Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:32 PM EDT

PDB ID	:	1Q90
Title	:	Structure of the cytochrome b6f (plastohydroquinone : plastocyanin oxidoreductase) from Chlamydomonas reinhardtii
Authors	:	Stroebel, D.; Choquet, Y.; Popot, J.-L.; Picot, D.
Deposited on	:	2003-08-22
Resolution	:	3.10 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:

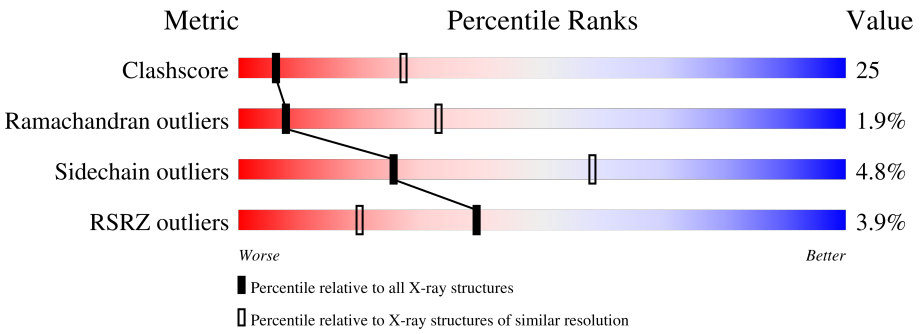
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	292	%, 59%, 37%, •
2	B	215	%, 57%, 40%, • •
3	C	127	24%, 42%, 53%, 5%, •
4	D	159	47%, 45%, 6%, •
5	R	49	6%, 57%, 16%, 6%, 20%
6	G	37	65%, 16%, 19%

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Mol	Chain	Length	Quality of chain
7	L	32	53% 34% 12%
8	M	39	46% 33% 8% 13%
9	N	31	65% 35%

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
14	CLA	D	910	X	-	-	-
16	LMG	D	953	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 7778 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 Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	2266	1457	387	417	5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	HIS	-	expression tag	UNP P23577
A	288	HIS	-	expression tag	UNP P23577
A	289	HIS	-	expression tag	UNP P23577
A	290	HIS	-	expression tag	UNP P23577
A	291	HIS	-	expression tag	UNP P23577
A	292	HIS	-	expression tag	UNP P23577

- Molecule 2 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	1681	1117	270	281	13	0	0	0

- Molecule 3 is a protein called Cytochrome B6-F complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	126	955	606	163	181	5	0	0	0

- Molecule 4 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	156	1201	807	185	204	5	0	0	0

- Molecule 5 is a protein called Cytochrome B6-F complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	R	39	283	184	46	51	2	0	0	0

- Molecule 6 is a protein called Cytochrome b6f complex subunit petG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	G	30	224	154	31	37	2	0	0	0

- Molecule 7 is a protein called Cytochrome b6f complex subunit petL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	L	32	242	168	34	39	1	0	0	0

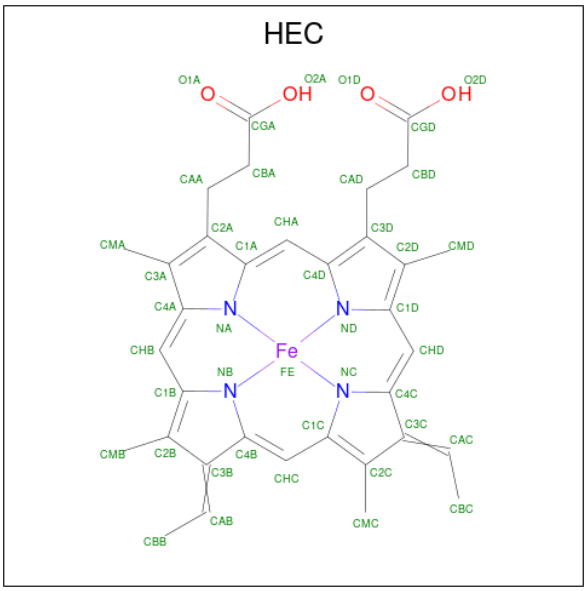
- Molecule 8 is a protein called Cytochrome b6f complex subunit PETM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	M	34	247	162	37	46	2	0	0	0

- Molecule 9 is a protein called Cytochrome b6f complex subunit PETN.

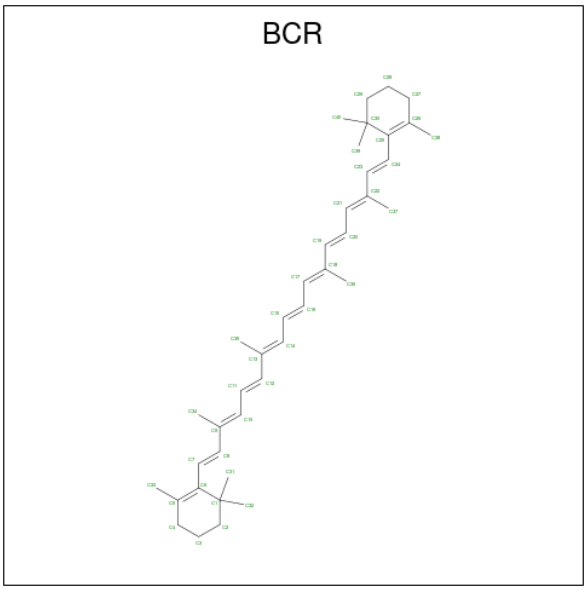
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	N	31	231	152	37	40	2	0	0	0

- Molecule 10 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



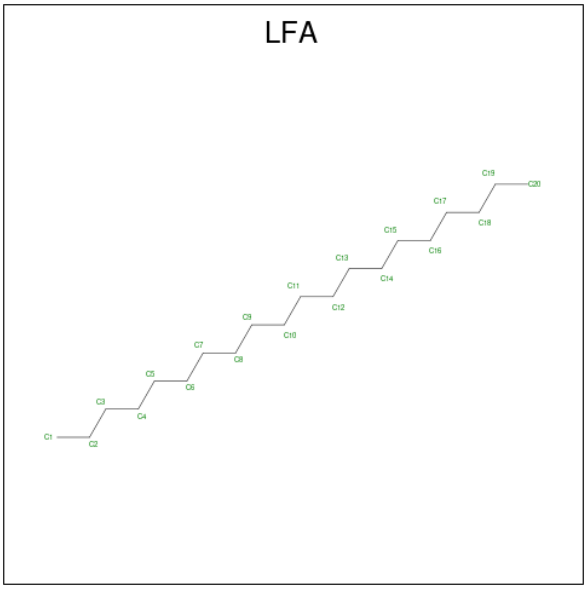
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
10	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
10	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
10	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
10	B	1	43	34	1	4	4	0	0

- Molecule 11 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



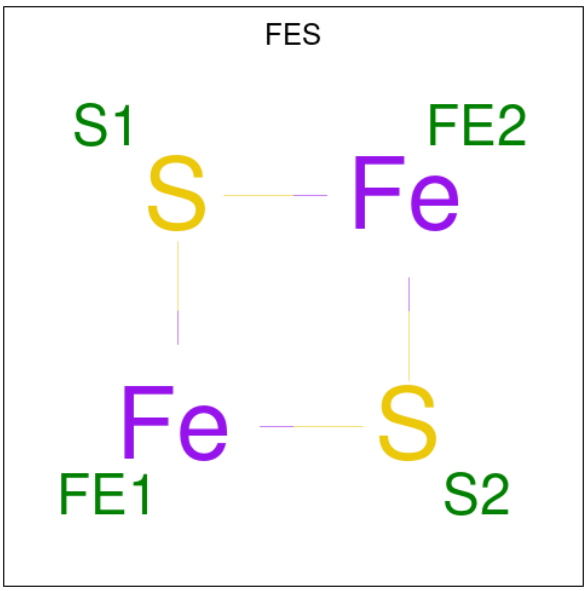
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C 27 27	0	0

- Molecule 12 is EICOSANE (three-letter code: LFA) (formula: $C_{20}H_{42}$).



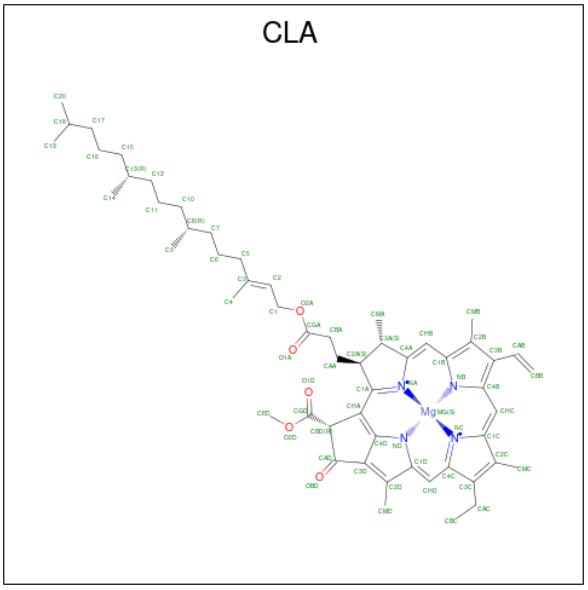
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C 20 20	0	0

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



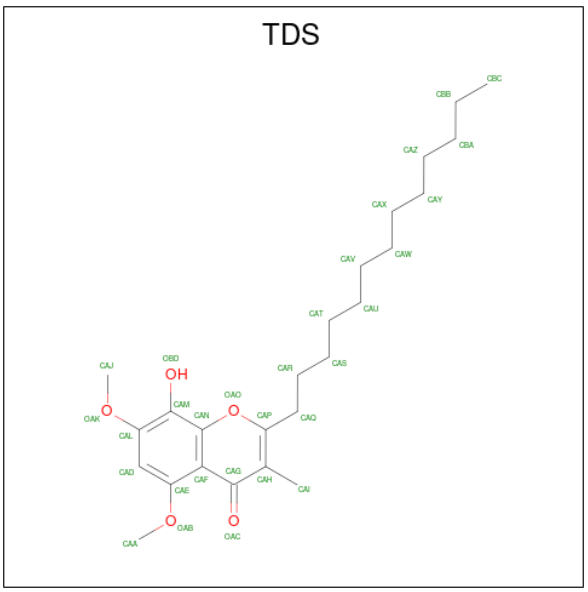
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
13	C	1	4	2	2	0	0

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



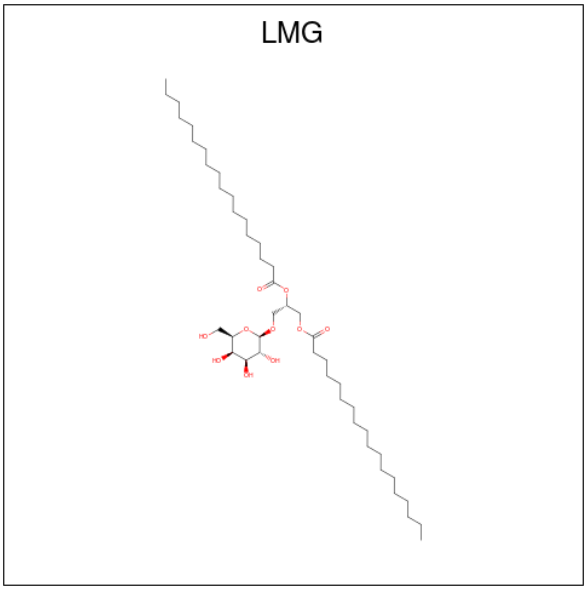
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
14	D	1	65	55	1	4	5	0	0

- Molecule 15 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROMEN-4-ONE (three-letter code: TDS) (formula: $C_{25}H_{38}O_5$).



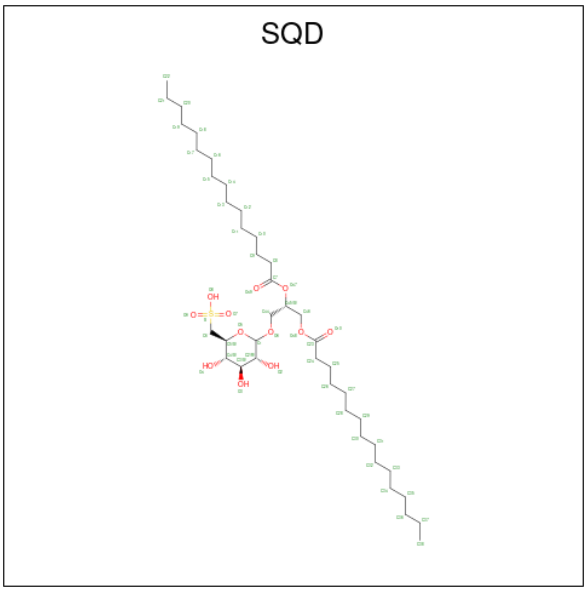
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	D	1	30	25	5	0	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
16	D	1	53	43	10	0	0
			Total	C	O		
16	L	1	42	32	10	0	0

- Molecule 17 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
17	R	1	33	20	12	1	0	0

- Molecule 18 is water.

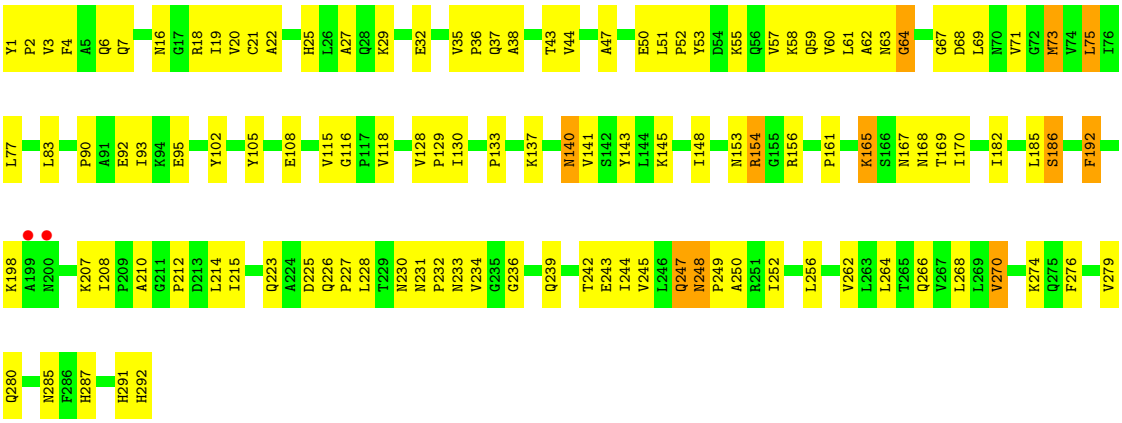
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	B	2	2	2	0	0

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.

