Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 03:00 PM EDT

PDB ID	:	3HYV
Title	:	3-D X-Ray structure of the sulfide:quinone oxidoreductase from the hyperthermophilic bacterium Aquifex aeolicus
Authors	:	Marcia, M.; Ermler, U.; Peng, G.H.; Michel, H.
Deposited on	:	2009-06-23
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

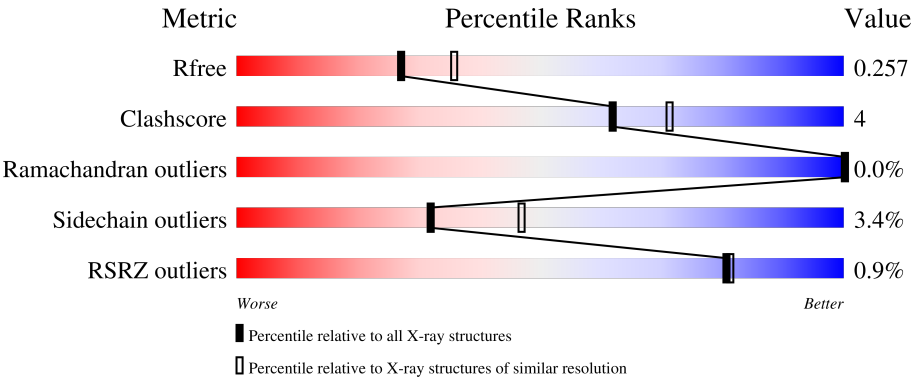
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	430	% 90% 10%
1	B	430	90% 10%
1	C	430	% 87% 12% •
1	D	430	% 89% 10% •
1	E	430	91% 8%

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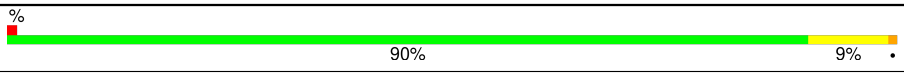
Mol	Chain	Length	Quality of chain
1	F	430	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PS9	A	800	-	-	X	-
5	PS9	B	800	-	-	X	-
7	SO4	C	432	-	-	X	-

2 Entry composition (i)

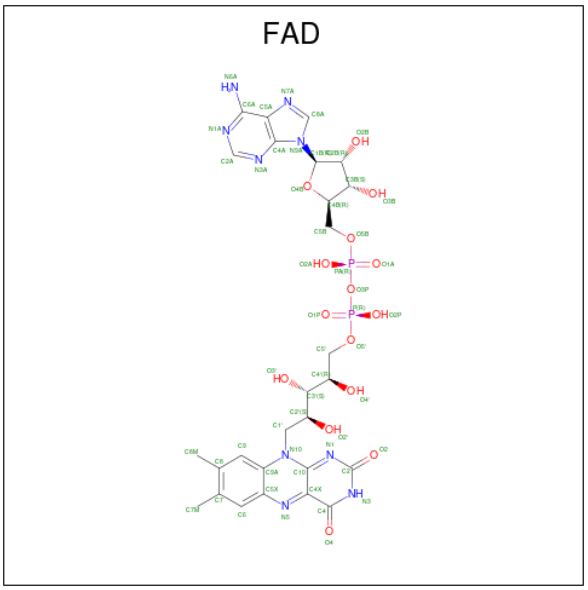
There are 8 unique types of molecules in this entry. The entry contains 21480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sulfide-quinone reductase.

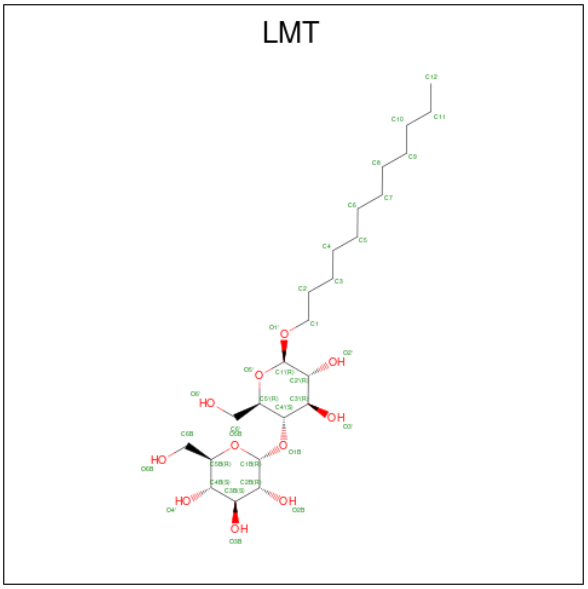
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	8	0
			3370	2182	556	609	23			
1	B	429	Total	C	N	O	S	0	7	0
			3364	2179	556	606	23			
1	C	429	Total	C	N	O	S	0	6	0
			3358	2174	555	606	23			
1	D	429	Total	C	N	O	S	0	6	0
			3357	2175	555	604	23			
1	E	429	Total	C	N	O	S	0	4	0
			3346	2166	555	602	23			
1	F	429	Total	C	N	O	S	0	4	0
			3346	2166	555	602	23			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		
3	D	1	Total	C	O	0	0
			35	24	11		
3	E	1	Total	C	O	0	0
			35	24	11		

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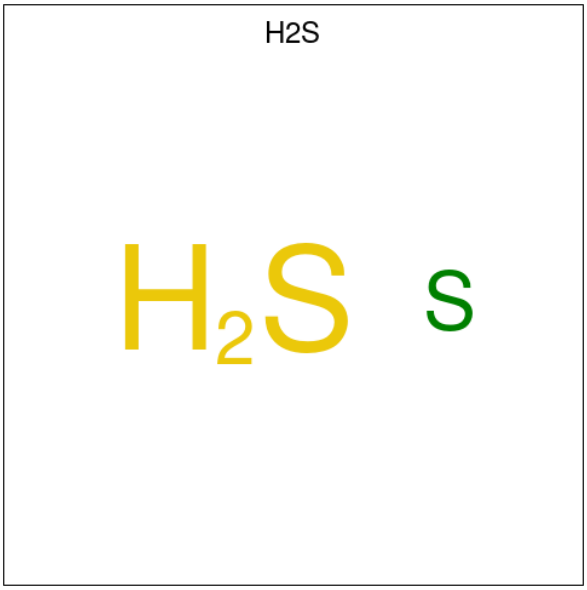
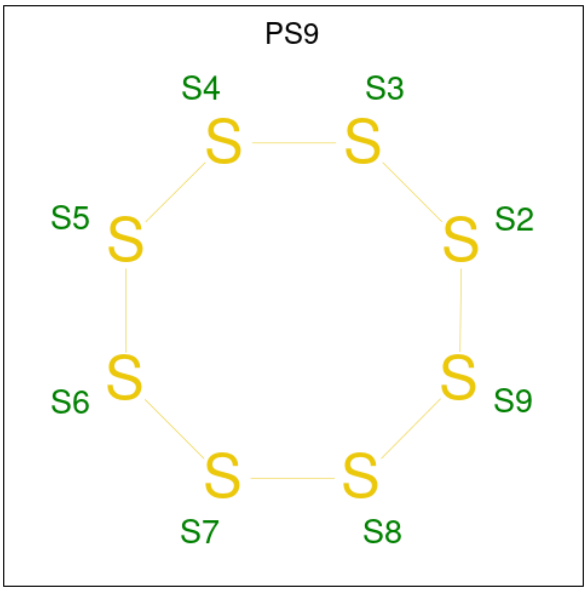
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 35 24 11	0	0

- Molecule 4 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S).



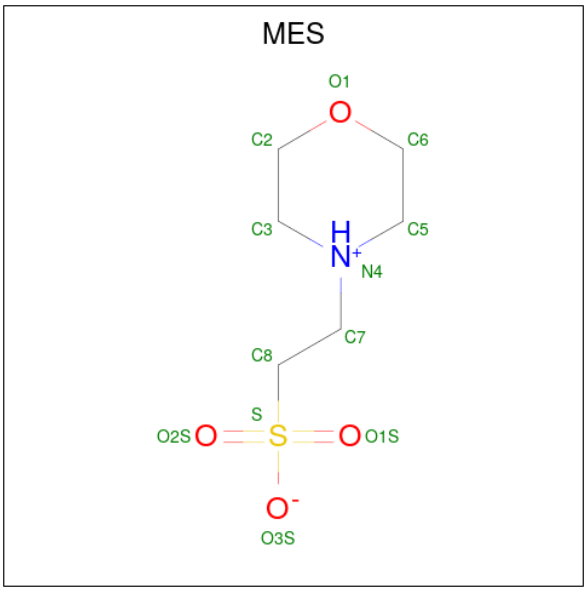
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total S 1 1	0	0
4	B	1	Total S 1 1	0	0
4	C	1	Total S 1 1	0	0
4	D	1	Total S 1 1	0	0
4	E	1	Total S 1 1	0	0
4	F	1	Total S 1 1	0	0

- Molecule 5 is octathiocane (three-letter code: PS9) (formula: S_8).



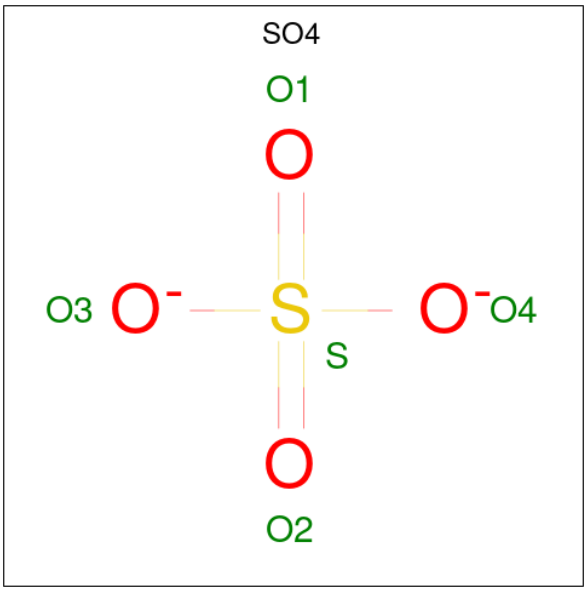
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total S 8 8	0	0
5	B	1	Total S 6 6	0	0
5	C	1	Total S 6 6	0	0
5	D	1	Total S 1 1	0	0
5	D	1	Total S 5 5	0	0
5	E	1	Total S 8 8	0	0
5	F	1	Total S 8 8	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total O S 5 4 1	0	0
7	D	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	E	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0
7	F	1	Total O S 5 4 1	0	0

- Molecule 8 is water.

