGD	2.51	0.41
2:L:60:ILE:HD13	2:L:79:MET:HE1	2.02	0.41
2:L:74:TYR:O	2:L:78:ARG:HG3	2.20	0.41
1:A:63:TYR:CD1	1:A:65:TYR:HE1	2.38	0.41
1:A:105:LEU:HD21	1:A:159:ILE:HD11	2.02	0.41
2:B:115:GLU:CD	2:B:115:GLU:H	2.29	0.41
2:L:114:LYS:HD2	2:L:176:VAL:C	2.46	0.41
2:B:88:ILE:HG21	5:B:181:CYC:CAB	2.44	0.41
2:L:105:LEU:HG	2:L:110:LEU:CD1	2.50	0.41
5:L:181:CYC:HMA1	3:H:2:PHE:HB2	2.03	0.41
1:K:138:LEU:HA	5:K:168:CYC:HMB2	2.03	0.41
2:B:97:LEU:HD22	2:B:165:ILE:HD13	2.02	0.40
2:B:114:LYS:HB2	2:B:176:VAL:HA	2.02	0.40
2:B:54:ASP:OD2	6:B:179:PUB:HHC1	2.21	0.40
2:B:154:ILE:O	2:B:154:ILE:HG13	2.22	0.40
1:K:15:ALA:HB3	1:K:17:ARG:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	10	7
1	K	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	10	7
2	B	174/177 (98%)	167 (96%)	5 (3%)	2 (1%)	11	8
2	L	174/177 (98%)	168 (97%)	5 (3%)	1 (1%)	21	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
3	H	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	679/694 (98%)	646 (95%)	26 (4%)	7 (1%)	12	10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	75	THR
1	K	140	GLY
2	L	69	PRO
1	A	140	GLY
2	B	69	PRO
1	A	141	PRO
1	K	141	PRO

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	129/129 (100%)	115 (89%)	14 (11%)	6	4
1	K	129/129 (100%)	115 (89%)	14 (11%)	6	4
2	B	138/138 (100%)	121 (88%)	17 (12%)	4	3
2	L	138/138 (100%)	122 (88%)	16 (12%)	5	3
3	G	2/2 (100%)	2 (100%)	0	100	100
3	H	2/2 (100%)	2 (100%)	0	100	100
All	All	538/538 (100%)	477 (89%)	61 (11%)	5	3

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	8	VAL

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Mol	Chain	Res	Type
1	A	9	ILE
1	A	10	SER
1	A	43	LYS
1	A	67	LYS
1	A	79	ILE
1	A	99	ILE
1	A	114	ARG
1	A	124	THR
1	A	144	MET
1	A	160	ILE
1	A	164	SER
2	B	1	MET
2	B	9	ILE
2	B	23	ASP
2	B	37	ARG
2	B	45	VAL
2	B	48	SER
2	B	50	CYS
2	B	56	ILE
2	B	57	SER
2	B	68	THR
2	B	78	ARG
2	B	94	SER
2	B	118	ILE
2	B	129	ARG
2	B	152	GLU
2	B	172	ILE
2	B	176	VAL
1	K	1	MET
1	K	2	LYS
1	K	8	VAL
1	K	24	LEU
1	K	43	LYS
1	K	67	LYS
1	K	77	GLU
1	K	79	ILE
1	K	99	ILE
1	K	118	ARG
1	K	124	THR
1	K	142	ARG
1	K	144	MET
1	K	164	SER

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Mol	Chain	Res	Type
2	L	1	MET
2	L	9	ILE
2	L	37	ARG
2	L	45	VAL
2	L	46	SER
2	L	48	SER
2	L	50	CYS
2	L	56	ILE
2	L	57	SER
2	L	68	THR
2	L	78	ARG
2	L	94	SER
2	L	118	ILE
2	L	154	ILE
2	L	172	ILE
2	L	176	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	80	ASN
2	B	125	ASN
2	B	144	ASN
1	K	28	GLN
1	K	32	GLN
1	K	88	HIS
2	L	144	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	L	72	2	7,8,9	0.67	0	4,9,11	0.37	0
2	MEN	B	72	2	7,8,9	0.65	0	4,9,11	0.67	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	L	72	2	-	4/7/8/10	-
2	MEN	B	72	2	-	4/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	72	MEN	OD1-CG-ND2-CE2
2	L	72	MEN	N-CA-CB-CG
2	B	72	MEN	CA-CB-CG-OD1
2	B	72	MEN	CA-CB-CG-ND2
2	L	72	MEN	CA-CB-CG-ND2
2	L	72	MEN	CA-CB-CG-OD1
2	L	72	MEN	OD1-CG-ND2-CE2
2	B	72	MEN	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	72	MEN	2	0
2	B	72	MEN	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PUB	L	179	2	45,46,46	2.93	18 (40%)	45,67,67	2.99	13 (28%)
4	SO4	A	201	-	4,4,4	0.70	0	6,6,6	0.08	0
5	CYC	B	181	2	46,46,46	2.88	15 (32%)	63,67,67	2.33	23 (36%)
5	CYC	A	168	1	46,46,46	2.92	15 (32%)	63,67,67	2.25	17 (26%)
5	CYC	K	166	1	46,46,46	2.92	16 (34%)	63,67,67	2.36	24 (38%)
5	CYC	L	181	2	46,46,46	2.89	13 (28%)	63,67,67	2.40	23 (36%)
5	CYC	L	183	2	46,46,46	2.89	15 (32%)	63,67,67	2.24	17 (26%)
6	PUB	B	179	2	45,46,46	2.95	19 (42%)	45,67,67	3.03	13 (28%)
5	CYC	A	166	1	46,46,46	2.86	16 (34%)	63,67,67	2.49	23 (36%)
5	CYC	K	168	1	46,46,46	2.85	14 (30%)	63,67,67	2.21	16 (25%)
5	CYC	B	183	2	46,46,46	2.87	16 (34%)	63,67,67	2.17	17 (26%)
4	SO4	B	202	-	4,4,4	0.73	0	6,6,6	0.08	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
6	PUB	L	179	2	-	9/26/74/74	0/4/4/4
5	CYC	B	181	2	-	13/26/74/74	0/4/4/4
5	CYC	A	168	1	1/1/14/19	12/26/74/74	0/4/4/4
5	CYC	K	166	1	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CYC	L	181	2	-	15/26/74/74	0/4/4/4
5	CYC	L	183	2	-	15/26/74/74	0/4/4/4
6	PUB	B	179	2	-	9/26/74/74	0/4/4/4
5	CYC	A	166	1	-	8/26/74/74	0/4/4/4
5	CYC	K	168	1	1/1/14/19	13/26/74/74	0/4/4/4
5	CYC	B	183	2	-	15/26/74/74	0/4/4/4

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	168	CYC	C2C-C1C	-13.70	1.39	1.52
5	L	183	CYC	C2C-C1C	-13.65	1.39	1.52
5	L	181	CYC	C2C-C1C	-13.56	1.40	1.52
5	K	166	CYC	C2C-C1C	-13.52	1.40	1.52
5	B	181	CYC	C2C-C1C	-13.47	1.40	1.52
5	B	183	CYC	C2C-C1C	-13.39	1.40	1.52
5	A	166	CYC	C2C-C1C	-13.21	1.40	1.52
5	K	168	CYC	C2C-C1C	-13.12	1.40	1.52
6	B	179	PUB	CBA-CAA	-8.79	1.14	1.51
6	L	179	PUB	CBA-CAA	-8.62	1.14	1.51
5	A	168	CYC	O1D-CGD	7.21	1.45	1.22
5	A	166	CYC	O1D-CGD	7.15	1.45	1.22
6	L	179	PUB	O1B-CGB	7.14	1.45	1.22
6	B	179	PUB	O1B-CGB	7.07	1.45	1.22
5	K	166	CYC	O1D-CGD	7.06	1.45	1.22
5	K	168	CYC	O1D-CGD	7.06	1.45	1.22
5	B	181	CYC	O1D-CGD	7.04	1.45	1.22
5	L	181	CYC	O1D-CGD	7.03	1.45	1.22
5	L	183	CYC	O1D-CGD	7.00	1.45	1.22
5	B	183	CYC	O1D-CGD	6.96	1.44	1.22
