Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 05:33 AM EDT

PDB ID	:	1B8D
Title	:	CRYSTAL STRUCTURE OF A PHYCOUROBILIN-CONTAINING PHYCOERYTHRIN
Authors	:	Ritter, S.; Hiller, R.G.; Wrench, P.M.; Welte, W.; Diederichs, K.
Deposited on	:	1999-01-29
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

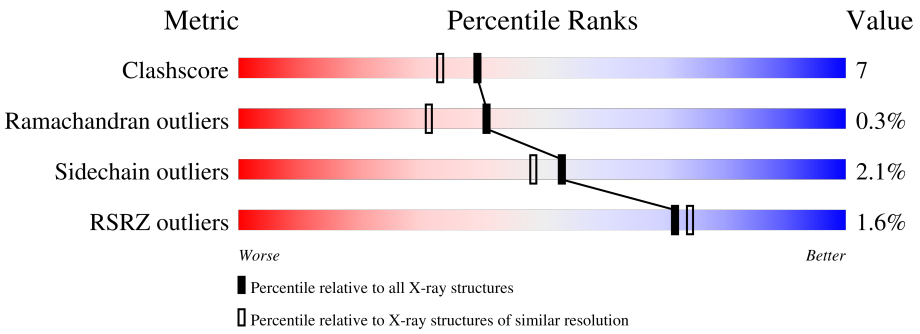
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	.% 82% 17% •
1	K	164	.% 86% 14%
2	B	177	2% 91% 9%
2	L	177	2% 88% 11% •
3	G	6	17% 83% 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7734 atoms, of which 1879 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 PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (ALPHA CHAIN)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	164	1530	771	290	217	245	7	290	0	0
1	K	164	1530	771	290	217	245	7	290	0	0

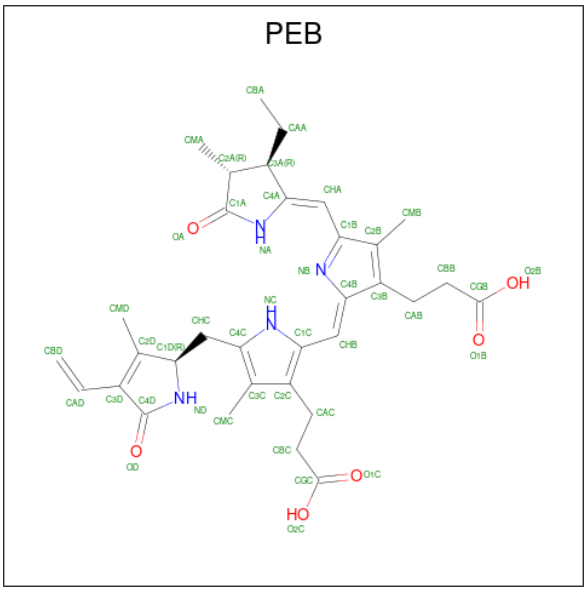
- Molecule 2 is a protein called PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (BETA CHAIN)).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	177	1590	797	299	223	261	10	299	0	0
2	L	177	1590	797	299	223	261	10	299	0	0

- Molecule 3 is a protein called PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (GAMMA CHAIN)).

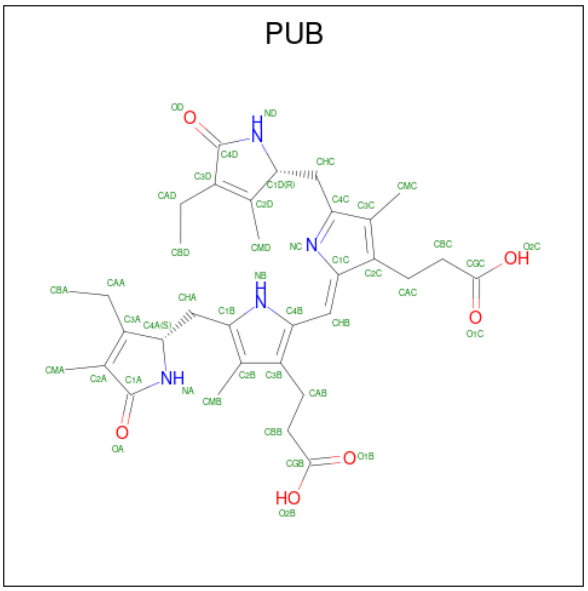
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	G	5	35	20	5	5	5	5	0	2

- Molecule 4 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	A	1	46	33	3	4	6	3	0
			Total	C	H	N	O		
4	A	1	46	33	3	4	6	3	0
			Total	C	H	N	O		
4	B	1	46	33	3	4	6	3	0
			Total	C	H	N	O		
4	B	1	46	33	3	4	6	3	0
			Total	C	H	N	O		
4	K	1	46	33	3	4	6	3	0
			Total	C	H	N	O		
4	K	1	46	33	3	4	6	3	0
			Total	C	H	N	O		
4	L	1	46	33	3	4	6	3	0
			Total	C	H	N	O		
4	L	1	46	33	3	4	6	3	0

- Molecule 5 is PHYCOUROBILIN (three-letter code: PUB) (formula: $C_{33}H_{42}N_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
5	B	1	46	33	3	4	6	3	0
			Total	C	H	N	O		
5	L	1	46	33	3	4	6	3	0

- Molecule 6 is water.

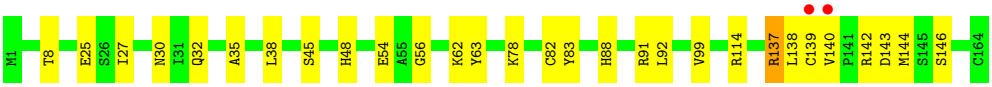
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
6	A	80	240	160	80	160	0
			Total	H	O		
6	B	74	222	148	74	148	0
			Total	H	O		
6	K	80	240	160	80	160	0
			Total	H	O		
6	L	99	297	198	99	198	0

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.

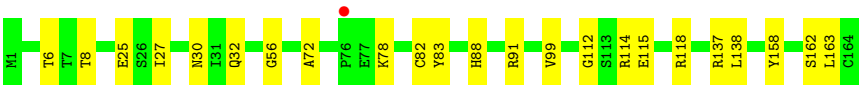
• Molecule 1: PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (ALPHA CHAIN))

Chain A:



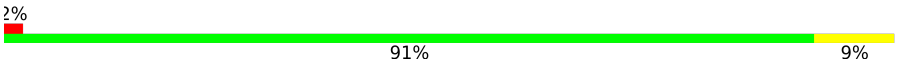
• Molecule 1: PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (ALPHA CHAIN))

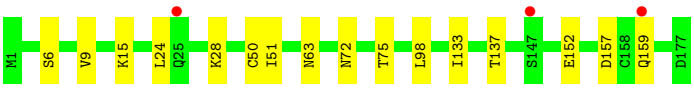
Chain K:



• Molecule 2: PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (BETA CHAIN))

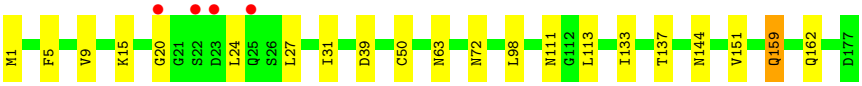
Chain B:





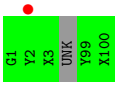
• Molecule 2: PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (BETA CHAIN))

Chain L:



• Molecule 3: PROTEIN (RHODOPHYTAN PHYCOERYTHRIN (GAMMA CHAIN))

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	187.35Å 187.35Å 59.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 1.90 31.53 – 1.82	Depositor EDS
% Data completeness (in resolution range)	97.0 (100.00-1.90) 73.9 (31.53-1.82)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.175 , 0.227 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.8	EDS
L-test for twinning[1]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.004 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7734	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ 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, PUB, PEB

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	0.46	0/1261	0.63	0/1704
1	K	0.46	0/1261	0.61	0/1704
2	B	0.46	0/1294	0.63	0/1748
2	L	0.46	0/1294	0.63	0/1748
3	G	0.89	0/28	0.86	0/35
All	All	0.46	0/5138	0.62	0/6939