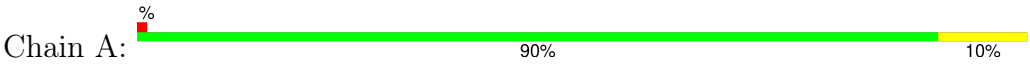
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	97	Total O 97 97	0	0
8	B	107	Total O 107 107	0	0
8	C	105	Total O 105 105	0	0
8	D	57	Total O 57 57	0	0
8	E	92	Total O 92 92	0	0
8	F	113	Total O 113 113	0	0

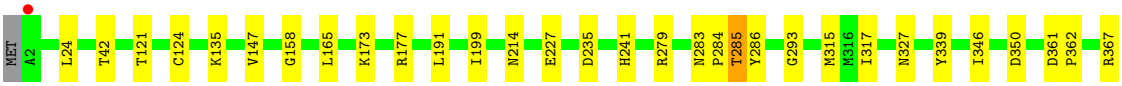
3 Residue-property plots (i)

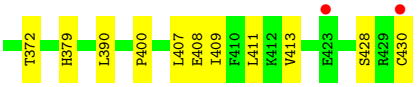
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sulfide-quinone reductase

Chain A:

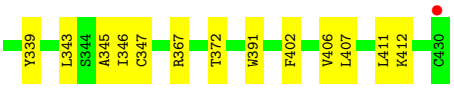






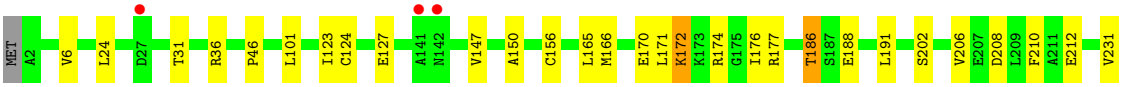
• Molecule 1: Sulfide-quinone reductase

Chain B:



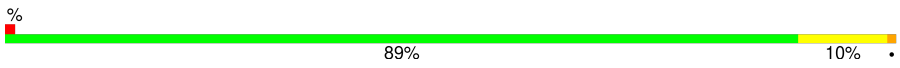
• Molecule 1: Sulfide-quinone reductase

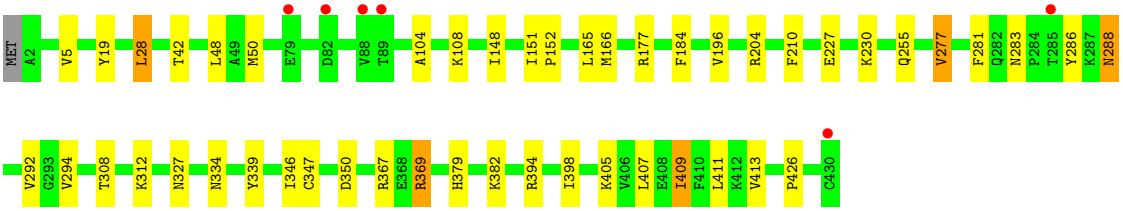
Chain C:



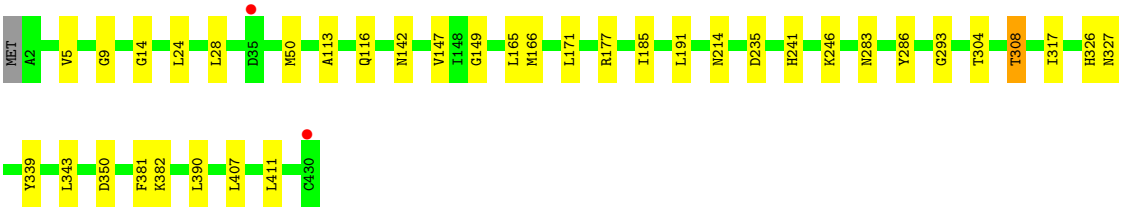
• Molecule 1: Sulfide-quinone reductase

Chain D:

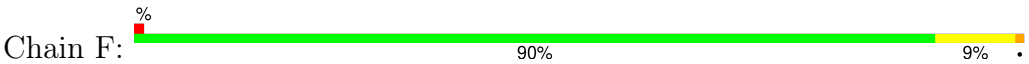


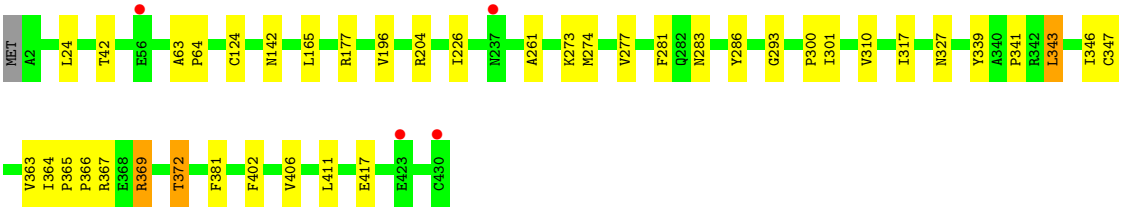


• Molecule 1: Sulfide-quinone reductase



• Molecule 1: Sulfide-quinone reductase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	112.85Å 154.92Å 178.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.04 – 2.30 20.04 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (20.04-2.30) 97.8 (20.04-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.235 0.217 , 0.257	Depositor DCC
R_{free} test set	6821 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21480	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, H2S, LMT, SO4, PS9, FAD, CSS

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	0.52	0/3477	0.57	0/4720
1	B	0.50	0/3468	0.58	0/4707
1	C	0.50	0/3459	0.58	0/4696
1	D	0.47	0/3458	0.54	0/4695
1	E	0.48	0/3441	0.57	0/4672
1	F	0.50	0/3441	0.57	0/4672
All	All	0.49	0/20744	0.57	0/28162

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

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	3370	0	3373	25	0
1	B	3364	0	3372	26	0
1	C	3358	0	3359	33	0
1	D	3357	0	3364	31	0
1	E	3346	0	3347	18	0
1	F	3346	0	3347	27	0
2	A	53	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	29	0	0
2	C	53	0	29	0	0
2	D	53	0	29	1	0
2	E	53	0	29	1	0
2	F	53	0	29	1	0
3	A	35	0	46	0	0
3	B	35	0	46	0	0
3	C	35	0	46	2	0
3	D	35	0	46	0	0
3	E	35	0	46	8	0
3	F	35	0	46	9	0
4	A	1	0	0	1	0
4	B	1	0	0	1	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	1	0
5	A	8	0	0	2	0
5	B	6	0	0	2	0
5	C	6	0	0	1	0
5	D	6	0	0	1	0
5	E	8	0	0	0	0
5	F	8	0	0	1	0
6	A	12	0	12	0	0
6	B	12	0	12	0	0
6	C	12	0	12	1	0
6	D	12	0	12	0	0
6	E	12	0	12	0	0
6	F	12	0	12	0	0
7	A	20	0	0	0	0
7	B	25	0	0	1	0
7	C	20	0	0	2	0
7	D	15	0	0	1	0
7	E	25	0	0	0	0
7	F	15	0	0	1	0
8	A	97	0	0	2	0
8	B	107	0	0	3	0
8	C	105	0	0	4	0
8	D	57	0	0	0	0
8	E	92	0	0	1	0
8	F	113	0	0	1	0
All	All	21480	0	20685	168	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 4.