6	L	179	PUB	C3A-C2A	6.84	1.44	1.33
6	B	179	PUB	C3A-C2A	6.77	1.44	1.33
6	L	179	PUB	O2C-CGC	5.07	1.47	1.30
6	B	179	PUB	O2C-CGC	4.89	1.47	1.30
5	K	166	CYC	O2A-CGA	4.61	1.46	1.30
5	L	183	CYC	O2A-CGA	4.61	1.46	1.30
5	K	168	CYC	O2A-CGA	4.60	1.46	1.30
5	A	166	CYC	O2A-CGA	4.56	1.45	1.30
5	L	181	CYC	O2A-CGA	4.53	1.45	1.30
5	B	183	CYC	O2A-CGA	4.52	1.45	1.30
6	B	179	PUB	CHA-C1B	-4.52	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	181	CYC	O2A-CGA	4.51	1.45	1.30
5	A	168	CYC	O2A-CGA	4.45	1.45	1.30
6	B	179	PUB	CHC-C1D	-4.38	1.44	1.53
6	L	179	PUB	C4D-C3D	-4.29	1.40	1.48
6	L	179	PUB	CHA-C1B	-4.19	1.45	1.50
6	B	179	PUB	C4D-C3D	-4.18	1.40	1.48
6	L	179	PUB	CHC-C1D	-4.15	1.45	1.53
6	B	179	PUB	CHA-C4A	-4.11	1.45	1.53
6	L	179	PUB	CHC-C4C	-4.06	1.44	1.50
6	B	179	PUB	C2C-C3C	3.97	1.45	1.36
6	B	179	PUB	CHC-C4C	-3.96	1.44	1.50
6	L	179	PUB	C2C-C3C	3.95	1.45	1.36
5	L	181	CYC	C2A-C3A	3.89	1.45	1.36
6	L	179	PUB	CHA-C4A	-3.88	1.45	1.53
5	A	166	CYC	C2A-C3A	3.87	1.45	1.36
5	L	183	CYC	C2A-C3A	3.80	1.45	1.36
5	K	166	CYC	CAC-C3C	3.77	1.61	1.54
5	B	181	CYC	C2A-C3A	3.74	1.44	1.36
5	K	166	CYC	C2A-C3A	3.71	1.44	1.36
5	A	168	CYC	C2A-C3A	3.68	1.44	1.36
5	B	183	CYC	C2A-C3A	3.67	1.44	1.36
5	K	168	CYC	C2A-C3A	3.65	1.44	1.36
5	A	168	CYC	C4C-NC	3.55	1.44	1.37
5	K	168	CYC	C4B-C3B	-3.48	1.41	1.48
5	A	166	CYC	C4B-C3B	-3.47	1.41	1.48
5	L	181	CYC	C4C-NC	3.45	1.44	1.37
5	A	168	CYC	C4B-C3B	-3.45	1.41	1.48
5	B	181	CYC	C4C-NC	3.44	1.44	1.37
5	L	181	CYC	C4B-C3B	-3.44	1.41	1.48
5	K	166	CYC	C4B-C3B	-3.37	1.42	1.48
5	B	181	CYC	C3B-C2B	3.35	1.44	1.36
5	A	168	CYC	CAC-C3C	3.34	1.60	1.54
5	L	181	CYC	C3B-C2B	3.34	1.44	1.36
5	B	183	CYC	C4C-NC	3.31	1.43	1.37
5	B	181	CYC	C4B-C3B	-3.29	1.42	1.48
5	B	183	CYC	CAC-C3C	3.28	1.60	1.54
5	L	183	CYC	CAC-C3C	3.27	1.60	1.54
5	L	183	CYC	C4C-NC	3.26	1.43	1.37
5	L	183	CYC	C4B-C3B	-3.26	1.42	1.48
6	L	179	PUB	C1B-C2B	3.25	1.42	1.38
5	A	166	CYC	C3B-C2B	3.24	1.43	1.36
5	B	183	CYC	C4B-C3B	-3.24	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	179	PUB	C4C-NC	3.20	1.40	1.35
6	L	179	PUB	C4C-NC	3.20	1.40	1.35
5	K	166	CYC	C3B-C2B	3.19	1.43	1.36
5	K	168	CYC	C4C-NC	3.17	1.43	1.37
5	K	168	CYC	C3B-C2B	3.15	1.43	1.36
5	A	166	CYC	C4C-NC	3.15	1.43	1.37
5	K	166	CYC	C4C-NC	3.13	1.43	1.37
6	B	179	PUB	C4B-NB	3.09	1.43	1.37
6	B	179	PUB	C1B-C2B	3.08	1.42	1.38
6	L	179	PUB	C4B-NB	3.07	1.43	1.37
5	L	183	CYC	C3B-C2B	3.03	1.43	1.36
5	B	183	CYC	C3B-C2B	2.98	1.43	1.36
5	A	168	CYC	C3B-C2B	2.94	1.43	1.36
5	B	181	CYC	CHB-C1B	2.90	1.44	1.37
5	A	166	CYC	CHB-C1B	2.88	1.44	1.37
5	K	168	CYC	CHB-C1B	2.87	1.44	1.37
6	L	179	PUB	C4A-C3A	-2.79	1.42	1.51
5	B	183	CYC	CHB-C1B	2.75	1.44	1.37
5	K	166	CYC	CHB-C1B	2.75	1.44	1.37
5	L	183	CYC	CHB-C1B	2.73	1.44	1.37
5	L	181	CYC	CHB-C1B	2.72	1.44	1.37
6	L	179	PUB	C1A-C2A	-2.72	1.41	1.48
5	B	181	CYC	CAC-C3C	2.70	1.59	1.54
6	L	179	PUB	C1B-NB	2.68	1.43	1.37
6	B	179	PUB	C1A-C2A	-2.67	1.41	1.48
5	K	168	CYC	CAC-C3C	2.64	1.59	1.54
6	B	179	PUB	C4A-C3A	-2.63	1.42	1.51
5	L	181	CYC	CAC-C3C	2.62	1.59	1.54
5	K	168	CYC	CHD-C4C	2.62	1.40	1.36
5	A	168	CYC	CHD-C4C	2.57	1.40	1.36
5	B	181	CYC	CHD-C4C	2.56	1.40	1.36
6	B	179	PUB	C1B-NB	2.56	1.42	1.37
5	L	181	CYC	CHD-C4C	2.55	1.40	1.36
5	B	183	CYC	CHD-C4C	2.50	1.40	1.36
5	A	166	CYC	CAC-C3C	2.41	1.58	1.54
5	A	168	CYC	C1B-NB	2.41	1.41	1.37
5	K	166	CYC	CHD-C4C	2.41	1.40	1.36
5	A	166	CYC	C1B-NB	2.38	1.41	1.37
5	K	168	CYC	C1C-NC	-2.36	1.34	1.37
5	A	168	CYC	CHB-C1B	2.35	1.43	1.37
5	L	181	CYC	C4A-NA	2.35	1.42	1.36
5	L	183	CYC	C4A-NA	2.34	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	181	CYC	C1B-NB	2.33	1.41	1.37
5	L	183	CYC	CHD-C4C	2.32	1.40	1.36
5	K	166	CYC	C1C-NC	-2.31	1.34	1.37
5	B	183	CYC	C1B-NB	2.31	1.41	1.37
5	L	183	CYC	C1C-NC	-2.30	1.34	1.37
5	A	168	CYC	C1C-NC	-2.30	1.34	1.37
5	B	183	CYC	C4A-NA	2.28	1.41	1.36
5	K	168	CYC	C4A-NA	2.27	1.41	1.36
5	B	181	CYC	C1C-NC	-2.27	1.34	1.37
5	K	166	CYC	C4B-NB	-2.27	1.32	1.38
5	K	166	CYC	C1B-NB	2.26	1.41	1.37
5	L	181	CYC	C1B-NB	2.25	1.41	1.37
6	L	179	PUB	O2B-CGB	-2.25	1.23	1.30
5	K	166	CYC	O2D-CGD	-2.25	1.23	1.30
5	B	183	CYC	C4B-NB	-2.23	1.32	1.38
5	B	183	CYC	C1C-NC	-2.22	1.34	1.37
5	A	166	CYC	C1C-NC	-2.22	1.34	1.37
6	B	179	PUB	C3B-C2B	2.22	1.44	1.38
5	A	166	CYC	C4A-NA	2.21	1.41	1.36
5	L	181	CYC	C1C-NC	-2.20	1.34	1.37
5	A	168	CYC	C4B-NB	-2.20	1.32	1.38
5	A	168	CYC	C4A-NA	2.20	1.41	1.36
5	L	183	CYC	C4B-NB	-2.19	1.33	1.38
5	B	183	CYC	C4D-ND	2.18	1.41	1.37
6	L	179	PUB	C3B-C2B	2.18	1.44	1.38
5	K	168	CYC	O2D-CGD	-2.17	1.23	1.30
5	B	181	CYC	C4D-ND	2.17	1.41	1.37
5	B	183	CYC	O2D-CGD	-2.16	1.23	1.30
5	A	166	CYC	CBA-CGA	2.16	1.55	1.50
5	B	181	CYC	C4A-NA	2.16	1.41	1.36
5	K	166	CYC	CBA-CGA	2.16	1.55	1.50
5	A	166	CYC	O2D-CGD	-2.15	1.23	1.30
6	B	179	PUB	O2B-CGB	-2.14	1.23	1.30
5	A	168	CYC	O2D-CGD	-2.13	1.23	1.30
5	K	168	CYC	C4B-NB	-2.12	1.33	1.38
5	B	181	CYC	O2D-CGD	-2.12	1.23	1.30
5	L	183	CYC	O2D-CGD	-2.11	1.23	1.30
5	L	183	CYC	C1B-NB	2.10	1.41	1.37
6	B	179	PUB	C1D-C2D	-2.04	1.44	1.50
5	A	166	CYC	CHD-C4C	2.04	1.39	1.36
5	K	166	CYC	C4A-NA	2.01	1.41	1.36
5	A	166	CYC	C4B-NB	-2.00	1.33	1.38