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	1240	290	1211	26	0
1	K	1240	290	1211	21	0
2	B	1291	299	1286	15	0
2	L	1291	299	1286	19	0
3	G	30	5	22	0	0
4	A	86	6	74	7	0
4	B	86	6	74	6	0
4	K	86	6	74	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	86	6	74	7	0
5	B	43	3	38	4	0
5	L	43	3	38	2	0
6	A	80	160	0	3	0
6	B	74	148	0	1	0
6	K	80	160	0	2	0
6	L	99	198	0	3	0
All	All	5855	1879	5388	81	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 7.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLN:HG3	1:K:32:GLN:HG3	1.48	0.93
2:B:137:THR:HG21	6:B:364:HOH:O	1.82	0.79
1:A:88:HIS:CD2	1:A:91:ARG:HH21	2.04	0.75
4:B:203:PEB:HNA	4:B:203:PEB:HMB2	1.52	0.73
2:L:137:THR:HG21	6:L:401:HOH:O	1.88	0.73
1:A:140:VAL:HG11	1:A:146:SER:HA	1.72	0.72
1:A:32:GLN:CG	1:K:32:GLN:HG3	2.21	0.71
2:L:137:THR:HG22	5:L:210:PUB:C4B	2.21	0.70
2:B:137:THR:HG22	5:B:205:PUB:C4B	2.22	0.69
4:L:209:PEB:HBC2	6:L:525:HOH:O	1.95	0.67
1:A:32:GLN:HG3	1:K:32:GLN:CG	2.23	0.64
2:L:133:ILE:O	2:L:137:THR:HG23	1.98	0.64
1:A:38:LEU:HD22	2:B:24:LEU:HD22	1.84	0.60
2:L:1:MET:SD	6:L:597:HOH:O	2.56	0.60
1:A:88:HIS:HD2	1:A:91:ARG:HH21	1.48	0.59
2:B:133:ILE:O	2:B:137:THR:HG23	2.02	0.58
1:K:88:HIS:CD2	1:K:91:ARG:HH21	2.21	0.58
2:L:159:GLN:HE21	2:L:159:GLN:HA	1.69	0.57
4:A:202:PEB:HMB2	4:A:202:PEB:NA	2.20	0.57
2:L:144:ASN:HD21	2:L:151:VAL:H	1.52	0.57
1:A:27:ILE:O	1:A:30:ASN:HB2	2.05	0.56
1:A:82:CYS:HA	4:A:201:PEB:HHA1	1.88	0.56
2:B:157:ASP:OD1	2:B:159:GLN:HG2	2.06	0.55
2:B:137:THR:HG22	5:B:205:PUB:NB	2.22	0.54
1:K:27:ILE:HD12	2:L:98:LEU:HD11	1.89	0.54
1:A:54:GLU:OE1	1:A:137:ARG:HD3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:208:PEB:HMB2	4:L:208:PEB:HNA	1.72	0.53
2:L:137:THR:HG22	5:L:210:PUB:NB	2.23	0.53
4:B:204:PEB:HMB2	4:B:204:PEB:NA	2.24	0.52
1:A:62:LYS:HD3	1:A:63:TYR:CE2	2.45	0.52
2:B:72:MEN:HB2	4:B:203:PEB:OA	2.09	0.51
1:A:56:GLY:HA3	1:A:83:TYR:CE2	2.46	0.50
2:B:51:ILE:HG23	2:B:137:THR:OG1	2.12	0.50
1:A:139:CYS:HB2	4:A:202:PEB:HHA1	1.92	0.50
1:A:25:GLU:OE2	1:K:30:ASN:HA	2.12	0.49
1:A:27:ILE:HD13	2:B:98:LEU:HD11	1.95	0.48
1:K:137:ARG:HG3	4:K:207:PEB:HHC1	1.94	0.48
1:K:82:CYS:HA	4:K:206:PEB:HHA1	1.94	0.48
1:K:56:GLY:HA3	1:K:83:TYR:CE2	2.48	0.48
1:A:45:SER:O	1:A:48:HIS:HD2	1.97	0.48
1:A:114:ARG:HH11	1:A:114:ARG:HB3	1.79	0.48
1:K:114:ARG:HB3	1:K:114:ARG:NH1	2.28	0.48
1:K:138:LEU:HA	4:K:207:PEB:HMD2	1.97	0.47
1:A:30:ASN:HA	1:K:25:GLU:OE2	2.15	0.47
1:K:114:ARG:HB3	1:K:114:ARG:HH11	1.80	0.47
4:B:204:PEB:OD	4:B:204:PEB:HBD1	2.14	0.46
1:A:88:HIS:HE1	6:A:406:HOH:O	1.98	0.46
2:B:15:LYS:HE3	2:B:15:LYS:HB2	1.58	0.46
1:K:6:THR:HG22	2:L:1:MET:HG3	1.98	0.46
1:A:140:VAL:HG13	1:A:144:MET:O	2.16	0.46
1:A:88:HIS:O	1:A:92:LEU:HG	2.16	0.46
1:K:158:TYR:HA	6:K:574:HOH:O	2.15	0.45
1:K:118:ARG:NH1	6:K:535:HOH:O	2.48	0.45
1:K:99:VAL:HG23	2:L:9:VAL:HG21	1.99	0.44
2:L:113:LEU:CD1	4:L:208:PEB:HMD3	2.47	0.44
2:B:137:THR:HG22	5:B:205:PUB:C1B	2.48	0.44
4:B:203:PEB:HBD1	4:B:203:PEB:OD	2.18	0.44
1:K:162:SER:OG	1:K:163:LEU:HD22	2.18	0.44
2:L:5:PHE:CZ	2:L:31:ILE:HD11	2.53	0.44
2:L:15:LYS:HE3	2:L:15:LYS:HB2	1.81	0.44
1:A:78:LYS:HE3	4:A:201:PEB:O1B	2.18	0.44
4:A:202:PEB:HHC2	6:A:546:HOH:O	2.17	0.44
2:B:24:LEU:O	2:B:28:LYS:HG3	2.18	0.43
1:A:35:ALA:HB3	6:A:367:HOH:O	2.19	0.43
2:L:27:LEU:O	2:L:31:ILE:HG12	2.19	0.43
1:A:99:VAL:HG23	2:B:9:VAL:HG21	1.99	0.43
1:K:27:ILE:O	1:K:30:ASN:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:72:MEN:HB2	4:L:208:PEB:OA	2.19	0.42
2:L:20:GLY:HA2	2:L:24:LEU:HG	2.01	0.42
1:K:112:GLY:HA2	1:K:115:GLU:OE1	2.20	0.42
4:L:209:PEB:HHB1	4:L:209:PEB:HBC1	2.01	0.42
2:B:137:THR:HG22	5:B:205:PUB:C3B	2.51	0.41
2:L:159:GLN:HA	2:L:159:GLN:NE2	2.34	0.41
2:L:72:MEN:HE22	4:L:208:PEB:HBB2	2.03	0.41
1:K:72:ALA:O	1:K:78:LYS:HB3	2.20	0.41
4:A:202:PEB:HMA1	4:A:202:PEB:HBA2	2.03	0.41
4:B:204:PEB:HBA3	4:B:204:PEB:HHA1	2.02	0.41
1:A:137:ARG:HG2	4:A:202:PEB:HHC1	2.03	0.40
1:A:142:ARG:NH1	1:A:143:ASP:OD1	2.54	0.40
2:L:39:ASP:OD2	4:L:209:PEB:NB	2.54	0.40
2:B:6:SER:HA	2:B:9:VAL:HB	2.02	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%)	157 (97%)	5 (3%)	0	100	100
1	K	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
2	B	174/177 (98%)	169 (97%)	4 (2%)	1 (1%)	25	15
2	L	174/177 (98%)	169 (97%)	4 (2%)	1 (1%)	25	15
3	G	1/6 (17%)	1 (100%)	0	0	100	100
All	All	673/688 (98%)	655 (97%)	16 (2%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	111	ASN
2	B	75	THR

5.3.2 Protein sidechains (i)

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%)	126 (98%)	3 (2%)	50	45
1	K	129/129 (100%)	128 (99%)	1 (1%)	81	82
2	B	137/137 (100%)	134 (98%)	3 (2%)	52	47
2	L	137/137 (100%)	133 (97%)	4 (3%)	42	35
3	G	2/2 (100%)	2 (100%)	0	100	100
All	All	534/534 (100%)	523 (98%)	11 (2%)	53	48

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	137	ARG
1	A	138	LEU
2	B	50	CYS
2	B	63	ASN
2	B	152	GLU
1	K	8	THR
2	L	50	CYS
2	L	63	ASN
2	L	159	GLN
2	L	162	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	48	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	88	HIS
2	B	63	ASN
1	K	48	HIS
1	K	88	HIS
2	L	63	ASN
2	L	144	ASN
2	L	159	GLN
2	L	162	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	B	72	2	7,8,9	0.62	0	6,9,11	0.37	0
2	MEN	L	72	2	7,8,9	0.52	0	6,9,11	0.34	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	B	72	2	-	4/7/8/10	-
2	MEN	L	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	L	72	MEN	C-CA-CB-CG
2	B	72	MEN	N-CA-CB-CG
2	L	72	MEN	N-CA-CB-CG
2	L	72	MEN	CA-CB-CG-OD1
2	B	72	MEN	CA-CB-CG-OD1
2	B	72	MEN	C-CA-CB-CG
2	B	72	MEN	CA-CB-CG-ND2
2	L	72	MEN	CA-CB-CG-ND2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
4	PEB	B	203	2	43,46,46	1.58	6 (13%)	45,67,67	1.66	9 (20%)
4	PEB	A	201	1	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
4	PEB	K	207	1	43,46,46	2.00	9 (20%)	45,67,67	1.71	10 (22%)
5	PUB	B	205	2	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PEB	L	208	2	43,46,46	1.44	7 (16%)	45,67,67	1.69	10 (22%)
4	PEB	L	209	2	43,46,46	2.04	9 (20%)	45,67,67	1.47	6 (13%)
5	PUB	L	210	2	42,46,46	2.06	6 (14%)	37,67,67	2.53	7 (18%)
4	PEB	A	202	1	43,46,46	1.64	4 (9%)	45,67,67	1.16	2 (4%)
4	PEB	K	206	1	43,46,46	1.86	7 (16%)	45,67,67	1.60	8 (17%)
4	PEB	B	204	2	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)

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
4	PEB	B	203	2	-	6/24/74/74	0/4/4/4
4	PEB	A	201	1	-	8/24/74/74	0/4/4/4
4	PEB	K	207	1	-	7/24/74/74	0/4/4/4
5	PUB	B	205	2	-	7/24/74/74	0/4/4/4
4	PEB	L	208	2	-	5/24/74/74	0/4/4/4
4	PEB	L	209	2	-	11/24/74/74	0/4/4/4
5	PUB	L	210	2	-	5/24/74/74	0/4/4/4
4	PEB	A	202	1	-	8/24/74/74	0/4/4/4
4	PEB	K	206	1	-	6/24/74/74	0/4/4/4
4	PEB	B	204	2	-	7/24/74/74	0/4/4/4

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	205	PUB	C3A-C2A	10.46	1.46	1.34
5	L	210	PUB	C3A-C2A	9.95	1.45	1.34
4	B	204	PEB	C2D-C3D	9.30	1.46	1.34
4	K	207	PEB	C2D-C3D	8.02	1.44	1.34
4	A	202	PEB	C2D-C3D	7.50	1.44	1.34
4	K	206	PEB	C2D-C3D	7.44	1.44	1.34
4	L	209	PEB	C2D-C3D	7.39	1.44	1.34
4	A	201	PEB	C2D-C3D	6.69	1.43	1.34
4	B	203	PEB	C2D-C3D	6.22	1.42	1.34
4	K	206	PEB	C2A-C1A	-5.35	1.47	1.52
4	L	209	PEB	C4D-ND	5.24	1.42	1.35
4	L	208	PEB	C2D-C3D	4.96	1.41	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	PEB	C2A-C1A	-4.86	1.47	1.52
5	B	205	PUB	C4D-ND	4.70	1.41	1.35
4	K	207	PEB	C2A-C1A	-4.44	1.48	1.52
5	B	205	PUB	C1C-C2C	-4.33	1.38	1.45
5	L	210	PUB	C4D-ND	4.04	1.40	1.35
4	L	209	PEB	C3B-C2B	3.87	1.44	1.36
4	K	207	PEB	C4D-ND	3.83	1.40	1.35
4	B	204	PEB	C2A-C1A	-3.76	1.48	1.52
4	L	209	PEB	CAD-C3D	-3.66	1.37	1.47
4	L	209	PEB	C3C-C4C	3.65	1.47	1.42
5	L	210	PUB	C1C-C2C	-3.44	1.40	1.45
4	B	203	PEB	CAD-C3D	-3.43	1.38	1.47
4	L	209	PEB	C2A-C1A	-3.41	1.49	1.52
4	A	201	PEB	C4D-ND	3.40	1.39	1.35
4	K	207	PEB	CMD-C2D	3.37	1.55	1.50
4	B	204	PEB	CAD-C3D	-3.32	1.38	1.47
4	B	203	PEB	C4D-ND	3.29	1.39	1.35
4	A	201	PEB	CAD-C3D	-3.17	1.38	1.47
4	A	202	PEB	CAD-C3D	-3.10	1.39	1.47
4	K	207	PEB	CAD-C3D	-3.10	1.39	1.47
5	L	210	PUB	C4D-C3D	-3.08	1.42	1.48
4	L	208	PEB	CAD-C3D	-3.01	1.39	1.47
4	K	206	PEB	CAD-C3D	-2.98	1.39	1.47
4	B	204	PEB	C3C-C4C	2.94	1.46	1.42
5	B	205	PUB	CHC-C1D	2.87	1.59	1.53
4	B	204	PEB	C4D-ND	2.82	1.38	1.35
5	L	210	PUB	C1A-NA	2.81	1.38	1.35
4	K	206	PEB	C3C-C4C	2.78	1.46	1.42
4	K	207	PEB	C3A-C4A	2.77	1.54	1.50
4	K	207	PEB	CAC-C2C	-2.72	1.48	1.52
5	B	205	PUB	C1A-NA	2.72	1.38	1.35
5	B	205	PUB	C4D-C3D	-2.63	1.43	1.48
4	B	203	PEB	C3B-C2B	2.60	1.42	1.36
4	B	203	PEB	C3A-C4A	2.56	1.54	1.50
4	A	202	PEB	C2A-C1A	-2.52	1.49	1.52
4	L	208	PEB	C4D-ND	2.50	1.38	1.35
4	A	202	PEB	C3C-C4C	2.48	1.45	1.42
4	K	206	PEB	OD-C4D	-2.47	1.18	1.23
4	L	208	PEB	C2A-C1A	-2.43	1.49	1.52
4	L	209	PEB	CHC-C1D	2.42	1.60	1.54
4	L	208	PEB	C3C-C4C	2.36	1.45	1.42
5	B	205	PUB	C2C-C3C	2.31	1.41	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	204	PEB	C3B-C2B	2.29	1.41	1.36
4	L	209	PEB	C4B-C3B	-2.24	1.42	1.45
5	B	205	PUB	C4C-NC	2.22	1.39	1.35
4	B	203	PEB	OA-C1A	2.17	1.27	1.23
4	K	207	PEB	OA-C1A	2.16	1.27	1.23
4	L	208	PEB	C2C-C3C	2.10	1.43	1.37
4	L	208	PEB	OD-C4D	-2.09	1.19	1.23
4	B	204	PEB	C2C-C3C	2.05	1.43	1.37
5	B	205	PUB	C3B-C2B	2.04	1.43	1.37
4	K	206	PEB	C3B-C2B	2.03	1.41	1.36
4	L	209	PEB	C1B-C2B	2.03	1.50	1.45
4	K	206	PEB	C2C-C3C	2.02	1.43	1.37
5	L	210	PUB	C4C-NC	2.02	1.38	1.35
4	K	207	PEB	CHB-C4B	2.00	1.36	1.35