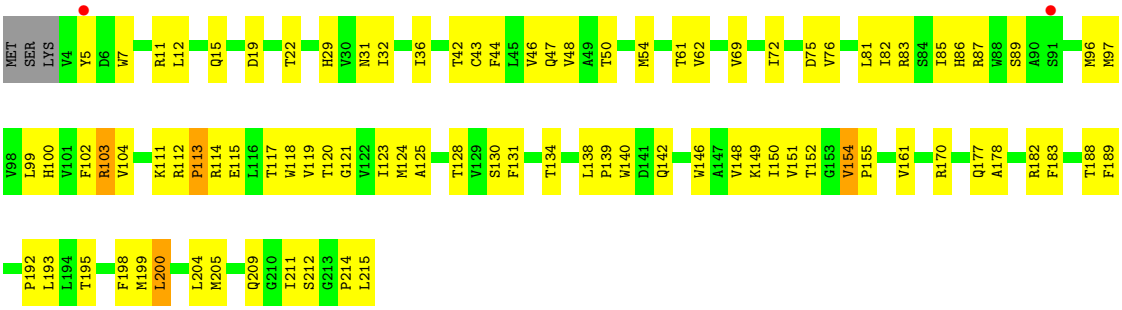
- Molecule 1: Apocytochrome f

Chain A:



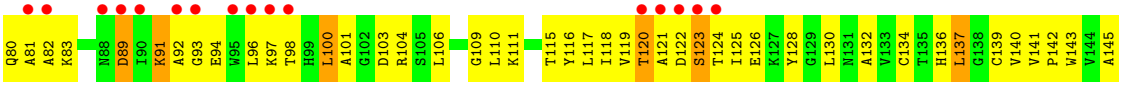
- Molecule 2: Cytochrome b6

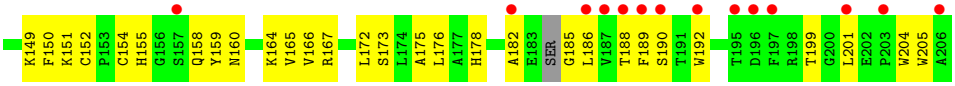
Chain B:



- Molecule 3: Cytochrome B6-F complex iron-sulfur subunit

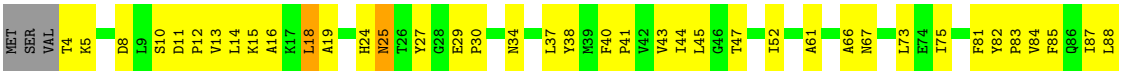
Chain C:

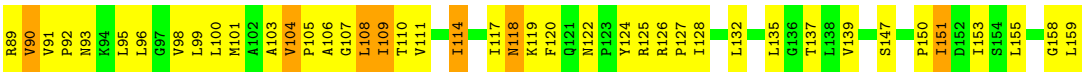




• Molecule 4: Cytochrome b6-f complex subunit 4

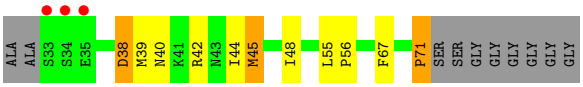
Chain D:





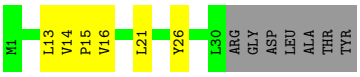
• Molecule 5: Cytochrome B6-F complex iron-sulfur subunit

Chain R:



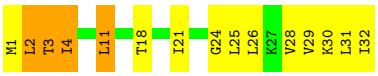
• Molecule 6: Cytochrome b6f complex subunit petG

Chain G:



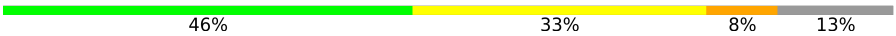
• Molecule 7: Cytochrome b6f complex subunit petL

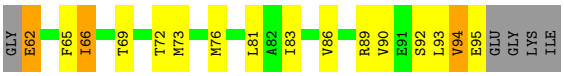
Chain L:



• Molecule 8: Cytochrome b6f complex subunit PETM

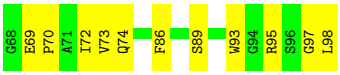
Chain M:





• Molecule 9: Cytochrome b6f complex subunit PETN

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	102.45Å 171.21Å 351.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.42 – 3.10 35.14 – 2.97	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.42-3.10) 92.7 (35.14-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.29 (at 2.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.261 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	62.5	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 77.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7778	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]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: HEC, SQD, CLA, TDS, FES, LMG, LFA, BCR

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	0.36	0/2318	0.64	0/3148
2	B	0.48	0/1732	0.64	0/2360
3	C	0.29	0/979	0.55	0/1333
4	D	0.38	0/1238	0.62	0/1698
5	R	0.46	0/289	0.94	1/393 (0.3%)
6	G	0.42	0/228	0.60	0/313
7	L	0.39	0/244	0.61	0/329
8	M	0.42	0/248	0.64	0/335
9	N	0.56	0/237	0.57	0/321
All	All	0.40	0/7513	0.63	1/10230 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	71	PRO	CA-N-CD	-13.91	92.03	111.50

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	2266	0	2301	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1681	0	1692	105	0
3	C	955	0	922	67	0
4	D	1201	0	1256	88	0
5	R	283	0	291	13	0
6	G	224	0	248	9	0
7	L	242	0	286	12	0
8	M	247	0	263	19	0
9	N	231	0	230	19	0
10	A	43	0	30	4	0
10	B	129	0	95	8	0
11	B	27	0	35	3	0
12	B	20	0	42	2	0
13	C	4	0	0	1	0
14	D	65	0	72	5	0
15	D	30	0	38	2	0
16	D	53	0	79	3	0
16	L	42	0	54	4	0
17	R	33	0	29	1	0
18	B	2	0	0	0	0
All	All	7778	0	7963	386	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 25.