All (168) 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:D:347[B]:CYS:SG	5:D:802:PS9:S9	2.39	1.19
1:C:420:LYS:HD3	1:C:420:LYS:H	1.28	0.98
3:E:600:LMT:H1B	3:F:600:LMT:O2B	1.64	0.97
1:D:327:ASN:HD21	1:D:339:TYR:H	1.17	0.92
3:F:600:LMT:O2B	3:F:600:LMT:H4'	1.72	0.89
1:C:327:ASN:HD21	1:C:339:TYR:H	1.24	0.84
1:E:327:ASN:HD21	1:E:339:TYR:H	1.24	0.84
3:E:600:LMT:C1B	3:F:600:LMT:O2B	2.26	0.84
1:C:420:LYS:H	1:C:420:LYS:CD	1.91	0.83
1:C:283:ASN:HD22	1:C:286:TYR:H	1.27	0.82
1:F:283:ASN:HD22	1:F:286:TYR:H	1.28	0.79
1:A:283:ASN:HD22	1:A:286:TYR:H	1.31	0.77
1:E:283:ASN:HD22	1:E:286:TYR:H	1.29	0.77
1:B:283:ASN:HD22	1:B:286:TYR:H	1.29	0.75
1:F:274:MET:HE1	8:F:822:HOH:O	1.87	0.74
1:F:42:THR:HG21	2:F:441:FAD:O4'	1.88	0.73
1:F:327:ASN:HD21	1:F:339:TYR:H	1.35	0.72
1:B:327:ASN:HD21	1:B:339:TYR:H	1.39	0.70
3:E:600:LMT:H2B	3:F:600:LMT:O2B	1.92	0.69
1:C:186:THR:HG21	1:C:188:GLU:OE1	1.93	0.69
1:A:327:ASN:HD21	1:A:339:TYR:H	1.41	0.68
3:E:600:LMT:C2B	3:F:600:LMT:O2B	2.41	0.68
1:A:124[A]:CYS:SG	4:A:700:H2S:S	2.67	0.64
1:B:169:TYR:CE2	1:B:173[B]:LYS:HD2	2.33	0.63
1:F:346:ILE:HD11	1:F:411:LEU:CD1	2.29	0.63
1:B:196:VAL:HG22	1:B:367:ARG:NH1	2.14	0.62
1:B:285:THR:HG23	8:B:451:HOH:O	1.99	0.61
1:A:367:ARG:H	1:E:214:ASN:HD22	1.47	0.61
1:D:288:ASN:HD22	1:D:288:ASN:H	1.47	0.61
1:D:346:ILE:HD11	1:D:411:LEU:CD1	2.31	0.61
1:B:81:ILE:HG23	1:B:263:ALA:HB2	1.82	0.61
1:B:199:ILE:O	1:B:372:THR:HG21	2.00	0.60
1:D:196:VAL:HG13	1:D:367:ARG:NH1	2.16	0.60
1:E:283:ASN:ND2	1:E:286:TYR:H	1.99	0.60
1:D:346:ILE:HD11	1:D:411:LEU:HD13	1.84	0.60
1:A:367:ARG:H	1:E:214:ASN:ND2	2.01	0.59
1:E:411:LEU:HD21	3:E:600:LMT:H62	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ASP:OD1	1:C:379:HIS:HD2	1.88	0.56
1:E:327:ASN:HD21	1:E:339:TYR:N	1.99	0.56
1:A:283:ASN:ND2	1:A:286:TYR:H	2.02	0.56
1:D:283:ASN:HD22	1:D:286:TYR:H	1.51	0.56
1:F:402:PHE:O	1:F:406:VAL:HG23	2.06	0.56
1:A:285:THR:HG23	8:A:438:HOH:O	2.04	0.56
1:F:124[A]:CYS:SG	4:F:700:H2S:S	2.91	0.56
1:C:147:VAL:HG11	1:C:231:VAL:HG21	1.88	0.56
1:D:327:ASN:HD21	1:D:339:TYR:N	1.96	0.56
1:D:350:ASP:OD1	1:D:379:HIS:HD2	1.88	0.55
1:C:166:MET:HE3	1:C:350:ASP:HB3	1.89	0.55
1:A:199:ILE:O	1:A:372:THR:HG21	2.07	0.55
1:C:394:ARG:NH1	7:C:432:SO4:S	2.79	0.55
1:D:196:VAL:CG1	1:D:367:ARG:NH1	2.70	0.55
1:D:19:TYR:CD2	1:D:398:ILE:HG12	2.42	0.54
1:C:394:ARG:NH1	7:C:432:SO4:O1	2.41	0.53
1:F:346:ILE:HD11	1:F:411:LEU:HD11	1.90	0.53
1:C:420:LYS:CD	1:C:420:LYS:N	2.69	0.53
1:A:293:GLY:HA2	1:A:317:ILE:HG12	1.91	0.53
3:F:600:LMT:H4'	3:F:600:LMT:H2O1	1.74	0.53
1:D:19:TYR:HD2	1:D:398:ILE:HG12	1.74	0.52
1:B:124[A]:CYS:SG	4:B:700:H2S:S	2.98	0.52
1:B:346:ILE:HD11	1:B:411:LEU:CD1	2.39	0.52
1:E:293:GLY:HA2	1:E:317:ILE:HG12	1.91	0.52
1:F:196:VAL:HG22	1:F:367:ARG:NH1	2.25	0.52
1:D:108:LYS:HB3	1:D:255:GLN:O	2.10	0.52
1:D:294:VAL:HA	1:D:312:LYS:HD3	1.91	0.52
1:B:196:VAL:HG22	1:B:367:ARG:HH11	1.74	0.51
1:C:293:GLY:HA2	1:C:317:ILE:HG12	1.92	0.51
3:E:600:LMT:H6'1	3:F:600:LMT:H2'	1.92	0.51
1:D:50:MET:HG3	1:D:166:MET:HE2	1.92	0.51
1:D:394:ARG:NH1	7:D:432:SO4:O3	2.44	0.50
3:E:600:LMT:H2B	3:F:600:LMT:H2O1	1.77	0.50
1:B:235:ASP:OD2	1:B:241:HIS:HE1	1.94	0.50
1:E:350:ASP:HB2	1:E:382:LYS:HD3	1.94	0.50
1:F:283:ASN:ND2	1:F:286:TYR:H	2.03	0.50
1:E:327:ASN:ND2	1:E:339:TYR:H	2.02	0.50
1:F:300:PRO:HA	1:F:310:VAL:HG23	1.94	0.50
1:C:6:VAL:HG12	1:C:31:THR:CG2	2.41	0.49
1:D:227:GLU:HB2	1:D:230:LYS:HG2	1.95	0.49
1:F:327:ASN:HD21	1:F:339:TYR:N	2.07	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:THR:CG2	1:B:135:LYS:HD3	2.43	0.48
1:A:121:THR:CG2	1:A:135:LYS:HD3	2.43	0.48
1:B:283:ASN:ND2	1:B:286:TYR:H	2.05	0.48
1:D:405:LYS:O	1:D:409:ILE:HG23	2.13	0.48
1:D:196:VAL:CG1	1:D:367:ARG:HH12	2.26	0.48
1:C:283:ASN:ND2	1:C:286:TYR:H	2.05	0.48
1:E:304:THR:OG1	1:E:308:THR:HB	2.13	0.48
1:B:327:ASN:HD21	1:B:339:TYR:N	2.09	0.47
1:E:326:HIS:HD2	8:E:451:HOH:O	1.97	0.47
1:A:158:GLY:HA3	5:A:800:PS9:S7	2.55	0.47
1:C:165:LEU:HD21	1:C:210:PHE:HE1	1.79	0.47
1:C:346:ILE:HD11	1:C:411:LEU:CD1	2.45	0.47
1:C:208:ASP:O	1:C:212:GLU:HG3	2.15	0.47
1:B:313:THR:HG21	1:B:345:ALA:HB1	1.98	0.46
1:D:277:VAL:HG22	1:D:281:PHE:C	2.36	0.46
1:C:202:SER:O	1:C:206:VAL:HG23	2.15	0.46
1:D:104:ALA:HB2	1:D:292:VAL:HG22	1.98	0.46
1:E:235:ASP:OD2	1:E:241:HIS:HE1	1.99	0.46
1:E:50:MET:HG3	1:E:166:MET:HE2	1.98	0.46
1:B:308:THR:HG22	8:B:476:HOH:O	2.16	0.45
1:B:149:GLY:HA3	1:B:185:ILE:O	2.16	0.45
1:C:147:VAL:HG11	1:C:231:VAL:CG2	2.47	0.45
1:D:369:ARG:NH1	7:F:431:SO4:O2	2.50	0.45
1:C:36:ARG:NH1	1:C:127:GLU:OE1	2.49	0.44
1:C:407:LEU:HD13	3:C:600:LMT:H92	1.99	0.44
1:A:350:ASP:OD1	1:A:379:HIS:HD2	2.00	0.44
1:C:353:GLU:CG	6:C:900:MES:H51	2.47	0.44
1:D:165:LEU:HD21	1:D:210:PHE:HE1	1.82	0.44
1:B:137:GLN:NE2	8:B:457:HOH:O	2.51	0.44
1:F:347[A]:CYS:HB3	5:F:800:PS9:S6	2.58	0.44
1:A:346:ILE:HD11	1:A:411:LEU:CD1	2.48	0.44
1:C:6:VAL:HG23	1:C:101:LEU:CD1	2.48	0.43
1:D:204:ARG:CZ	1:F:204:ARG:HD3	2.48	0.43
3:E:600:LMT:H3'	3:F:600:LMT:H6E	2.00	0.43
1:F:196:VAL:HG21	1:F:363:VAL:HG13	1.99	0.43
1:F:293:GLY:HA2	1:F:317:ILE:HG12	1.99	0.43
1:B:347[B]:CYS:SG	5:B:800:PS9:S5	3.15	0.43
1:D:350:ASP:HB2	1:D:382:LYS:HD3	2.00	0.43
1:C:147:VAL:HG12	1:C:248:THR:HG22	1.99	0.43
1:A:121:THR:HG22	1:A:135:LYS:HD3	2.00	0.43
1:D:5:VAL:HG12	1:D:28:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ASN:O	1:E:246:LYS:HE2	2.19	0.43
1:F:372:THR:O	1:F:372:THR:CG2	2.66	0.43
1:B:173[A]:LYS:HD3	1:B:173[A]:LYS:HA	1.86	0.43
1:B:214:ASN:HD21	1:F:366:PRO:HA	1.83	0.42
1:C:124[A]:CYS:HB2	8:C:743:HOH:O	2.19	0.42
1:E:113:ALA:HB3	1:E:116:GLN:HB2	2.02	0.42
1:F:261:ALA:HB2	1:F:273:LYS:HD3	2.00	0.42
1:F:341:PRO:HB2	1:F:343:LEU:HD13	2.01	0.42
1:B:402:PHE:O	1:B:406:VAL:HG23	2.19	0.42
1:C:46:PRO:HG3	1:C:123:ILE:HD12	2.01	0.42
1:A:283:ASN:HA	1:A:284:PRO:HD3	1.89	0.42
1:B:347[A]:CYS:HB3	5:B:800:PS9:S5	2.60	0.42
1:D:151:ILE:HB	1:D:152:PRO:HD2	2.02	0.42
1:A:158:GLY:HA3	5:A:800:PS9:S4	2.60	0.42
1:B:27:ASP:OD1	1:B:27:ASP:N	2.53	0.42
7:B:435:SO4:O3	1:F:369:ARG:HD3	2.20	0.42
1:A:315:MET:CE	1:A:346:ILE:HD12	2.50	0.42
1:D:50:MET:HG3	1:D:166:MET:CE	2.50	0.42
1:A:279:ARG:HD2	1:A:428:SER:OG	2.20	0.41
1:C:172:LYS:HE3	8:C:624:HOH:O	2.18	0.41
1:F:196:VAL:HG23	1:F:301:ILE:HD13	2.02	0.41
1:C:310:VAL:HG12	8:C:784:HOH:O	2.21	0.41
1:D:277:VAL:O	1:D:426:PRO:HD3	2.19	0.41
2:D:441:FAD:H9	2:D:441:FAD:H1'1	1.87	0.41
1:A:400:PRO:HB3	1:B:391:TRP:CZ2	2.55	0.41
1:C:170:GLU:O	1:C:174:ARG:HG2	2.19	0.41
1:D:148:ILE:O	1:D:184:PHE:HA	2.19	0.41
1:C:156[A]:CSS:SG	5:C:800:PS9:S2	3.18	0.41
1:F:196:VAL:HG22	1:F:367:ARG:HH11	1.84	0.41
2:A:441:FAD:H9	2:A:441:FAD:H1'1	1.77	0.41
1:A:361:ASP:HA	1:A:362:PRO:HA	1.94	0.41
1:A:407:LEU:HB3	1:A:413:VAL:CG1	2.51	0.41
1:C:124[B]:CYS:HB2	8:C:743:HOH:O	2.21	0.41
1:C:388:TYR:CZ	1:C:392:LYS:HD2	2.56	0.41
1:E:9:GLY:O	1:E:14:GLY:HA3	2.21	0.41
2:E:441:FAD:H9	2:E:441:FAD:H1'1	1.85	0.41
1:B:79:GLU:HG3	1:B:91:GLN:HA	2.03	0.41
1:F:277:VAL:HB	1:F:281:PHE:HA	2.03	0.41
1:A:279:ARG:NH1	1:A:430:CYS:HA	2.37	0.40
1:E:149:GLY:HA3	1:E:185:ILE:O	2.22	0.40
1:F:372:THR:O	1:F:372:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124[A]:CYS:HB2	8:A:510:HOH:O	2.22	0.40
1:A:173:LYS:HD3	1:A:173:LYS:HA	1.92	0.40
1:C:150:ALA:HB3	1:C:186:THR:HG22	2.03	0.40
1:D:151:ILE:HB	1:D:152:PRO:CD	2.52	0.40
1:F:364:ILE:HA	1:F:365:PRO:HD3	1.95	0.40
1:A:235:ASP:OD2	1:A:241:HIS:HE1	2.04	0.40
3:C:600:LMT:O2B	3:C:600:LMT:H6E	2.22	0.40
1:F:63:ALA:HB3	1:F:64:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/430 (101%)	427 (99%)	6 (1%)	0	100	100
1	B	432/430 (100%)	426 (99%)	6 (1%)	0	100	100
1	C	431/430 (100%)	423 (98%)	8 (2%)	0	100	100
1	D	431/430 (100%)	421 (98%)	9 (2%)	1 (0%)	44	55
1	E	429/430 (100%)	417 (97%)	12 (3%)	0	100	100
1	F	429/430 (100%)	422 (98%)	7 (2%)	0	100	100
All	All	2585/2580 (100%)	2536 (98%)	48 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	334	ASN