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	205	PUB	CHB-C1C-NC	-11.93	112.28	128.83
5	L	210	PUB	CHB-C1C-NC	-11.85	112.39	128.83
4	K	207	PEB	C1C-CHB-C4B	6.60	136.69	128.81
4	L	208	PEB	C1C-CHB-C4B	5.61	135.51	128.81
4	B	204	PEB	C1C-CHB-C4B	5.58	135.47	128.81
4	B	203	PEB	C1C-CHB-C4B	5.46	135.34	128.81
4	L	209	PEB	C1C-CHB-C4B	5.06	134.85	128.81
4	K	206	PEB	C1C-CHB-C4B	4.96	134.73	128.81
5	B	205	PUB	C4B-CHB-C1C	4.55	134.25	128.81
5	L	210	PUB	C4B-CHB-C1C	4.03	133.63	128.81
4	A	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
5	L	210	PUB	CHB-C1C-C2C	3.79	134.09	125.32
4	L	209	PEB	CMD-C2D-C3D	-3.63	124.94	130.06
5	B	205	PUB	CHB-C1C-C2C	3.45	133.29	125.32
4	L	208	PEB	CMD-C2D-C3D	-3.19	125.56	130.06
5	B	205	PUB	OD-C4D-C3D	-3.17	124.60	128.04
4	A	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
5	L	210	PUB	OD-C4D-C3D	-3.02	124.76	128.04
4	A	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
4	B	203	PEB	C4B-NB-C1B	3.00	112.16	106.51
5	L	210	PUB	CHC-C1D-ND	-2.98	109.95	113.72
5	B	205	PUB	C2C-C1C-NC	2.93	114.31	110.05
4	K	207	PEB	CBC-CAC-C2C	-2.93	107.63	112.62
4	B	203	PEB	CMD-C2D-C3D	-2.87	126.02	130.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	203	PEB	CHA-C4A-NA	2.81	128.54	125.20
4	K	206	PEB	C4B-NB-C1B	2.80	111.79	106.51
5	B	205	PUB	CHC-C1D-ND	-2.78	110.21	113.72
4	L	208	PEB	CHA-C4A-NA	2.78	128.51	125.20
4	B	204	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
4	L	208	PEB	CMB-C2B-C1B	2.73	129.26	125.06
4	L	209	PEB	C4B-NB-C1B	2.70	111.59	106.51
4	B	203	PEB	CMB-C2B-C1B	2.68	129.19	125.06
4	A	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
4	K	207	PEB	OA-C1A-C2A	-2.68	124.04	126.17
4	K	206	PEB	CMD-C2D-C3D	-2.68	126.29	130.06
4	B	204	PEB	C4B-NB-C1B	2.66	111.53	106.51
4	B	203	PEB	C2A-C3A-C4A	2.63	105.27	101.34
4	A	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
4	K	207	PEB	CMD-C2D-C3D	-2.62	126.37	130.06
5	B	205	PUB	CHA-C4A-NA	-2.57	110.96	113.95
4	K	206	PEB	C3B-C4B-NB	-2.57	106.31	110.05
4	B	203	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
4	A	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
4	L	208	PEB	C2A-C3A-C4A	2.51	105.11	101.34
4	L	208	PEB	C4B-NB-C1B	2.51	111.24	106.51
5	B	205	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
4	L	209	PEB	CBC-CAC-C2C	-2.48	108.39	112.62
4	A	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
4	L	208	PEB	C3B-C4B-NB	-2.38	106.59	110.05
4	L	208	PEB	CHA-C1B-C2B	2.37	131.00	124.90
4	K	206	PEB	CHC-C4C-C3C	-2.36	126.32	130.34
5	L	210	PUB	C2C-C1C-NC	2.34	113.46	110.05
4	A	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
4	B	204	PEB	CHC-C1D-ND	-2.27	111.31	113.95
4	L	209	PEB	C2A-C3A-C4A	2.25	104.72	101.34
4	K	206	PEB	OA-C1A-C2A	-2.25	124.38	126.17
4	B	204	PEB	C3B-C4B-NB	-2.21	106.83	110.05
5	L	210	PUB	C2A-C1A-NA	2.20	109.16	107.21
4	L	208	PEB	CHC-C4C-C3C	-2.20	126.59	130.34
4	A	202	PEB	CHC-C1D-ND	-2.19	111.40	113.95
4	K	207	PEB	C4B-NB-C1B	2.18	110.62	106.51
4	A	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
4	K	207	PEB	C2A-C3A-C4A	2.18	104.60	101.34
4	K	207	PEB	CHC-C4C-C3C	-2.17	126.64	130.34
4	K	206	PEB	CMB-C2B-C1B	2.16	128.40	125.06
4	L	209	PEB	C2B-C1B-NB	-2.16	105.90	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	207	PEB	CMB-C2B-C1B	2.16	128.40	125.06
4	A	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
4	B	203	PEB	C3B-C4B-NB	-2.14	106.94	110.05
4	B	203	PEB	CHA-C1B-C2B	2.09	130.27	124.90
4	K	206	PEB	C2A-C3A-C4A	2.07	104.44	101.34
4	B	204	PEB	CMB-C2B-C1B	2.07	128.25	125.06
4	K	207	PEB	C3B-C4B-NB	-2.06	107.05	110.05
4	K	207	PEB	CHB-C4B-NB	2.03	131.65	128.83
5	B	205	PUB	CMA-C2A-C1A	2.01	126.12	121.39
4	L	208	PEB	C4B-C3B-C2B	2.01	109.01	106.78

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	PEB	NA-C4A-CHA-C1B
4	A	201	PEB	C3A-C4A-CHA-C1B
4	A	201	PEB	NB-C1B-CHA-C4A
4	A	201	PEB	C2B-C1B-CHA-C4A
4	A	202	PEB	NB-C1B-CHA-C4A
4	A	202	PEB	C2B-C1B-CHA-C4A
4	B	203	PEB	NB-C1B-CHA-C4A
4	B	203	PEB	C2B-C1B-CHA-C4A
4	B	204	PEB	C1C-C2C-CAC-CBC
4	B	204	PEB	C3C-C2C-CAC-CBC
4	B	204	PEB	NB-C1B-CHA-C4A
4	B	204	PEB	C2B-C1B-CHA-C4A
4	K	206	PEB	NA-C4A-CHA-C1B
4	K	206	PEB	C3A-C4A-CHA-C1B
4	K	206	PEB	NB-C1B-CHA-C4A
4	K	206	PEB	C2B-C1B-CHA-C4A
4	K	207	PEB	NB-C1B-CHA-C4A
4	K	207	PEB	C2B-C1B-CHA-C4A
4	L	208	PEB	NB-C1B-CHA-C4A
4	L	208	PEB	C2B-C1B-CHA-C4A
4	L	209	PEB	C2A-C3A-CAA-CBA
4	L	209	PEB	C4A-C3A-CAA-CBA
4	L	209	PEB	NB-C1B-CHA-C4A
4	L	209	PEB	C2B-C1B-CHA-C4A
5	B	205	PUB	NB-C4B-CHB-C1C
4	A	202	PEB	C3B-CAB-CBB-CGB
4	L	209	PEB	C2C-CAC-CBC-CGC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	205	PUB	C2A-C3A-CAA-CBA
5	B	205	PUB	C4A-C3A-CAA-CBA
5	B	205	PUB	C2D-C3D-CAD-CBD
4	B	204	PEB	C4A-C3A-CAA-CBA
4	A	202	PEB	NA-C4A-CHA-C1B
4	L	209	PEB	C3C-C2C-CAC-CBC
4	B	204	PEB	NA-C4A-CHA-C1B
4	K	207	PEB	NA-C4A-CHA-C1B
4	L	209	PEB	NA-C4A-CHA-C1B
5	L	210	PUB	C4A-C3A-CAA-CBA
4	A	201	PEB	CAC-CBC-CGC-O2C
4	A	202	PEB	CAB-CBB-CGB-O2B
4	K	207	PEB	CAC-CBC-CGC-O1C
4	A	201	PEB	CAC-CBC-CGC-O1C
4	K	206	PEB	CAC-CBC-CGC-O2C
5	B	205	PUB	NC-C1C-CHB-C4B
4	A	202	PEB	CAC-CBC-CGC-O2C
4	K	207	PEB	CAB-CBB-CGB-O2B
4	B	203	PEB	CAC-CBC-CGC-O1C
4	K	206	PEB	CAC-CBC-CGC-O1C
5	L	210	PUB	CAC-CBC-CGC-O2C
4	B	203	PEB	CAB-CBB-CGB-O1B
4	K	207	PEB	CAB-CBB-CGB-O1B
5	L	210	PUB	CAC-CBC-CGC-O1C
4	A	202	PEB	CAC-CBC-CGC-O1C
5	L	210	PUB	CAB-CBB-CGB-O1B
4	L	209	PEB	CAC-CBC-CGC-O2C
4	A	202	PEB	CAB-CBB-CGB-O1B
5	L	210	PUB	CAB-CBB-CGB-O2B
4	B	203	PEB	CAB-CBB-CGB-O2B
4	K	207	PEB	CAC-CBC-CGC-O2C
4	L	209	PEB	CAC-CBC-CGC-O1C
4	L	208	PEB	CAC-CBC-CGC-O2C
4	L	208	PEB	CAC-CBC-CGC-O1C
4	B	203	PEB	CAC-CBC-CGC-O2C
5	B	205	PUB	CAB-CBB-CGB-O1B
5	B	205	PUB	CAB-CBB-CGB-O2B
4	A	201	PEB	CAB-CBB-CGB-O1B
4	A	201	PEB	CAB-CBB-CGB-O2B
4	L	209	PEB	CAB-CBB-CGB-O2B
4	L	209	PEB	CAB-CBB-CGB-O1B
4	L	208	PEB	C2C-CAC-CBC-CGC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	204	PEB	CAB-CBB-CGB-O1B