All (386) 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:31:ASN:HA	9:N:98:LEU:HD22	1.24	1.18
3:C:178:HIS:HB2	3:C:190:SER:HB2	1.34	1.10
2:B:50:THR:HG23	2:B:86:HIS:HD1	1.07	1.07
1:A:59:GLN:HE22	1:A:156:ARG:HG3	1.27	1.00
2:B:142:GLN:NE2	4:D:67:ASN:H	1.63	0.96
2:B:50:THR:CG2	2:B:86:HIS:HD1	1.82	0.93
4:D:118:ASN:ND2	4:D:120:PHE:H	1.67	0.93
3:C:92:ALA:H	3:C:185:GLY:HA2	1.33	0.92
3:C:158:GLN:HB2	3:C:167:ARG:HB3	1.49	0.92
2:B:61:THR:HA	2:B:177:GLN:HE22	1.36	0.91
1:A:247:GLN:HE21	1:A:248:ASN:H	1.20	0.89
1:A:116:GLY:HA2	1:A:118:VAL:HG13	1.55	0.88
1:A:2:PRO:HG3	10:A:900:HEC:HMB2	1.58	0.86
2:B:47:GLN:NE2	2:B:89:SER:HB3	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:THR:HG23	2:B:86:HIS:ND1	1.90	0.85
1:A:92:GLU:CD	1:A:92:GLU:H	1.83	0.82
4:D:118:ASN:HD22	4:D:119:LYS:N	1.77	0.82
1:A:248:ASN:C	1:A:248:ASN:HD22	1.83	0.82
2:B:152:THR:HG23	2:B:170:ARG:HE	1.43	0.81
2:B:124:MET:HE1	2:B:199:MET:HG3	1.61	0.81
4:D:117:ILE:HD12	4:D:118:ASN:H	1.47	0.80
4:D:117:ILE:HD12	4:D:118:ASN:N	1.97	0.79
2:B:31:ASN:HA	9:N:98:LEU:CD2	2.09	0.77
1:A:247:GLN:HE21	1:A:248:ASN:N	1.84	0.76
3:C:143:TRP:HE1	3:C:145:ALA:HB2	1.50	0.76
2:B:214:PRO:O	2:B:215:LEU:HB2	1.86	0.75
1:A:59:GLN:OE1	1:A:69:LEU:HG	1.87	0.75
2:B:32:ILE:N	9:N:98:LEU:HD13	2.01	0.75
2:B:119:VAL:HG13	4:D:109:ILE:HD11	1.69	0.75
1:A:73:MET:HG3	1:A:115:VAL:HG12	1.69	0.74
1:A:280:GLN:HE22	4:D:34:ASN:HD21	1.36	0.74
2:B:215:LEU:CD1	4:D:122:ASN:HD22	2.01	0.73
4:D:106:ALA:O	4:D:109:ILE:HG22	1.89	0.73
3:C:106:LEU:H	3:C:106:LEU:HD12	1.54	0.73
1:A:90:PRO:HD2	1:A:93:ILE:HD12	1.71	0.73
2:B:104:VAL:HG11	10:B:901:HEC:HMD2	1.71	0.72
1:A:247:GLN:NE2	1:A:248:ASN:H	1.89	0.71
8:M:92:SER:O	8:M:95:GLU:HB3	1.91	0.70
2:B:31:ASN:CA	9:N:98:LEU:HD22	2.14	0.70
1:A:3:VAL:O	1:A:7:GLN:HG3	1.90	0.69
3:C:182:ALA:O	3:C:186:LEU:HD12	1.93	0.69
4:D:81:PHE:HE2	14:D:910:CLA:H52	1.57	0.69
3:C:134:CYS:HB2	3:C:141:VAL:HG23	1.74	0.69
4:D:4:THR:HG22	4:D:5:LYS:H	1.56	0.69
2:B:47:GLN:HE21	2:B:89:SER:HB3	1.56	0.68
4:D:118:ASN:HD22	4:D:118:ASN:C	1.95	0.68
3:C:92:ALA:N	3:C:185:GLY:HA2	2.09	0.68
1:A:143:TYR:CE2	1:A:248:ASN:HB2	2.28	0.68
4:D:137:THR:HA	16:D:953:LMG:H242	1.76	0.68
1:A:60:VAL:HG12	1:A:167:ASN:ND2	2.10	0.68
2:B:152:THR:CG2	2:B:170:ARG:HE	2.07	0.68
1:A:59:GLN:HE22	1:A:156:ARG:CG	2.05	0.67
2:B:113:PRO:HB2	2:B:209:GLN:HE22	1.59	0.67
2:B:124:MET:CE	2:B:199:MET:HG3	2.23	0.67
2:B:215:LEU:HD12	4:D:122:ASN:HD22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:21:ILE:O	7:L:25:LEU:HB2	1.94	0.67
2:B:215:LEU:HG	4:D:125:ARG:HH12	1.60	0.66
1:A:27:ALA:HB3	1:A:236:GLY:HA2	1.76	0.66
1:A:53:TYR:HB3	1:A:154:ARG:HD2	1.77	0.66
1:A:27:ALA:HB2	1:A:233:ASN:ND2	2.10	0.66
2:B:154:VAL:HB	2:B:155:PRO:HD3	1.77	0.65
3:C:118:ILE:HD12	3:C:118:ILE:H	1.61	0.65
4:D:30:PRO:HG2	4:D:34:ASN:ND2	2.12	0.64
2:B:81:LEU:O	2:B:85:ILE:HG13	1.97	0.64
7:L:4:ILE:HD13	7:L:4:ILE:O	1.96	0.64
3:C:143:TRP:NE1	3:C:145:ALA:HB2	2.13	0.64
2:B:113:PRO:HB2	2:B:209:GLN:NE2	2.13	0.64
1:A:266:GLN:O	1:A:270:VAL:HG12	1.98	0.63
2:B:124:MET:HB3	10:B:901:HEC:HBB3	1.79	0.63
3:C:104:ARG:HD2	3:C:143:TRP:CE2	2.34	0.63
5:R:44:ILE:CG2	7:L:31:LEU:HD21	2.28	0.63
1:A:27:ALA:HB2	1:A:233:ASN:HD21	1.63	0.63
1:A:71:VAL:HG12	1:A:154:ARG:HB3	1.80	0.63
1:A:71:VAL:HG12	1:A:154:ARG:CB	2.29	0.62
4:D:104:VAL:HB	4:D:105:PRO:CD	2.30	0.62
3:C:104:ARG:HD2	3:C:143:TRP:CD2	2.35	0.61
3:C:103:ASP:HB3	3:C:119:VAL:CG2	2.30	0.61
4:D:85:PHE:HD2	4:D:147:SER:HB2	1.66	0.60
4:D:4:THR:HG22	4:D:5:LYS:N	2.15	0.60
4:D:95:LEU:HG	4:D:99:LEU:CD2	2.31	0.60
2:B:36:ILE:HG22	2:B:100:HIS:HB2	1.84	0.60
3:C:172:LEU:HD13	3:C:204:TRP:CG	2.36	0.60
4:D:95:LEU:HG	4:D:99:LEU:HD23	1.84	0.60
9:N:72:ILE:HG23	9:N:73:VAL:N	2.17	0.60
4:D:128:ILE:O	4:D:132:LEU:HD23	2.01	0.59
2:B:215:LEU:CG	4:D:125:ARG:HH12	2.15	0.59
3:C:141:VAL:HG22	3:C:152:CYS:HB2	1.83	0.59
1:A:36:PRO:O	1:A:244:ILE:HD12	2.02	0.59
3:C:83:LYS:HA	3:C:89:ASP:HA	1.85	0.59
1:A:143:TYR:CD2	1:A:248:ASN:HB2	2.37	0.59
8:M:89:ARG:HH21	8:M:93:LEU:HD21	1.68	0.59
1:A:60:VAL:HG12	1:A:167:ASN:HD22	1.66	0.59
1:A:2:PRO:HA	10:A:900:HEC:HBB2	1.84	0.59
2:B:151:VAL:HG13	15:D:920:TDS:HAT1	1.84	0.58
3:C:116:TYR:OH	3:C:142:PRO:HA	2.03	0.58
1:A:248:ASN:C	1:A:248:ASN:ND2	2.53	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:PRO:HA	4:D:15:LYS:HE3	1.85	0.58
4:D:158:GLY:O	4:D:159:LEU:HD23	2.04	0.58
2:B:150:ILE:HD11	3:C:139:CYS:SG	2.43	0.58
16:L:951:LMG:H112	8:M:69:THR:HG23	1.85	0.58
4:D:150:PRO:HD2	4:D:153:ILE:HD11	1.85	0.57
2:B:11:ARG:O	2:B:12:LEU:HD23	2.04	0.57
2:B:154:VAL:HA	3:C:137:LEU:HD11	1.85	0.57
4:D:88:LEU:HD22	15:D:920:TDS:HAI1	1.85	0.57
4:D:4:THR:HA	4:D:29:GLU:OE2	2.03	0.57
1:A:92:GLU:O	1:A:95:GLU:HB2	2.05	0.57
3:C:93:GLY:O	3:C:97:LYS:HG3	2.05	0.57
3:C:110:LEU:O	3:C:111:LYS:HB2	2.04	0.57
1:A:145:LYS:HD2	4:D:61:ALA:HB2	1.85	0.57
3:C:109:GLY:HA3	3:C:115:THR:OG1	2.05	0.57
1:A:285:ASN:OD1	1:A:287:HIS:HB2	2.04	0.57
16:D:953:LMG:H292	8:M:66:ILE:HD11	1.87	0.57
2:B:15:GLN:OE1	2:B:15:GLN:HA	2.05	0.56
2:B:102:PHE:HE1	6:G:14:VAL:HG13	1.70	0.56
2:B:47:GLN:HE21	2:B:89:SER:CB	2.17	0.56
3:C:136:HIS:NE2	3:C:137:LEU:HD22	2.20	0.56
2:B:120:THR:HG21	2:B:205:MET:CE	2.35	0.56
3:C:92:ALA:H	3:C:185:GLY:CA	2.13	0.55
3:C:100:LEU:O	3:C:119:VAL:HG11	2.06	0.55
2:B:121:GLY:O	10:B:901:HEC:HMC3	2.06	0.55
4:D:108:LEU:O	4:D:111:VAL:HG23	2.07	0.55
2:B:103:ARG:HA	6:G:21:LEU:HD11	1.88	0.55
4:D:93:ASN:HB2	4:D:96:LEU:HB3	1.87	0.55
4:D:16:ALA:O	4:D:19:ALA:HB3	2.07	0.55
2:B:104:VAL:CG1	10:B:901:HEC:HMD2	2.37	0.54
2:B:32:ILE:CA	9:N:98:LEU:HD13	2.36	0.54
2:B:152:THR:HG23	2:B:170:ARG:NE	2.17	0.54
3:C:120:THR:HG22	3:C:121:ALA:N	2.23	0.54
2:B:142:GLN:HE21	4:D:66:ALA:HA	1.73	0.54
6:G:13:LEU:HA	6:G:16:VAL:HG12	1.88	0.54
1:A:63:ASN:OD1	1:A:64:GLY:N	2.39	0.54
1:A:291:HIS:O	1:A:292:HIS:HB2	2.08	0.53
2:B:211:ILE:HG23	2:B:212:SER:O	2.07	0.53
3:C:118:ILE:HD12	3:C:118:ILE:N	2.22	0.53
4:D:91:VAL:HG11	4:D:96:LEU:HD12	1.90	0.53
9:N:95:ARG:HE	9:N:98:LEU:HD11	1.72	0.53
1:A:16:ASN:HD22	4:D:73:LEU:HD21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:TYR:OH	2:B:15:GLN:HG2	2.08	0.53
3:C:82:ALA:HB2	3:C:189:PHE:CD2	2.43	0.53
5:R:40:ASN:O	5:R:44:ILE:HG12	2.09	0.53
2:B:47:GLN:NE2	2:B:89:SER:CB	2.70	0.53
3:C:173:SER:O	3:C:204:TRP:HZ2	1.91	0.53
1:A:1:TYR:H3	1:A:4:PHE:HD2	1.57	0.53
2:B:72:ILE:HA	2:B:76:VAL:CG2	2.39	0.53
3:C:106:LEU:HD12	3:C:106:LEU:N	2.22	0.53
1:A:61:LEU:HD11	1:A:67:GLY:HA3	1.90	0.53
2:B:214:PRO:HD2	4:D:24:HIS:CE1	2.43	0.53
1:A:192:PHE:CD1	1:A:192:PHE:N	2.76	0.53
4:D:100:LEU:O	4:D:103:ALA:HB3	2.09	0.53
1:A:248:ASN:HD22	1:A:249:PRO:N	2.07	0.52
3:C:172:LEU:HD13	3:C:204:TRP:CD2	2.43	0.52
5:R:45:MET:HE2	5:R:45:MET:HA	1.91	0.52
1:A:59:GLN:NE2	1:A:156:ARG:HG3	2.09	0.52
1:A:268:LEU:HD13	5:R:48:ILE:HG22	1.90	0.52
1:A:248:ASN:ND2	1:A:250:ALA:H	2.08	0.52
3:C:143:TRP:HB2	3:C:150:PHE:CE1	2.45	0.52
4:D:108:LEU:C	4:D:110:THR:H	2.12	0.52
4:D:124:TYR:HE1	6:G:26:TYR:CA	2.23	0.52
1:A:44:VAL:HA	1:A:130:ILE:O	2.09	0.52
2:B:215:LEU:HD13	4:D:122:ASN:HD22	1.74	0.52
4:D:11:ASP:OD1	4:D:13:VAL:N	2.43	0.52
2:B:42:THR:O	2:B:46:VAL:HG23	2.09	0.52
8:M:73:MET:HA	8:M:76:MET:HE3	1.92	0.52
3:C:101:ALA:HA	3:C:119:VAL:CG1	2.40	0.51
1:A:32:GLU:HB2	1:A:50:GLU:HB2	1.92	0.51
3:C:103:ASP:O	3:C:118:ILE:HA	2.10	0.51
4:D:85:PHE:CD2	4:D:147:SER:HB2	2.44	0.51
8:M:86:VAL:O	8:M:90:VAL:HG23	2.11	0.51
7:L:24:GLY:O	7:L:28:VAL:HB	2.08	0.51
2:B:188:THR:HG22	10:B:902:HEC:HMB2	1.92	0.51
2:B:31:ASN:C	9:N:98:LEU:HD13	2.30	0.51
4:D:118:ASN:HD21	4:D:120:PHE:HD1	1.57	0.51
3:C:192:TRP:HB3	3:C:205:TRP:HE1	1.75	0.51
5:R:45:MET:HA	5:R:45:MET:CE	2.40	0.50
1:A:51:LEU:N	1:A:51:LEU:HD12	2.26	0.50
2:B:130:SER:HA	14:D:910:CLA:H143	1.92	0.50
4:D:75:ILE:HG23	4:D:75:ILE:O	2.12	0.50
5:R:55:LEU:HB2	5:R:56:PRO:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:PHE:O	2:B:48:VAL:HG23	2.12	0.50
3:C:116:TYR:HH	3:C:142:PRO:HA	1.76	0.50
4:D:110:THR:HG22	4:D:114:ILE:HG12	1.93	0.50
2:B:149:LYS:O	2:B:152:THR:HG22	2.12	0.50
3:C:126:GLU:HG3	3:C:128:TYR:H	1.77	0.50
1:A:182:ILE:HG21	1:A:214:LEU:HD13	1.92	0.49
1:A:21:CYS:O	1:A:25:HIS:HB2	2.13	0.49
1:A:223:GLN:O	1:A:226:GLN:HB2	2.12	0.49
2:B:72:ILE:HA	2:B:76:VAL:HG23	1.92	0.49
3:C:155:HIS:HB2	13:C:210:FES:S1	2.52	0.49
8:M:90:VAL:O	8:M:94:VAL:HG23	2.12	0.49
8:M:94:VAL:HG12	8:M:94:VAL:O	2.11	0.49
2:B:142:GLN:NE2	4:D:67:ASN:N	2.46	0.49
8:M:93:LEU:C	8:M:95:GLU:H	2.14	0.49
14:D:910:CLA:HHC	14:D:910:CLA:HBB1	1.93	0.49
1:A:37:GLN:HB2	16:L:951:LMG:HC4	1.94	0.49
2:B:103:ARG:NH1	10:B:901:HEC:O1A	2.46	0.49
1:A:2:PRO:HG3	10:A:900:HEC:CMB	2.37	0.49
4:D:118:ASN:ND2	4:D:118:ASN:C	2.63	0.49
1:A:108:GLU:OE2	1:A:108:GLU:N	2.45	0.49