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	362/356 (102%)	350 (97%)	12 (3%)	33	48
1	B	361/356 (101%)	350 (97%)	11 (3%)	36	52
1	C	360/356 (101%)	343 (95%)	17 (5%)	22	32
1	D	360/356 (101%)	349 (97%)	11 (3%)	35	51
1	E	358/356 (101%)	345 (96%)	13 (4%)	30	44
1	F	358/356 (101%)	348 (97%)	10 (3%)	38	55
All	All	2159/2136 (101%)	2085 (97%)	74 (3%)	32	47

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	42	THR
1	A	147	VAL
1	A	165	LEU
1	A	177	ARG
1	A	191	LEU
1	A	214	ASN
1	A	227	GLU
1	A	285	THR
1	A	390	LEU
1	A	408	GLU
1	A	409	ILE
1	B	24	LEU
1	B	28	LEU
1	B	64	PRO
1	B	81	ILE
1	B	177	ARG
1	B	191	LEU
1	B	308	THR
1	B	334	ASN
1	B	343	LEU
1	B	407	LEU

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Mol	Chain	Res	Type
1	B	412	LYS
1	C	24	LEU
1	C	171	LEU
1	C	172	LYS
1	C	176	ILE
1	C	177	ARG
1	C	186	THR
1	C	191	LEU
1	C	240	THR
1	C	243	VAL
1	C	285	THR
1	C	338	LYS
1	C	343	LEU
1	C	347[A]	CYS
1	C	347[B]	CYS
1	C	390	LEU
1	C	407	LEU
1	C	420	LYS
1	D	28	LEU
1	D	42	THR
1	D	48	LEU
1	D	177	ARG
1	D	277	VAL
1	D	288	ASN
1	D	308	THR
1	D	369	ARG
1	D	407	LEU
1	D	409	ILE
1	D	413	VAL
1	E	5	VAL
1	E	24	LEU
1	E	28	LEU
1	E	147	VAL
1	E	165	LEU
1	E	171	LEU
1	E	177	ARG
1	E	191	LEU
1	E	308	THR
1	E	343	LEU
1	E	381	PHE
1	E	390	LEU
1	E	407	LEU

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Mol	Chain	Res	Type
1	F	24	LEU
1	F	142	ASN
1	F	165	LEU
1	F	177	ARG
1	F	226	ILE
1	F	343	LEU
1	F	369	ARG
1	F	372	THR
1	F	381	PHE
1	F	417	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	241	HIS
1	A	283	ASN
1	A	327	ASN
1	A	379	HIS
1	B	128	HIS
1	B	214	ASN
1	B	241	HIS
1	B	283	ASN
1	B	327	ASN
1	B	334	ASN
1	B	379	HIS
1	C	23	ASN
1	C	128	HIS
1	C	133	GLN
1	C	137	GLN
1	C	214	ASN
1	C	237	ASN
1	C	241	HIS
1	C	283	ASN
1	C	327	ASN
1	C	379	HIS
1	C	395	ASN
1	D	70	ASN
1	D	214	ASN
1	D	283	ASN
1	D	288	ASN
1	D	327	ASN

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Mol	Chain	Res	Type
1	D	379	HIS
1	E	128	HIS
1	E	214	ASN
1	E	237	ASN
1	E	241	HIS
1	E	283	ASN
1	E	327	ASN
1	E	379	HIS
1	E	395	ASN
1	F	128	HIS
1	F	133	GLN
1	F	214	ASN
1	F	241	HIS
1	F	283	ASN
1	F	327	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

12 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	$\#\|Z\| > 2$
1	CSS	F	156[B]	5	4,6,7	1.10	0	2,6,8	0.76	0
1	CSS	C	156[A]	-	4,5,7	1.07	0	2,5,8	0.71	0
1	CSS	B	156[A]	-	4,5,7	1.01	0	2,5,8	0.37	0
1	CSS	A	156[A]	-	4,5,7	0.84	0	2,5,8	0.09	0
1	CSS	D	156[A]	-	4,5,7	1.14	0	2,5,8	1.11	0
1	CSS	D	156[B]	5	4,6,7	1.04	0	2,6,8	0.40	0
1	CSS	E	156[A]	-	4,5,7	1.06	0	2,5,8	0.36	0
1	CSS	B	156[B]	5	4,6,7	1.01	0	2,6,8	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	CSS	C	156[B]	5	4,6,7	1.10	0	2,6,8	0.74	0
1	CSS	E	156[B]	5	4,6,7	1.05	0	2,6,8	0.48	0
1	CSS	A	156[B]	5	4,6,7	0.89	0	2,6,8	0.29	0
1	CSS	F	156[A]	-	4,5,7	1.05	0	2,5,8	0.15	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
1	CSS	F	156[B]	5	-	1/1/5/7	-
1	CSS	C	156[A]	-	-	1/1/4/7	-
1	CSS	B	156[A]	-	-	0/1/4/7	-
1	CSS	A	156[A]	-	-	1/1/4/7	-
1	CSS	D	156[A]	-	-	1/1/4/7	-
1	CSS	D	156[B]	5	-	0/1/5/7	-
1	CSS	E	156[A]	-	-	1/1/4/7	-
1	CSS	B	156[B]	5	-	1/1/5/7	-
1	CSS	C	156[B]	5	-	0/1/5/7	-
1	CSS	E	156[B]	5	-	0/1/5/7	-
1	CSS	A	156[B]	5	-	0/1/5/7	-
1	CSS	F	156[A]	-	-	1/1/4/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	156[B]	CSS	N-CA-CB-SG
1	D	156[A]	CSS	N-CA-CB-SG
1	F	156[B]	CSS	N-CA-CB-SG
1	A	156[A]	CSS	N-CA-CB-SG
1	C	156[A]	CSS	N-CA-CB-SG
1	E	156[A]	CSS	N-CA-CB-SG
1	F	156[A]	CSS	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	156[A]	CSS	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 7 are modelled with single atom - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	SO4	E	433	-	4,4,4	0.24	0	6,6,6	0.16	0
7	SO4	F	434	-	4,4,4	0.23	0	6,6,6	0.13	0
7	SO4	B	432	-	4,4,4	0.27	0	6,6,6	0.12	0
5	PS9	C	800	1	3,5,8	0.85	0	2,4,8	1.19	0
7	SO4	C	432	-	4,4,4	0.18	0	6,6,6	0.19	0
2	FAD	B	441	4	54,58,58	1.30	4 (7%)	71,89,89	1.49	11 (15%)
2	FAD	E	441	4	54,58,58	1.39	5 (9%)	71,89,89	1.45	11 (15%)
5	PS9	F	800	1	8,8,8	0.89	0	8,8,8	1.32	1 (12%)
3	LMT	E	600	-	36,36,36	0.53	0	47,47,47	0.98	3 (6%)
6	MES	C	900	-	12,12,12	2.33	1 (8%)	15,16,16	2.39	5 (33%)
2	FAD	D	441	4	54,58,58	1.36	6 (11%)	71,89,89	1.42	12 (16%)
2	FAD	A	441	4	54,58,58	1.33	5 (9%)	71,89,89	1.45	11 (15%)
7	SO4	B	434	-	4,4,4	0.23	0	6,6,6	0.11	0
6	MES	B	900	-	12,12,12	2.28	1 (8%)	15,16,16	2.35	6 (40%)
7	SO4	A	434	-	4,4,4	0.23	0	6,6,6	0.12	0
7	SO4	F	431	-	4,4,4	0.24	0	6,6,6	0.09	0
7	SO4	E	435	-	4,4,4	0.22	0	6,6,6	0.11	0
3	LMT	F	600	-	36,36,36	0.49	0	47,47,47	0.97	1 (2%)
7	SO4	A	433	-	4,4,4	0.22	0	6,6,6	0.19	0
5	PS9	A	800	1	8,8,8	0.90	0	8,8,8	1.53	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SO4	A	432	-	4,4,4	0.22	0	6,6,6	0.16	0
7	SO4	D	434	-	4,4,4	0.24	0	6,6,6	0.16	0
7	SO4	A	431	-	4,4,4	0.25	0	6,6,6	0.10	0
3	LMT	C	600	-	36,36,36	0.52	0	47,47,47	1.05	4 (8%)
7	SO4	D	433	-	4,4,4	0.23	0	6,6,6	0.06	0
6	MES	E	900	-	12,12,12	2.31	1 (8%)	15,16,16	2.44	7 (46%)
7	SO4	C	434	-	4,4,4	0.26	0	6,6,6	0.16	0
6	MES	D	900	-	12,12,12	2.38	1 (8%)	15,16,16	2.33	4 (26%)
7	SO4	B	433	-	4,4,4	0.29	0	6,6,6	0.24	0
5	PS9	B	800	1	3,5,8	0.84	0	2,4,8	0.81	0
3	LMT	D	600	-	36,36,36	0.48	0	47,47,47	0.88	1 (2%)
7	SO4	F	433	-	4,4,4	0.24	0	6,6,6	0.29	0
7	SO4	B	435	-	4,4,4	0.24	0	6,6,6	0.12	0
7	SO4	C	431	-	4,4,4	0.22	0	6,6,6	0.18	0
7	SO4	E	434	-	4,4,4	0.26	0	6,6,6	0.17	0
7	SO4	D	432	-	4,4,4	0.25	0	6,6,6	0.16	0
7	SO4	C	433	-	4,4,4	0.26	0	6,6,6	0.36	0
6	MES	F	900	-	12,12,12	2.25	1 (8%)	15,16,16	2.38	7 (46%)
2	FAD	C	441	4	54,58,58	1.36	7 (12%)	71,89,89	1.41	10 (14%)
5	PS9	D	802	-	2,4,8	0.85	0	1,3,8	1.52	0
7	SO4	B	431	-	4,4,4	0.22	0	6,6,6	0.19	0
5	PS9	E	800	1	8,8,8	0.85	0	8,8,8	1.31	1 (12%)
3	LMT	A	600	-	36,36,36	0.53	0	47,47,47	0.94	2 (4%)
7	SO4	E	432	-	4,4,4	0.23	0	6,6,6	0.09	0
2	FAD	F	441	4	54,58,58	1.30	4 (7%)	71,89,89	1.45	11 (15%)
3	LMT	B	600	-	36,36,36	0.62	1 (2%)	47,47,47	1.33	4 (8%)
7	SO4	E	431	-	4,4,4	0.27	0	6,6,6	0.14	0
6	MES	A	900	-	12,12,12	2.28	1 (8%)	15,16,16	2.34	6 (40%)