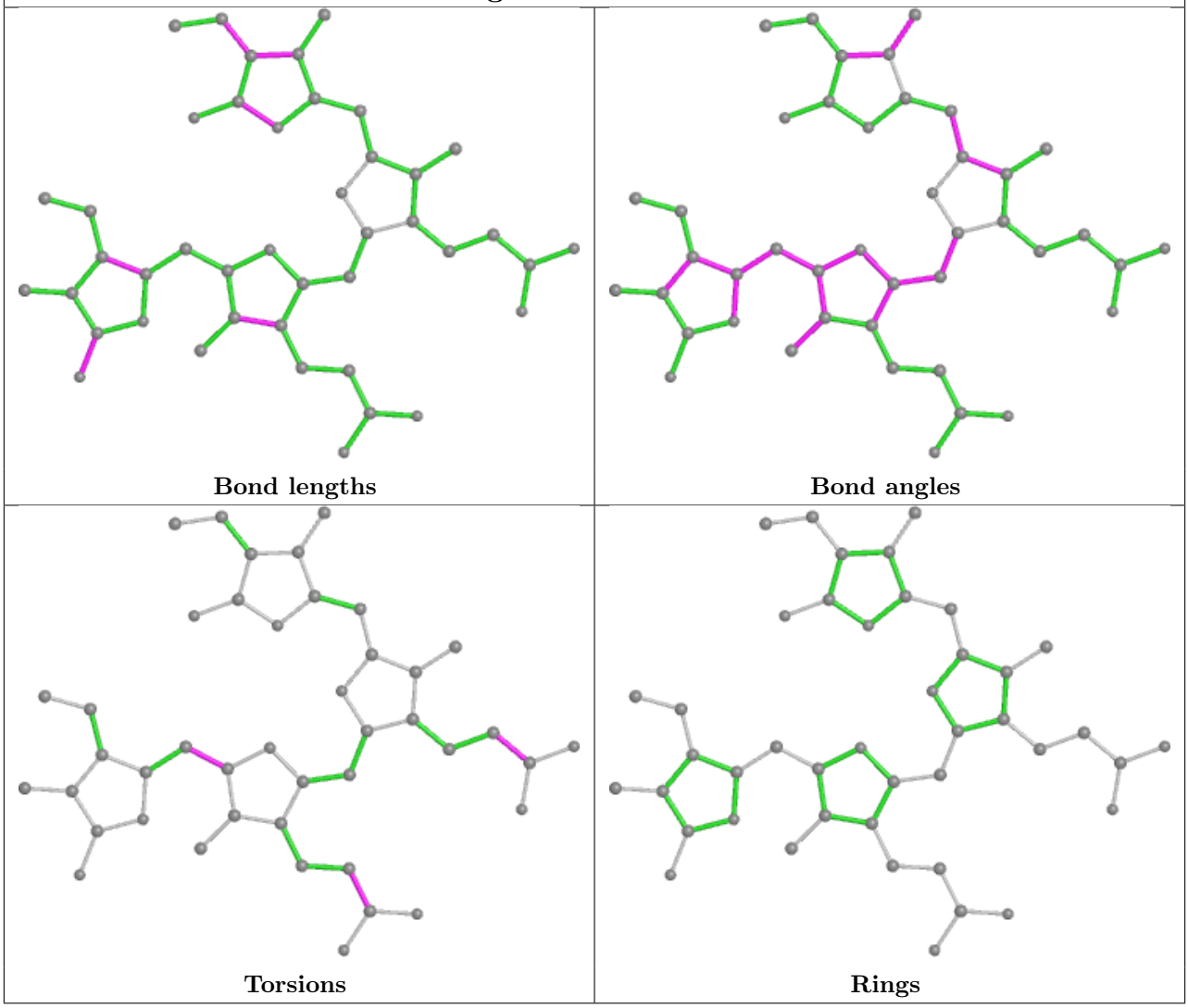
There are no ring outliers.

10 monomers are involved in 29 short contacts:

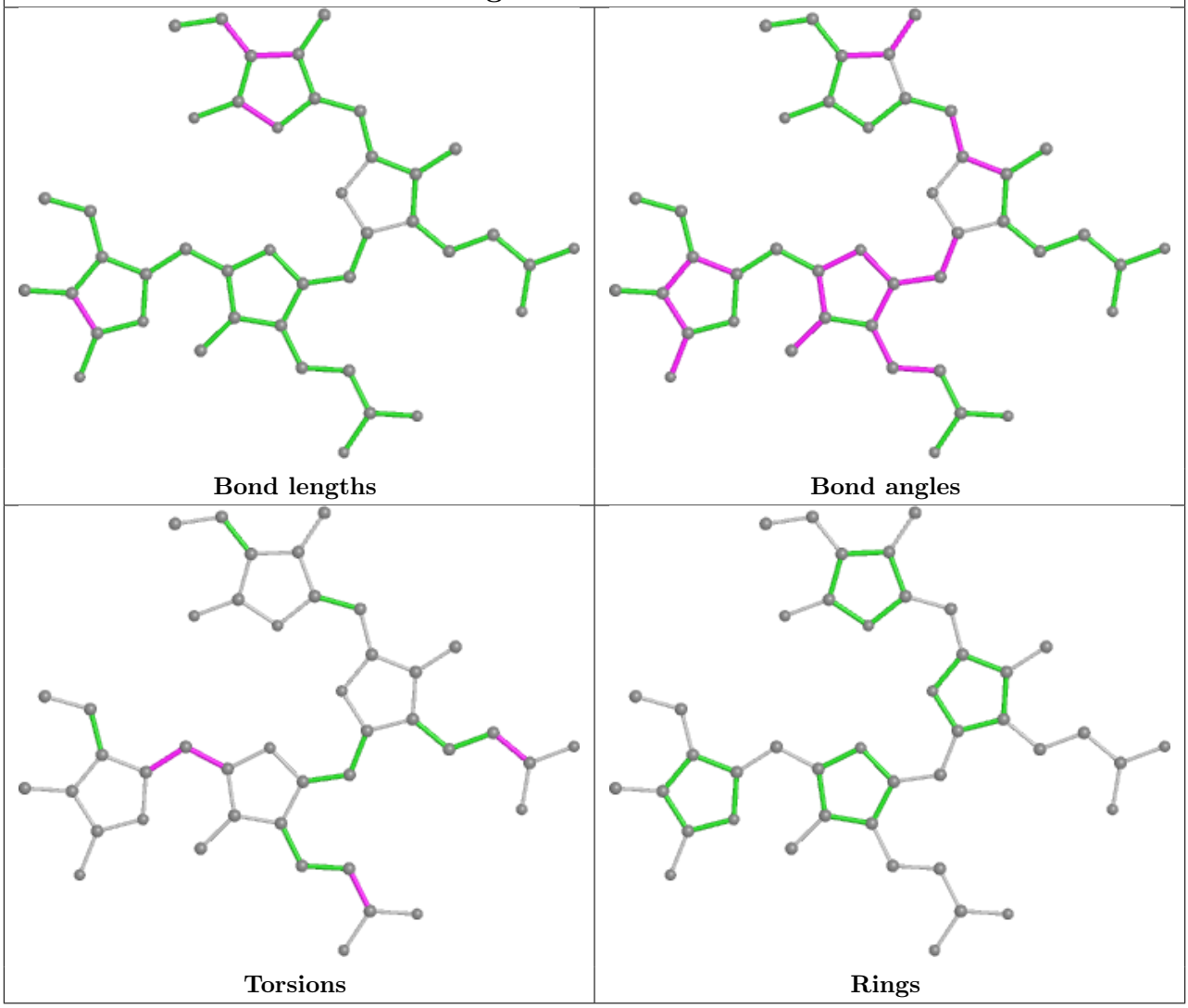
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	203	PEB	3	0
4	A	201	PEB	2	0
4	K	207	PEB	2	0
5	B	205	PUB	4	0
4	L	208	PEB	4	0
4	L	209	PEB	3	0
5	L	210	PUB	2	0
4	A	202	PEB	5	0
4	K	206	PEB	1	0
4	B	204	PEB	3	0