2:B:142:GLN:HE21	4:D:67:ASN:H	1.57	0.49
4:D:137:THR:HA	16:D:953:LMG:C24	2.43	0.49
2:B:215:LEU:CD1	4:D:125:ARG:HH12	2.26	0.48
4:D:107:GLY:O	4:D:110:THR:HB	2.12	0.48
2:B:120:THR:HG21	2:B:205:MET:HE2	1.93	0.48
4:D:124:TYR:CE1	6:G:26:TYR:HA	2.48	0.48
1:A:274:LYS:HE3	9:N:93:TRP:NE1	2.29	0.48
3:C:96:LEU:HD11	3:C:124:THR:HA	1.96	0.48
4:D:81:PHE:CE2	14:D:910:CLA:H52	2.43	0.48
3:C:81:ALA:HA	3:C:188:THR:HG22	1.95	0.48
3:C:199:THR:C	3:C:201:LEU:H	2.17	0.48
2:B:61:THR:HA	2:B:177:GLN:NE2	2.17	0.48
3:C:160:ASN:HD21	3:C:164:LYS:HB3	1.79	0.48
1:A:16:ASN:HD22	4:D:73:LEU:CD2	2.27	0.48
2:B:7:TRP:CZ2	2:B:11:ARG:NH1	2.81	0.48
3:C:175:ALA:HA	3:C:205:TRP:CE3	2.48	0.48
8:M:73:MET:SD	8:M:76:MET:HE1	2.53	0.48
1:A:226:GLN:CG	1:A:227:PRO:HD2	2.44	0.48
2:B:112:ARG:HA	2:B:115:GLU:OE2	2.14	0.48
11:B:904:BCR:H15C	8:M:81:LEU:HD11	1.96	0.47
1:A:208:ILE:HD12	1:A:214:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:ARG:HA	6:G:21:LEU:CD1	2.44	0.47
1:A:53:TYR:CZ	1:A:55:LYS:HG2	2.49	0.47
2:B:62:VAL:HG13	2:B:140:TRP:NE1	2.29	0.47
2:B:113:PRO:HA	2:B:115:GLU:OE2	2.14	0.47
1:A:153:ASN:CG	1:A:154:ARG:N	2.66	0.47
8:M:89:ARG:NH2	8:M:93:LEU:HD21	2.29	0.47
7:L:1:MET:O	7:L:4:ILE:HG22	2.15	0.47
8:M:93:LEU:C	8:M:95:GLU:N	2.67	0.47
1:A:18:ARG:HB2	4:D:73:LEU:HD11	1.96	0.47
1:A:102:TYR:CZ	1:A:128:VAL:HG22	2.50	0.47
2:B:47:GLN:HA	2:B:50:THR:HG22	1.97	0.47
8:M:92:SER:O	8:M:95:GLU:CB	2.61	0.47
10:B:903:HEC:HBC2	4:D:44:ILE:HD11	1.97	0.46
1:A:133:PRO:CG	1:A:141:VAL:HG11	2.46	0.46
1:A:170:ILE:HD11	1:A:231:ASN:HB2	1.98	0.46
2:B:47:GLN:HE22	2:B:89:SER:HB3	1.75	0.46
1:A:1:TYR:O	1:A:4:PHE:HB2	2.15	0.46
2:B:54:MET:CE	2:B:83:ARG:HB2	2.46	0.46
1:A:83:LEU:HD12	1:A:129:PRO:O	2.15	0.46
1:A:262:VAL:HG13	4:D:45:LEU:HB3	1.97	0.46
3:C:151:LYS:HG2	3:C:158:GLN:HG2	1.97	0.46
9:N:69:GLU:OE1	9:N:69:GLU:N	2.42	0.46
2:B:82:ILE:HG13	5:R:67:PHE:CD1	2.50	0.46
1:A:83:LEU:HD22	1:A:102:TYR:HB2	1.97	0.46
3:C:122:ASP:O	3:C:123:SER:C	2.52	0.46
1:A:52:PRO:O	1:A:154:ARG:NH1	2.48	0.46
2:B:142:GLN:HE21	2:B:142:GLN:HA	1.80	0.46
2:B:150:ILE:HD11	3:C:154:CYS:SG	2.56	0.46
6:G:14:VAL:HB	6:G:15:PRO:CD	2.46	0.46
3:C:103:ASP:H	3:C:119:VAL:HB	1.81	0.46
8:M:62:GLU:O	8:M:65:PHE:HB3	2.16	0.46
3:C:125:ILE:HD12	3:C:125:ILE:N	2.31	0.46
2:B:114:ARG:CZ	2:B:212:SER:HA	2.46	0.46
1:A:16:ASN:ND2	4:D:73:LEU:HD21	2.32	0.45
1:A:57:VAL:HG12	1:A:58:LYS:N	2.31	0.45
3:C:141:VAL:CG1	3:C:150:PHE:HB3	2.46	0.45
8:M:93:LEU:O	8:M:95:GLU:N	2.49	0.45
5:R:45:MET:HE3	5:R:48:ILE:HD12	1.99	0.45
1:A:60:VAL:CG1	1:A:167:ASN:HD22	2.27	0.45
1:A:279:VAL:HG21	5:R:42:ARG:HD3	1.98	0.45
4:D:14:LEU:CD1	4:D:18:LEU:HD13	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:HG12	1:A:230:ASN:O	2.16	0.45
2:B:123:ILE:HD13	2:B:198:PHE:CE2	2.52	0.45
2:B:200:LEU:HD22	2:B:204:LEU:HG	1.99	0.45
4:D:40:PHE:HB2	4:D:41:PRO:HD3	1.99	0.45
9:N:72:ILE:CG2	9:N:73:VAL:N	2.79	0.45
1:A:226:GLN:HG3	1:A:227:PRO:HD2	1.99	0.45
2:B:96:MET:SD	16:L:951:LMG:H232	2.56	0.45
1:A:77:LEU:HD23	1:A:148:ILE:HG23	1.99	0.45
2:B:142:GLN:NE2	2:B:142:GLN:HA	2.32	0.45
3:C:91:LYS:HB2	3:C:94:GLU:HB2	1.99	0.45
7:L:26:LEU:O	7:L:30:LYS:HA	2.17	0.45
2:B:29:HIS:CG	2:B:214:PRO:HA	2.52	0.45
3:C:164:LYS:O	3:C:166:VAL:HG23	2.17	0.45
7:L:29:VAL:O	7:L:29:VAL:HG12	2.17	0.45
8:M:72:THR:HG22	8:M:76:MET:HE2	1.99	0.45
2:B:69:VAL:HG21	2:B:139:PRO:HB3	1.99	0.45
4:D:82:TYR:HB2	4:D:83:PRO:HD3	1.99	0.45
4:D:84:VAL:HG11	4:D:101:MET:SD	2.57	0.45
1:A:156:ARG:HH12	1:A:167:ASN:ND2	2.15	0.44
1:A:29:LYS:HG3	1:A:236:GLY:HA3	1.99	0.44
1:A:274:LYS:HE3	9:N:93:TRP:CE2	2.52	0.44
1:A:6:GLN:HE21	1:A:105:TYR:HA	1.82	0.44
2:B:54:MET:HE1	2:B:83:ARG:HB2	1.99	0.44
2:B:81:LEU:CD2	12:B:960:LFA:H121	2.48	0.44
2:B:148:VAL:O	2:B:152:THR:HG22	2.17	0.44
12:B:960:LFA:H101	4:D:52:ILE:HD13	1.99	0.44
8:M:89:ARG:O	8:M:92:SER:HB3	2.18	0.44
1:A:20:VAL:C	1:A:22:ALA:N	2.70	0.44
6:G:13:LEU:HA	6:G:16:VAL:CG1	2.47	0.44
1:A:232:PRO:O	1:A:234:VAL:HG13	2.18	0.44
3:C:141:VAL:HG22	3:C:152:CYS:CB	2.46	0.44
5:R:45:MET:HE2	5:R:48:ILE:HB	1.99	0.44
5:R:39:MET:O	5:R:42:ARG:HB2	2.17	0.44
4:D:38:TYR:O	4:D:41:PRO:HD2	2.18	0.44
11:B:904:BCR:HC41	4:D:43:VAL:HG13	2.00	0.43
2:B:102:PHE:CE1	6:G:14:VAL:HG13	2.53	0.43
1:A:247:GLN:HE21	1:A:247:GLN:CA	2.30	0.43
2:B:97:MET:SD	2:B:125:ALA:HA	2.58	0.43
3:C:130:LEU:HD23	3:C:176:LEU:HD23	2.00	0.43
1:A:133:PRO:HG2	1:A:141:VAL:HG11	2.00	0.43
7:L:1:MET:O	7:L:2:LEU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:HIS:ND1	1:A:292:HIS:CD2	2.87	0.43
4:D:104:VAL:HG11	14:D:910:CLA:H42	2.01	0.43
4:D:118:ASN:ND2	4:D:120:PHE:CD1	2.82	0.43
1:A:210:ALA:O	1:A:212:PRO:HD2	2.19	0.43
2:B:124:MET:HE2	10:B:901:HEC:CBB	2.49	0.42
3:C:119:VAL:HA	3:C:124:THR:O	2.19	0.42
3:C:149:LYS:HB2	3:C:159:TYR:O	2.19	0.42
1:A:19:ILE:N	1:A:239:GLN:OE1	2.35	0.42
1:A:145:LYS:HD3	1:A:243:GLU:CD	2.40	0.42
2:B:118:TRP:HZ2	4:D:108:LEU:HD22	1.83	0.42
2:B:178:ALA:O	2:B:182:ARG:HG3	2.18	0.42
4:D:25:ASN:N	4:D:25:ASN:HD22	2.17	0.42
4:D:87:ILE:O	4:D:90:VAL:HG12	2.19	0.42
4:D:118:ASN:HD22	4:D:120:PHE:H	1.58	0.42
2:B:152:THR:CG2	2:B:170:ARG:NE	2.79	0.42
4:D:104:VAL:CB	4:D:105:PRO:CD	2.97	0.42
2:B:118:TRP:CZ2	4:D:108:LEU:HD22	2.55	0.42
2:B:152:THR:HG23	2:B:170:ARG:HH21	1.85	0.42
7:L:3:THR:HG22	9:N:74:GLN:NE2	2.34	0.42
2:B:32:ILE:HD11	11:B:904:BCR:H333	2.00	0.42
2:B:215:LEU:HD12	4:D:125:ARG:NH1	2.34	0.42
3:C:91:LYS:HD2	3:C:91:LYS:N	2.35	0.42
3:C:134:CYS:HB2	3:C:141:VAL:CG2	2.48	0.42
9:N:97:GLY:O	9:N:98:LEU:HB2	2.20	0.42
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.89	0.42
2:B:211:ILE:HG13	2:B:212:SER:N	2.35	0.42
4:D:8:ASP:C	4:D:10:SER:H	2.23	0.42
1:A:4:PHE:CD1	1:A:161:PRO:HG2	2.55	0.42
4:D:96:LEU:C	4:D:96:LEU:HD13	2.40	0.42
1:A:35:VAL:HG12	1:A:47:ALA:HA	2.02	0.42
1:A:215:ILE:HG13	1:A:228:LEU:O	2.20	0.42
2:B:138:LEU:HA	2:B:138:LEU:HD23	1.81	0.42
3:C:117:LEU:HD13	3:C:189:PHE:HZ	1.84	0.42
3:C:141:VAL:HG12	3:C:150:PHE:HB3	2.01	0.42
1:A:38:ALA:HB2	1:A:245:VAL:HB	2.02	0.41
1:A:210:ALA:C	1:A:212:PRO:HD2	2.39	0.41
2:B:195:THR:O	2:B:199:MET:HB2	2.19	0.41
3:C:80:GLN:O	3:C:188:THR:HB	2.19	0.41
7:L:11:LEU:HD13	8:M:83:ILE:HD11	2.02	0.41
3:C:132:ALA:HB1	3:C:140:VAL:HG13	2.02	0.41
1:A:62:ALA:HA	1:A:156:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:THR:HG21	2:B:205:MET:HE1	2.02	0.41
2:B:146:TRP:HH2	3:C:140:VAL:HG23	1.85	0.41
3:C:103:ASP:HB3	3:C:119:VAL:HG23	2.01	0.41
3:C:136:HIS:HE1	3:C:155:HIS:CG	2.37	0.41
4:D:24:HIS:HA	4:D:27:TYR:CE2	2.55	0.41
9:N:86:PHE:O	9:N:89:SER:HB2	2.19	0.41
1:A:43:THR:HG22	1:A:44:VAL:N	2.36	0.41
1:A:75:LEU:HD21	1:A:148:ILE:CG2	2.51	0.41
1:A:148:ILE:HB	1:A:242:THR:HG23	2.02	0.41
1:A:276:PHE:HE1	5:R:42:ARG:NH1	2.17	0.41
4:D:11:ASP:OD1	4:D:13:VAL:HG23	2.21	0.41
9:N:97:GLY:O	9:N:98:LEU:CB	2.68	0.41
1:A:185:LEU:O	1:A:186:SER:C	2.59	0.41
1:A:215:ILE:HD11	1:A:227:PRO:O	2.21	0.41
2:B:43:CYS:O	2:B:47:GLN:HG2	2.21	0.41
2:B:134:THR:HG22	2:B:183:PHE:CD2	2.56	0.41
3:C:165:VAL:O	3:C:165:VAL:HG13	2.21	0.41
4:D:126:ARG:N	4:D:127:PRO:HD3	2.36	0.41
4:D:135:LEU:O	4:D:139:VAL:HG23	2.21	0.41
3:C:106:LEU:H	3:C:106:LEU:CD1	2.30	0.41
4:D:25:ASN:H	4:D:25:ASN:ND2	2.18	0.41
4:D:37:LEU:HD11	17:R:950:SQD:H261	2.03	0.41
1:A:61:LEU:O	1:A:167:ASN:ND2	2.54	0.41
1:A:223:GLN:O	1:A:226:GLN:CB	2.68	0.41
2:B:111:LYS:O	2:B:113:PRO:O	2.38	0.41
2:B:114:ARG:O	2:B:117:THR:HB	2.21	0.41
2:B:128:THR:O	2:B:131:PHE:HB2	2.21	0.41
3:C:178:HIS:CB	3:C:190:SER:HB2	2.25	0.41
4:D:90:VAL:HG21	4:D:155:LEU:HG	2.02	0.41
4:D:91:VAL:CG1	4:D:96:LEU:HD12	2.51	0.41
7:L:18:THR:HG1	9:N:86:PHE:HZ	1.64	0.41
9:N:69:GLU:HB3	9:N:70:PRO:HD2	2.02	0.41
2:B:113:PRO:HB2	2:B:114:ARG:H	1.68	0.41
5:R:38:ASP:O	5:R:39:MET:C	2.59	0.41
1:A:161:PRO:HG3	10:A:900:HEC:HBC2	2.01	0.40
2:B:99:LEU:O	2:B:102:PHE:HB2	2.21	0.40
4:D:4:THR:CG2	4:D:5:LYS:N	2.83	0.40
4:D:47:THR:HG23	16:L:951:LMG:C25	2.50	0.40
1:A:165:LYS:HB3	1:A:169:THR:HG21	2.04	0.40
4:D:89:ARG:NH2	4:D:151:ILE:HG12	2.35	0.40
4:D:98:VAL:O	4:D:101:MET:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:32:ILE:O	7:L:32:ILE:HG22	2.20	0.40
1:A:252:ILE:HD13	9:N:73:VAL:HA	2.02	0.40
2:B:189:PHE:C	2:B:192:PRO:HD2	2.42	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	290/292 (99%)	263 (91%)	21 (7%)	6 (2%)	7	30
2	B	210/215 (98%)	179 (85%)	29 (14%)	2 (1%)	15	49
3	C	122/127 (96%)	96 (79%)	22 (18%)	4 (3%)	4	21
4	D	154/159 (97%)	134 (87%)	15 (10%)	5 (3%)	4	22
5	R	37/49 (76%)	32 (86%)	5 (14%)	0	100	100
6	G	28/37 (76%)	24 (86%)	4 (14%)	0	100	100
7	L	30/32 (94%)	25 (83%)	5 (17%)	0	100	100
8	M	32/39 (82%)	31 (97%)	0	1 (3%)	4	23
9	N	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
All	All	932/981 (95%)	811 (87%)	103 (11%)	18 (2%)	8	33