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
5	PS9	C	800	1	-	1/3/3/8	-
2	FAD	B	441	4	-	5/30/50/50	0/6/6/6
2	FAD	E	441	4	-	5/30/50/50	0/6/6/6
5	PS9	F	800	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	E	600	-	-	14/21/61/61	0/2/2/2
6	MES	C	900	-	-	1/6/14/14	0/1/1/1
2	FAD	D	441	4	-	5/30/50/50	0/6/6/6
2	FAD	A	441	4	-	5/30/50/50	0/6/6/6
6	MES	B	900	-	-	3/6/14/14	0/1/1/1
3	LMT	F	600	-	-	13/21/61/61	0/2/2/2
5	PS9	A	800	1	-	-	0/1/1/1
3	LMT	C	600	-	-	9/21/61/61	0/2/2/2
6	MES	E	900	-	-	1/6/14/14	0/1/1/1
6	MES	D	900	-	-	1/6/14/14	0/1/1/1
5	PS9	B	800	1	-	2/3/3/8	-
3	LMT	D	600	-	-	13/21/61/61	0/2/2/2
6	MES	F	900	-	-	1/6/14/14	0/1/1/1
2	FAD	C	441	4	-	5/30/50/50	0/6/6/6
5	PS9	D	802	-	-	1/2/2/8	-
5	PS9	E	800	1	-	-	0/1/1/1
3	LMT	A	600	-	-	11/21/61/61	0/2/2/2
2	FAD	F	441	4	-	5/30/50/50	0/6/6/6
3	LMT	B	600	-	-	12/21/61/61	0/2/2/2
6	MES	A	900	-	-	4/6/14/14	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	900	MES	C8-S	-7.99	1.66	1.77
6	C	900	MES	C8-S	-7.76	1.66	1.77
6	E	900	MES	C8-S	-7.74	1.66	1.77
6	A	900	MES	C8-S	-7.62	1.66	1.77
6	B	900	MES	C8-S	-7.58	1.67	1.77
6	F	900	MES	C8-S	-7.52	1.67	1.77
2	E	441	FAD	O4-C4	6.73	1.36	1.23
2	C	441	FAD	O4-C4	6.69	1.36	1.23
2	A	441	FAD	O4-C4	6.53	1.36	1.23
2	D	441	FAD	O4-C4	6.45	1.35	1.23
2	F	441	FAD	O4-C4	6.38	1.35	1.23
2	B	441	FAD	O4-C4	6.09	1.35	1.23
3	B	600	LMT	O1'-C1'	2.82	1.44	1.40
2	D	441	FAD	O4B-C1B	2.70	1.44	1.40
2	C	441	FAD	P-O3P	2.67	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	441	FAD	P-O3P	2.62	1.62	1.59
2	B	441	FAD	C9A-N10	-2.60	1.36	1.41
2	F	441	FAD	C9A-N10	-2.58	1.36	1.41
2	E	441	FAD	O4B-C1B	2.53	1.44	1.40
2	B	441	FAD	C4X-N5	2.53	1.36	1.30
2	B	441	FAD	P-O3P	2.43	1.62	1.59
2	A	441	FAD	C4X-N5	2.40	1.35	1.30
2	E	441	FAD	C9A-N10	-2.37	1.37	1.41
2	A	441	FAD	O4B-C1B	2.36	1.44	1.40
2	D	441	FAD	C4X-N5	2.32	1.35	1.30
2	E	441	FAD	C5X-N5	-2.31	1.35	1.39
2	C	441	FAD	C9A-N10	-2.27	1.37	1.41
2	D	441	FAD	C9A-N10	-2.26	1.37	1.41
2	E	441	FAD	C4X-N5	2.17	1.35	1.30
2	F	441	FAD	O4B-C1B	2.16	1.43	1.40
2	A	441	FAD	C9A-N10	-2.16	1.37	1.41
2	D	441	FAD	P-O3P	2.16	1.61	1.59
2	F	441	FAD	C4X-N5	2.13	1.35	1.30
2	C	441	FAD	C5X-N5	-2.09	1.35	1.39
2	C	441	FAD	C2A-N3A	2.08	1.35	1.32
2	D	441	FAD	PA-O3P	2.07	1.61	1.59
2	C	441	FAD	C4X-N5	2.06	1.35	1.30
2	C	441	FAD	C4-N3	-2.02	1.35	1.38