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	166	CYC	C1D-CHD-C4C	10.12	145.04	127.76
5	K	166	CYC	C1D-CHD-C4C	9.90	144.66	127.76
6	L	179	PUB	CHA-C4A-NA	9.39	125.27	113.73
6	B	179	PUB	CHA-C4A-NA	9.12	124.94	113.73
5	L	181	CYC	C1D-CHD-C4C	8.08	141.56	127.76
5	B	181	CYC	C1D-CHD-C4C	7.93	141.30	127.76
6	B	179	PUB	C4A-CHA-C1B	7.85	126.54	113.32
6	L	179	PUB	C4A-CHA-C1B	7.69	126.26	113.32
6	L	179	PUB	CHC-C1D-ND	7.65	123.13	113.73
6	B	179	PUB	CAD-C3D-C4D	-7.64	109.55	121.37
6	B	179	PUB	CHC-C1D-ND	7.53	122.99	113.73
5	A	168	CYC	C1D-CHD-C4C	7.33	140.28	127.76
6	L	179	PUB	CAD-C3D-C4D	-7.19	110.26	121.37
5	K	168	CYC	C1D-CHD-C4C	6.86	139.48	127.76
5	B	183	CYC	C1D-CHD-C4C	6.64	139.11	127.76
5	L	183	CYC	C1D-CHD-C4C	6.14	138.25	127.76
6	B	179	PUB	C1D-CHC-C4C	6.05	127.91	113.74
5	A	168	CYC	CMC-C2C-C1C	6.01	125.36	112.40
5	A	166	CYC	CMC-C2C-C1C	5.89	125.10	112.40
5	K	168	CYC	CMC-C2C-C1C	5.67	124.62	112.40
5	B	181	CYC	CMC-C2C-C1C	5.58	124.42	112.40
5	L	181	CYC	CMC-C2C-C1C	5.54	124.35	112.40
6	B	179	PUB	C1D-ND-C4D	-5.51	104.95	113.42
5	L	181	CYC	C1B-C2B-C3B	-5.50	102.21	107.86
5	K	166	CYC	CMC-C2C-C1C	5.45	124.14	112.40
6	L	179	PUB	C1D-CHC-C4C	5.40	126.38	113.74
5	K	168	CYC	CAC-C3C-C4C	5.38	126.48	112.67
5	A	168	CYC	C1B-C2B-C3B	-5.34	102.38	107.86
5	L	181	CYC	CAC-C3C-C4C	5.32	126.33	112.67
6	L	179	PUB	C1D-ND-C4D	-5.23	105.38	113.42
5	A	166	CYC	C1B-C2B-C3B	-5.23	102.49	107.86
5	B	181	CYC	CAC-C3C-C4C	5.22	126.08	112.67
5	L	183	CYC	CMC-C2C-C1C	5.15	123.50	112.40
5	K	168	CYC	C1B-C2B-C3B	-5.14	102.58	107.86
5	K	166	CYC	C1B-C2B-C3B	-5.02	102.70	107.86
5	B	183	CYC	C1B-C2B-C3B	-5.02	102.70	107.86
5	B	181	CYC	C1B-C2B-C3B	-4.99	102.73	107.86
5	B	183	CYC	C1C-NC-C4C	-4.96	107.19	113.41
5	L	183	CYC	C1B-C2B-C3B	-4.94	102.78	107.86
5	B	183	CYC	CMC-C2C-C1C	4.82	122.79	112.40
5	A	166	CYC	CAC-C3C-C4C	4.82	125.04	112.67
5	B	183	CYC	C3B-C4B-NB	4.70	110.51	106.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	183	CYC	C1C-NC-C4C	-4.69	107.53	113.41
5	L	183	CYC	CAC-C3C-C4C	4.61	124.50	112.67
5	L	183	CYC	C3B-C4B-NB	4.55	110.39	106.77
6	B	179	PUB	C4A-NA-C1A	-4.52	106.47	113.42
5	A	168	CYC	C3B-C4B-NB	4.44	110.31	106.77
5	L	181	CYC	C3B-C4B-NB	4.44	110.31	106.77
5	L	181	CYC	C1C-NC-C4C	-4.43	107.85	113.41
5	A	168	CYC	C1C-NC-C4C	-4.36	107.94	113.41
5	A	166	CYC	C3B-C4B-NB	4.28	110.18	106.77
5	B	181	CYC	C1C-NC-C4C	-4.23	108.11	113.41
5	B	183	CYC	CAC-C3C-C4C	4.21	123.47	112.67
5	K	166	CYC	C3B-C4B-NB	4.11	110.04	106.77
5	L	181	CYC	C1B-NB-C4B	-3.99	105.76	110.66
5	K	168	CYC	C3B-C4B-NB	3.95	109.92	106.77
5	L	183	CYC	OC-C1C-C2C	-3.95	123.03	126.17
5	K	168	CYC	CMB-C2B-C1B	3.93	128.94	124.16
5	A	166	CYC	C1B-NB-C4B	-3.88	105.90	110.66
5	L	183	CYC	CBC-CAC-C3C	-3.86	105.22	113.41
6	L	179	PUB	C4A-NA-C1A	-3.85	107.50	113.42
5	K	166	CYC	O2A-CGA-O1A	-3.80	113.57	123.33
5	B	181	CYC	C3B-C4B-NB	3.79	109.79	106.77
5	A	168	CYC	C1B-NB-C4B	-3.74	106.07	110.66
5	A	166	CYC	O2A-CGA-O1A	-3.73	113.74	123.33
5	K	166	CYC	C1B-NB-C4B	-3.73	106.09	110.66
5	K	168	CYC	C1C-NC-C4C	-3.71	108.76	113.41
5	A	168	CYC	CAC-C3C-C4C	3.70	122.18	112.67
5	B	181	CYC	O2A-CGA-O1A	-3.65	113.94	123.33
5	A	168	CYC	O2A-CGA-O1A	-3.59	114.10	123.33
6	L	179	PUB	CBA-CAA-C3A	-3.57	107.48	112.93
5	B	181	CYC	C1B-NB-C4B	-3.57	106.28	110.66
5	B	183	CYC	O2A-CGA-O1A	-3.57	114.15	123.33
5	L	183	CYC	O2A-CGA-O1A	-3.51	114.31	123.33
5	K	166	CYC	CBC-CAC-C3C	-3.50	105.99	113.41
5	K	166	CYC	CMB-C2B-C1B	3.50	128.41	124.16
5	K	168	CYC	CBC-CAC-C3C	-3.48	106.02	113.41
5	B	183	CYC	CBC-CAC-C3C	-3.46	106.07	113.41
5	K	168	CYC	O2A-CGA-O1A	-3.46	114.44	123.33
5	L	183	CYC	C1B-NB-C4B	-3.41	106.48	110.66
6	B	179	PUB	O2B-CGB-O1B	-3.41	114.57	123.33
5	K	166	CYC	OC-C1C-C2C	-3.40	123.47	126.17
5	L	181	CYC	CMB-C2B-C1B	3.37	128.26	124.16
5	L	181	CYC	O2A-CGA-CBA	3.36	124.62	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	168	CYC	CMB-C2B-C1B	3.36	128.24	124.16
5	L	181	CYC	CBC-CAC-C3C	-3.33	106.35	113.41
5	B	181	CYC	CBC-CAC-C3C	-3.31	106.39	113.41
5	K	166	CYC	CAC-C3C-C4C	3.31	121.16	112.67
5	A	166	CYC	CBC-CAC-C3C	-3.30	106.41	113.41
5	K	168	CYC	C1B-NB-C4B	-3.29	106.62	110.66
5	B	181	CYC	CMB-C2B-C1B	3.28	128.15	124.16
5	A	166	CYC	CMC-C2C-C3C	3.28	126.66	113.98
6	B	179	PUB	CBA-CAA-C3A	-3.27	107.94	112.93
5	L	181	CYC	O2A-CGA-O1A	-3.27	114.92	123.33
5	A	168	CYC	CMC-C2C-C3C	3.27	126.63	113.98
5	B	183	CYC	C1B-NB-C4B	-3.24	106.69	110.66
5	A	168	CYC	CBC-CAC-C3C	-3.21	106.60	113.41
5	B	183	CYC	C3C-C4C-NC	-3.19	103.84	107.94
5	A	166	CYC	CMB-C2B-C1B	3.17	128.01	124.16
5	A	168	CYC	O2A-CGA-CBA	3.13	123.89	114.00
5	K	168	CYC	CMC-C2C-C3C	3.12	126.06	113.98
6	L	179	PUB	O2B-CGB-O1B	-3.11	115.33	123.33
5	L	181	CYC	CMC-C2C-C3C	3.06	125.82	113.98
5	B	183	CYC	O2A-CGA-CBA	3.01	123.52	114.00
5	B	181	CYC	CHA-C4D-C3D	-3.01	120.75	127.22
5	K	168	CYC	O2A-CGA-CBA	2.97	123.39	114.00
5	L	183	CYC	C3C-C4C-NC	-2.97	104.11	107.94
5	L	181	CYC	C3C-C4C-NC	-2.95	104.15	107.94
5	A	166	CYC	CHD-C1D-C2D	2.90	134.63	127.53
5	B	183	CYC	CBB-CAB-C3B	2.89	120.25	112.42
5	L	183	CYC	CBB-CAB-C3B	2.88	120.23	112.42
5	A	166	CYC	CHD-C4C-NC	2.87	129.21	125.63
5	L	183	CYC	O2A-CGA-CBA	2.82	122.91	114.00
5	B	183	CYC	CMB-C2B-C1B	2.80	127.56	124.16
5	L	183	CYC	CMC-C2C-C3C	2.79	124.77	113.98
5	B	181	CYC	O2A-CGA-CBA	2.79	122.81	114.00
5	A	166	CYC	O2A-CGA-CBA	2.78	122.80	114.00
5	A	166	CYC	C3C-C4C-NC	-2.78	104.36	107.94
5	B	181	CYC	C3C-C4C-NC	-2.77	104.37	107.94
5	B	181	CYC	CMC-C2C-C3C	2.76	124.66	113.98
5	K	166	CYC	CBB-CAB-C3B	2.74	119.85	112.42
5	A	166	CYC	CBB-CAB-C3B	2.73	119.83	112.42
5	L	181	CYC	CBB-CAB-C3B	2.73	119.83	112.42
5	L	181	CYC	CAA-CBA-CGA	2.71	120.86	113.67
5	A	168	CYC	C3C-C4C-NC	-2.65	104.53	107.94
5	K	166	CYC	O2A-CGA-CBA	2.64	122.34	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	179	PUB	OD-C4D-ND	-2.62	122.42	126.02
5	A	166	CYC	CHB-C4A-NA	-2.61	119.33	124.95
5	B	181	CYC	CBB-CAB-C3B	2.59	119.45	112.42
5	K	168	CYC	CBB-CAB-C3B	2.58	119.43	112.42
5	K	166	CYC	CHD-C1D-ND	-2.56	119.50	125.29
5	K	166	CYC	CMC-C2C-C3C	2.54	123.81	113.98
5	K	168	CYC	CAA-CBA-CGA	2.49	120.28	113.67
5	B	183	CYC	CHB-C4A-NA	-2.48	119.60	124.95
5	B	181	CYC	CHB-C4A-NA	-2.48	119.60	124.95
5	A	166	CYC	C1C-NC-C4C	-2.43	110.35	113.41
5	K	166	CYC	C1C-NC-C4C	-2.43	110.35	113.41
5	K	166	CYC	CHD-C1D-C2D	2.43	133.49	127.53
5	A	168	CYC	CAA-CBA-CGA	2.42	120.09	113.67
5	A	168	CYC	CHD-C1D-ND	-2.42	119.82	125.29
5	L	181	CYC	CHD-C1D-ND	-2.42	119.83	125.29
5	B	181	CYC	CHB-C1B-NB	-2.41	120.92	126.06
5	B	183	CYC	CMC-C2C-C3C	2.40	123.25	113.98
5	L	181	CYC	OC-C1C-C2C	-2.39	124.27	126.17
5	L	183	CYC	CHA-C4D-C3D	-2.38	122.11	127.22
5	L	183	CYC	CMB-C2B-C1B	2.38	127.05	124.16
5	K	166	CYC	CHD-C4C-NC	2.38	128.60	125.63
5	A	168	CYC	CBB-CAB-C3B	2.32	118.71	112.42
5	K	168	CYC	C3C-C4C-NC	-2.30	104.98	107.94
5	K	166	CYC	C3C-C4C-NC	-2.30	104.98	107.94
6	B	179	PUB	O2C-CGC-CBC	2.30	121.25	114.00
5	K	166	CYC	C4D-ND-C1D	-2.29	105.76	109.78
5	A	166	CYC	CHD-C1D-ND	-2.28	120.15	125.29
5	B	181	CYC	C4D-ND-C1D	-2.26	105.81	109.78
5	K	166	CYC	CMD-C2D-C1D	2.25	128.89	125.62
6	L	179	PUB	O2C-CGC-CBC	2.25	121.11	114.00
5	K	166	CYC	CHB-C1B-NB	-2.23	121.30	126.06
5	A	166	CYC	C2D-C1D-ND	-2.21	104.41	107.43
5	A	166	CYC	C4D-ND-C1D	-2.21	105.90	109.78
5	B	183	CYC	CHB-C1B-NB	-2.21	121.35	126.06
5	A	166	CYC	OC-C1C-C2C	-2.21	124.42	126.17
5	L	181	CYC	CHB-C4A-NA	-2.20	120.19	124.95
5	B	181	CYC	CMD-C2D-C1D	2.20	128.81	125.62
5	L	181	CYC	CMD-C2D-C1D	2.19	128.80	125.62
5	B	181	CYC	OC-C1C-C2C	-2.17	124.44	126.17
5	A	166	CYC	CHB-C4A-C3A	2.17	130.45	124.87
5	K	168	CYC	CHB-C4A-NA	-2.16	120.28	124.95
5	A	168	CYC	CHB-C4A-NA	-2.16	120.29	124.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	166	CYC	CHB-C1B-NB	-2.16	121.46	126.06
6	B	179	PUB	CHA-C1B-NB	2.15	123.98	121.10
5	L	183	CYC	C2C-C1C-NC	2.12	110.05	108.29
5	L	181	CYC	CHA-C4D-C3D	-2.11	122.68	127.22
6	B	179	PUB	C2B-C1B-NB	2.11	110.02	108.31
5	K	166	CYC	CHB-C4A-NA	-2.10	120.42	124.95
5	B	181	CYC	CHD-C1D-C2D	2.06	132.57	127.53
5	B	181	CYC	CAA-CBA-CGA	2.05	119.11	113.67
5	L	181	CYC	CHB-C4A-C3A	2.05	130.14	124.87
5	K	166	CYC	CMA-C3A-C4A	2.05	128.28	125.10
5	K	166	CYC	CHA-C4D-C3D	-2.05	122.82	127.22
6	L	179	PUB	CMB-C2B-C1B	-2.04	124.78	126.97
5	L	181	CYC	CHD-C1D-C2D	2.03	132.51	127.53
5	L	181	CYC	CHB-C1B-NB	-2.02	121.75	126.06
5	B	181	CYC	CHD-C1D-ND	-2.01	120.74	125.29
6	L	179	PUB	OA-C1A-NA	-2.01	123.25	126.02
6	B	179	PUB	OD-C4D-ND	-2.01	123.26	126.02
5	B	183	CYC	C4D-ND-C1D	-2.01	106.26	109.78