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	89	ASP
1	A	140	ASN
1	A	165	LYS
1	A	198	LYS
3	C	100	LEU

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Mol	Chain	Res	Type
4	D	104	VAL
1	A	186	SER
2	B	113	PRO
3	C	120	THR
4	D	109	ILE
4	D	114	ILE
1	A	137	LYS
2	B	154	VAL
3	C	123	SER
1	A	64	GLY
4	D	92	PRO
8	M	94	VAL
4	D	151	ILE

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	246/246 (100%)	233 (95%)	13 (5%)	22	54
2	B	179/182 (98%)	171 (96%)	8 (4%)	27	60
3	C	99/100 (99%)	96 (97%)	3 (3%)	41	71
4	D	131/134 (98%)	126 (96%)	5 (4%)	33	66
5	R	30/32 (94%)	27 (90%)	3 (10%)	7	28
6	G	25/30 (83%)	25 (100%)	0	100	100
7	L	27/27 (100%)	23 (85%)	4 (15%)	3	13
8	M	26/29 (90%)	24 (92%)	2 (8%)	13	41
9	N	24/24 (100%)	24 (100%)	0	100	100
All	All	787/804 (98%)	749 (95%)	38 (5%)	25	58

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASP

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Mol	Chain	Res	Type
1	A	73	MET
1	A	75	LEU
1	A	140	ASN
1	A	154	ARG
1	A	168	ASN
1	A	192	PHE
1	A	207	LYS
1	A	225	ASP
1	A	247	GLN
1	A	248	ASN
1	A	264	LEU
1	A	270	VAL
2	B	19	ASP
2	B	22	THR
2	B	75	ASP
2	B	87	ARG
2	B	103	ARG
2	B	161	VAL
2	B	193	LEU
2	B	200	LEU
3	C	91	LYS
3	C	98	THR
3	C	137	LEU
4	D	18	LEU
4	D	25	ASN
4	D	90	VAL
4	D	108	LEU
4	D	118	ASN
5	R	38	ASP
5	R	45	MET
5	R	71	PRO
7	L	2	LEU
7	L	3	THR
7	L	4	ILE
7	L	11	LEU
8	M	62	GLU
8	M	66	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN

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Mol	Chain	Res	Type
1	A	28	GLN
1	A	59	GLN
1	A	70	ASN
1	A	168	ASN
1	A	247	GLN
1	A	248	ASN
2	B	31	ASN
2	B	47	GLN
2	B	142	GLN
2	B	209	GLN
3	C	80	GLN
3	C	148	ASN
4	D	25	ASN
4	D	34	ASN
4	D	118	ASN
4	D	121	GLN
5	R	43	ASN
9	N	74	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)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
16	LMG	D	953	-	53,53,55	1.39	8 (15%)	61,61,63	1.46	6 (9%)
17	SQD	R	950	-	32,33,54	2.07	9 (28%)	41,44,65	3.06	11 (26%)
11	BCR	B	904	-	27,27,41	1.56	5 (18%)	34,35,56	1.93	11 (32%)
10	HEC	B	903	18,2	32,50,50	1.98	7 (21%)	24,82,82	2.25	9 (37%)
13	FES	C	210	3	0,4,4	-	-	-		
16	LMG	L	951	-	42,42,55	1.35	7 (16%)	50,50,63	1.50	5 (10%)
15	TDS	D	920	-	28,31,31	2.46	11 (39%)	35,40,40	2.62	14 (40%)
14	CLA	D	910	-	65,73,73	1.55	12 (18%)	76,113,113	1.93	11 (14%)
12	LFA	B	960	-	19,19,19	0.43	0	18,18,18	0.62	0
10	HEC	B	902	2	32,50,50	1.59	6 (18%)	24,82,82	1.58	5 (20%)
10	HEC	B	901	2	32,50,50	1.76	5 (15%)	24,82,82	1.50	4 (16%)
10	HEC	A	900	1	32,50,50	2.02	10 (31%)	24,82,82	2.08	8 (33%)

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
16	LMG	D	953	-	-	9/48/68/70	0/1/1/1
17	SQD	R	950	-	-	10/28/48/69	0/1/1/1
10	HEC	B	903	18,2	-	3/10/54/54	-
11	BCR	B	904	-	-	2/21/38/63	0/1/1/2
16	LMG	L	951	-	-	8/37/57/70	0/1/1/1
13	FES	C	210	3	-	-	0/1/1/1
15	TDS	D	920	-	-	6/16/17/17	0/2/2/2
14	CLA	D	910	-	2/2/15/20	9/37/115/115	-
12	LFA	B	960	-	-	11/17/17/17	-
10	HEC	B	902	2	-	4/10/54/54	-
10	HEC	B	901	2	-	3/10/54/54	-
10	HEC	A	900	1	-	3/10/54/54	-

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	950	SQD	C4-C3	6.81	1.69	1.52
10	A	900	HEC	C2B-C3B	-5.63	1.34	1.40
10	B	903	HEC	C2B-C3B	-5.55	1.35	1.40
10	A	900	HEC	C3C-C2C	-5.50	1.35	1.40
15	D	920	TDS	OAO-CAP	4.97	1.42	1.35
10	B	903	HEC	C3C-C2C	-4.95	1.35	1.40
10	B	901	HEC	CBB-CAB	-4.77	1.31	1.49
15	D	920	TDS	CAD-CAL	4.52	1.47	1.38
11	B	904	BCR	C1-C6	4.47	1.59	1.53
14	D	910	CLA	O2D-CGD	4.41	1.44	1.33
15	D	920	TDS	CAH-CAP	4.32	1.44	1.39
15	D	920	TDS	OAK-CAL	4.29	1.44	1.37
10	B	901	HEC	C2B-C3B	-4.28	1.36	1.40
15	D	920	TDS	OAB-CAE	4.27	1.44	1.36
10	B	902	HEC	CBB-CAB	-4.22	1.33	1.49
15	D	920	TDS	OAO-CAN	4.19	1.43	1.36
14	D	910	CLA	MG-NA	4.18	2.16	2.06
14	D	910	CLA	C4B-NB	4.11	1.38	1.35
17	R	950	SQD	O7-S	4.08	1.57	1.45
10	B	902	HEC	CBC-CAC	-4.05	1.34	1.49
16	L	951	LMG	O1-C7	-3.99	1.36	1.43
10	B	901	HEC	CBC-CAC	-3.86	1.35	1.49
16	D	953	LMG	C4-C5	3.80	1.61	1.53
16	D	953	LMG	O8-C28	3.79	1.44	1.33
16	L	951	LMG	O7-C8	-3.65	1.37	1.46
14	D	910	CLA	C1B-NB	3.63	1.38	1.35
10	B	903	HEC	C4B-C3B	3.55	1.49	1.43
15	D	920	TDS	CAH-CAG	3.46	1.51	1.41
11	B	904	BCR	C2-C1	3.32	1.61	1.54
16	D	953	LMG	O6-C1	3.27	1.50	1.41
14	D	910	CLA	CMC-C2C	3.24	1.57	1.50
17	R	950	SQD	O47-C7	3.21	1.43	1.34
15	D	920	TDS	CAL-CAM	3.17	1.44	1.40
16	D	953	LMG	O7-C10	3.10	1.43	1.34
10	B	903	HEC	C1B-NB	3.10	1.42	1.36
14	D	910	CLA	MG-NC	3.08	2.13	2.06
10	B	901	HEC	C3C-C4C	3.04	1.48	1.43
16	L	951	LMG	O8-C28	3.00	1.42	1.33
15	D	920	TDS	CAD-CAE	2.95	1.46	1.37
16	D	953	LMG	C3-C2	2.94	1.59	1.52
17	R	950	SQD	O48-C23	2.93	1.41	1.33
17	R	950	SQD	O5-C5	2.88	1.51	1.44
15	D	920	TDS	CAF-CAN	2.87	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	910	CLA	C2-C3	2.86	1.39	1.33
11	B	904	BCR	C5-C6	2.83	1.39	1.34
10	B	903	HEC	CMD-C2D	2.80	1.57	1.51
17	R	950	SQD	O6-C44	-2.79	1.38	1.43
10	A	900	HEC	CMD-C2D	2.77	1.57	1.51
16	D	953	LMG	O6-C5	2.76	1.51	1.44
14	D	910	CLA	O2A-CGA	2.75	1.41	1.33
15	D	920	TDS	CAE-CAF	2.72	1.48	1.42
16	L	951	LMG	O6-C1	2.69	1.48	1.41
10	A	900	HEC	C3A-C4A	2.69	1.48	1.42
14	D	910	CLA	CHC-C1C	2.59	1.41	1.35
10	B	901	HEC	CBA-CGA	2.57	1.56	1.50
17	R	950	SQD	C1-C2	2.55	1.59	1.52
16	L	951	LMG	C4-C3	2.53	1.58	1.52
14	D	910	CLA	O1D-CGD	2.51	1.27	1.21
10	A	900	HEC	C1B-NB	2.43	1.41	1.36
17	R	950	SQD	O3-C3	2.43	1.48	1.43
11	B	904	BCR	C14-C13	2.43	1.39	1.35
10	A	900	HEC	CBB-CAB	2.41	1.58	1.49
10	B	903	HEC	CBB-CAB	2.41	1.58	1.49
16	L	951	LMG	O7-C10	2.35	1.40	1.34
10	B	902	HEC	C3C-C4C	2.31	1.47	1.43
17	R	950	SQD	O8-S	2.29	1.55	1.47
16	D	953	LMG	C9-C8	2.28	1.57	1.50
10	B	902	HEC	C2A-C1A	2.28	1.47	1.42
10	A	900	HEC	CAD-C3D	-2.23	1.48	1.52
10	B	903	HEC	C3A-C4A	2.21	1.47	1.42
16	D	953	LMG	C4-C3	2.20	1.57	1.52
10	B	902	HEC	C3A-C4A	2.17	1.47	1.42
10	A	900	HEC	C4B-C3B	2.15	1.47	1.43
10	A	900	HEC	CAA-C2A	2.13	1.56	1.52
14	D	910	CLA	C5-C3	2.09	1.55	1.51
11	B	904	BCR	C21-C20	-2.06	1.41	1.49
10	A	900	HEC	C1B-CHB	-2.04	1.35	1.41
10	B	902	HEC	C2B-C3B	-2.02	1.38	1.40
14	D	910	CLA	CMD-C2D	2.02	1.55	1.50
16	L	951	LMG	C4-C5	2.01	1.57	1.53