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

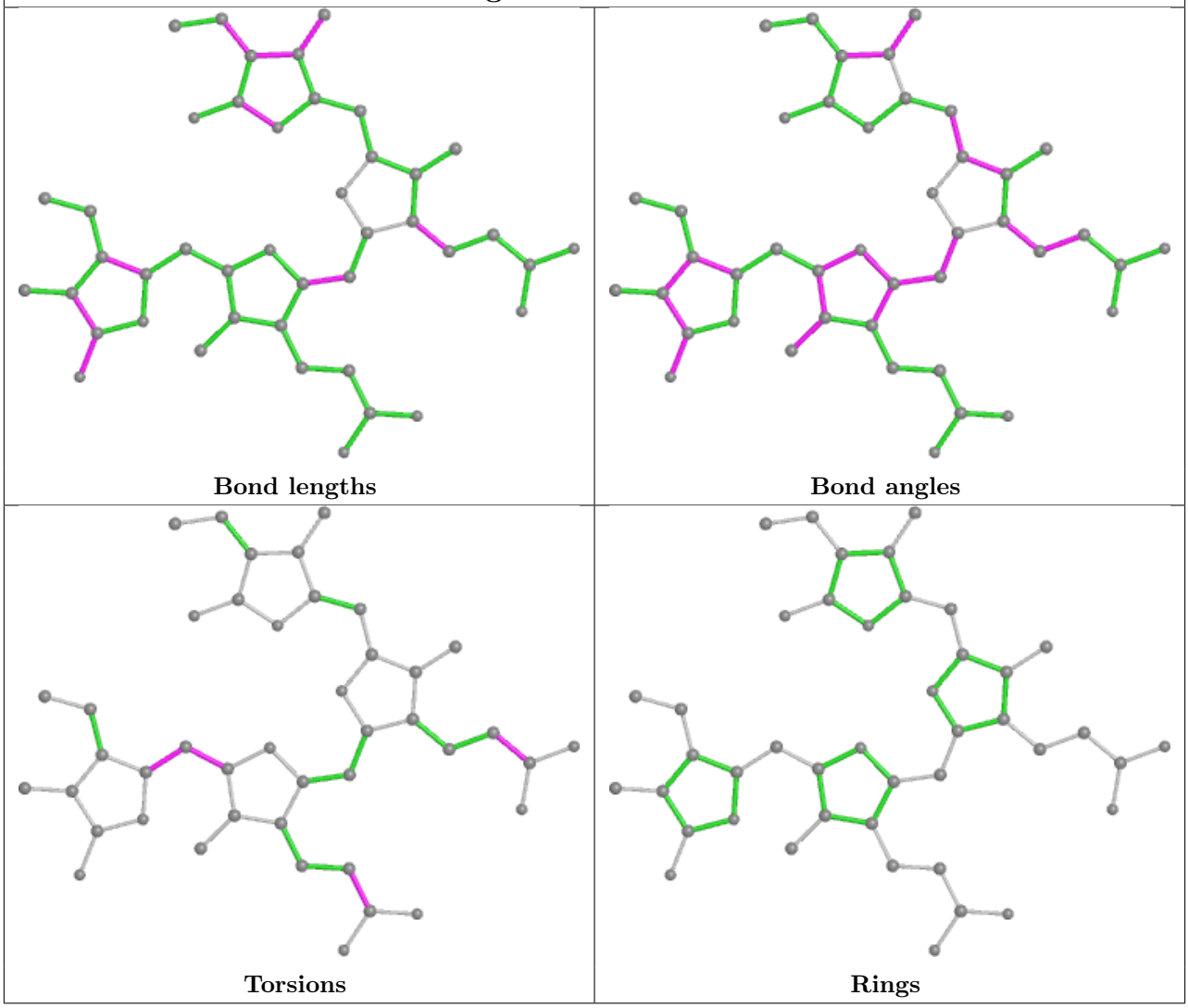
Ligand PEB B 203



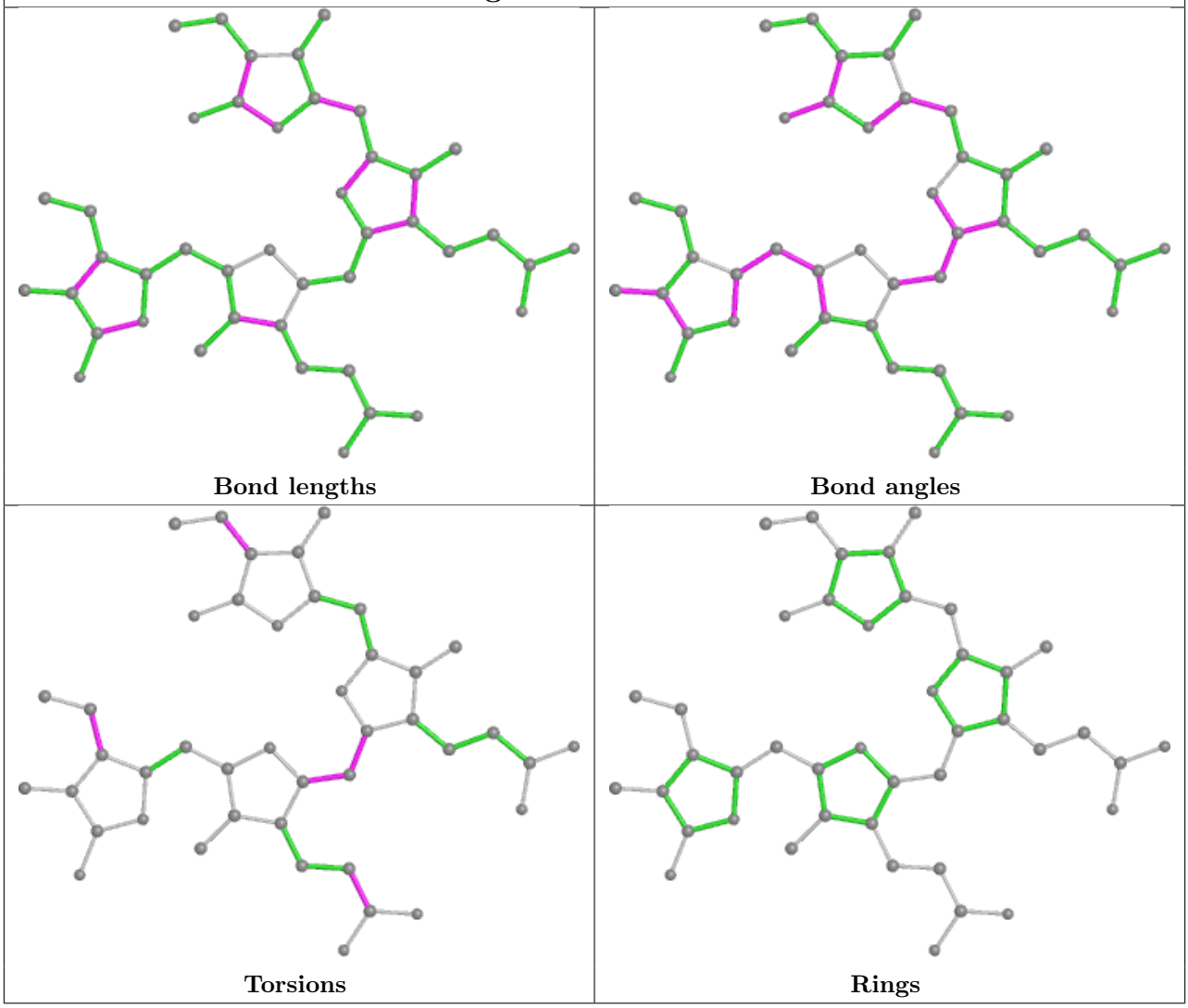
Ligand PEB A 201



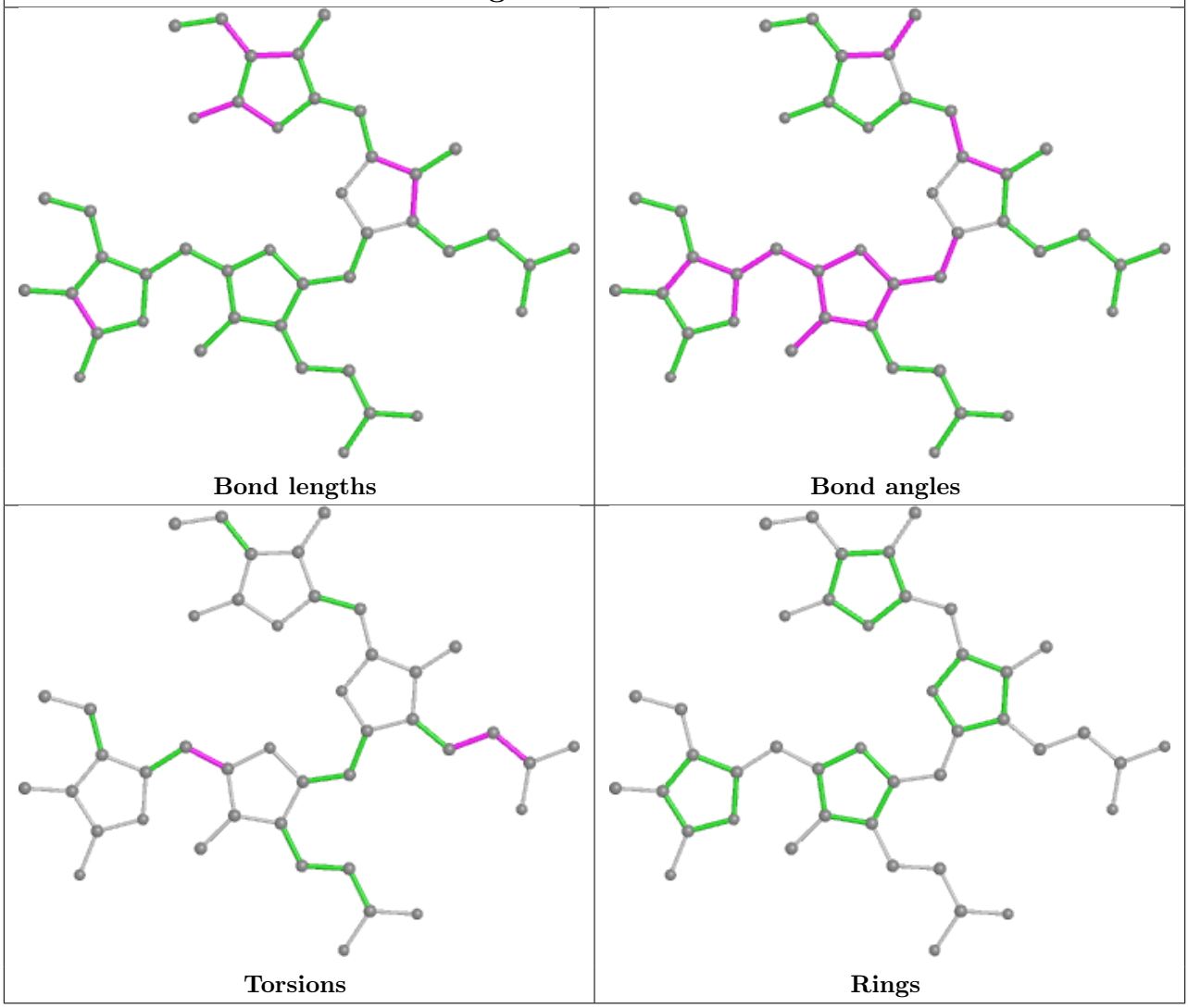
Ligand PEB K 207



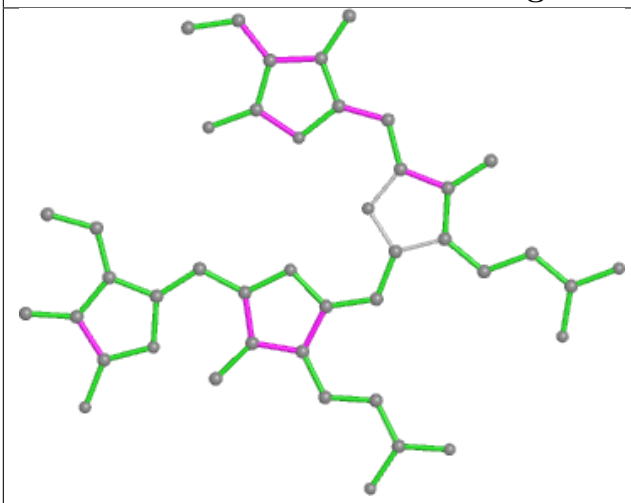
Ligand PUB B 205



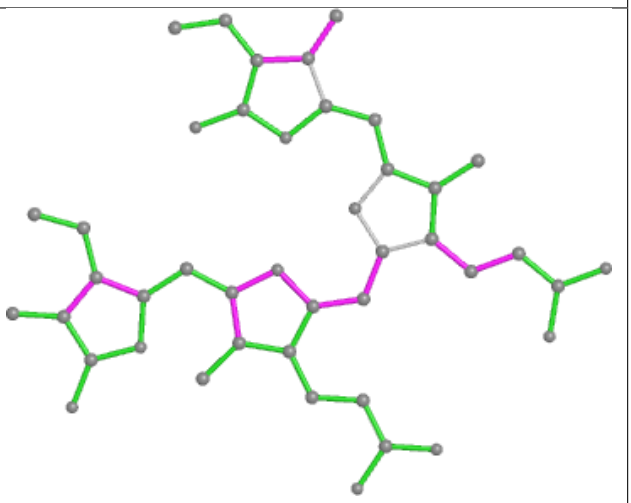
Ligand PEB L 208



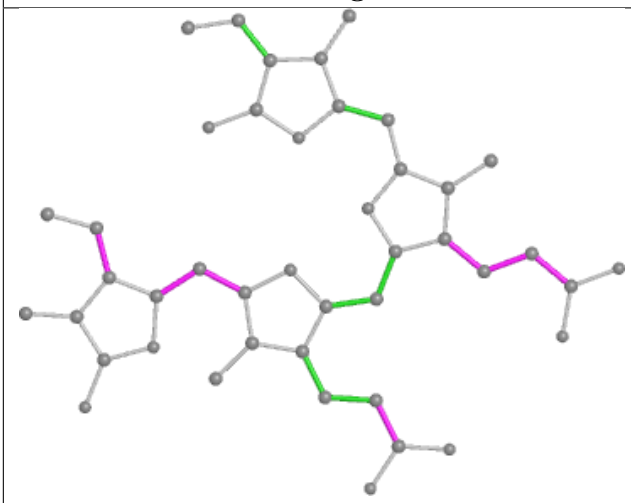
Ligand PEB L 209



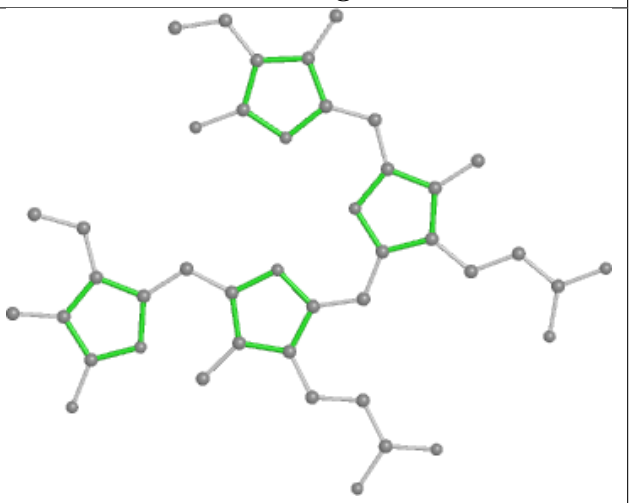
Bond lengths



Bond angles

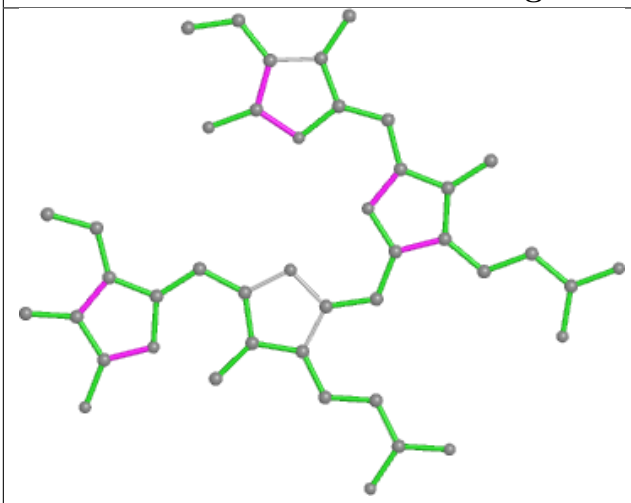


Torsions

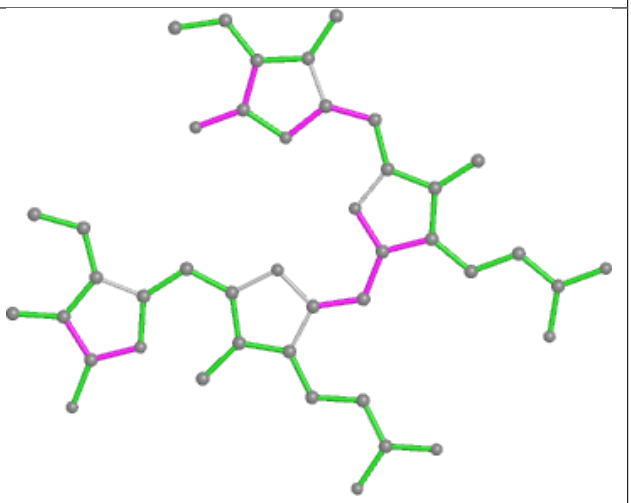


Rings

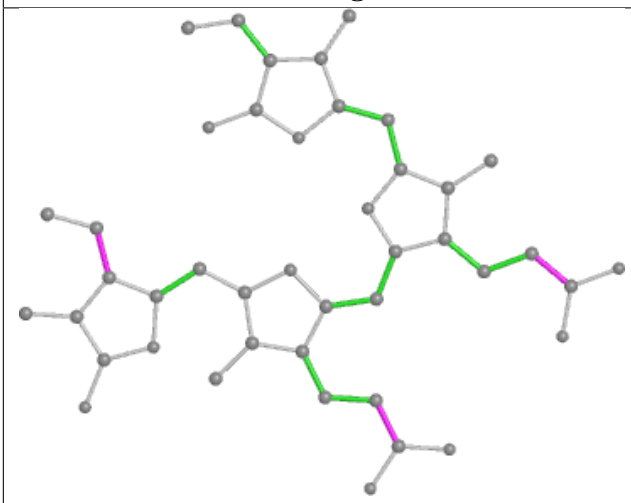
Ligand PUB L 210



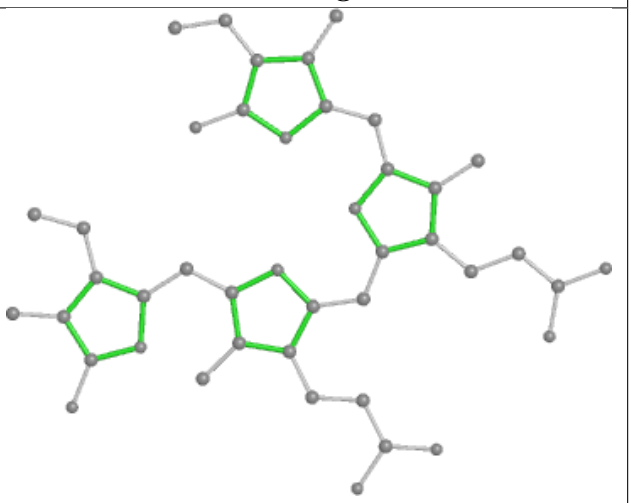
Bond lengths



Bond angles

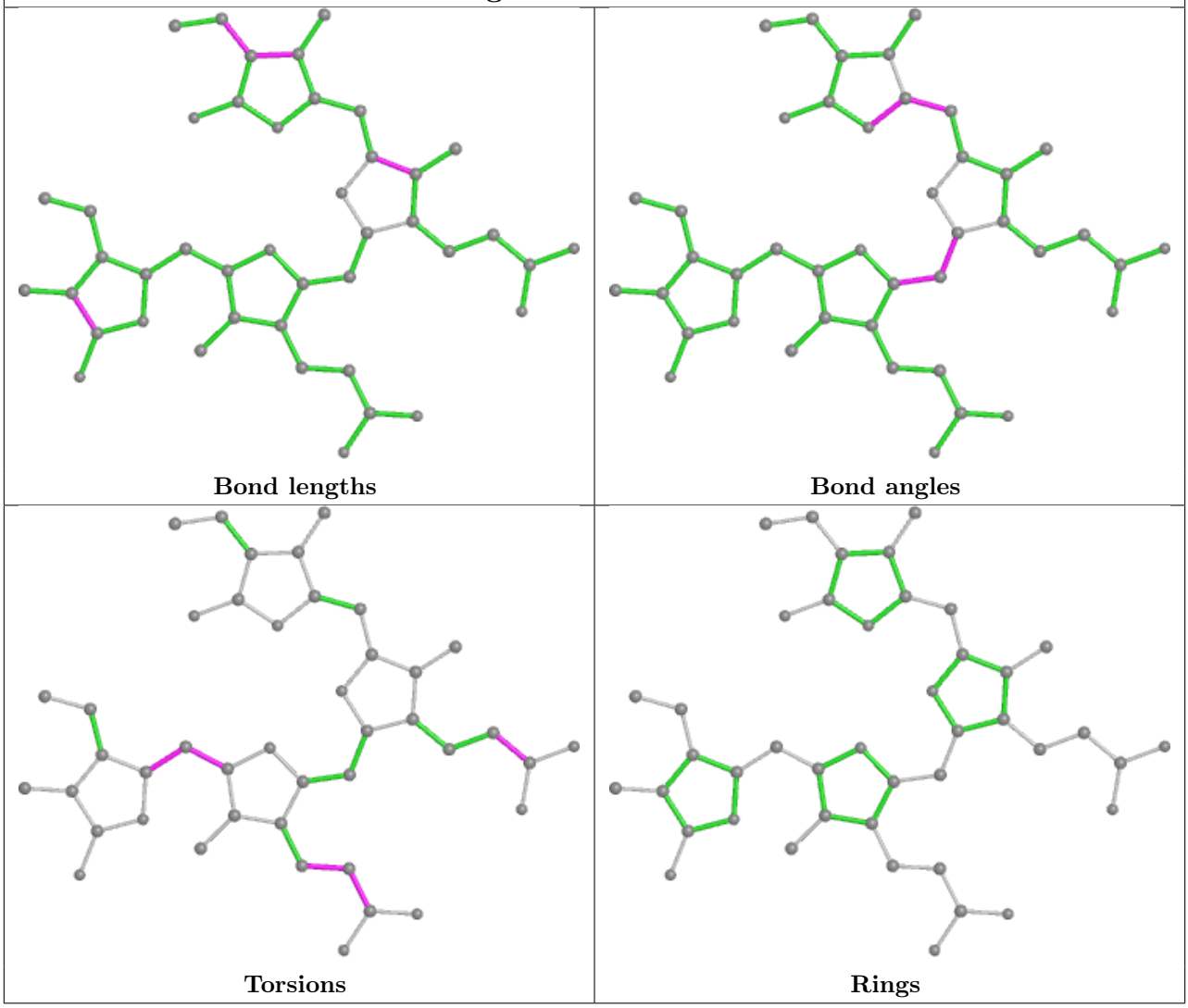


Torsions

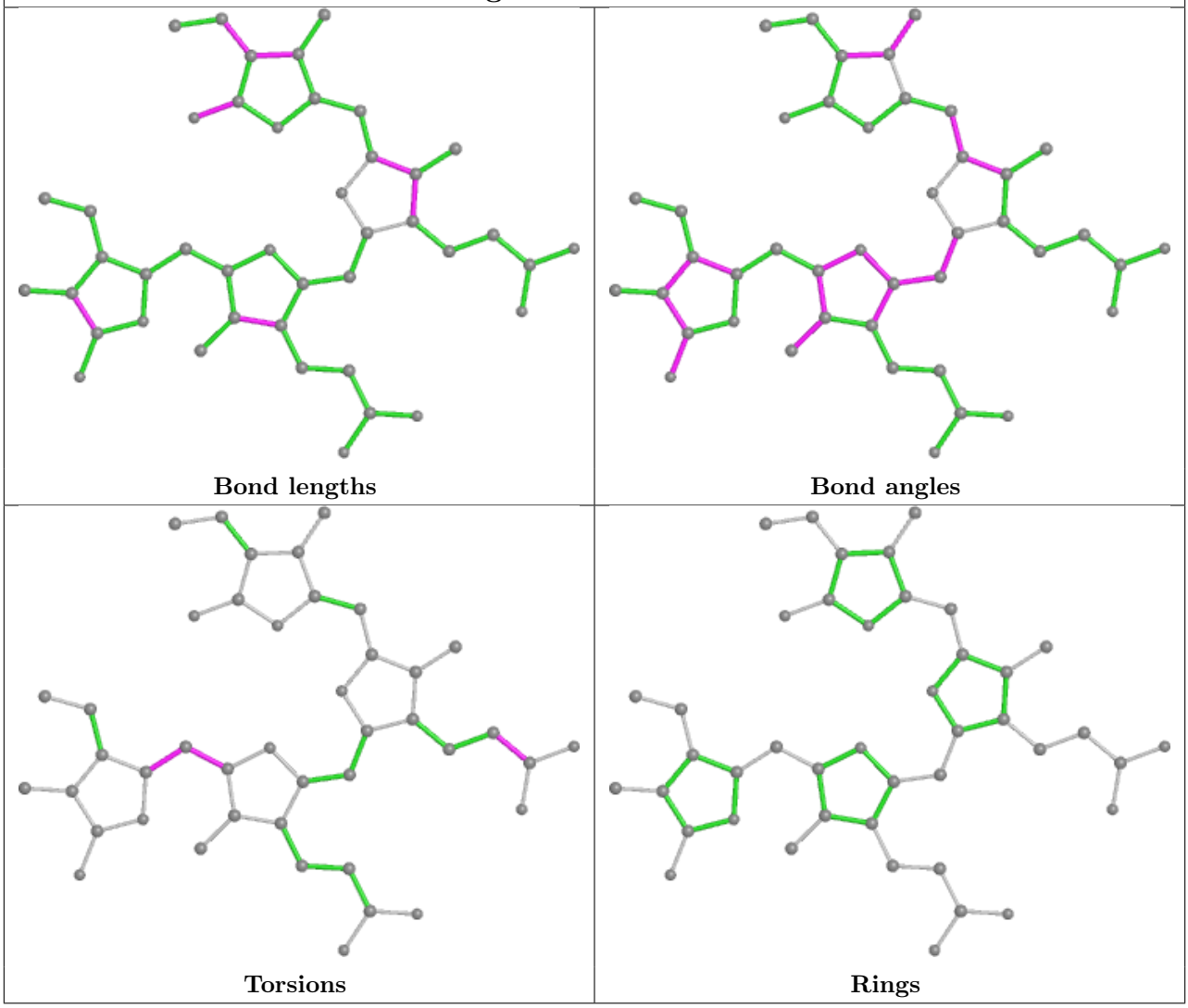


Rings

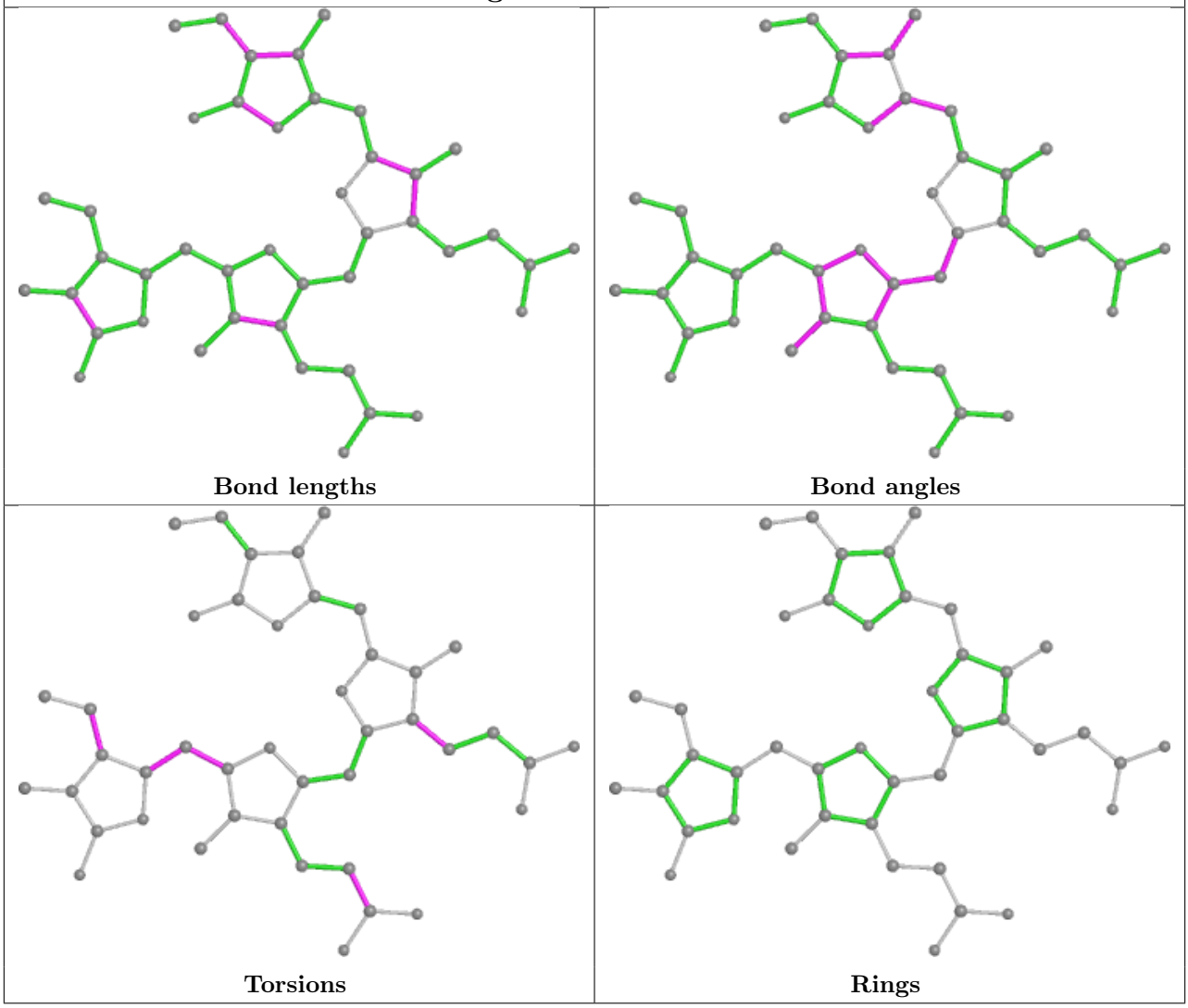
Ligand PEB A 202



Ligand PEB K 206



Ligand PEB B 204



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%)	-0.32	2 (1%)	79	81	12, 20, 34, 45	0