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	168	CYC	C2C
5	K	168	CYC	C2C

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	166	CYC	NA-C4A-CHB-C1B
5	A	166	CYC	C3A-C4A-CHB-C1B
5	A	168	CYC	NA-C4A-CHB-C1B
5	A	168	CYC	C3A-C4A-CHB-C1B
5	A	168	CYC	C2C-C3C-CAC-CBC
5	A	168	CYC	C4C-C3C-CAC-CBC
5	A	168	CYC	C2D-C1D-CHD-C4C
5	A	168	CYC	C2D-C3D-CAD-CBD
5	B	181	CYC	NA-C4A-CHB-C1B
5	B	181	CYC	C3A-C4A-CHB-C1B
5	B	181	CYC	C2C-C3C-CAC-CBC
5	B	181	CYC	C4C-C3C-CAC-CBC
5	B	183	CYC	NA-C4A-CHB-C1B
5	B	183	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
5	B	183	CYC	NC-C4C-CHD-C1D
5	K	166	CYC	NA-C4A-CHB-C1B
5	K	166	CYC	C3A-C4A-CHB-C1B
5	K	166	CYC	C4B-C3B-CAB-CBB
5	K	166	CYC	NC-C4C-CHD-C1D
5	K	166	CYC	C3C-C4C-CHD-C1D
5	K	166	CYC	ND-C1D-CHD-C4C
5	K	168	CYC	NA-C4A-CHB-C1B
5	K	168	CYC	C3A-C4A-CHB-C1B
5	K	168	CYC	C2C-C3C-CAC-CBC
5	K	168	CYC	C4C-C3C-CAC-CBC
5	K	168	CYC	C3C-C4C-CHD-C1D
5	K	168	CYC	C2D-C3D-CAD-CBD
5	L	181	CYC	NA-C4A-CHB-C1B
5	L	181	CYC	C3A-C4A-CHB-C1B
5	L	181	CYC	C2C-C3C-CAC-CBC
5	L	181	CYC	C4C-C3C-CAC-CBC
5	L	183	CYC	NA-C4A-CHB-C1B
5	L	183	CYC	C3A-C4A-CHB-C1B
5	L	183	CYC	NC-C4C-CHD-C1D
5	L	183	CYC	C3C-C4C-CHD-C1D
6	B	179	PUB	ND-C1D-CHC-C4C
6	B	179	PUB	C4D-C3D-CAD-CBD
6	B	179	PUB	NA-C4A-CHA-C1B
6	L	179	PUB	ND-C1D-CHC-C4C
6	L	179	PUB	C4D-C3D-CAD-CBD
6	L	179	PUB	NA-C4A-CHA-C1B
5	K	166	CYC	C2B-C3B-CAB-CBB
6	L	179	PUB	C2D-C3D-CAD-CBD
5	A	166	CYC	C2B-C3B-CAB-CBB
5	L	181	CYC	C2B-C3B-CAB-CBB
5	L	183	CYC	C2B-C3B-CAB-CBB
6	B	179	PUB	C2D-C3D-CAD-CBD
5	B	181	CYC	C2B-C3B-CAB-CBB
5	B	183	CYC	C2B-C3B-CAB-CBB
5	A	166	CYC	ND-C1D-CHD-C4C
5	K	166	CYC	C2D-C1D-CHD-C4C
5	L	183	CYC	C2D-C1D-CHD-C4C
5	B	181	CYC	C2A-CAA-CBA-CGA
5	L	181	CYC	C2A-CAA-CBA-CGA
6	L	179	PUB	C3B-CAB-CBB-CGB
5	A	168	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
5	B	181	CYC	ND-C1D-CHD-C4C
5	B	183	CYC	ND-C1D-CHD-C4C
5	K	168	CYC	ND-C1D-CHD-C4C
5	L	181	CYC	ND-C1D-CHD-C4C
5	L	183	CYC	ND-C1D-CHD-C4C
5	A	166	CYC	C2D-C1D-CHD-C4C
5	B	181	CYC	C2D-C1D-CHD-C4C
5	B	183	CYC	C2D-C1D-CHD-C4C
5	K	168	CYC	C2D-C1D-CHD-C4C
5	L	181	CYC	C2D-C1D-CHD-C4C
5	A	166	CYC	C4B-C3B-CAB-CBB
5	B	183	CYC	C4B-C3B-CAB-CBB
5	L	183	CYC	C4B-C3B-CAB-CBB
5	B	181	CYC	NB-C1B-CHB-C4A
5	B	183	CYC	C2A-CAA-CBA-CGA
5	L	183	CYC	C2A-CAA-CBA-CGA
6	B	179	PUB	C3B-CAB-CBB-CGB
5	B	183	CYC	NB-C1B-CHB-C4A
5	L	181	CYC	NB-C1B-CHB-C4A
5	L	183	CYC	NB-C1B-CHB-C4A
5	A	168	CYC	C3D-CAD-CBD-CGD
5	K	168	CYC	C3D-CAD-CBD-CGD
6	B	179	PUB	C1C-C2C-CAC-CBC
5	B	183	CYC	C4D-C3D-CAD-CBD
6	L	179	PUB	C2C-C1C-CHB-C4B
5	A	168	CYC	NA-C1A-CHA-C4D
5	B	183	CYC	C4C-C3C-CAC-CBC
5	L	183	CYC	C4C-C3C-CAC-CBC
5	L	183	CYC	C2C-C3C-CAC-CBC
5	A	168	CYC	C2A-CAA-CBA-CGA
5	K	168	CYC	NA-C1A-CHA-C4D
5	L	183	CYC	C2D-C3D-CAD-CBD
5	B	183	CYC	CAA-CBA-CGA-O1A
5	B	181	CYC	CAA-CBA-CGA-O1A
6	L	179	PUB	CAB-CBB-CGB-O1B
5	A	166	CYC	CAA-CBA-CGA-O2A
5	L	181	CYC	CAD-CBD-CGD-O1D
5	L	183	CYC	CAA-CBA-CGA-O1A
6	L	179	PUB	CAB-CBB-CGB-O2B
5	A	168	CYC	CAA-CBA-CGA-O2A
5	K	168	CYC	CAA-CBA-CGA-O1A
5	B	183	CYC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	K	168	CYC	CAA-CBA-CGA-O2A
5	L	181	CYC	CAA-CBA-CGA-O2A
6	B	179	PUB	CAB-CBB-CGB-O2B
5	B	181	CYC	CAD-CBD-CGD-O2D
6	B	179	PUB	CAB-CBB-CGB-O1B
5	A	168	CYC	CAA-CBA-CGA-O1A
5	B	181	CYC	CAD-CBD-CGD-O1D
5	K	166	CYC	CAA-CBA-CGA-O2A
5	B	183	CYC	CAA-CBA-CGA-O2A
5	L	181	CYC	CAD-CBD-CGD-O2D
5	L	181	CYC	CAA-CBA-CGA-O1A
5	B	181	CYC	CAA-CBA-CGA-O2A
5	B	183	CYC	C1A-C2A-CAA-CBA
5	A	166	CYC	CAA-CBA-CGA-O1A
5	K	166	CYC	CAA-CBA-CGA-O1A
5	L	183	CYC	CAA-CBA-CGA-O2A
5	K	168	CYC	C4D-C3D-CAD-CBD
6	B	179	PUB	CAC-CBC-CGC-O1C
5	L	181	CYC	NA-C1A-CHA-C4D
6	L	179	PUB	CAC-CBC-CGC-O2C
5	L	181	CYC	C3D-C4D-CHA-C1A
5	K	166	CYC	C2A-C1A-CHA-C4D

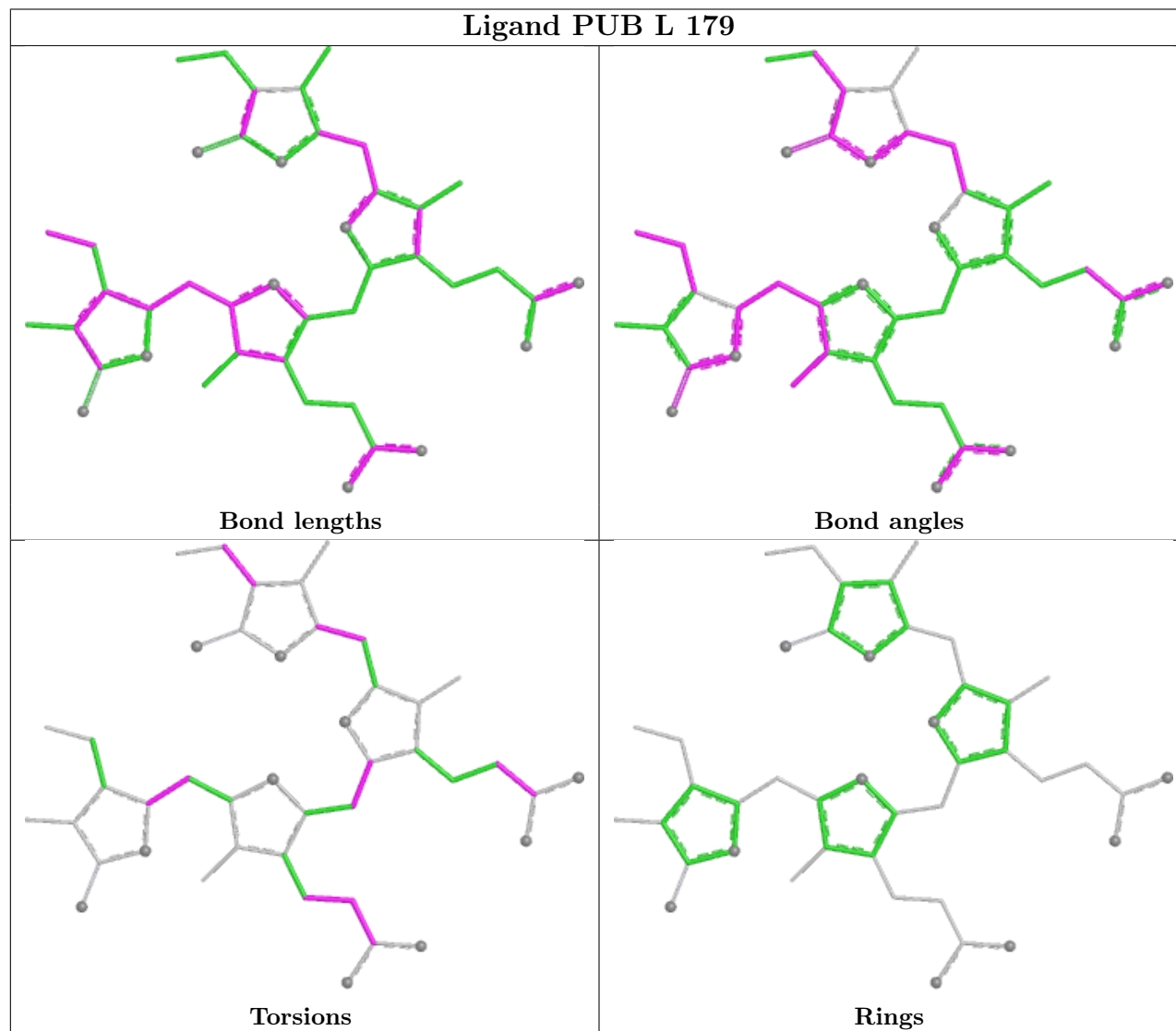
There are no ring outliers.

10 monomers are involved in 54 short contacts:

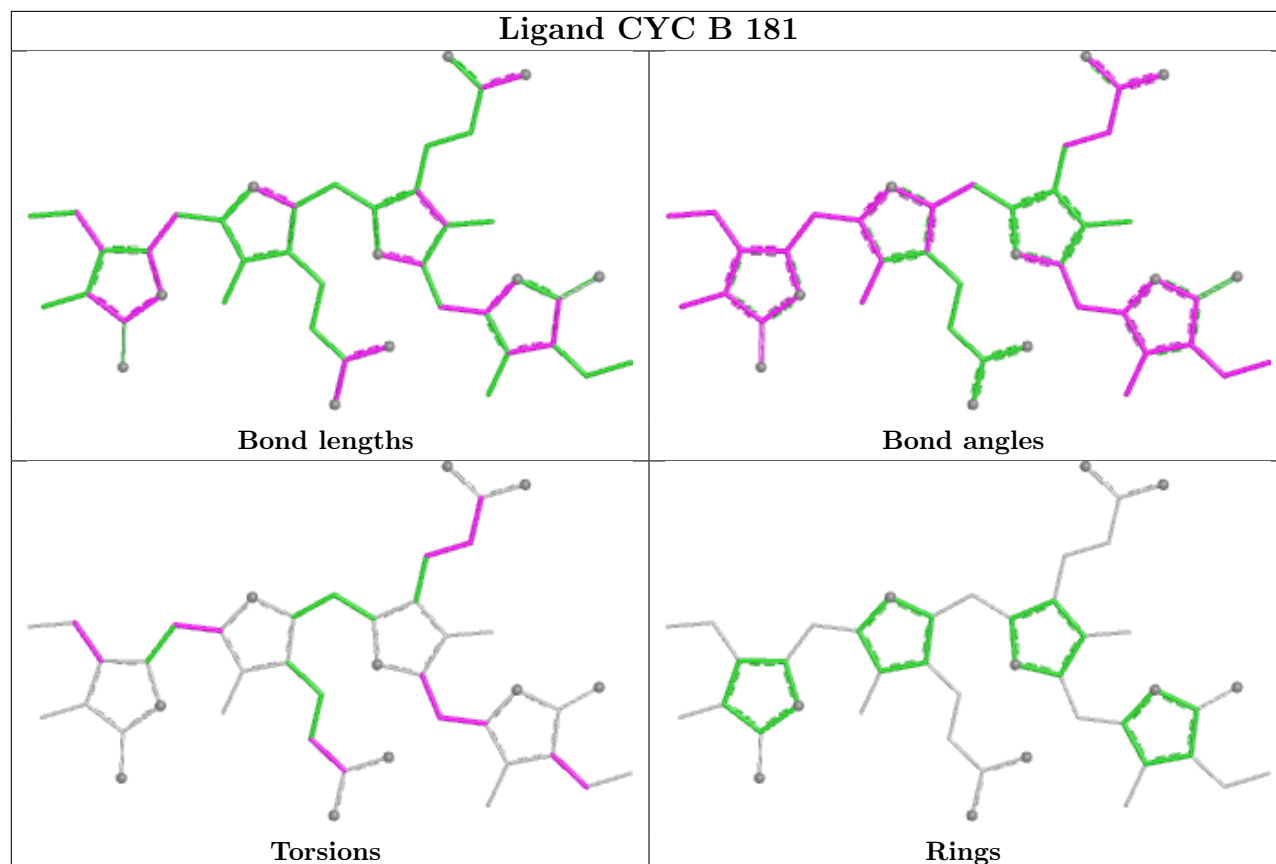
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	179	PUB	2	0
5	B	181	CYC	4	0
5	A	168	CYC	7	0
5	K	166	CYC	4	0
5	L	181	CYC	8	0
5	L	183	CYC	10	0
6	B	179	PUB	3	0
5	A	166	CYC	3	0
5	K	168	CYC	2	0
5	B	183	CYC	11	0