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	D	910	CLA	C4A-NA-C1A	12.42	112.29	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	920	TDS	CAQ-CAP-CAH	9.29	133.55	120.39
17	R	950	SQD	O7-S-C6	8.91	117.53	106.94
17	R	950	SQD	O5-C1-O6	8.66	130.49	109.97
17	R	950	SQD	O6-C1-C2	7.27	119.65	108.30
17	R	950	SQD	O8-S-C6	-7.22	94.23	105.74
15	D	920	TDS	CAR-CAQ-CAP	6.82	128.97	112.79
16	L	951	LMG	C30-C29-C28	6.59	137.60	113.62
16	D	953	LMG	C30-C29-C28	6.27	136.41	113.62
17	R	950	SQD	C25-C24-C23	6.07	135.70	113.62
11	B	904	BCR	C33-C5-C6	5.43	130.62	124.53
10	A	900	HEC	C1D-C2D-C3D	5.32	110.70	107.00
10	B	903	HEC	CMD-C2D-C1D	-5.20	120.47	128.46
10	A	900	HEC	CMD-C2D-C1D	-5.11	120.61	128.46
10	B	903	HEC	C1D-C2D-C3D	5.06	110.52	107.00
16	D	953	LMG	C7-O1-C1	4.50	122.54	113.74
10	B	903	HEC	CBA-CAA-C2A	-4.42	105.15	112.60
16	L	951	LMG	C12-C11-C10	-3.79	99.83	113.62
11	B	904	BCR	C33-C5-C4	-3.78	106.36	113.62
15	D	920	TDS	OAO-CAP-CAQ	-3.78	107.43	111.91
14	D	910	CLA	O2D-CGD-CBD	3.71	117.86	111.27
14	D	910	CLA	O2A-CGA-CBA	3.61	123.24	111.91
17	R	950	SQD	O48-C23-C24	3.48	122.82	111.91
10	B	903	HEC	CMB-C2B-C1B	-3.47	123.14	128.46
17	R	950	SQD	O3-C3-C2	-3.45	102.37	110.35
11	B	904	BCR	C2-C1-C6	3.45	115.79	110.48
10	B	902	HEC	CMC-C2C-C3C	3.35	129.76	125.82
16	D	953	LMG	O8-C28-C29	3.22	122.00	111.91
14	D	910	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
17	R	950	SQD	C44-O6-C1	3.16	119.91	113.74
10	B	901	HEC	CMC-C2C-C3C	3.09	129.45	125.82
11	B	904	BCR	C1-C6-C5	-3.06	118.31	122.61
11	B	904	BCR	C8-C7-C6	3.04	135.74	127.20
10	A	900	HEC	CMB-C2B-C1B	-3.03	123.80	128.46
14	D	910	CLA	C1-C2-C3	2.99	131.22	126.04
15	D	920	TDS	OAO-CAN-CAM	2.95	119.82	116.12
10	B	902	HEC	CMC-C2C-C1C	-2.94	123.95	128.46
16	D	953	LMG	O7-C10-C11	2.93	117.81	111.50
10	A	900	HEC	CMC-C2C-C3C	2.88	129.20	125.82
17	R	950	SQD	O5-C5-C4	2.87	114.91	109.69
10	B	902	HEC	CMB-C2B-C3B	2.87	129.19	125.82
15	D	920	TDS	CAI-CAH-CAP	2.86	126.39	122.30
10	B	901	HEC	CAA-CBA-CGA	2.84	121.72	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	920	TDS	CAY-CAZ-CBA	2.81	128.70	114.42
15	D	920	TDS	CAI-CAH-CAG	-2.81	115.38	120.40
10	B	901	HEC	CMC-C2C-C1C	-2.78	124.20	128.46
16	L	951	LMG	O8-C28-C29	2.76	120.58	111.91
10	A	900	HEC	CMB-C2B-C3B	2.71	129.01	125.82
10	B	903	HEC	CMB-C2B-C3B	2.67	128.96	125.82
17	R	950	SQD	O4-C4-C5	2.57	115.69	109.30
15	D	920	TDS	CAV-CAW-CAX	2.54	127.31	114.42
11	B	904	BCR	C32-C1-C6	2.52	114.38	110.30
10	A	900	HEC	CMA-C3A-C2A	2.49	129.65	124.94
17	R	950	SQD	O47-C7-C8	2.46	117.65	110.80
15	D	920	TDS	CAJ-OAK-CAL	2.43	121.20	117.53
10	B	903	HEC	CMA-C3A-C2A	2.43	129.53	124.94
10	B	903	HEC	CMC-C2C-C3C	2.41	128.65	125.82
14	D	910	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
10	B	903	HEC	CMC-C2C-C1C	-2.36	124.83	128.46
10	A	900	HEC	CBD-CAD-C3D	-2.36	108.60	112.62
15	D	920	TDS	CAW-CAX-CAY	2.35	126.37	114.42
15	D	920	TDS	CAD-CAL-CAM	-2.32	118.32	120.60
10	A	900	HEC	CMC-C2C-C1C	-2.29	124.94	128.46
10	B	902	HEC	CMD-C2D-C1D	-2.29	124.94	128.46
14	D	910	CLA	C4D-CHA-C1A	2.29	124.04	121.25
16	L	951	LMG	C21-C20-C19	-2.28	102.86	114.42
10	B	901	HEC	CMB-C2B-C3B	2.26	128.47	125.82
16	D	953	LMG	C12-C11-C10	-2.22	105.54	113.62
11	B	904	BCR	C16-C17-C18	2.22	130.48	127.31
14	D	910	CLA	CHD-C1D-ND	-2.22	122.42	124.45
15	D	920	TDS	CAE-CAF-CAN	2.21	119.79	115.15
11	B	904	BCR	C36-C18-C19	2.18	121.51	118.08
10	B	903	HEC	CMD-C2D-C3D	2.16	129.01	124.94
14	D	910	CLA	C2A-C1A-CHA	2.12	127.56	123.86
14	D	910	CLA	CMB-C2B-C3B	2.10	128.61	124.68
11	B	904	BCR	C11-C10-C9	2.09	130.29	127.31
15	D	920	TDS	CBC-CBB-CBA	2.07	129.16	113.42
10	B	902	HEC	CMB-C2B-C1B	-2.07	125.28	128.46
15	D	920	TDS	CAA-OAB-CAE	2.06	120.63	117.75
11	B	904	BCR	C1-C6-C7	2.05	121.57	115.78
16	L	951	LMG	C14-C13-C12	-2.04	104.05	114.42
14	D	910	CLA	CED-O2D-CGD	2.04	120.56	115.94
16	D	953	LMG	C14-C13-C12	-2.02	104.18	114.42
11	B	904	BCR	C7-C8-C9	2.01	129.27	126.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	D	910	CLA	C8
14	D	910	CLA	ND

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	901	HEC	C2A-CAA-CBA-CGA
15	D	920	TDS	CAH-CAP-CAQ-CAR
17	R	950	SQD	O5-C1-O6-C44
17	R	950	SQD	C5-C6-S-O7
17	R	950	SQD	C5-C6-S-O8
17	R	950	SQD	C5-C6-S-O9
14	D	910	CLA	O1A-CGA-O2A-C1
14	D	910	CLA	CBA-CGA-O2A-C1
14	D	910	CLA	C3-C5-C6-C7
16	L	951	LMG	C4-C5-C6-O5
15	D	920	TDS	CAP-CAQ-CAR-CAS
16	L	951	LMG	O6-C5-C6-O5
10	B	902	HEC	C3D-CAD-CBD-CGD
17	R	950	SQD	C24-C23-O48-C46
16	L	951	LMG	O6-C1-O1-C7
12	B	960	LFA	C5-C6-C7-C8
12	B	960	LFA	C9-C10-C11-C12
16	D	953	LMG	C21-C22-C23-C24
12	B	960	LFA	C12-C13-C14-C15
17	R	950	SQD	O10-C23-O48-C46
16	D	953	LMG	C16-C17-C18-C19
16	D	953	LMG	C31-C32-C33-C34
17	R	950	SQD	C24-C25-C26-C27
12	B	960	LFA	C16-C17-C18-C19
17	R	950	SQD	C25-C26-C27-C28
16	D	953	LMG	C40-C41-C42-C43
12	B	960	LFA	C15-C16-C17-C18
16	D	953	LMG	C15-C16-C17-C18
12	B	960	LFA	C10-C11-C12-C13
10	B	903	HEC	C3D-CAD-CBD-CGD
10	B	902	HEC	C2A-CAA-CBA-CGA
16	D	953	LMG	O6-C5-C6-O5
15	D	920	TDS	CAX-CAY-CAZ-CBA
15	D	920	TDS	CAS-CAT-CAU-CAV
16	D	953	LMG	C35-C36-C37-C38
14	D	910	CLA	O2A-C1-C2-C3
12	B	960	LFA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
16	L	951	LMG	C31-C32-C33-C34
12	B	960	LFA	C17-C18-C19-C20
16	L	951	LMG	C7-C8-C9-O8
15	D	920	TDS	CAR-CAS-CAT-CAU
12	B	960	LFA	C11-C12-C13-C14
12	B	960	LFA	C13-C14-C15-C16
16	L	951	LMG	C29-C30-C31-C32
14	D	910	CLA	C11-C12-C13-C15
16	L	951	LMG	C15-C16-C17-C18
10	B	901	HEC	CAA-CBA-CGA-O2A
16	D	953	LMG	C41-C42-C43-C44
10	A	900	HEC	C3D-CAD-CBD-CGD
10	B	901	HEC	CAA-CBA-CGA-O1A
11	B	904	BCR	C11-C10-C9-C34
10	B	902	HEC	CAD-CBD-CGD-O2D
10	B	902	HEC	CAD-CBD-CGD-O1D
11	B	904	BCR	C11-C10-C9-C8
16	L	951	LMG	O7-C8-C9-O8
12	B	960	LFA	C7-C8-C9-C10
10	A	900	HEC	CAD-CBD-CGD-O1D
10	A	900	HEC	CAD-CBD-CGD-O2D
14	D	910	CLA	C11-C12-C13-C14
10	B	903	HEC	CAA-CBA-CGA-O2A
14	D	910	CLA	CHA-CBD-CGD-O1D
14	D	910	CLA	CHA-CBD-CGD-O2D
16	D	953	LMG	O7-C8-C9-O8
17	R	950	SQD	O6-C44-C45-O47
10	B	903	HEC	CAA-CBA-CGA-O1A
15	D	920	TDS	CAW-CAX-CAY-CAZ
17	R	950	SQD	C27-C28-C29-C30
14	D	910	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

12 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	953	LMG	3	0
17	R	950	SQD	1	0
11	B	904	BCR	3	0
10	B	903	HEC	1	0
13	C	210	FES	1	0
16	L	951	LMG	4	0

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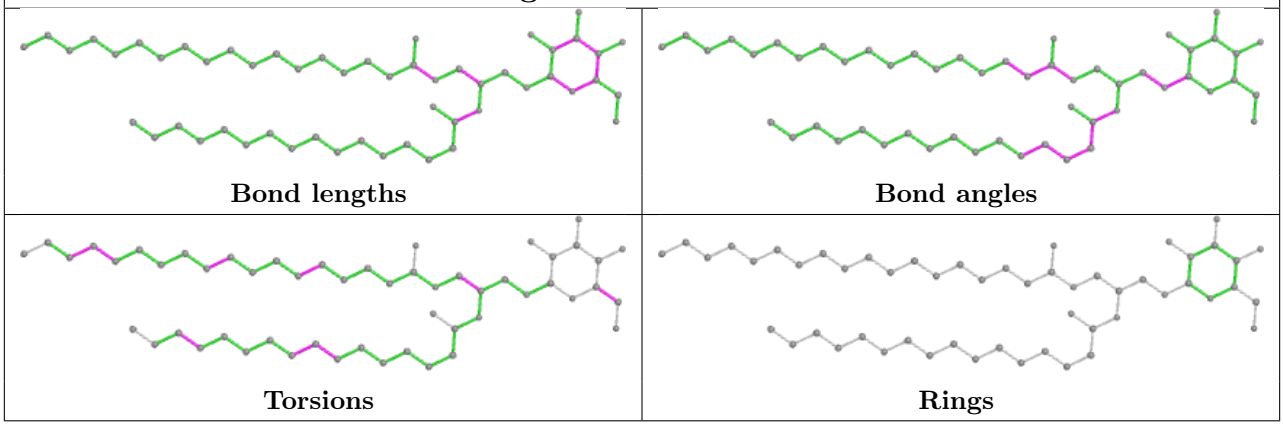
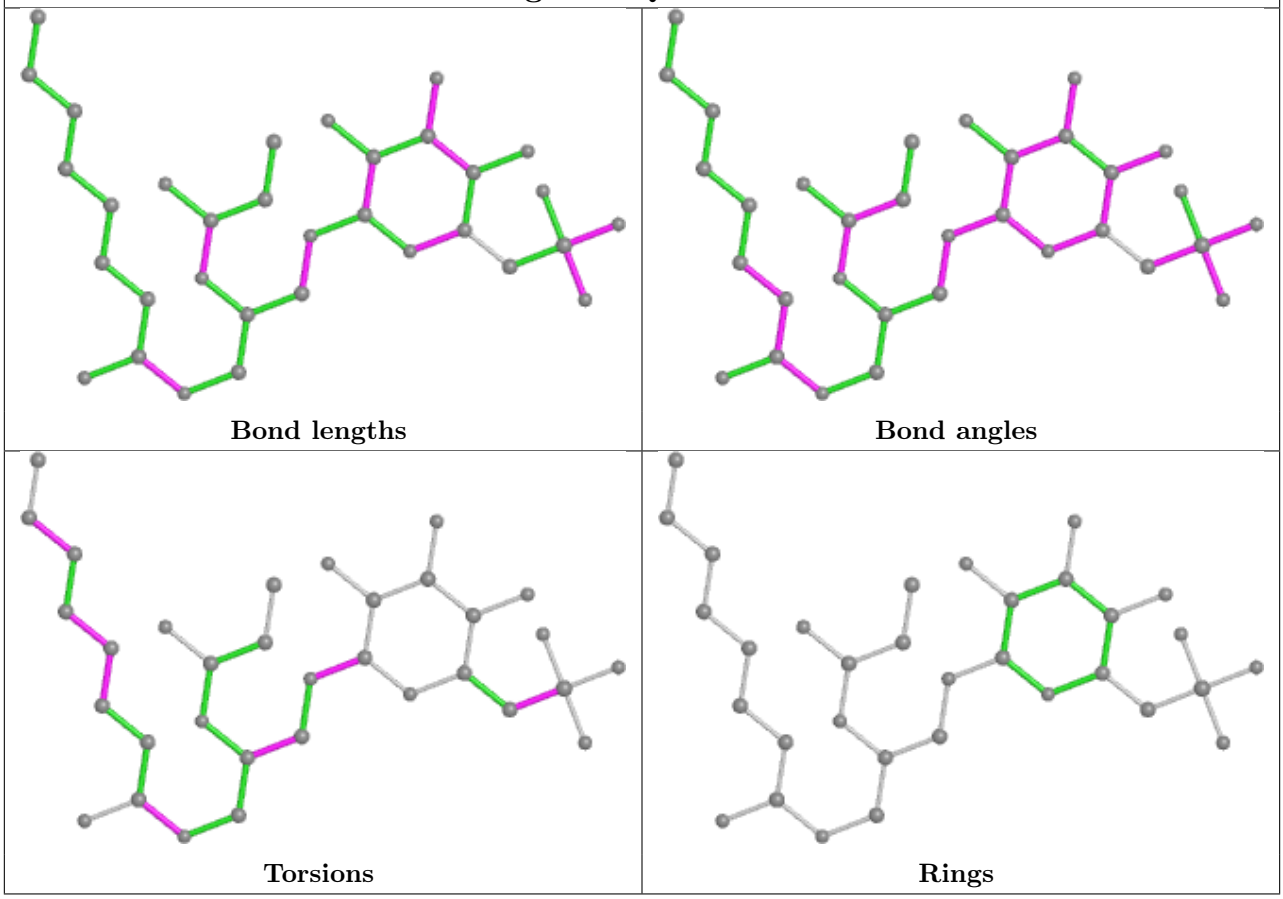
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	D	920	TDS	2	0
14	D	910	CLA	5	0
12	B	960	LFA	2	0
10	B	902	HEC	1	0
10	B	901	HEC	6	0
10	A	900	HEC	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 LMG D 953