1	K	164/164 (100%)	-0.29	1 (0%)	89	90	12, 19, 34, 45	0
2	B	176/177 (99%)	-0.36	3 (1%)	70	72	12, 20, 39, 57	0
2	L	176/177 (99%)	-0.36	4 (2%)	60	63	11, 20, 39, 57	0
3	G	3/6 (50%)	1.33	1 (33%)	0	0	36, 36, 40, 40	0
All	All	683/688 (99%)	-0.33	11 (1%)	72	74	11, 20, 38, 57	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	25	GLN	3.7
2	L	22	SER	2.7
2	B	147	SER	2.6
1	A	140	VAL	2.5
3	G	2	TYR	2.4
2	B	25	GLN	2.3
1	A	139	CYS	2.3
1	K	76	PRO	2.3
2	B	159	GLN	2.2
2	L	20	GLY	2.1
2	L	23	ASP	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	B	72	9/10	0.96	0.07	0,19,23,24	1
2	MEN	L	72	9/10	0.96	0.07	0,19,23,24	1

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

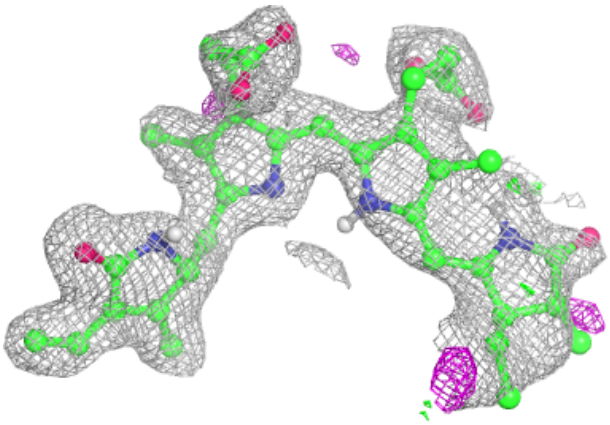
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

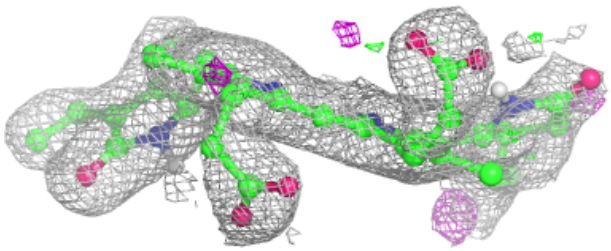
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEB	A	202	43/43	0.89	0.19	0,47,59,63	3
4	PEB	B	204	43/43	0.91	0.12	0,19,44,52	3
4	PEB	L	209	43/43	0.93	0.11	0,18,43,56	3
5	PUB	B	205	43/43	0.93	0.08	0,26,38,49	3