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

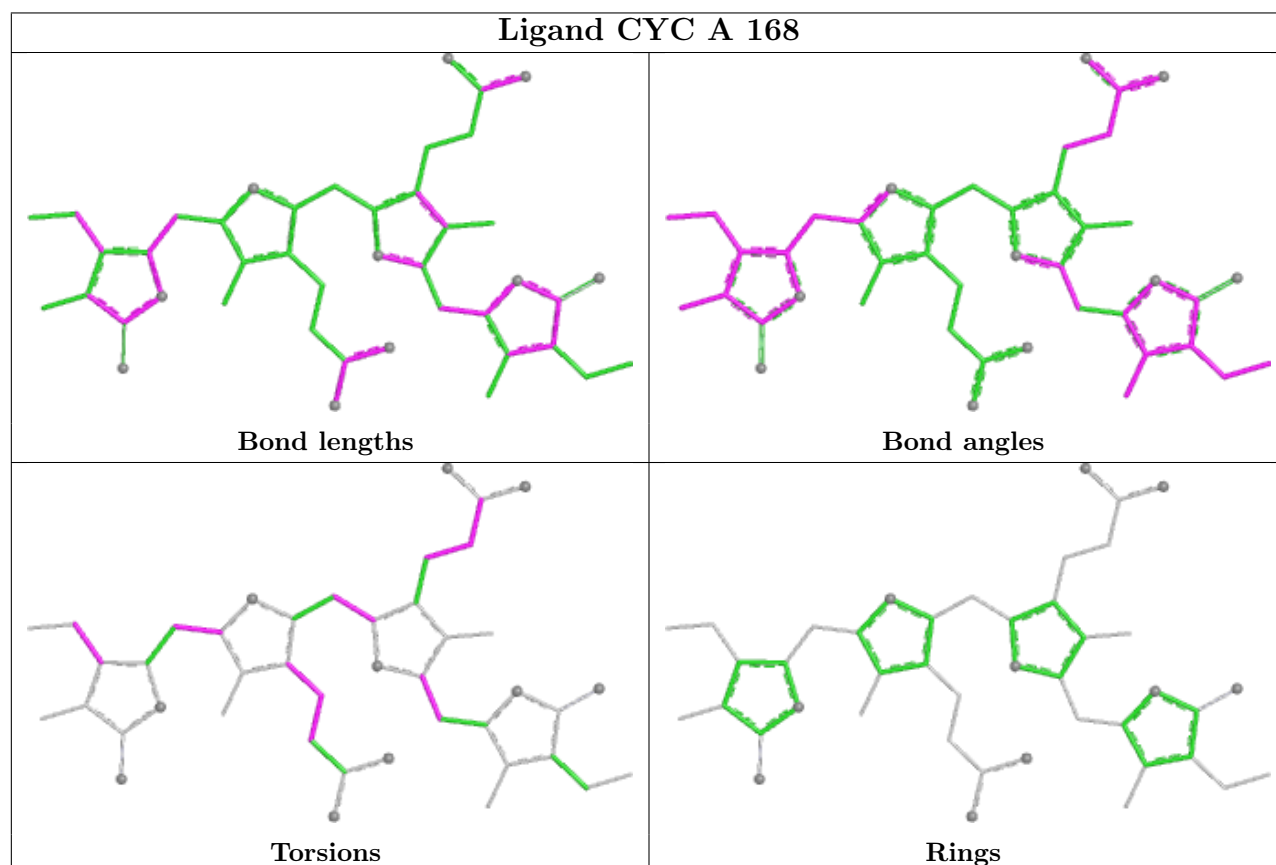
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

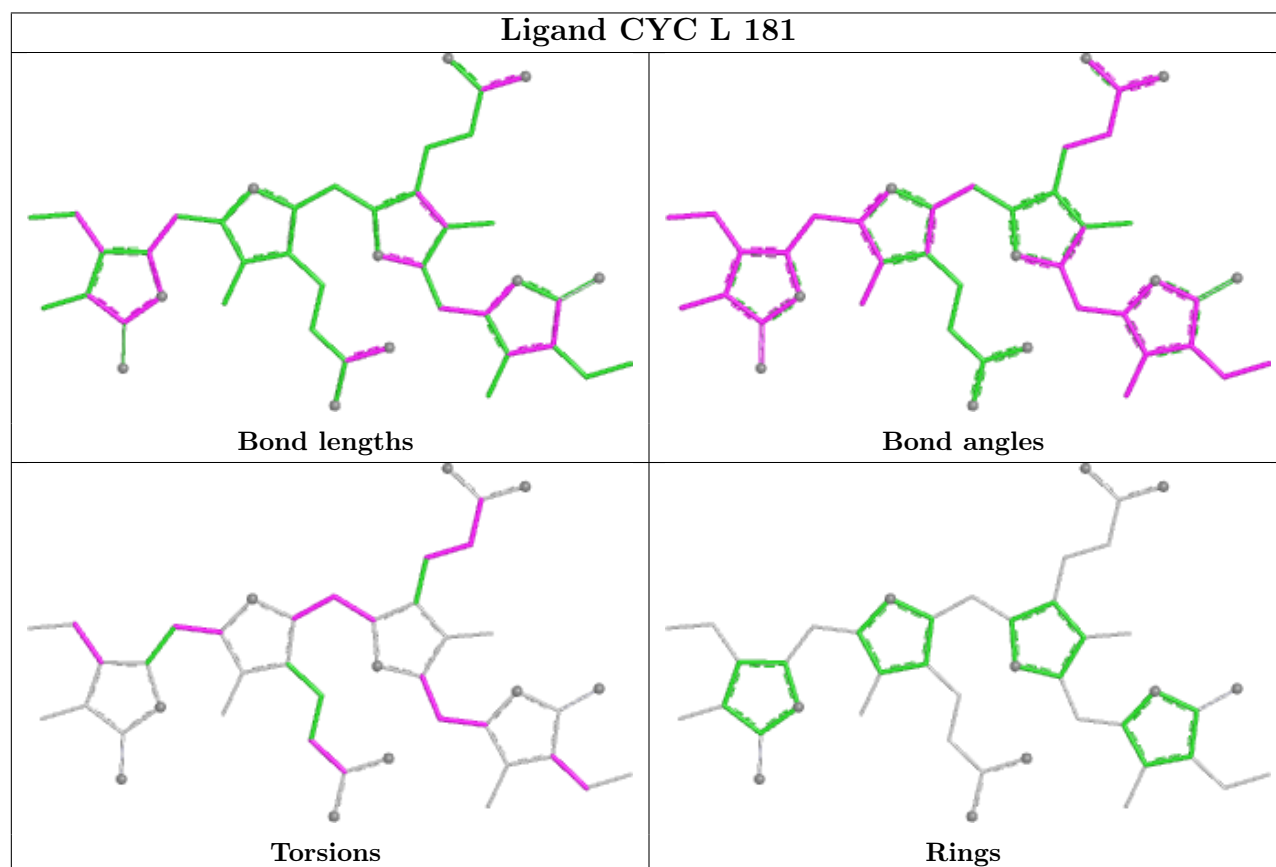
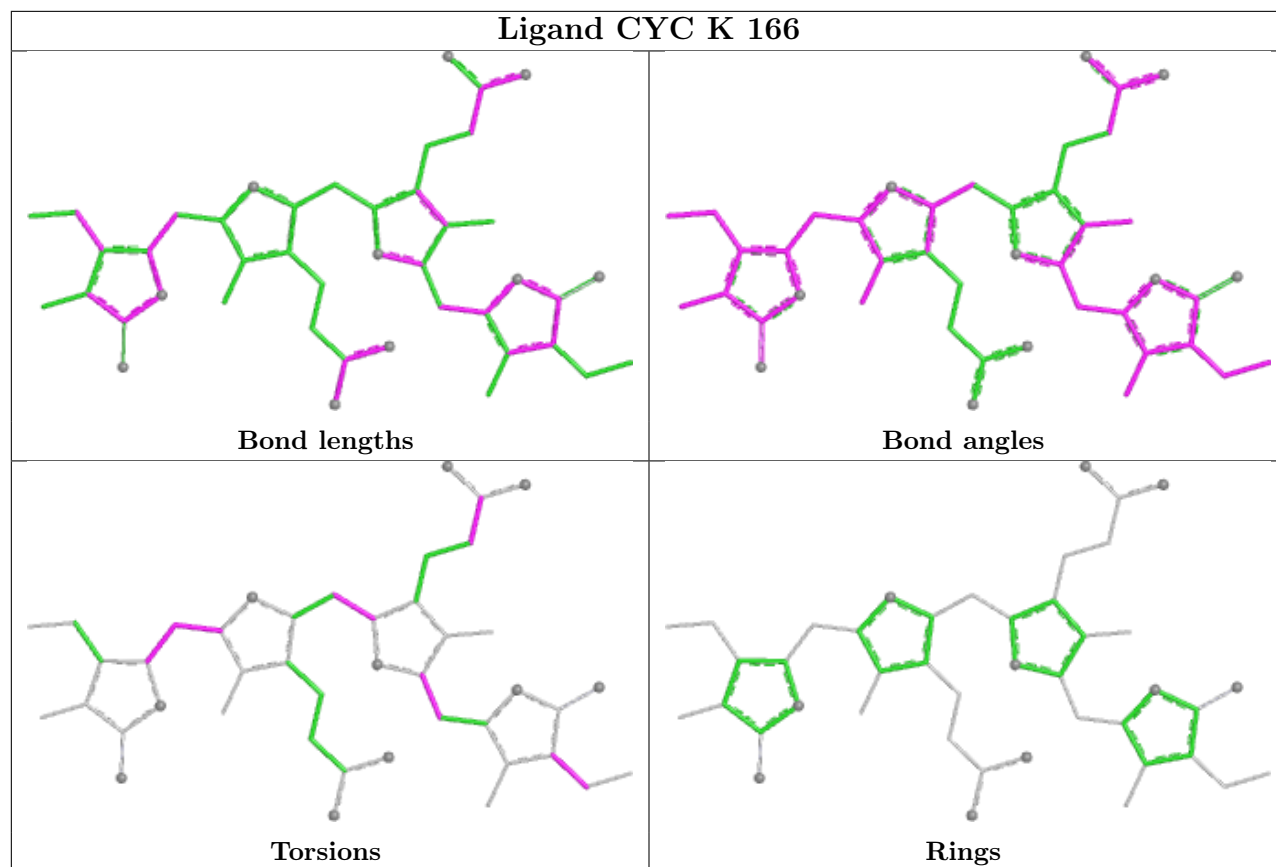