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	900	MES	C5-N4-C3	6.54	122.92	108.84
6	C	900	MES	C5-N4-C3	6.54	122.92	108.84
2	E	441	FAD	N3A-C2A-N1A	-6.14	120.33	128.67
3	B	600	LMT	O1'-C1'-C2'	5.81	117.09	108.27
2	F	441	FAD	N3A-C2A-N1A	-5.74	120.88	128.67
2	A	441	FAD	N3A-C2A-N1A	-5.70	120.94	128.67
2	C	441	FAD	N3A-C2A-N1A	-5.65	121.00	128.67
2	D	441	FAD	N3A-C2A-N1A	-5.57	121.11	128.67
2	B	441	FAD	N3A-C2A-N1A	-5.44	121.28	128.67
6	A	900	MES	C5-N4-C3	5.37	120.41	108.84
6	F	900	MES	C5-N4-C3	5.36	120.40	108.84
6	B	900	MES	C5-N4-C3	5.18	120.00	108.84
6	E	900	MES	C5-N4-C3	5.03	119.67	108.84
3	F	600	LMT	O1B-C1B-C2B	3.86	117.59	108.09
2	A	441	FAD	C4-N3-C2	-3.62	119.20	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	441	FAD	C4-N3-C2	-3.57	119.30	125.64
3	C	600	LMT	O1B-C4'-C3'	3.51	116.16	107.23
6	E	900	MES	C7-N4-C3	3.48	120.50	111.24
2	F	441	FAD	C4-N3-C2	-3.42	119.58	125.64
6	B	900	MES	C7-N4-C5	3.39	120.28	111.24
6	F	900	MES	C7-N4-C3	3.39	120.26	111.24
6	A	900	MES	C7-N4-C3	3.37	120.22	111.24
3	B	600	LMT	C1B-O5B-C5B	3.37	120.30	113.72
6	E	900	MES	C6-C5-N4	-3.32	105.07	110.12
6	D	900	MES	O3S-S-C8	3.29	112.44	106.00
6	E	900	MES	C7-N4-C5	3.22	119.82	111.24
3	B	600	LMT	C1-O1'-C1'	3.21	119.16	113.68
2	E	441	FAD	C2'-C1'-N10	3.20	125.33	110.20
6	E	900	MES	C2-C3-N4	-3.19	105.27	110.12
6	B	900	MES	O2S-S-C8	3.19	111.55	106.73
6	B	900	MES	C7-N4-C3	3.18	119.72	111.24
6	D	900	MES	C7-N4-C3	3.13	119.58	111.24
2	B	441	FAD	C4X-C10-N10	3.13	120.96	116.48
2	C	441	FAD	C4-N3-C2	-3.10	120.13	125.64
2	C	441	FAD	C4X-C10-N10	3.10	120.92	116.48
2	D	441	FAD	C4-N3-C2	-3.08	120.17	125.64
3	E	600	LMT	O1B-C4'-C3'	3.06	115.00	107.23
6	A	900	MES	C7-N4-C5	3.05	119.38	111.24
6	F	900	MES	C7-N4-C5	3.04	119.34	111.24
6	C	900	MES	C7-N4-C3	3.03	119.31	111.24
2	B	441	FAD	C4X-C4-N3	3.01	120.90	113.25
2	D	441	FAD	C4X-C10-N10	2.98	120.75	116.48
3	C	600	LMT	C1B-O5B-C5B	2.98	119.53	113.72
2	B	441	FAD	C4X-C10-N1	-2.92	117.42	124.59
2	B	441	FAD	C5X-C9A-N10	2.91	120.60	117.97
2	E	441	FAD	C4-N3-C2	-2.91	120.47	125.64
2	F	441	FAD	C4X-C4-N3	2.91	120.65	113.25
2	E	441	FAD	C5X-C9A-N10	2.88	120.58	117.97
6	F	900	MES	O1S-S-C8	2.87	111.07	106.73
2	D	441	FAD	C4X-C4-N3	2.83	120.45	113.25
6	F	900	MES	C6-C5-N4	-2.83	105.82	110.12
2	A	441	FAD	C4X-C10-N10	2.81	120.51	116.48
2	F	441	FAD	C2'-C1'-N10	2.78	123.34	110.20
6	C	900	MES	O1S-S-C8	2.77	110.91	106.73
2	F	441	FAD	C4X-C10-N1	-2.77	117.80	124.59
2	A	441	FAD	C4X-C4-N3	2.76	120.28	113.25
2	A	441	FAD	C5X-C9A-N10	2.75	120.45	117.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	600	LMT	C1B-O1B-C4'	-2.74	111.48	117.98
2	B	441	FAD	C2'-C1'-N10	2.73	123.10	110.20
2	A	441	FAD	C4X-C10-N1	-2.73	117.90	124.59
2	F	441	FAD	C5X-C9A-N10	2.68	120.39	117.97
2	D	441	FAD	C5X-C9A-N10	2.67	120.38	117.97
6	B	900	MES	C2-C3-N4	-2.66	106.07	110.12
2	E	441	FAD	C4X-C4-N3	2.66	120.02	113.25
2	F	441	FAD	C9A-C5X-N5	-2.66	119.64	122.45
2	E	441	FAD	C9A-C5X-N5	-2.65	119.64	122.45
3	D	600	LMT	C1B-O5B-C5B	2.62	118.85	113.72
2	C	441	FAD	C4X-C4-N3	2.62	119.93	113.25
2	D	441	FAD	C4X-C10-N1	-2.62	118.17	124.59
6	A	900	MES	C6-C5-N4	-2.59	106.18	110.12
6	A	900	MES	O2S-S-C8	2.59	110.64	106.73
6	F	900	MES	C2-C3-N4	-2.59	106.18	110.12
2	A	441	FAD	C2'-C1'-N10	2.58	122.42	110.20
2	C	441	FAD	C4X-C10-N1	-2.58	118.27	124.59
2	C	441	FAD	C5X-C9A-N10	2.56	120.28	117.97
2	F	441	FAD	C4X-C10-N10	2.55	120.13	116.48
2	E	441	FAD	C4X-C10-N1	-2.55	118.35	124.59
5	A	800	PS9	S7-S6-S5	2.54	115.49	107.68
3	E	600	LMT	O1B-C4'-C5'	2.54	116.13	109.48
3	C	600	LMT	O1B-C4'-C5'	2.51	116.06	109.48
6	E	900	MES	O3S-S-C8	2.49	110.88	106.00
6	C	900	MES	O2S-S-C8	2.48	110.48	106.73
6	A	900	MES	C2-C3-N4	-2.48	106.36	110.12
3	A	600	LMT	C1B-C2B-C3B	2.47	115.20	110.01
6	C	900	MES	C7-N4-C5	2.45	117.77	111.24
2	D	441	FAD	C2'-C1'-N10	2.41	121.58	110.20
2	A	441	FAD	O4B-C1B-N9A	2.40	111.92	108.75
2	E	441	FAD	C4X-C10-N10	2.39	119.91	116.48
2	B	441	FAD	C10-C4X-N5	-2.37	119.97	124.81
2	B	441	FAD	C10-N1-C2	2.36	121.96	116.85
2	A	441	FAD	C9A-C5X-N5	-2.36	119.95	122.45
6	D	900	MES	C7-N4-C5	2.35	117.50	111.24
6	B	900	MES	C6-C5-N4	-2.35	106.55	110.12
2	D	441	FAD	C9A-C5X-N5	-2.30	120.01	122.45
2	C	441	FAD	C10-C4X-N5	-2.30	120.11	124.81
5	A	800	PS9	S6-S5-S4	2.28	114.70	107.68
2	B	441	FAD	C4A-C5A-N7A	-2.26	106.95	109.34
2	F	441	FAD	C10-N1-C2	2.25	121.72	116.85
2	A	441	FAD	C10-C4X-N5	-2.24	120.23	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	441	FAD	C10-C4X-N5	-2.24	120.23	124.81
2	D	441	FAD	C10-N1-C2	2.23	121.68	116.85
6	E	900	MES	O1S-S-C8	2.23	110.09	106.73
3	B	600	LMT	O5B-C5B-C6B	2.22	111.95	106.44
6	F	900	MES	O2S-S-C8	2.22	110.08	106.73
2	A	441	FAD	O4-C4-C4X	-2.20	120.74	126.53
3	E	600	LMT	C1B-O5B-C5B	2.19	117.99	113.72
2	C	441	FAD	O4-C4-C4X	-2.14	120.89	126.53
2	C	441	FAD	C9A-C5X-N5	-2.13	120.19	122.45
2	D	441	FAD	C10-C4X-N5	-2.13	120.46	124.81
5	F	800	PS9	S8-S9-S2	2.12	114.20	107.68
2	F	441	FAD	O4-C4-C4X	-2.12	120.95	126.53
3	C	600	LMT	C3'-C4'-C5'	-2.11	106.24	110.93
2	D	441	FAD	O4-C4-C4X	-2.09	121.02	126.53
2	E	441	FAD	C10-C4X-N5	-2.09	120.55	124.81
2	D	441	FAD	C4B-O4B-C1B	2.08	111.83	109.92
5	E	800	PS9	S7-S6-S5	2.06	114.01	107.68
2	E	441	FAD	C4A-C5A-N7A	-2.05	107.17	109.34
2	E	441	FAD	O4-C4-C4X	-2.04	121.14	126.53
2	B	441	FAD	C4-C4X-N5	2.04	121.03	118.21
2	C	441	FAD	C10-N1-C2	2.04	121.26	116.85

There are no chirality outliers.

All (117) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	LMT	O5'-C1'-O1'-C1
3	B	600	LMT	C2'-C1'-O1'-C1
3	F	600	LMT	C2B-C1B-O1B-C4'
5	C	800	PS9	S2-S3-S4-S5
6	A	900	MES	C7-C8-S-O1S
6	A	900	MES	C7-C8-S-O2S
6	B	900	MES	C7-C8-S-O1S
6	D	900	MES	C8-C7-N4-C5
3	E	600	LMT	C4'-C5'-C6'-O6'
3	E	600	LMT	O5'-C5'-C6'-O6'
3	C	600	LMT	C3'-C4'-O1B-C1B
3	D	600	LMT	O5B-C5B-C6B-O6B
3	D	600	LMT	C4'-C5'-C6'-O6'
3	A	600	LMT	C4'-C5'-C6'-O6'
3	E	600	LMT	O5'-C1'-O1'-C1
3	A	600	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
3	D	600	LMT	O5'-C5'-C6'-O6'
3	F	600	LMT	O5B-C5B-C6B-O6B
3	E	600	LMT	C3'-C4'-O1B-C1B
3	E	600	LMT	C2'-C1'-O1'-C1
3	B	600	LMT	C4B-C5B-C6B-O6B
3	F	600	LMT	C4B-C5B-C6B-O6B
3	B	600	LMT	C4'-C5'-C6'-O6'
3	B	600	LMT	O5B-C5B-C6B-O6B
3	F	600	LMT	O5'-C5'-C6'-O6'
6	A	900	MES	C7-C8-S-O3S
3	B	600	LMT	O1'-C1-C2-C3
3	B	600	LMT	O5'-C5'-C6'-O6'
3	E	600	LMT	C5-C6-C7-C8
3	E	600	LMT	O5B-C5B-C6B-O6B
3	F	600	LMT	C5-C6-C7-C8
3	C	600	LMT	C2-C1-O1'-C1'
3	D	600	LMT	C2-C3-C4-C5
3	F	600	LMT	C2-C3-C4-C5
3	C	600	LMT	C1-C2-C3-C4
3	C	600	LMT	C2-C3-C4-C5
3	A	600	LMT	O5B-C5B-C6B-O6B
2	D	441	FAD	O3'-C3'-C4'-O4'
3	F	600	LMT	C3-C4-C5-C6
3	F	600	LMT	C11-C10-C9-C8
3	E	600	LMT	C7-C8-C9-C10
3	A	600	LMT	C1-C2-C3-C4
3	D	600	LMT	C4-C5-C6-C7
3	E	600	LMT	C1-C2-C3-C4
3	C	600	LMT	C3-C4-C5-C6
3	A	600	LMT	C7-C8-C9-C10
3	D	600	LMT	C7-C8-C9-C10
3	B	600	LMT	C4-C5-C6-C7
2	D	441	FAD	C2'-C3'-C4'-O4'
3	B	600	LMT	C6-C7-C8-C9
3	D	600	LMT	C4B-C5B-C6B-O6B
3	C	600	LMT	O5B-C5B-C6B-O6B
2	B	441	FAD	O4B-C4B-C5B-O5B
3	F	600	LMT	C4-C5-C6-C7
2	D	441	FAD	C2'-C3'-C4'-C5'
3	B	600	LMT	C3-C4-C5-C6
3	C	600	LMT	C4-C5-C6-C7
3	E	600	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
6	A	900	MES	C8-C7-N4-C5
6	B	900	MES	C8-C7-N4-C3
6	C	900	MES	C8-C7-N4-C5
6	E	900	MES	C8-C7-N4-C5
6	F	900	MES	C8-C7-N4-C5
2	B	441	FAD	C3B-C4B-C5B-O5B
2	B	441	FAD	C2'-C3'-C4'-O4'
3	A	600	LMT	C4-C5-C6-C7
3	D	600	LMT	C3-C4-C5-C6
3	E	600	LMT	C9-C10-C11-C12
3	F	600	LMT	C7-C8-C9-C10
3	E	600	LMT	C11-C10-C9-C8
2	A	441	FAD	C2'-C3'-C4'-C5'
3	B	600	LMT	C2-C1-O1'-C1'
3	A	600	LMT	C11-C10-C9-C8
3	D	600	LMT	C2'-C1'-O1'-C1
2	A	441	FAD	C2'-C3'-C4'-O4'
2	C	441	FAD	C2'-C3'-C4'-O4'
2	E	441	FAD	C2'-C3'-C4'-O4'
3	F	600	LMT	C9-C10-C11-C12
3	A	600	LMT	C5-C6-C7-C8
3	E	600	LMT	C6-C7-C8-C9
3	C	600	LMT	C5'-C4'-O1B-C1B
3	E	600	LMT	C4-C5-C6-C7
2	B	441	FAD	C2'-C3'-C4'-C5'
2	C	441	FAD	C2'-C3'-C4'-C5'
2	E	441	FAD	C2'-C3'-C4'-C5'
3	D	600	LMT	O5'-C1'-O1'-C1
5	D	802	PS9	S9-S2-S3-S4
2	C	441	FAD	O3'-C3'-C4'-O4'
2	F	441	FAD	O4B-C4B-C5B-O5B
2	A	441	FAD	C5B-O5B-PA-O3P
2	F	441	FAD	C2'-C3'-C4'-O4'
2	F	441	FAD	C2'-C3'-C4'-C5'
3	F	600	LMT	C6-C7-C8-C9
3	A	600	LMT	C9-C10-C11-C12
3	A	600	LMT	C6-C7-C8-C9
2	E	441	FAD	O3'-C3'-C4'-O4'
6	B	900	MES	C7-C8-S-O3S
3	D	600	LMT	C5-C6-C7-C8
2	D	441	FAD	O3'-C3'-C4'-C5'
2	A	441	FAD	O3'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
2	B	441	FAD	O3'-C3'-C4'-O4'
3	F	600	LMT	C1-C2-C3-C4
2	F	441	FAD	C3B-C4B-C5B-O5B
2	D	441	FAD	O4B-C4B-C5B-O5B
3	D	600	LMT	C2-C1-O1'-C1'
3	B	600	LMT	O5'-C1'-O1'-C1
2	A	441	FAD	O3'-C3'-C4'-C5'
3	C	600	LMT	C6-C7-C8-C9
5	B	800	PS9	S4-S5-S6-S7
2	F	441	FAD	O3'-C3'-C4'-O4'
3	B	600	LMT	C5-C6-C7-C8
2	C	441	FAD	O3'-C3'-C4'-C5'
5	B	800	PS9	S3-S4-S5-S6
3	D	600	LMT	C11-C10-C9-C8
2	E	441	FAD	O4B-C4B-C5B-O5B
2	E	441	FAD	O3'-C3'-C4'-C5'
2	C	441	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