4	PEB	K	207	43/43	0.94	0.10	0,23,38,47	3
4	PEB	L	208	43/43	0.94	0.09	0,17,29,37	3
5	PUB	L	210	43/43	0.94	0.09	0,19,32,35	3
4	PEB	A	201	43/43	0.95	0.09	0,19,27,40	3
4	PEB	B	203	43/43	0.95	0.08	0,17,28,38	3
4	PEB	K	206	43/43	0.96	0.08	0,16,27,34	3

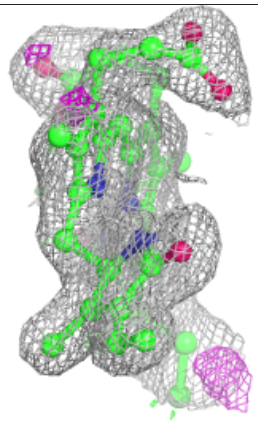
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEB A 202:

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

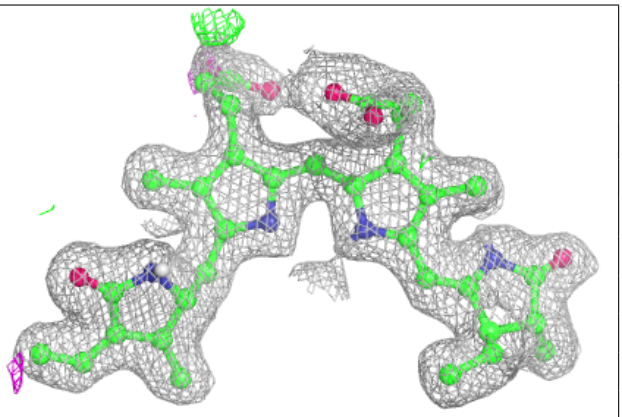


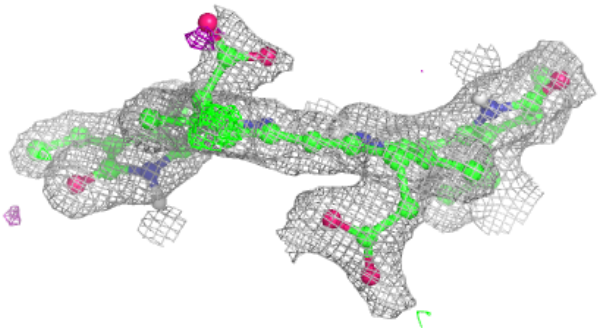


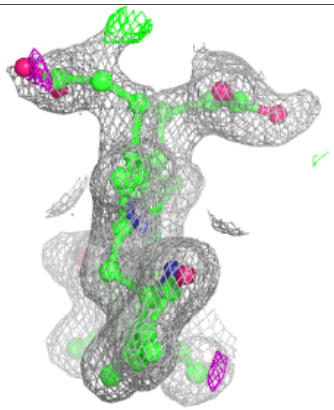


Electron density around PEB B 204:

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

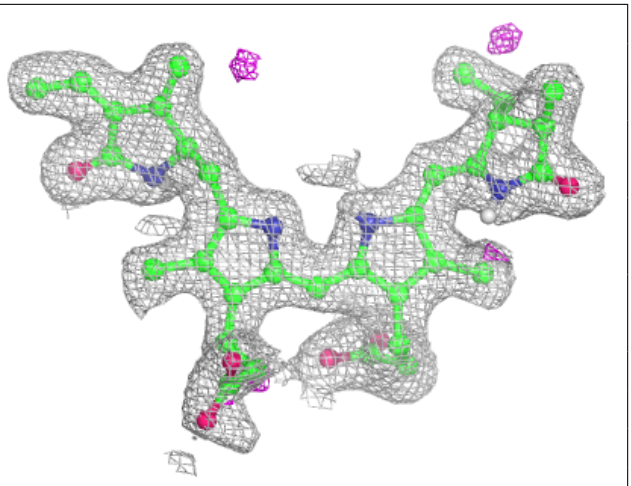


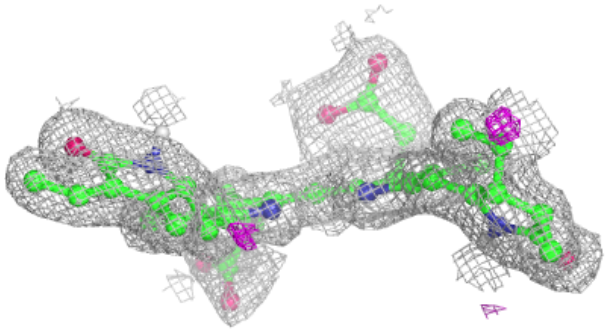


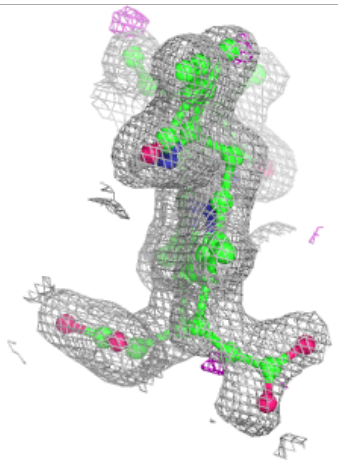


Electron density around PEB L 209:

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

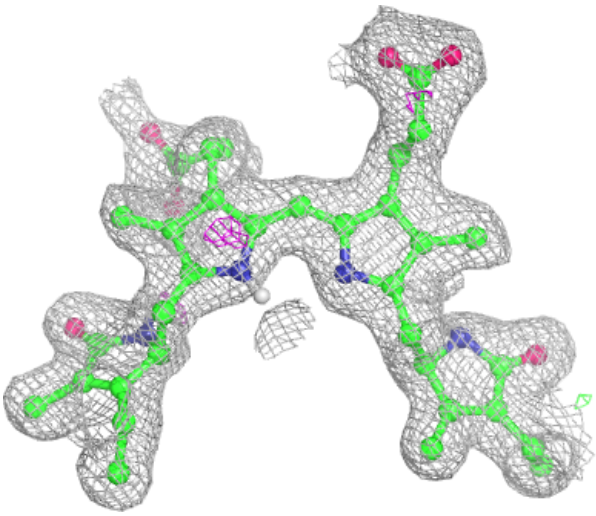


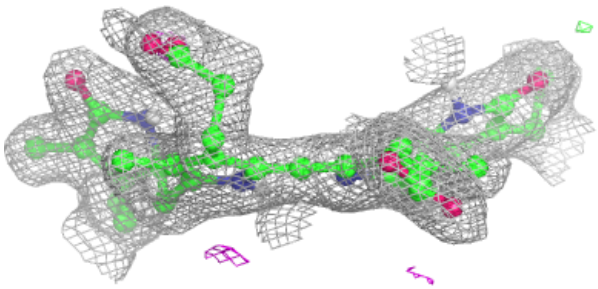


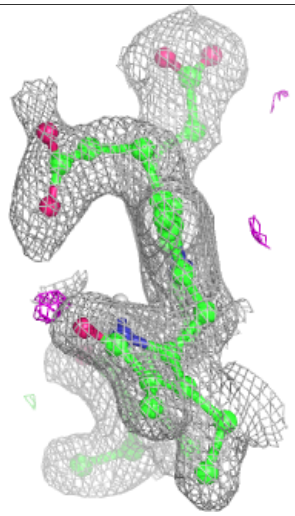


Electron density around PUB B 205:

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

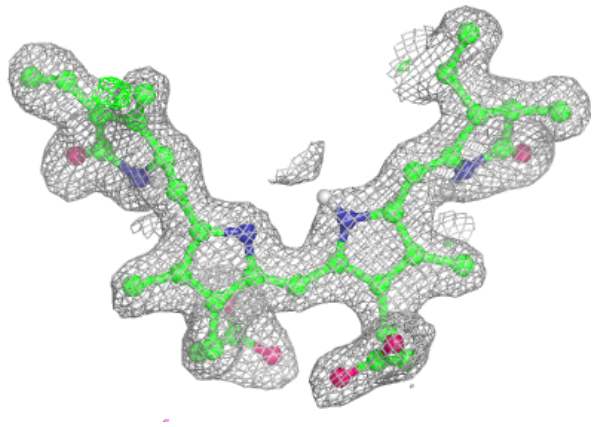


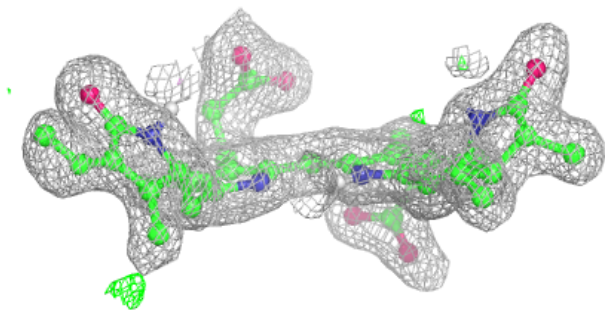


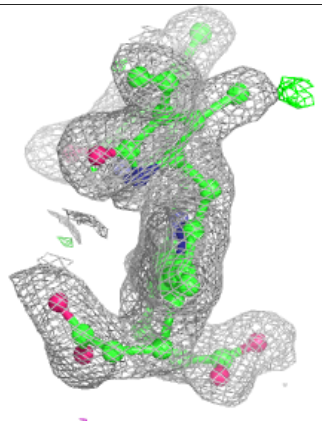


Electron density around PEB K 207:

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

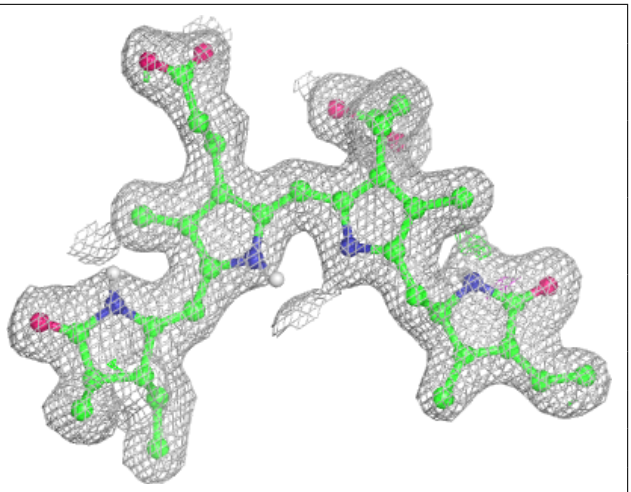


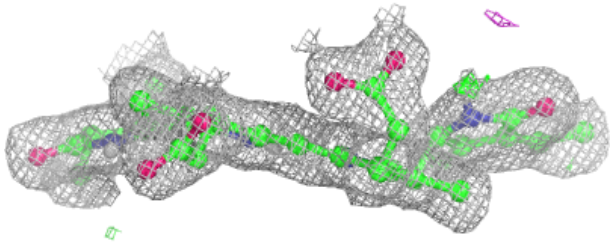


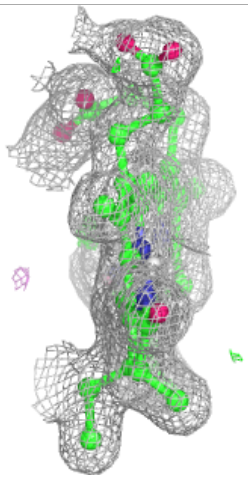


Electron density around PEB L 208:

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

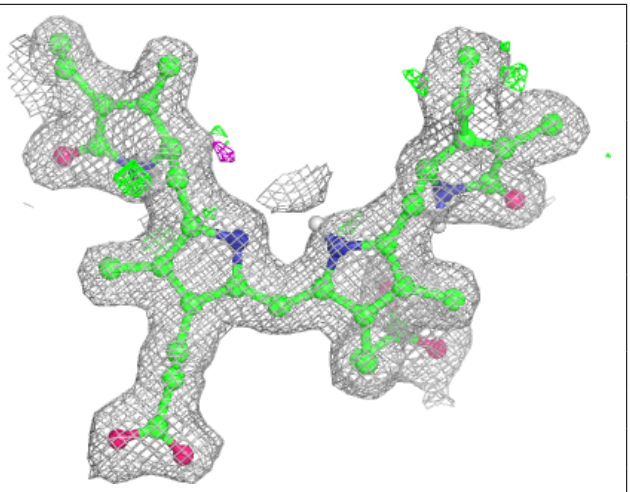


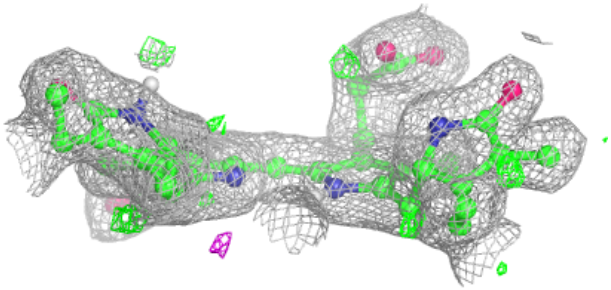


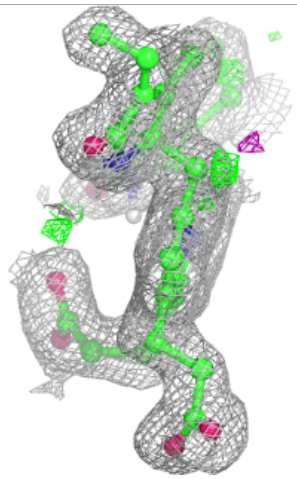


Electron density around PUB L 210:

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

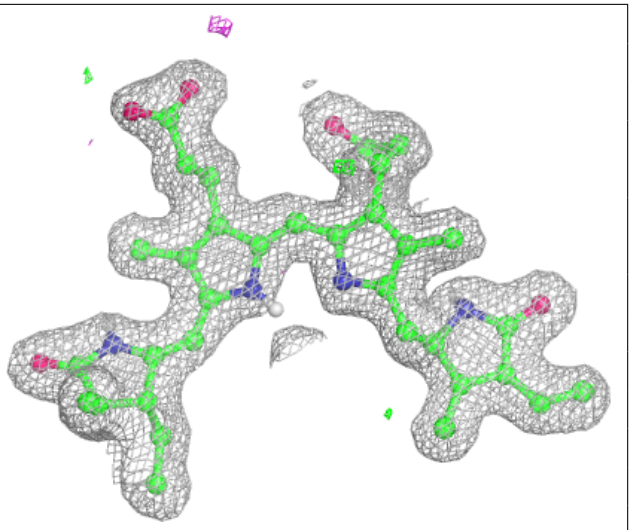


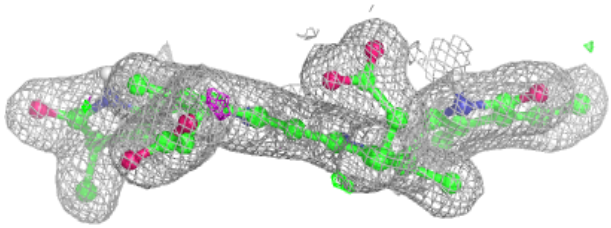




Electron density around PEB A 201:

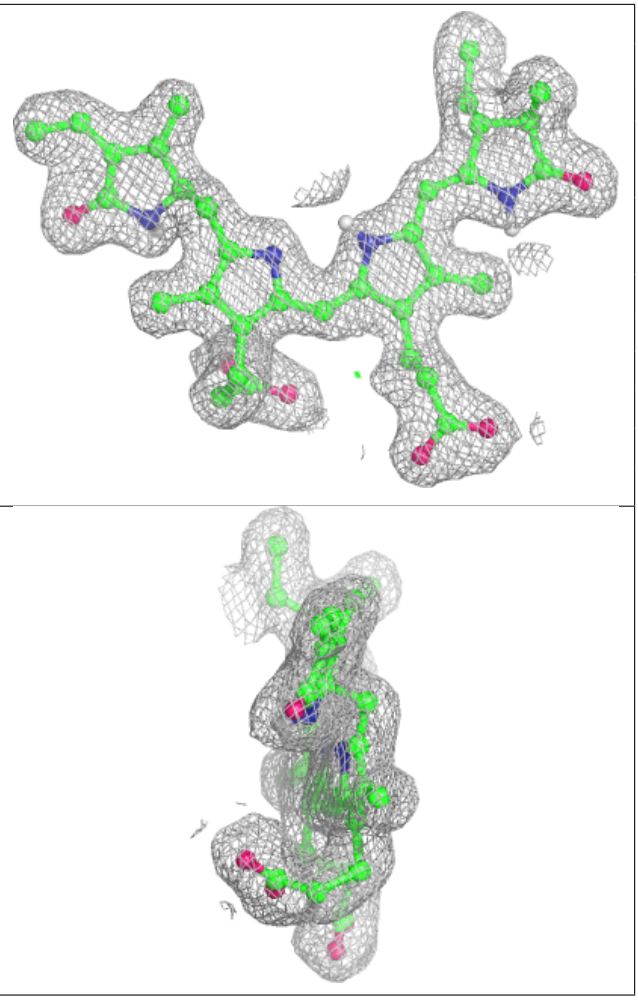
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





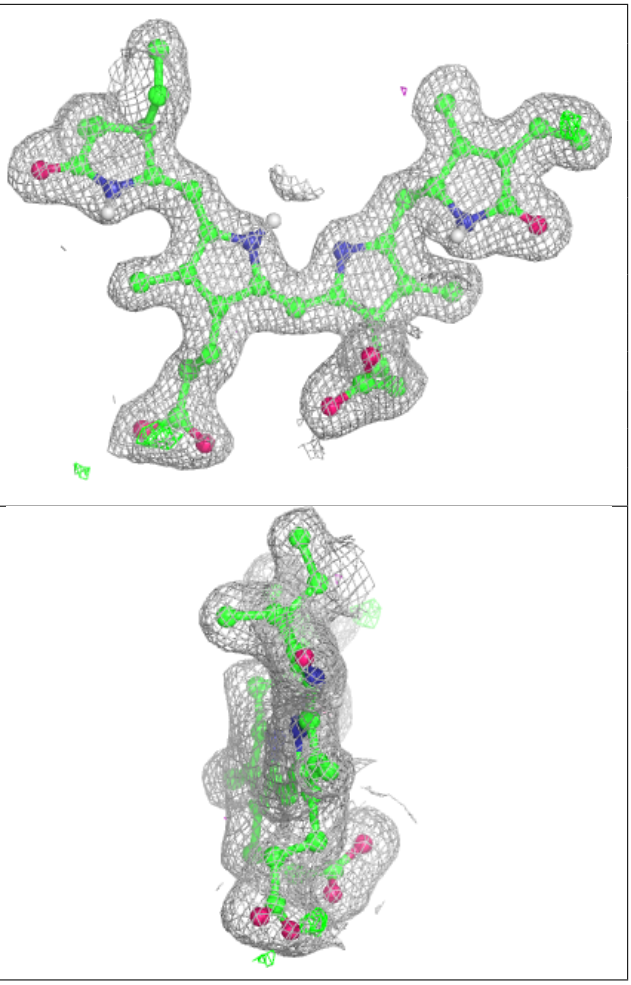
Electron density around PEB B 203:

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



Electron density around PEB K 206:

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.