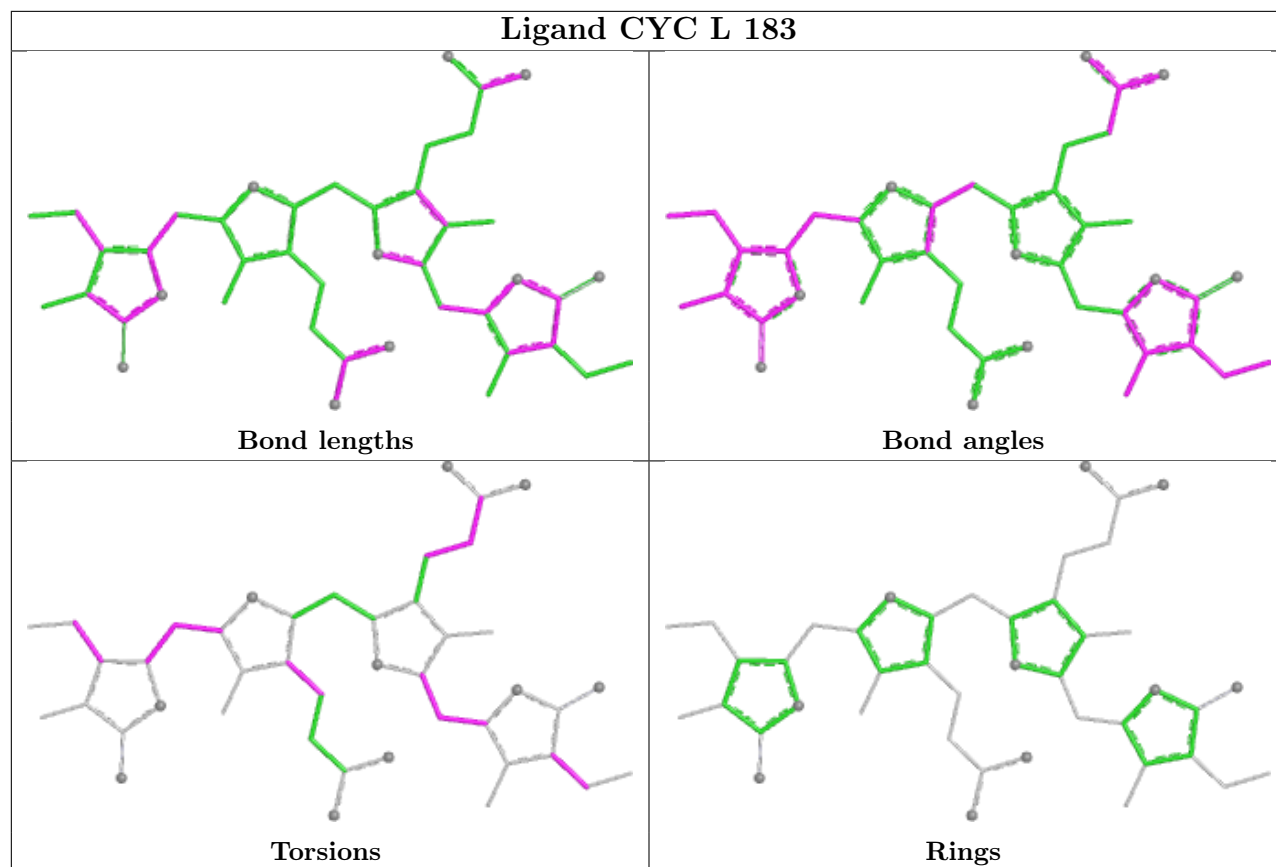
Ligand CYC B 181

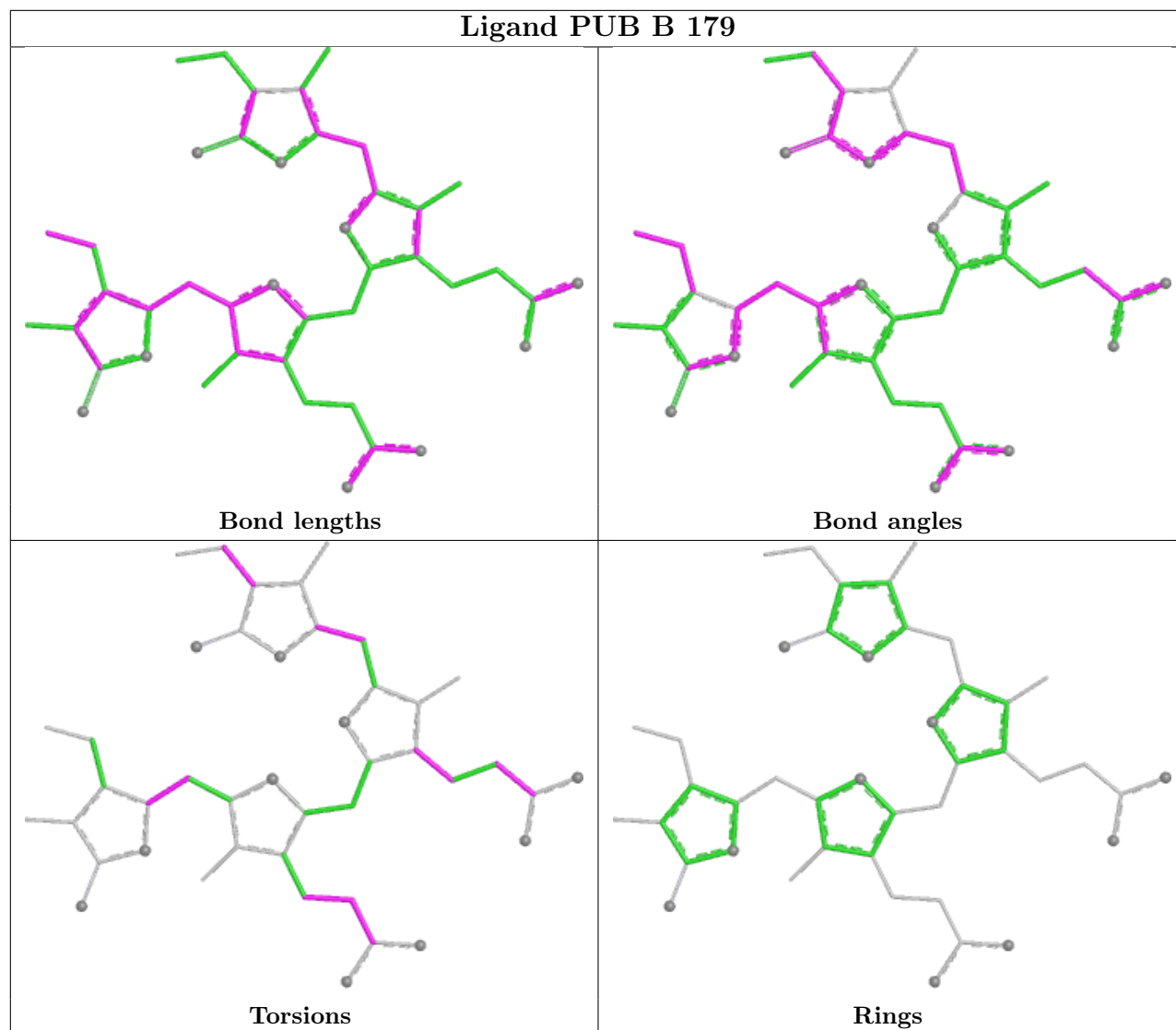


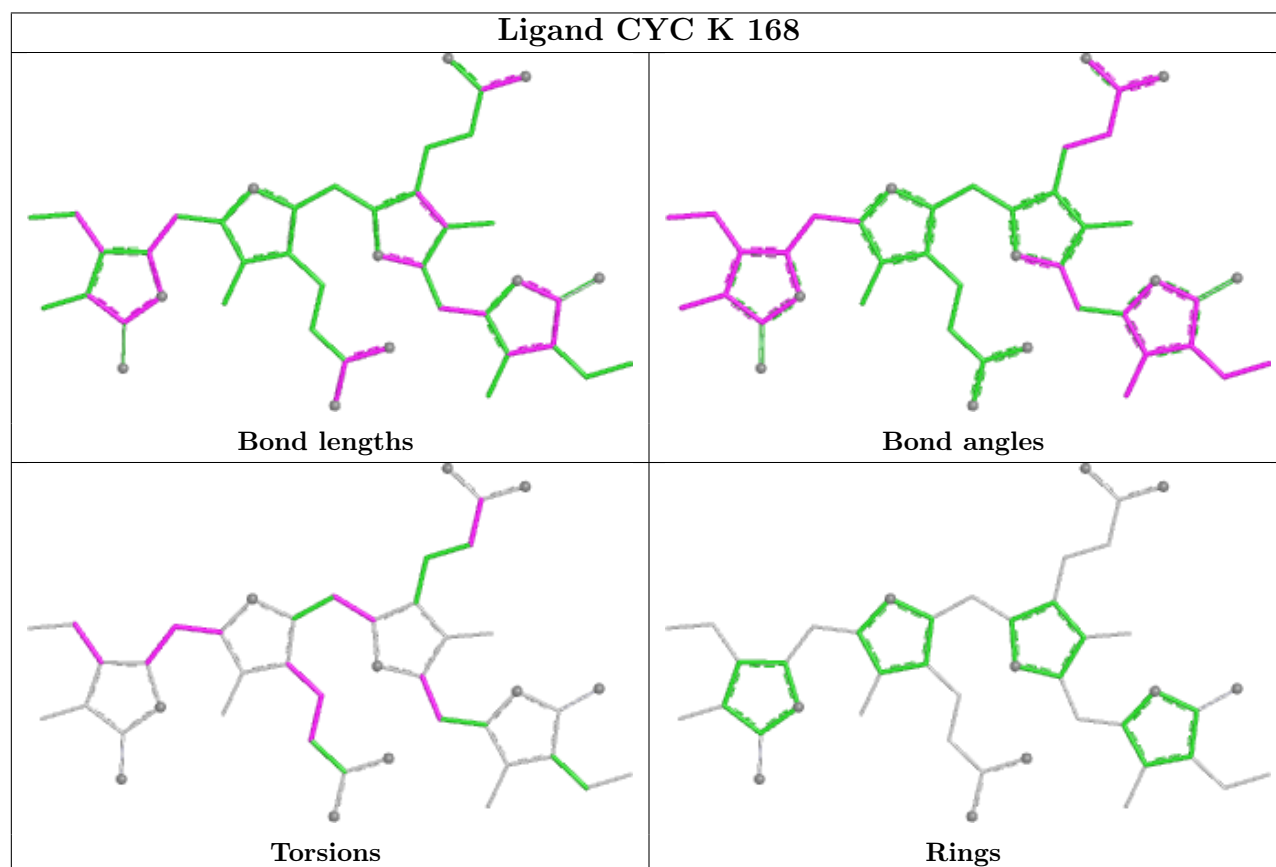
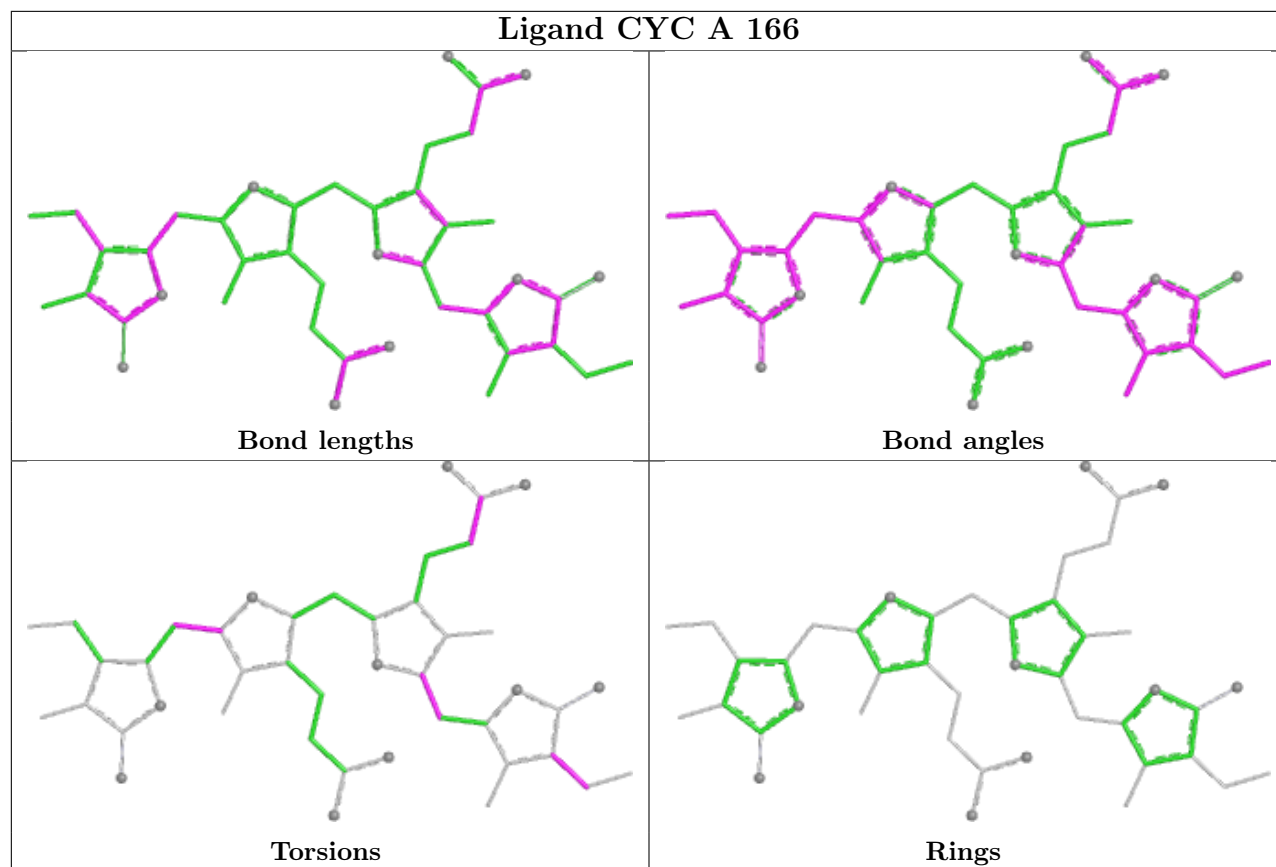
Ligand CYC A 168