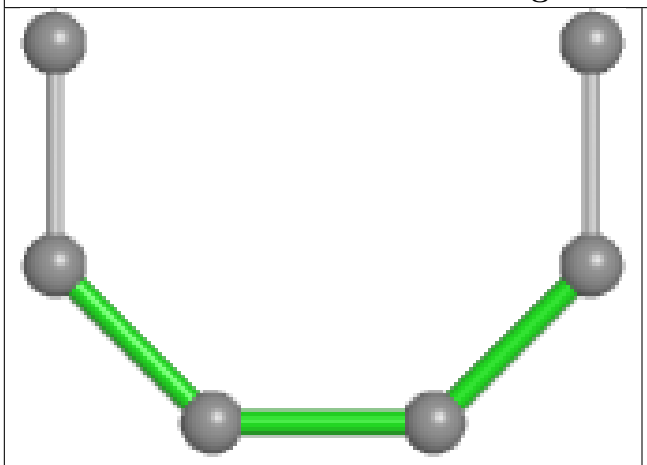
17 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	800	PS9	1	0
7	C	432	SO4	2	0
2	E	441	FAD	1	0
5	F	800	PS9	1	0
3	E	600	LMT	8	0
6	C	900	MES	1	0
2	D	441	FAD	1	0
2	A	441	FAD	1	0
7	F	431	SO4	1	0
3	F	600	LMT	9	0
5	A	800	PS9	2	0
3	C	600	LMT	2	0
5	B	800	PS9	2	0
7	B	435	SO4	1	0
7	D	432	SO4	1	0
5	D	802	PS9	1	0
2	F	441	FAD	1	0

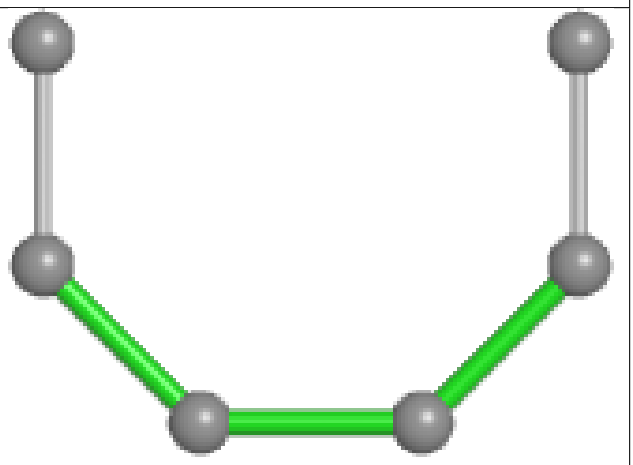
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

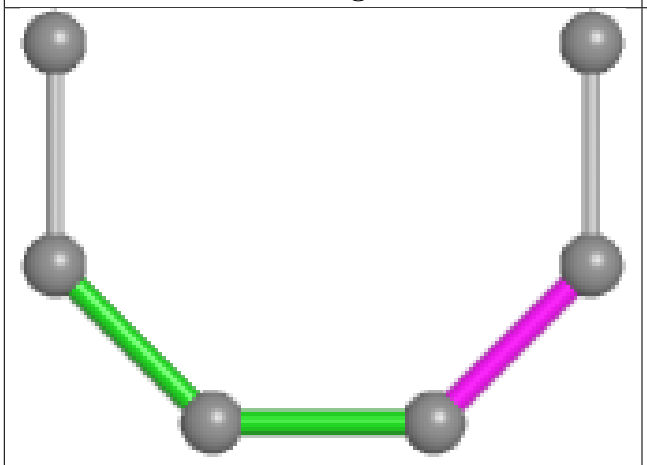
Ligand PS9 C 800



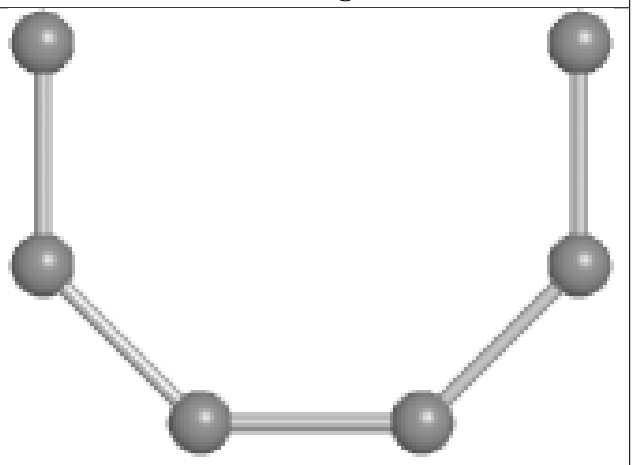
Bond lengths



Bond angles

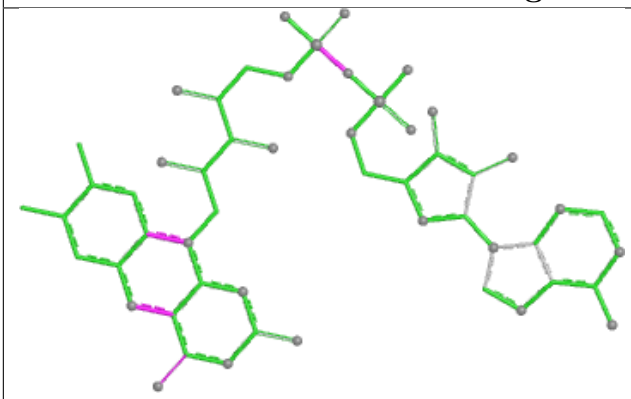


Torsions



Rings

Ligand FAD B 441



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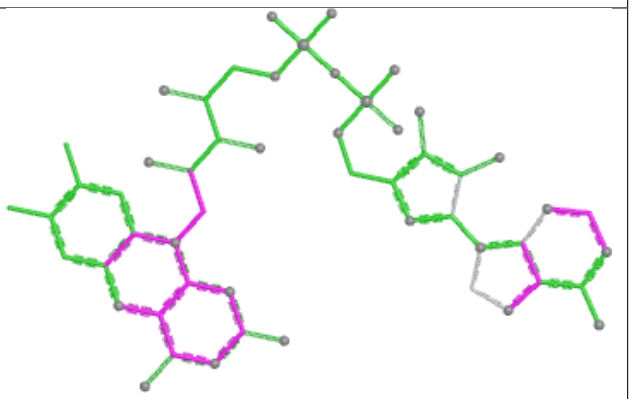