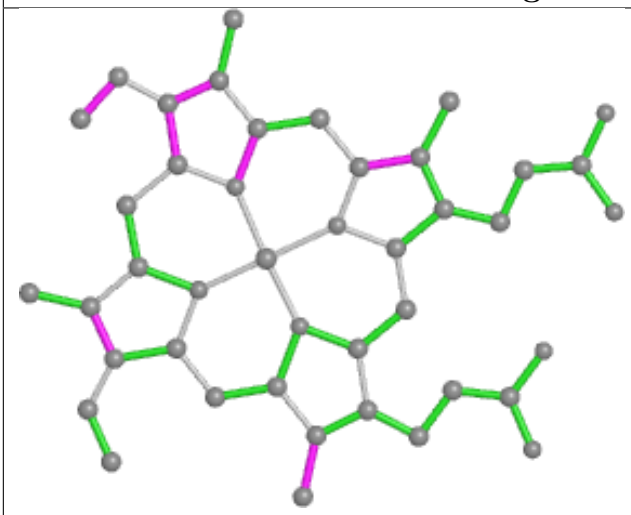


Ligand SQD R 950

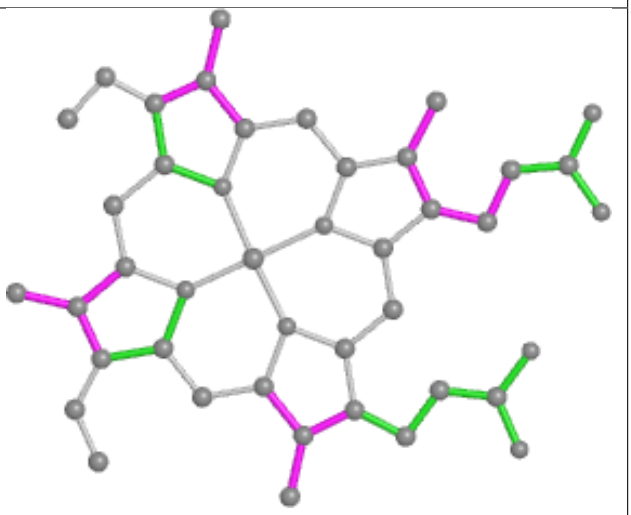


Ligand BCR B 904

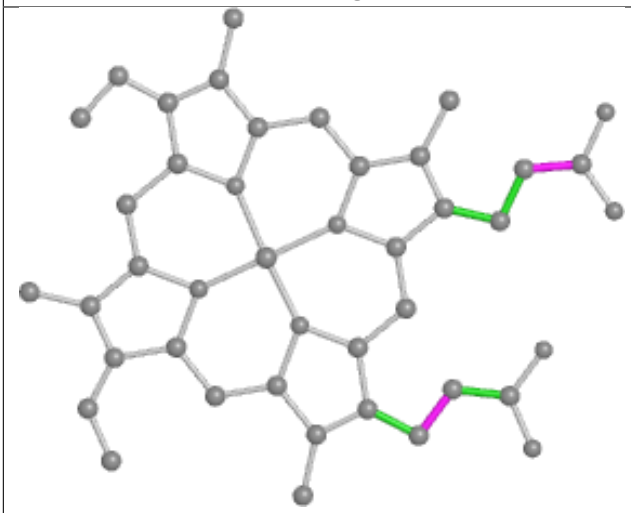
Ligand HEC B 903



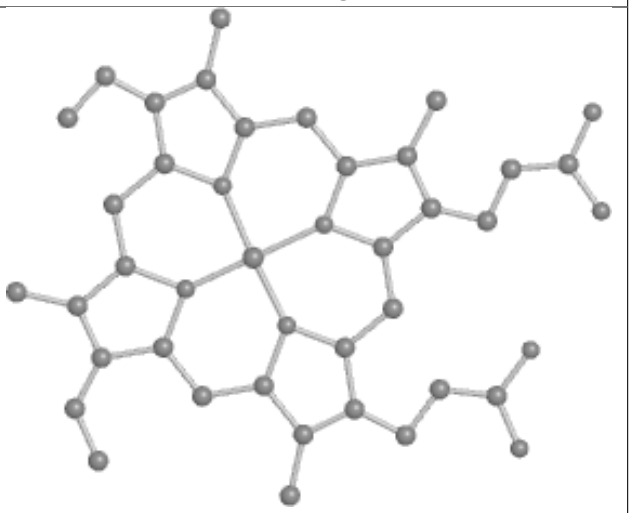
Bond lengths



Bond angles

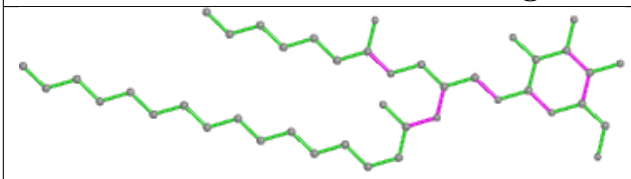


Torsions

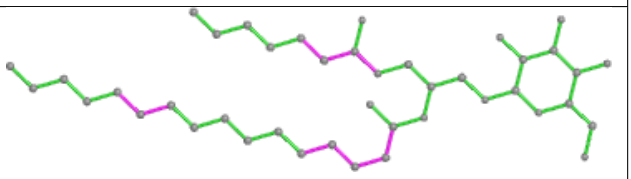


Rings

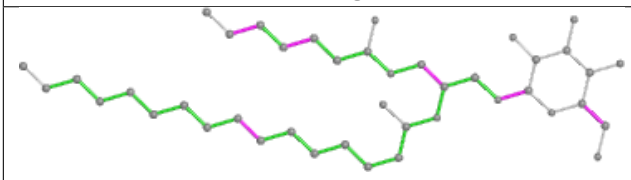
Ligand LMG L 951



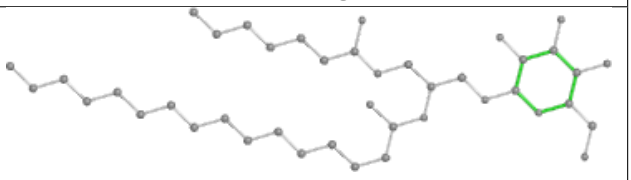
Bond lengths



Bond angles

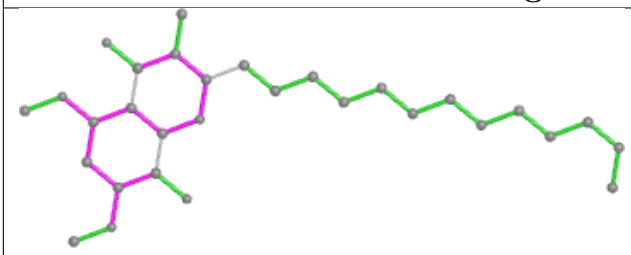


Torsions

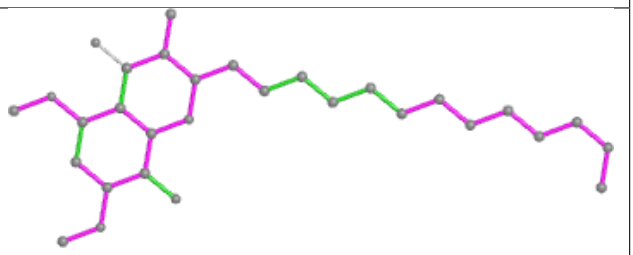


Rings

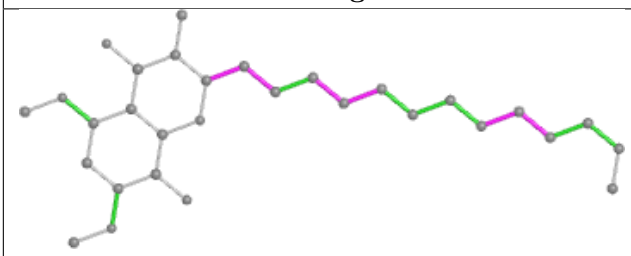
Ligand TDS D 920



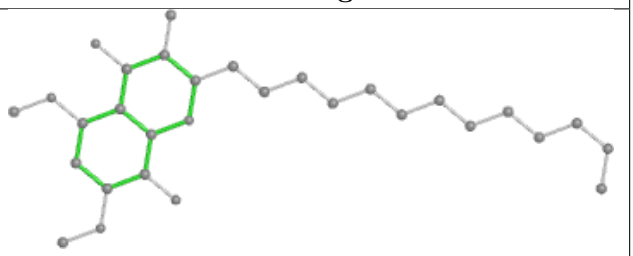
Bond lengths



Bond angles

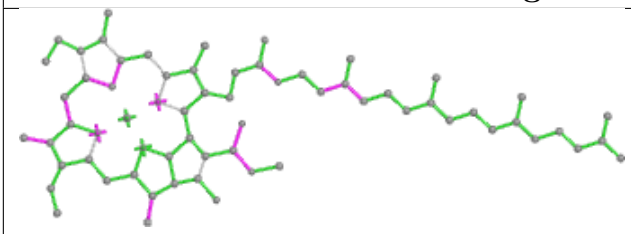


Torsions

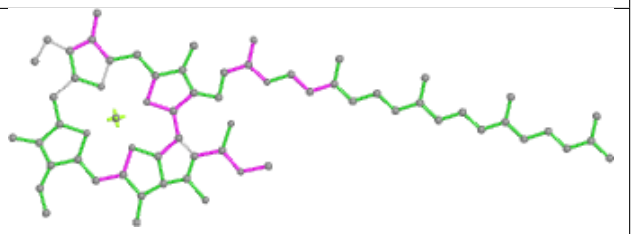


Rings

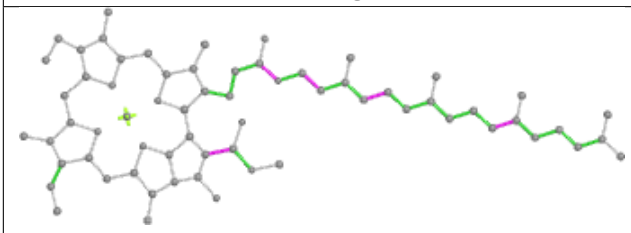
Ligand CLA D 910



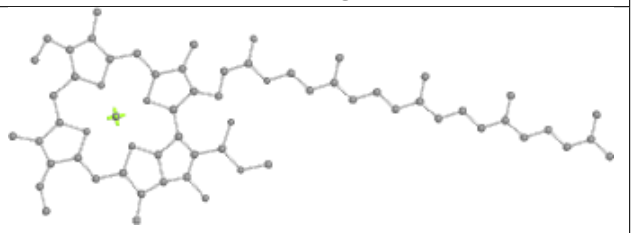
Bond lengths



Bond angles

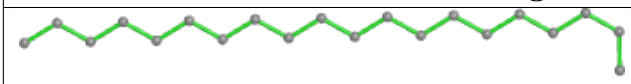


Torsions

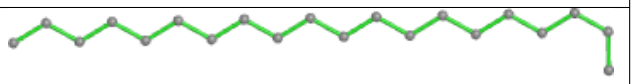


Rings

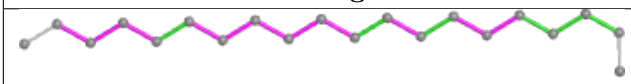
Ligand LFA B 960



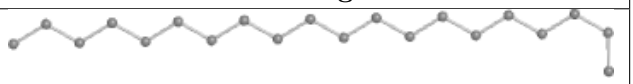
Bond lengths



Bond angles

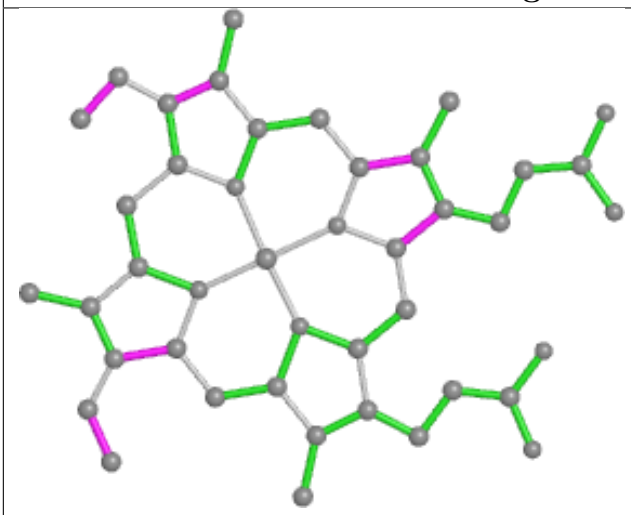


Torsions

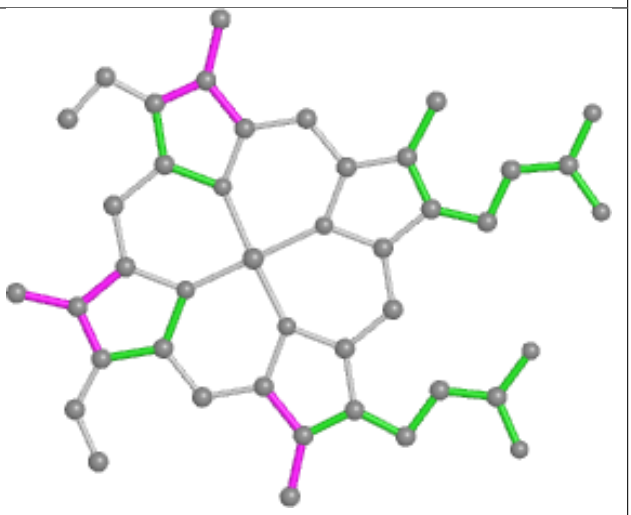


Rings

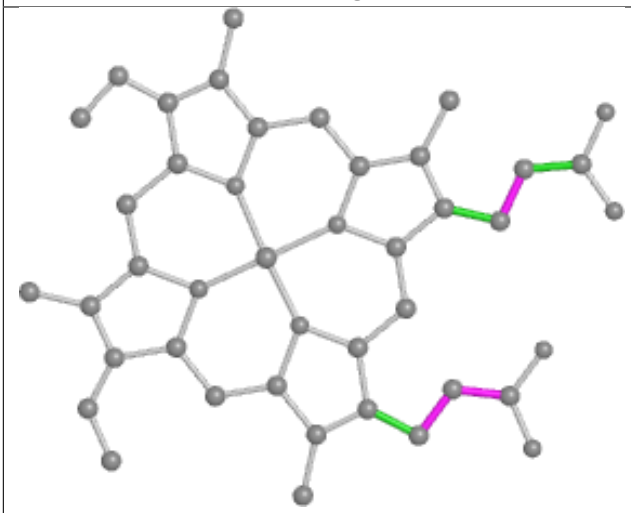
Ligand HEC B 902



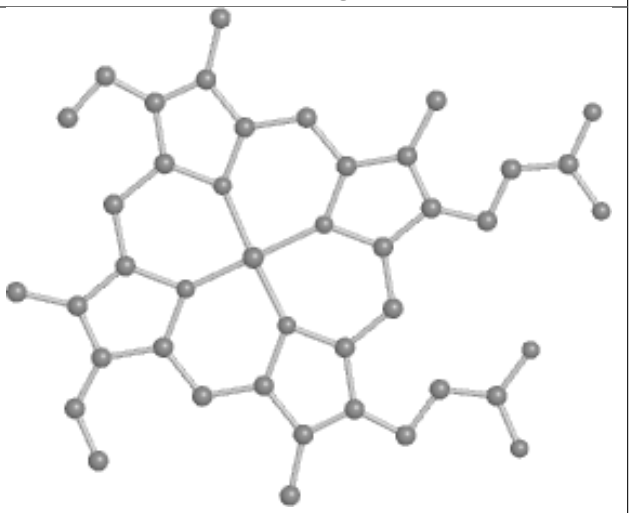
Bond lengths



Bond angles

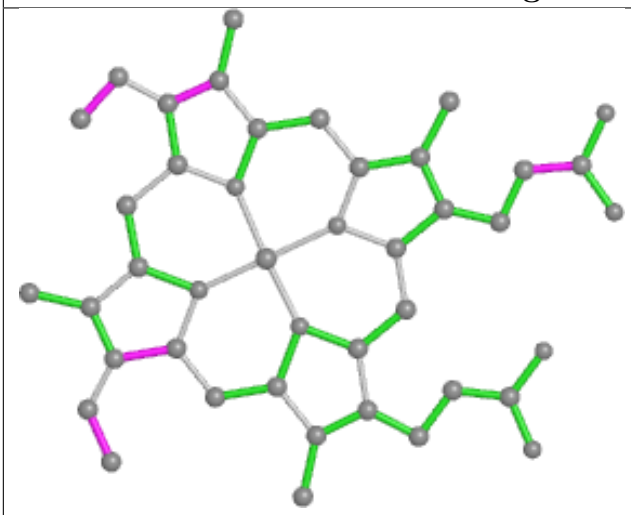


Torsions

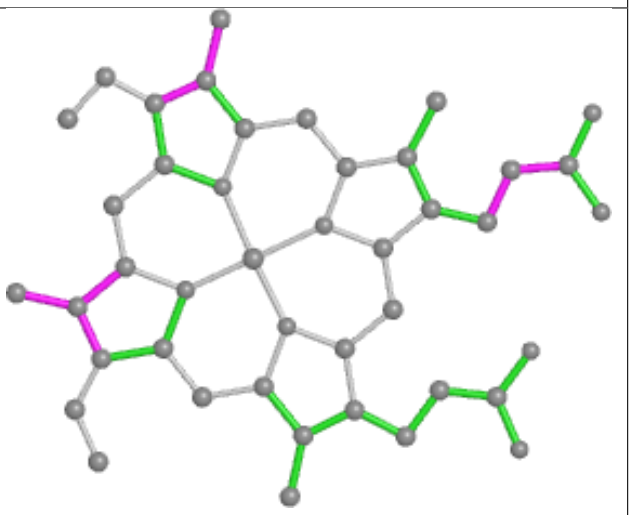


Rings

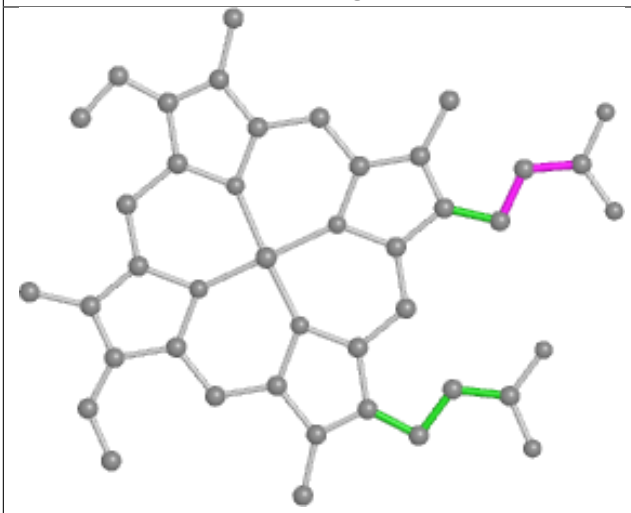
Ligand HEC B 901



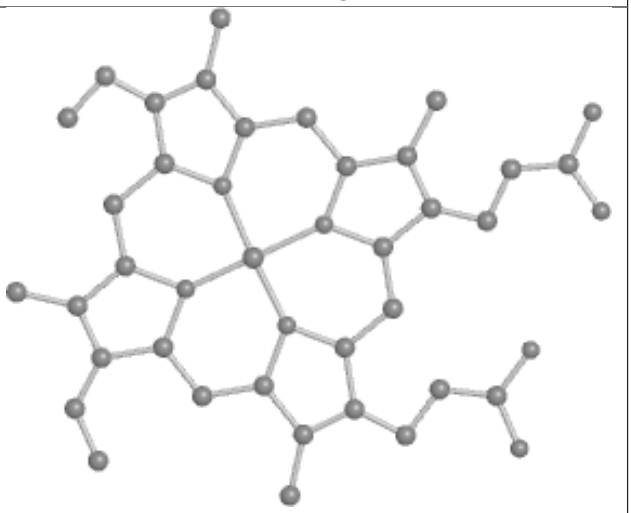
Bond lengths



Bond angles

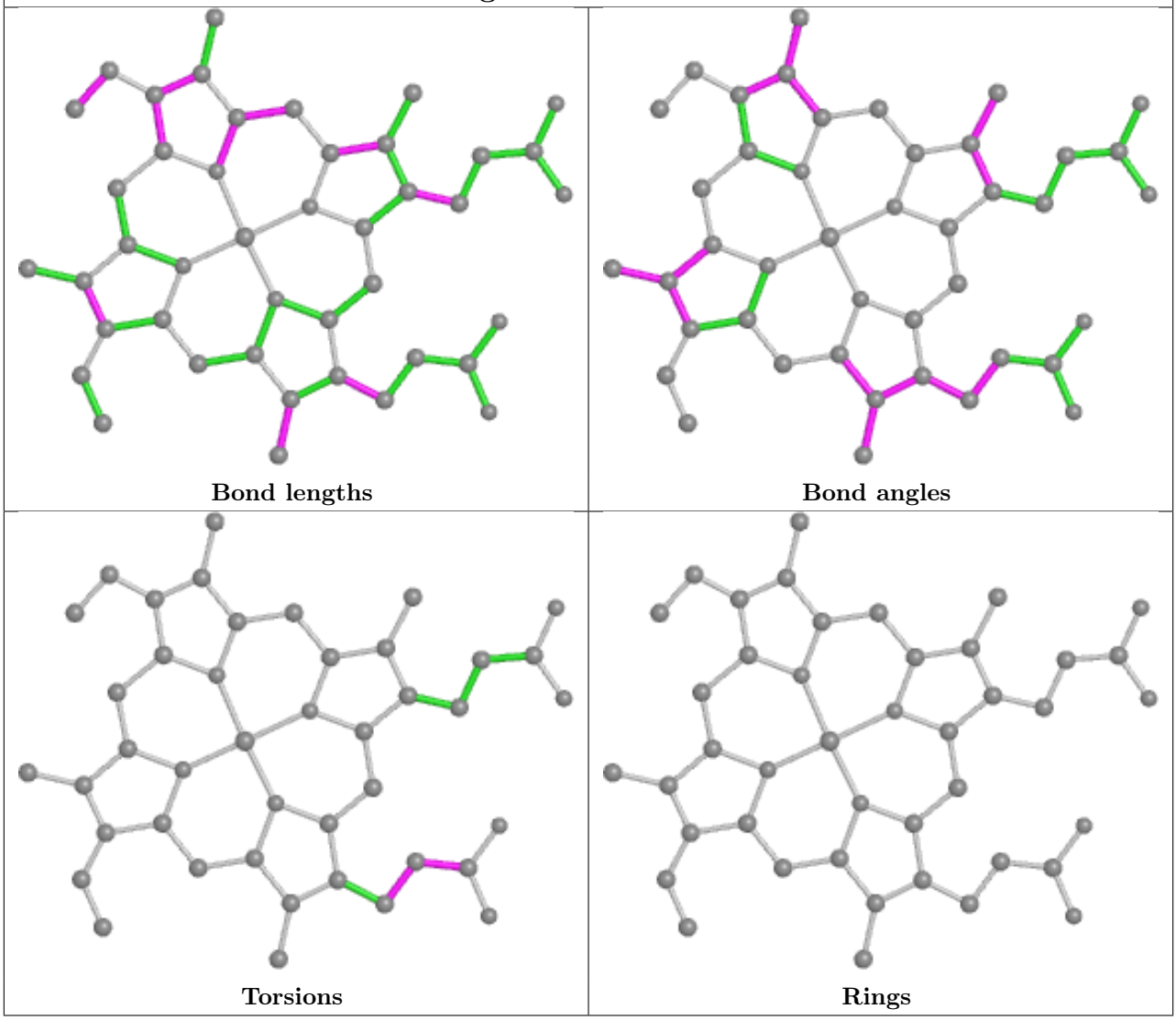


Torsions



Rings

Ligand HEC A 900



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	292/292 (100%)	-0.16	2 (0%)	87	75	42, 66, 102, 131	3 (1%)
2	B	212/215 (98%)	-0.10	2 (0%)	84	69	29, 47, 76, 114	0
3	C	126/127 (99%)	1.00	30 (23%)	0	0	70, 121, 159, 180	0
4	D	156/159 (98%)	-0.19	0	100	100	37, 62, 96, 131	0
5	R	39/49 (79%)	-0.10	3 (7%)	13	5	37, 51, 135, 159	0
6	G	30/37 (81%)	-0.21	0	100	100	41, 54, 77, 97	0
7	L	32/32 (100%)	-0.31	0	100	100	46, 65, 86, 126	0
8	M	34/39 (87%)	-0.40	0	100	100	41, 57, 83, 130	0
9	N	31/31 (100%)	-0.35	0	100	100	36, 50, 68, 91	0
All	All	952/981 (97%)	-0.02	37 (3%)	39	20	29, 62, 135, 180	3 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	33	SER	4.1
3	C	186	LEU	3.7
3	C	196	ASP	3.6
3	C	93	GLY	3.6
3	C	81	ALA	3.3
3	C	97	LYS	3.3
3	C	89	ASP	3.2
3	C	98	THR	3.2
1	A	200	ASN	3.0
3	C	157	SER	3.0
2	B	5	TYR	2.9
3	C	206	ALA	2.8
3	C	203	PRO	2.7
3	C	120	THR	2.7
3	C	123	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	197	PHE	2.7
3	C	88	ASN	2.6
3	C	190	SER	2.6
3	C	192	TRP	2.6
3	C	187	VAL	2.5
3	C	195	THR	2.4
3	C	182	ALA	2.4
3	C	82	ALA	2.4
3	C	95	TRP	2.3
3	C	122	ASP	2.3
3	C	96	LEU	2.3
5	R	34	SER	2.3
3	C	189	PHE	2.3
3	C	124	THR	2.3
3	C	201	LEU	2.2
3	C	121	ALA	2.2
3	C	90	ILE	2.2
3	C	188	THR	2.2
1	A	199	ALA	2.1
3	C	92	ALA	2.1
2	B	91	SER	2.1
5	R	35	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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
16	LMG	D	953	53/55	0.63	0.43	88,88,107,107	0

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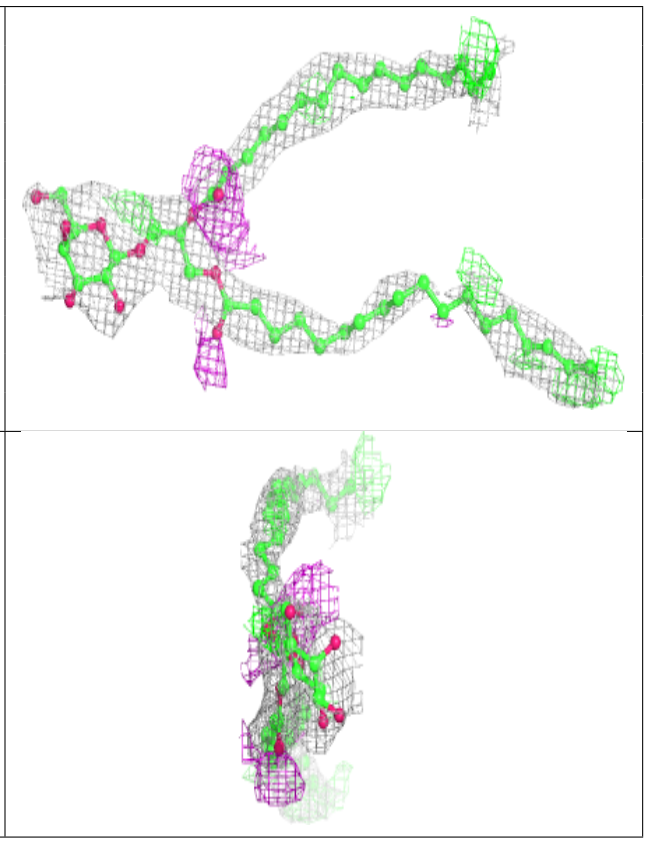
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	LMG	L	951	42/55	0.77	0.33	78,85,85,85	0
11	BCR	B	904	27/40	0.85	0.40	49,49,64,64	0
15	TDS	D	920	30/30	0.87	0.30	87,89,89,89	0
14	CLA	D	910	65/65	0.88	0.28	63,70,92,94	0
12	LFA	B	960	20/20	0.91	0.29	59,59,59,59	0
17	SQD	R	950	33/54	0.93	0.19	62,62,111,111	0
10	HEC	B	903	43/43	0.95	0.21	53,53,53,53	0
10	HEC	A	900	43/43	0.95	0.22	63,67,77,80	0
10	HEC	B	902	43/43	0.97	0.19	35,43,48,50	0
10	HEC	B	901	43/43	0.97	0.21	30,37,45,50	0
13	FES	C	210	4/4	0.99	0.09	62,62,63,65	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.

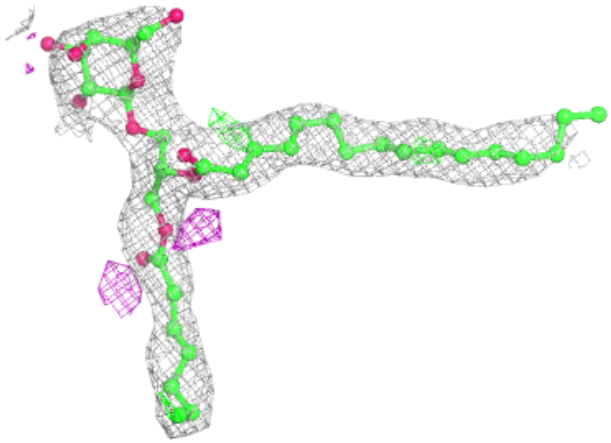
Electron density around LMG D 953:

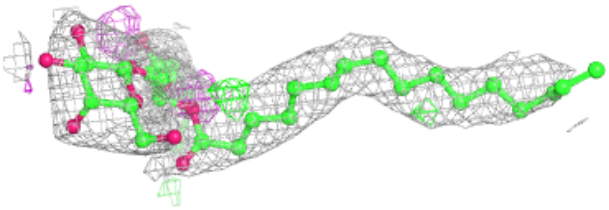
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

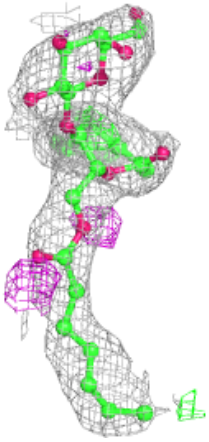


Electron density around LMG L 951:

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

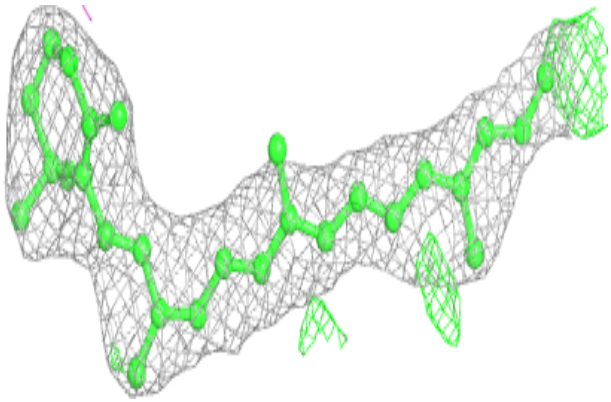


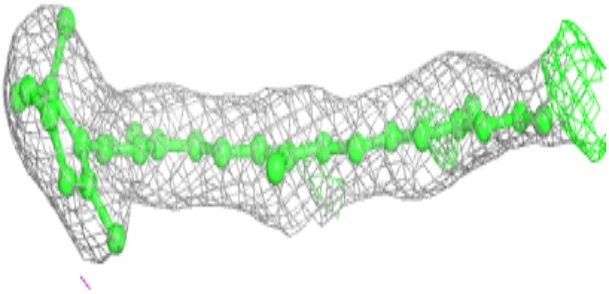


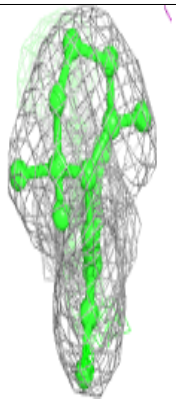


Electron density around BCR B 904:

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

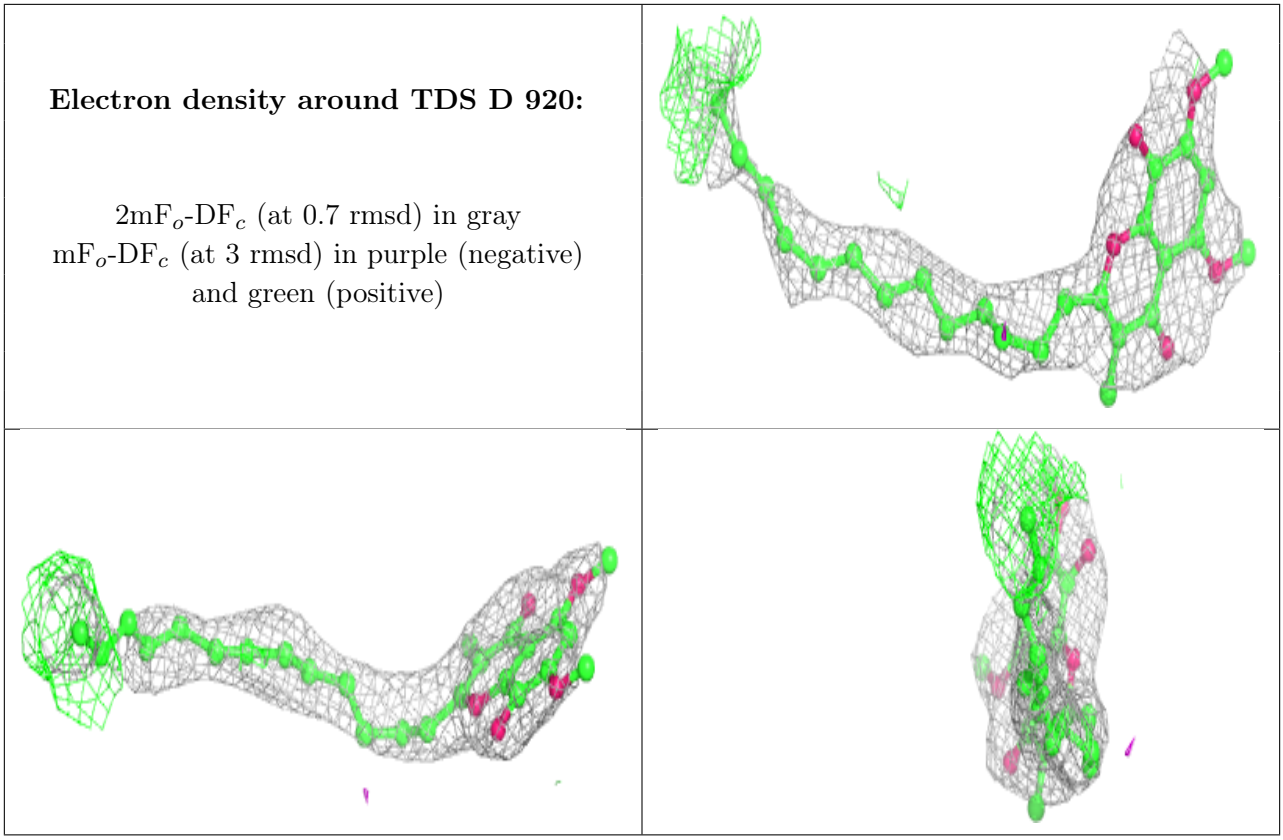






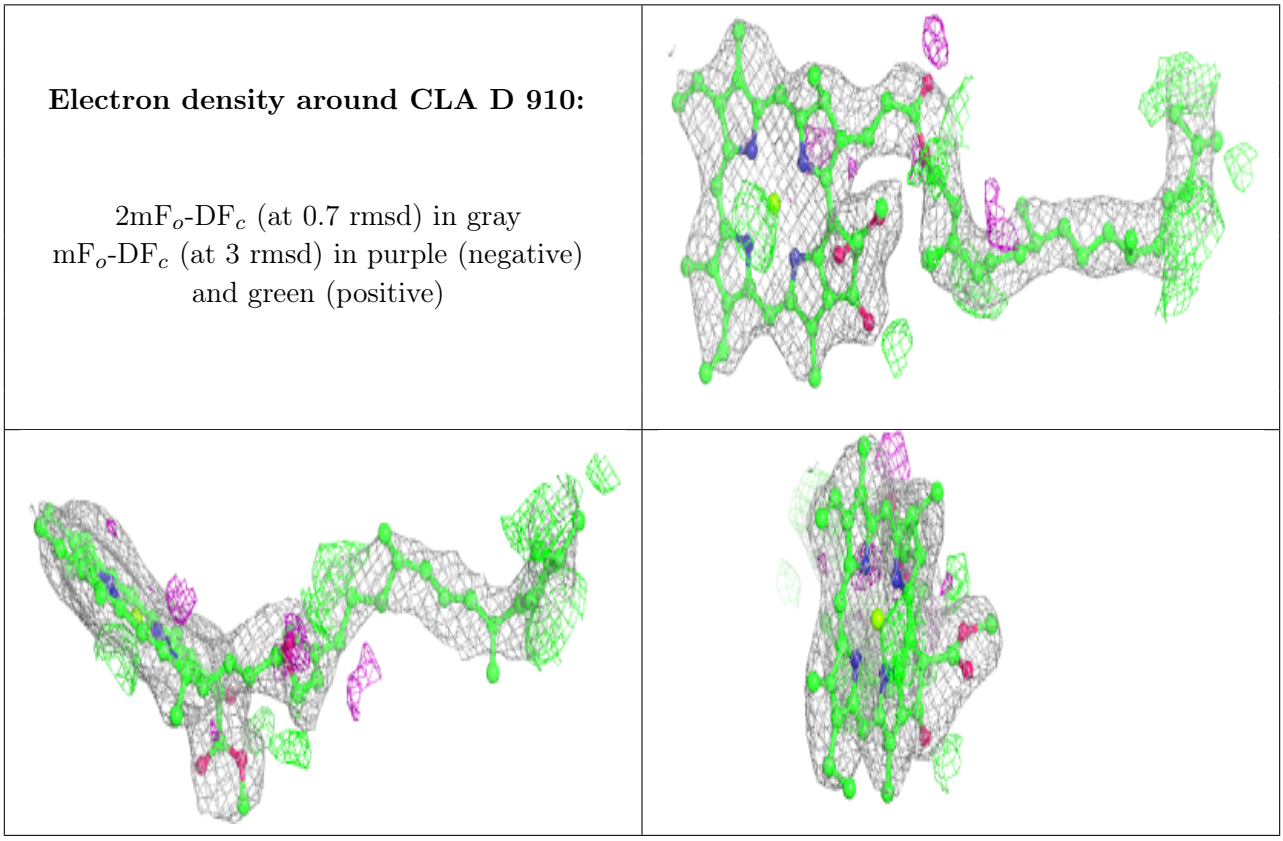
Electron density around TDS D 920:

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



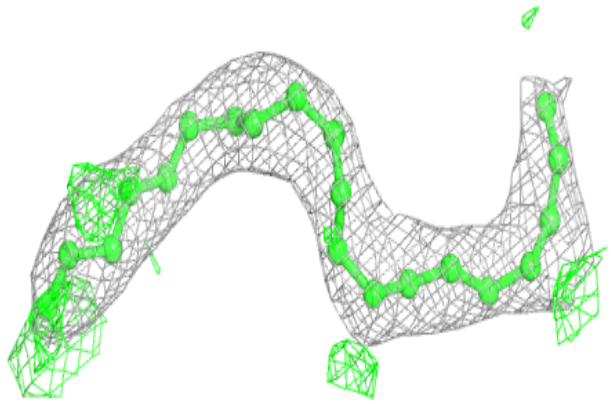
Electron density around CLA D 910:

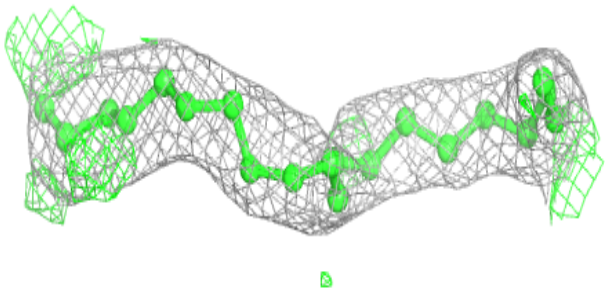
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

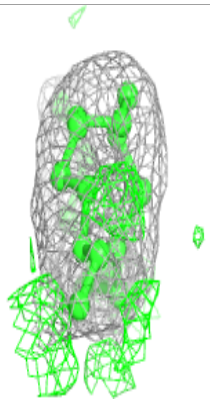


Electron density around LFA B 960:

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

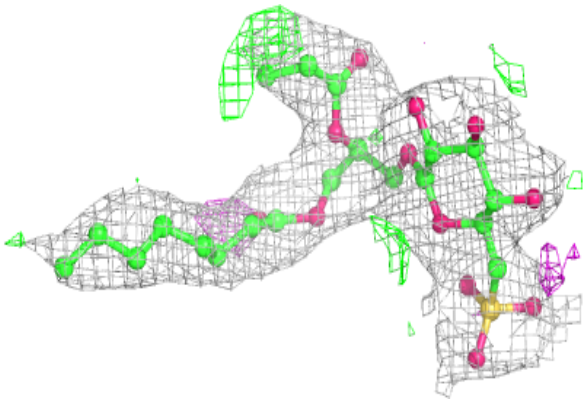


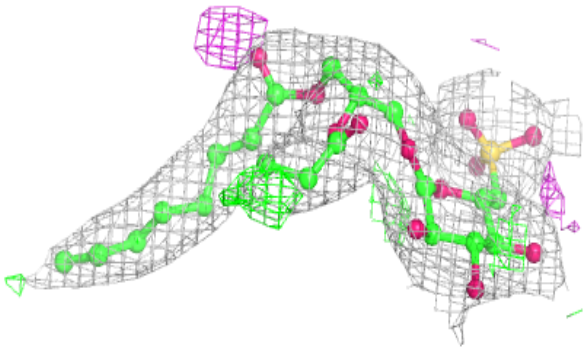


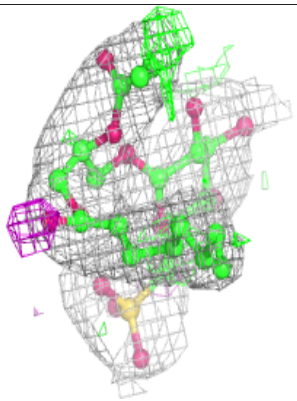


Electron density around SQD R 950:

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

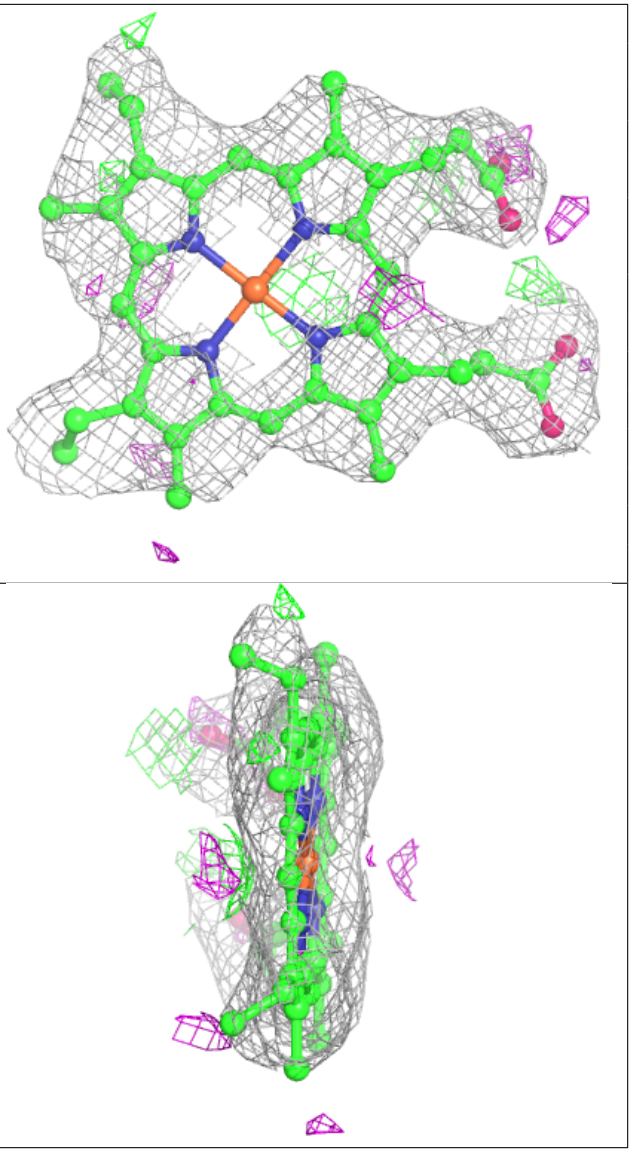






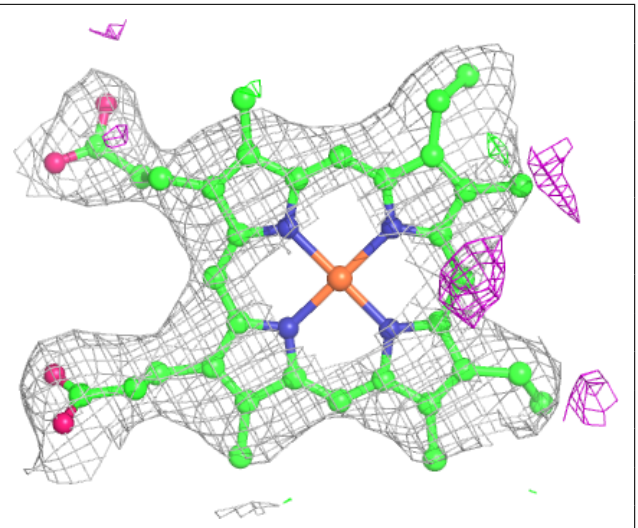
Electron density around HEC B 903:

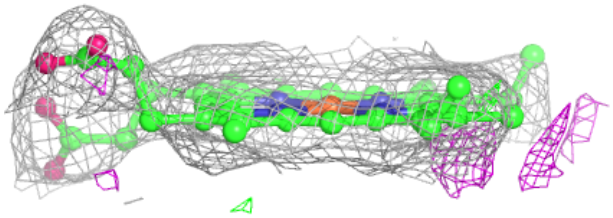
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

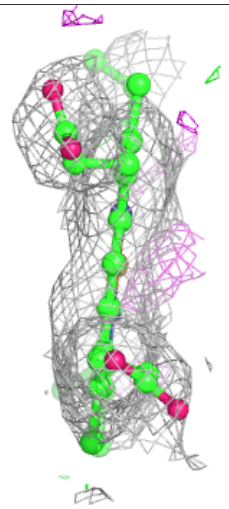


Electron density around HEC A 900:

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

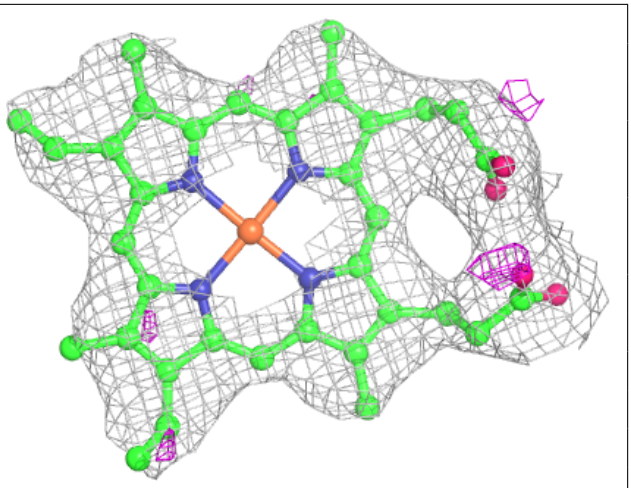


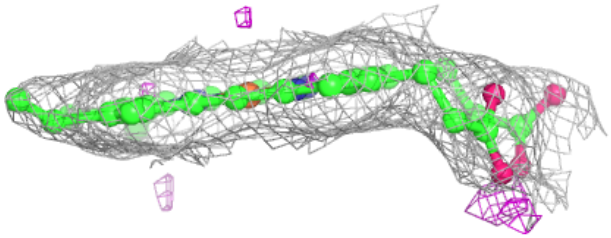


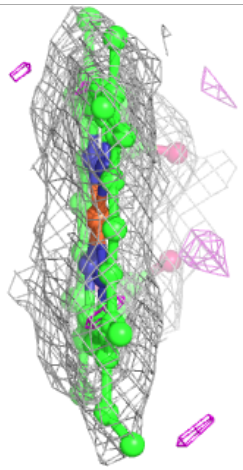


Electron density around HEC B 902:

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

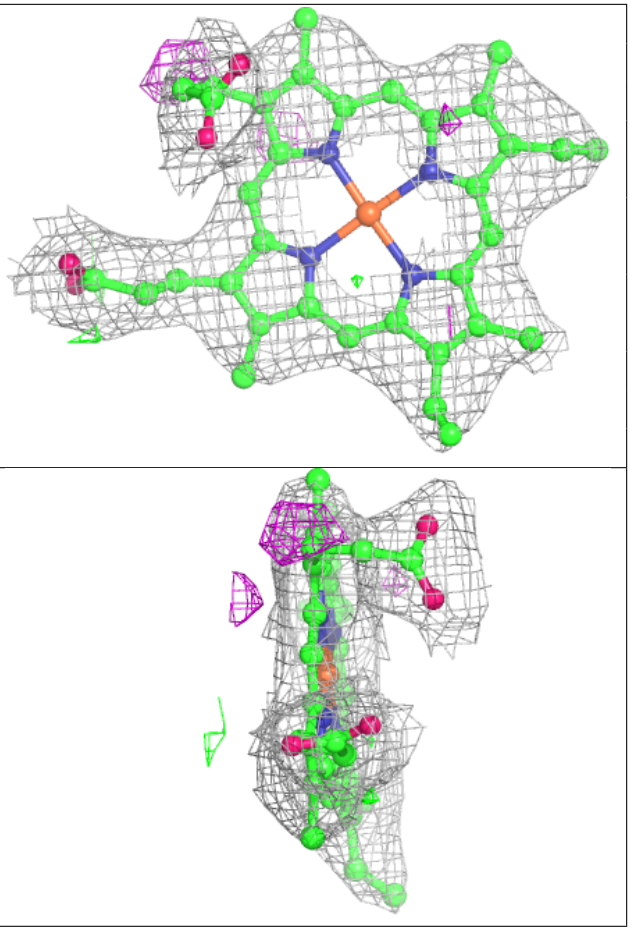






Electron density around HEC B 901:

$2mF_o$-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.