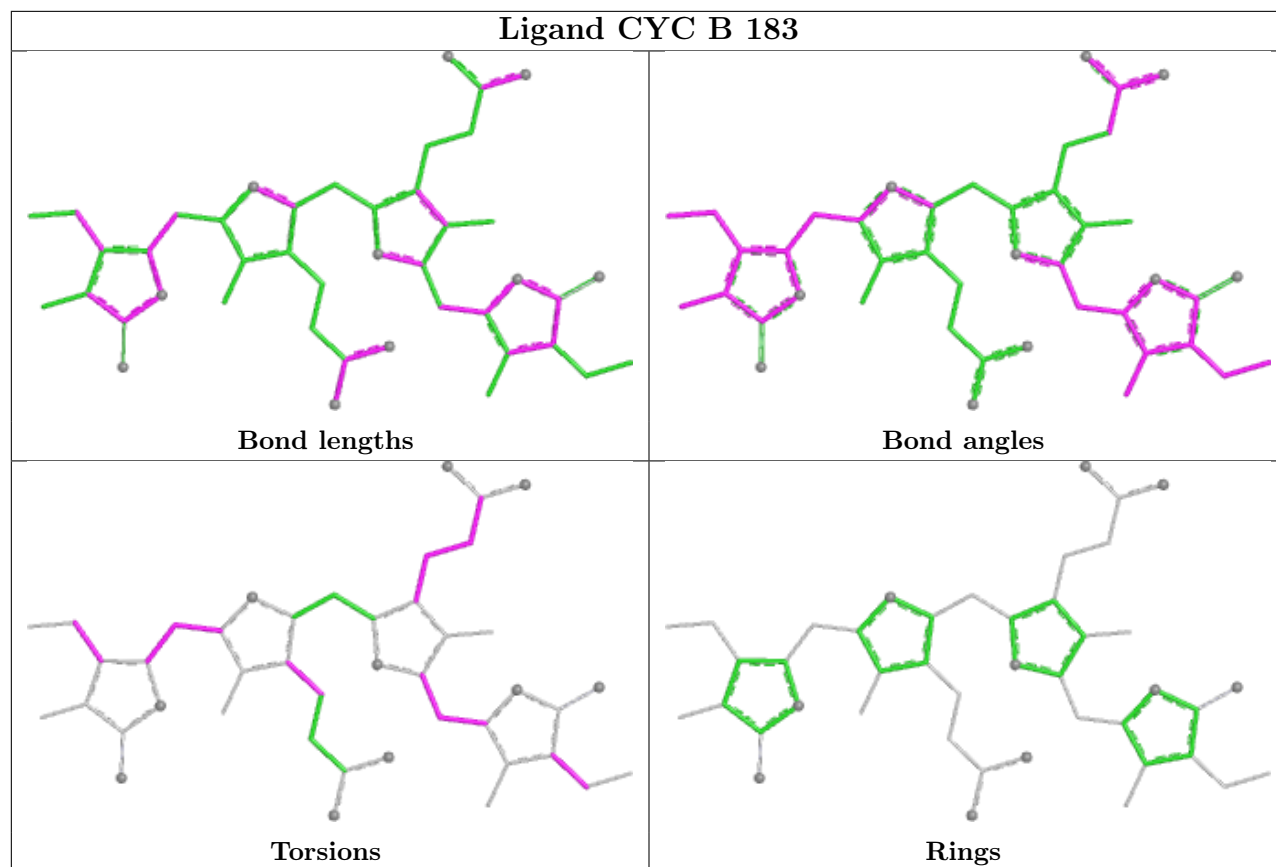












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	164/164 (100%)	-1.46	0 100 100	7, 20, 36, 53	0
1	K	164/164 (100%)	-1.45	0 100 100	7, 20, 36, 53	0
2	B	176/177 (99%)	-1.40	0 100 100	10, 20, 42, 62	5 (2%)
2	L	176/177 (99%)	-1.38	0 100 100	10, 20, 42, 87	4 (2%)
3	G	6/6 (100%)	0.46	1 (16%) 4 3	5, 9, 11, 23	6 (100%)
3	H	5/6 (83%)	1.79	1 (20%) 3 2	1, 6, 14, 28	4 (80%)
All	All	691/694 (99%)	-1.38	2 (0%) 90 90	1, 20, 40, 87	19 (2%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	4	ALA	8.0
3	G	1	ALA	2.3

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	B	72	9/10	0.99	0.05	0,9,27,29	0
2	MEN	L	72	9/10	0.99	0.03	0,9,27,27	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

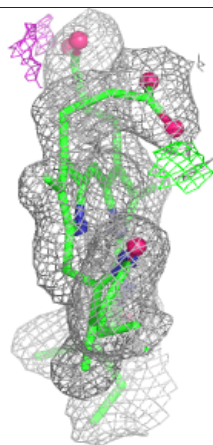
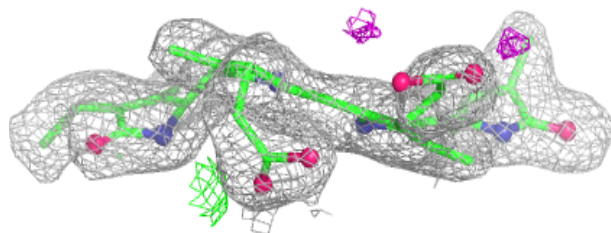
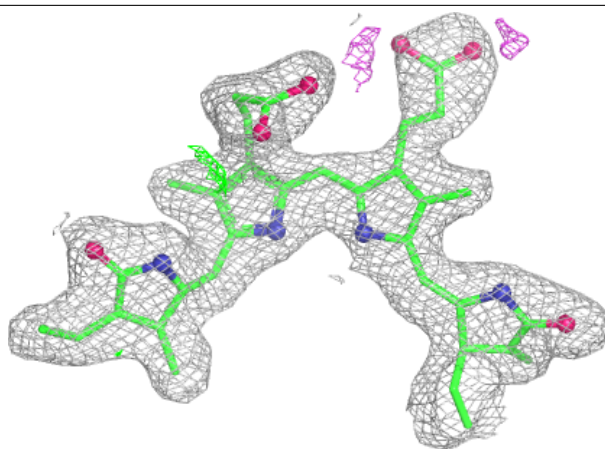
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	201	5/5	0.98	0.06	22,23,27,42	5
4	SO4	B	202	5/5	0.99	0.04	12,23,36,55	5
5	CYC	A	166	43/43	0.99	0.03	3,19,30,57	0
5	CYC	A	168	43/43	0.99	0.04	15,31,57,62	0
5	CYC	B	181	43/43	0.99	0.03	7,14,32,37	0
5	CYC	B	183	43/43	0.99	0.03	4,20,37,57	0
5	CYC	K	166	43/43	0.99	0.03	3,18,30,57	0
5	CYC	K	168	43/43	0.99	0.04	15,32,57,62	0
5	CYC	L	181	43/43	0.99	0.03	6,14,32,37	0
5	CYC	L	183	43/43	0.99	0.04	3,20,36,57	0
6	PUB	B	179	43/43	0.99	0.04	5,25,39,60	0
6	PUB	L	179	43/43	0.99	0.04	4,24,39,60	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.

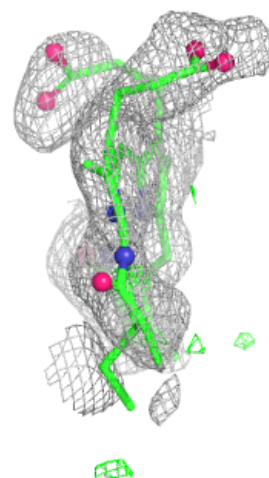
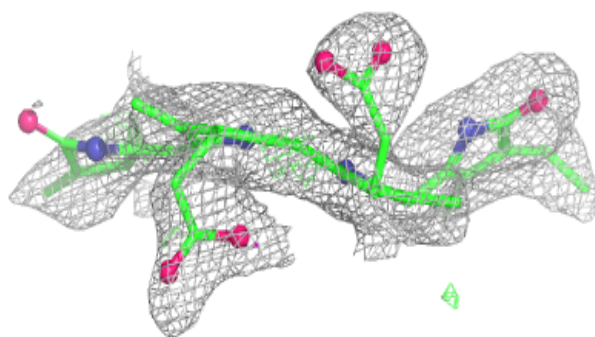
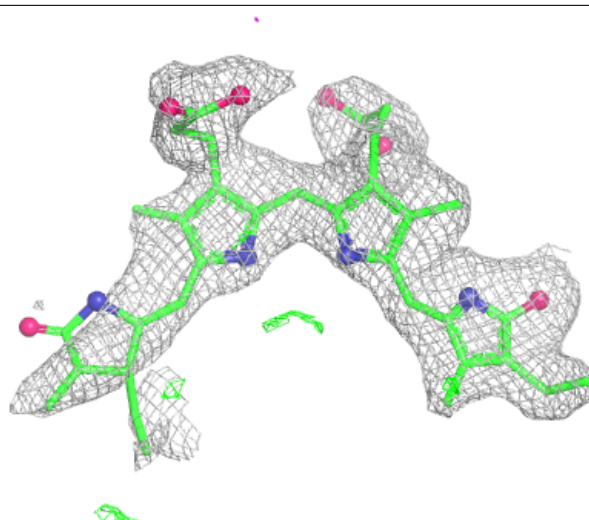
Electron density around CYC A 166:

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



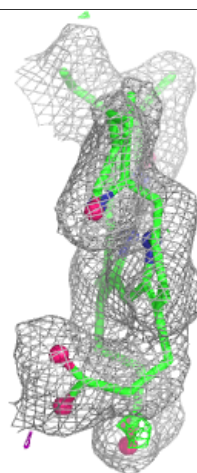
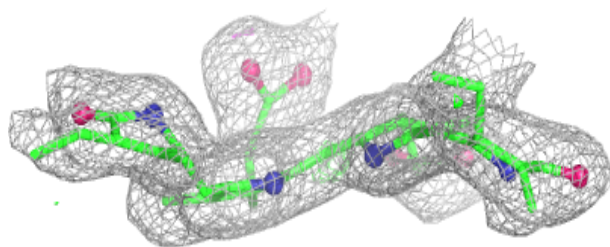
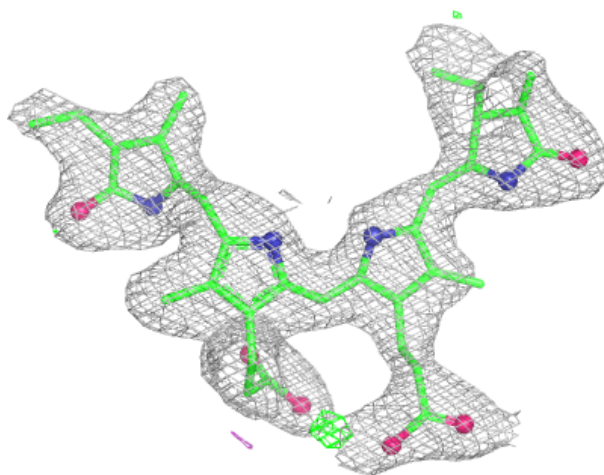
Electron density around CYC A 168:

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



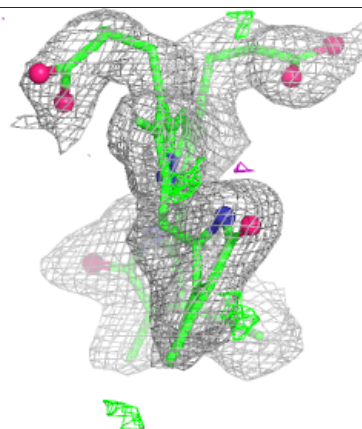
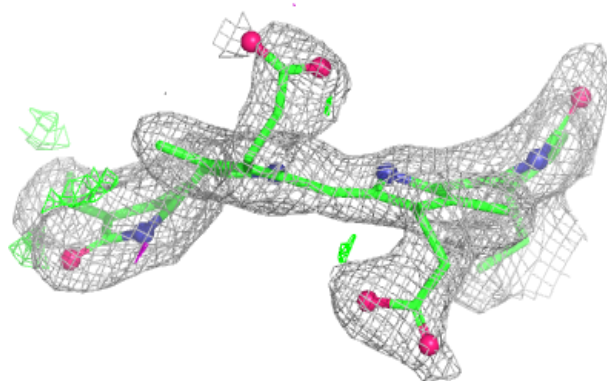
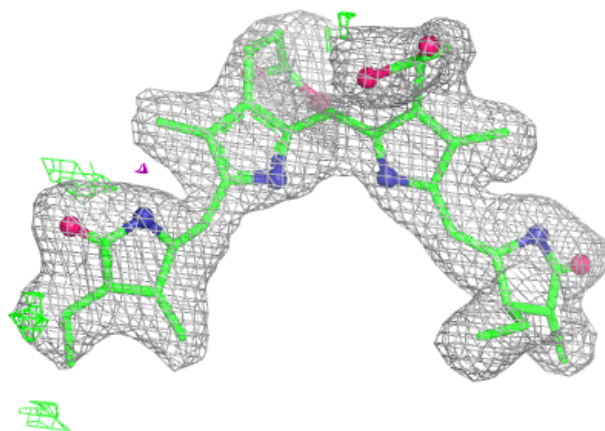
Electron density around CYC B 181:

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and green (positive)



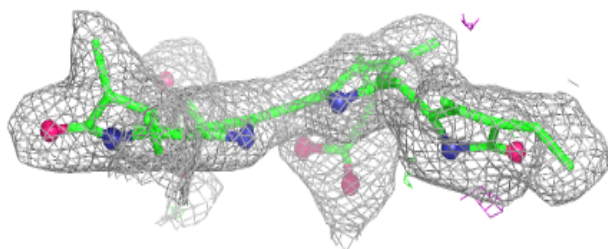
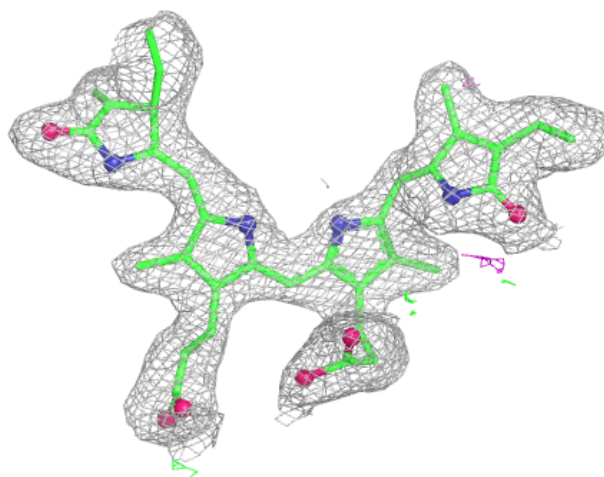
Electron density around CYC B 183:

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and green (positive)



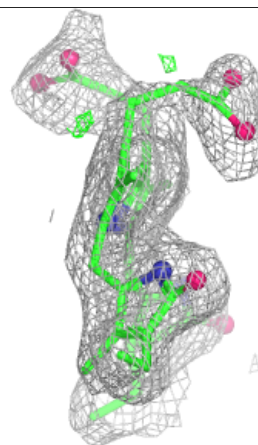
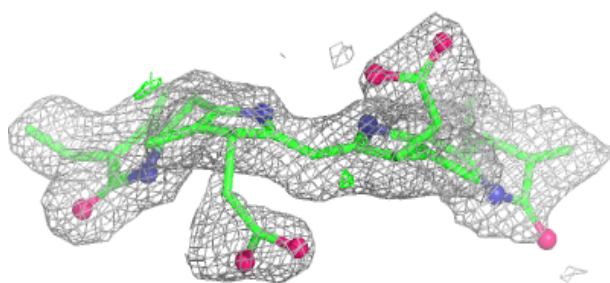
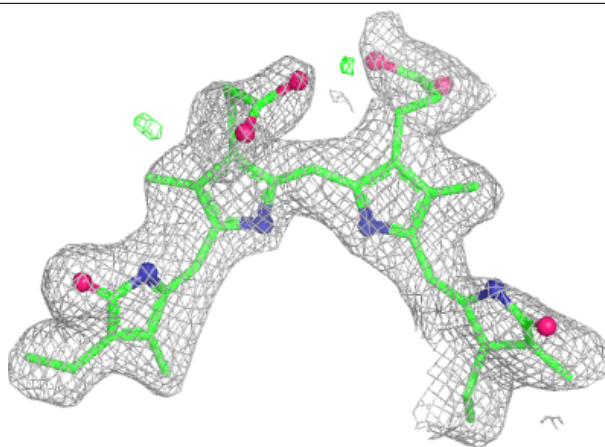
Electron density around CYC K 166:

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and green (positive)



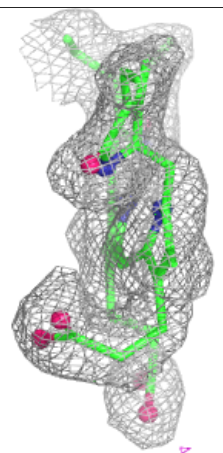
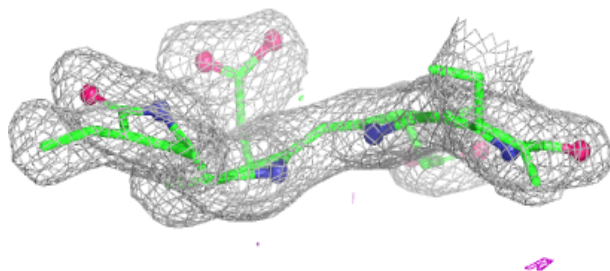
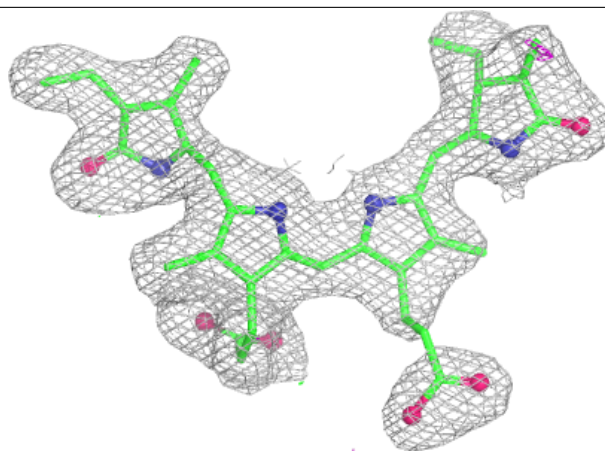
Electron density around CYC K 168:

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and green (positive)



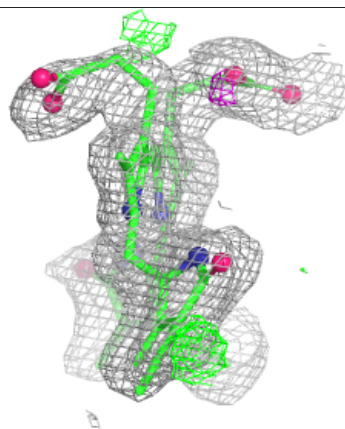
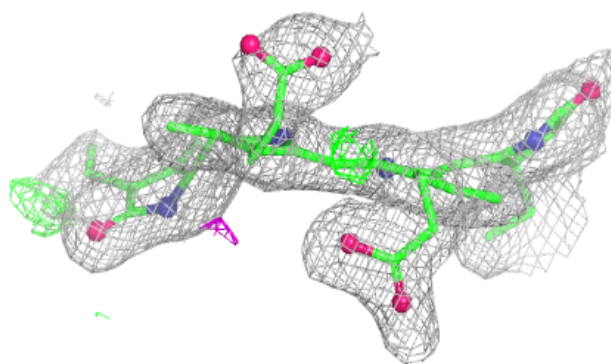
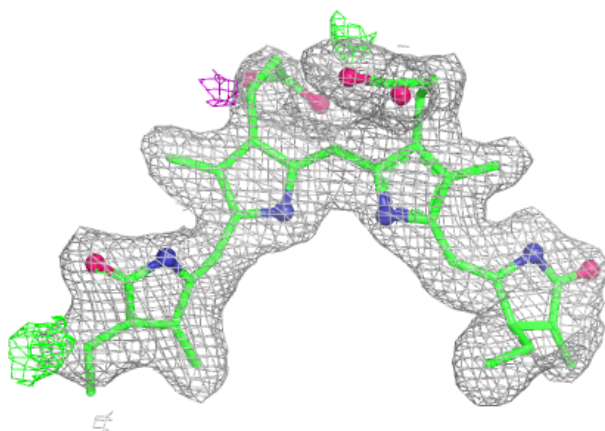
Electron density around CYC L 181:

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



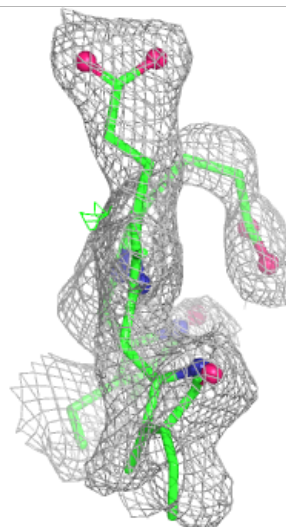
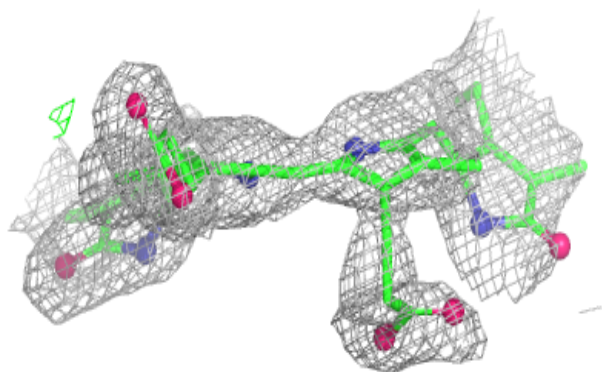
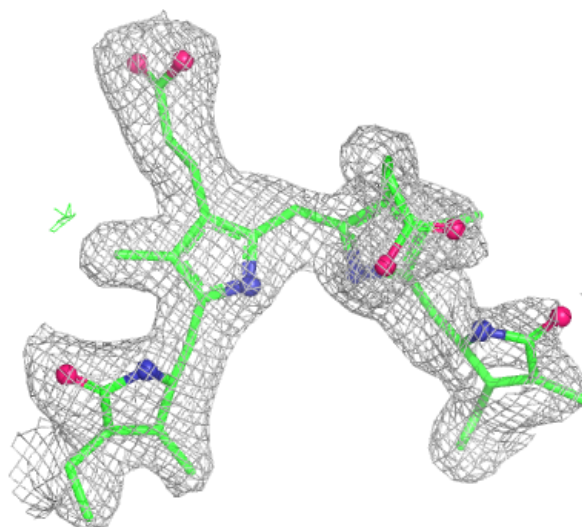
Electron density around CYC L 183:

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



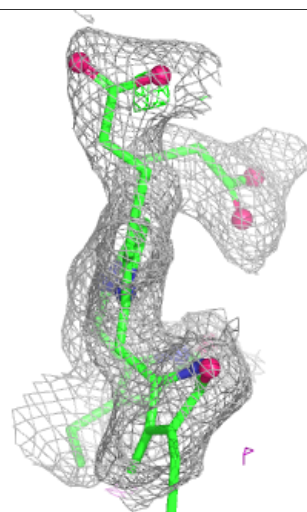
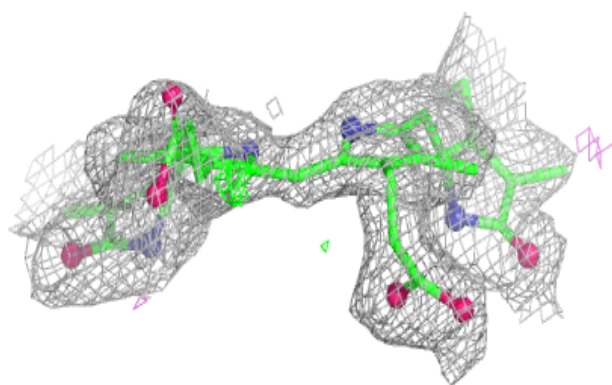
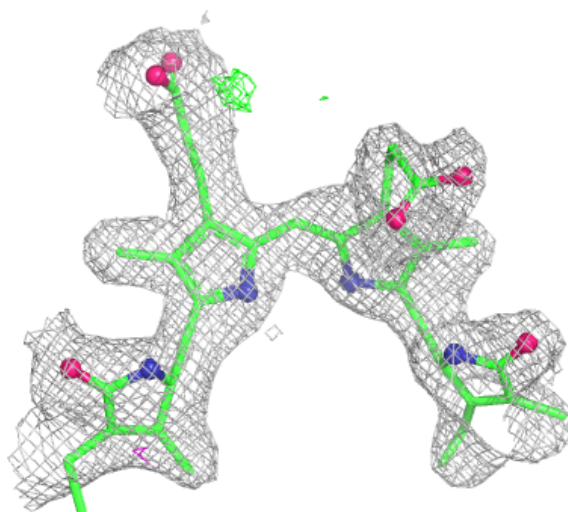
Electron density around PUB B 179:

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



Electron density around PUB L 179:

$2mF_o-DF_c$ (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.