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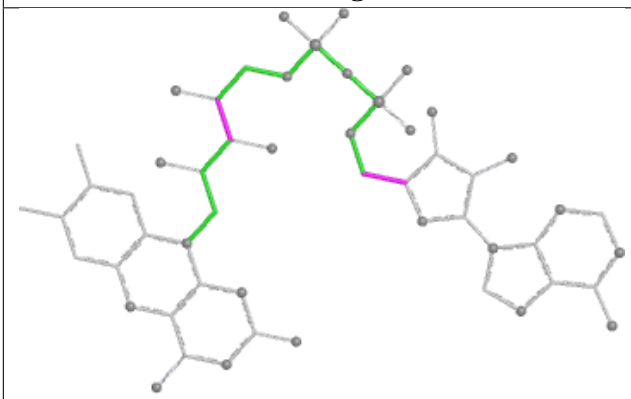

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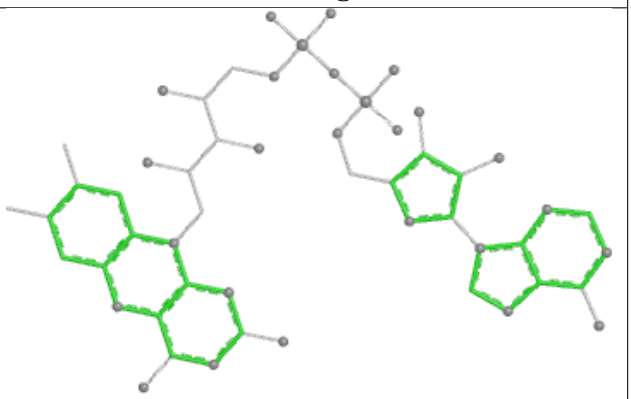
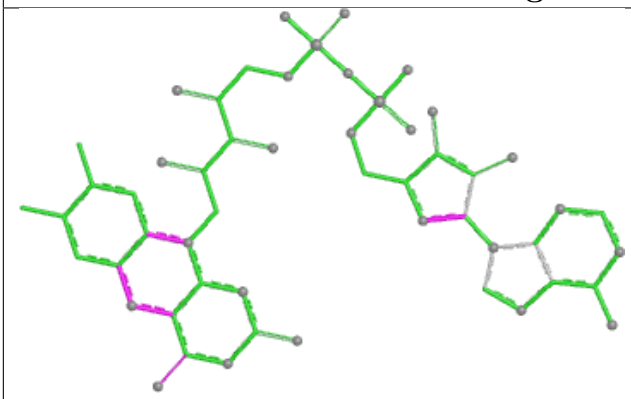
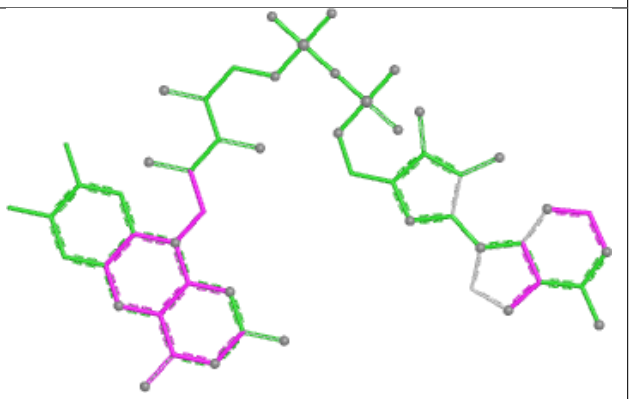


Rings

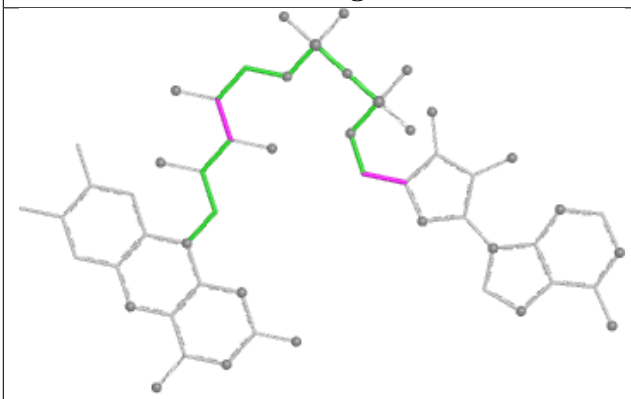
Ligand FAD E 441



Bond lengths



Bond angles



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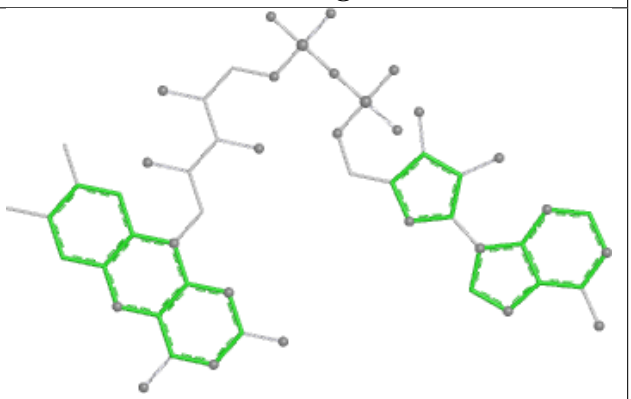
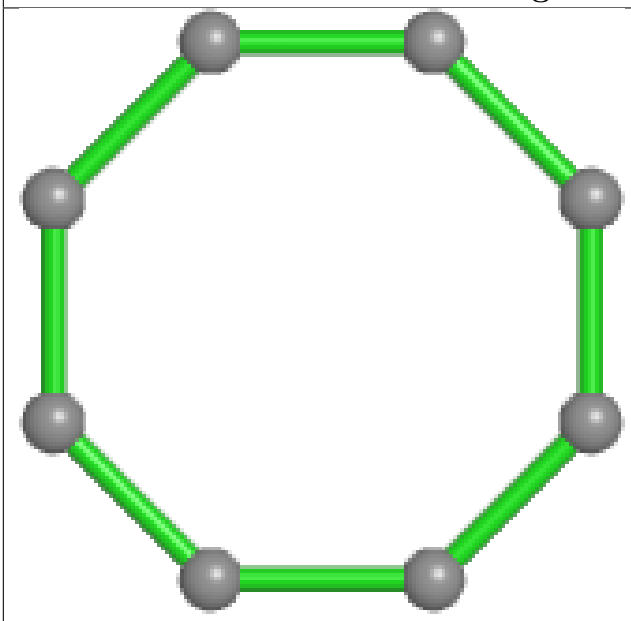


Rings

Ligand PS9 F 800



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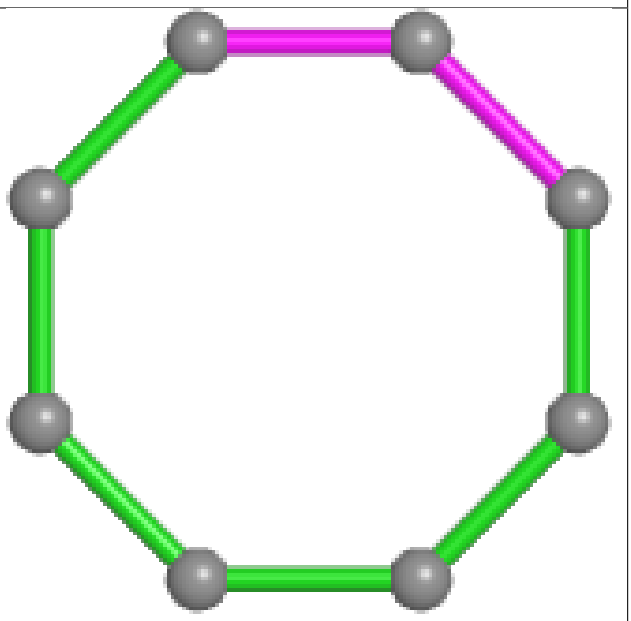

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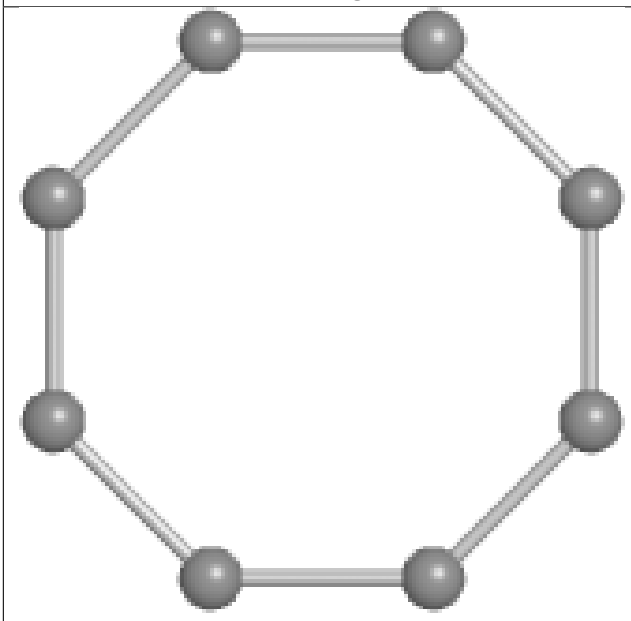

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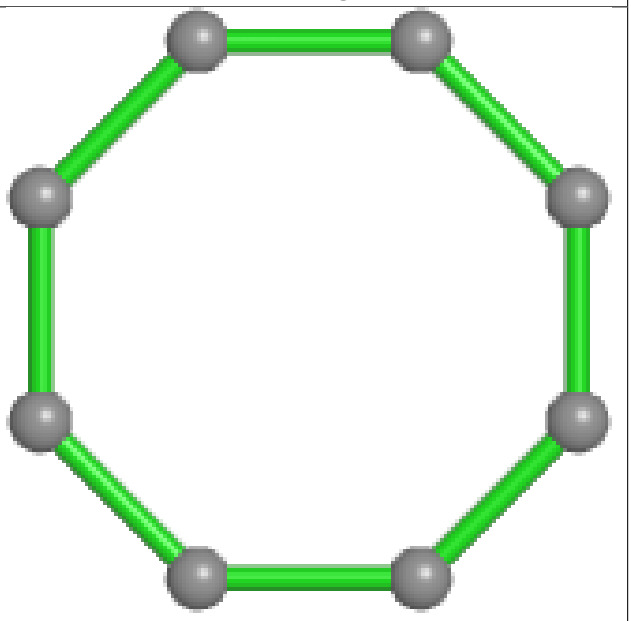
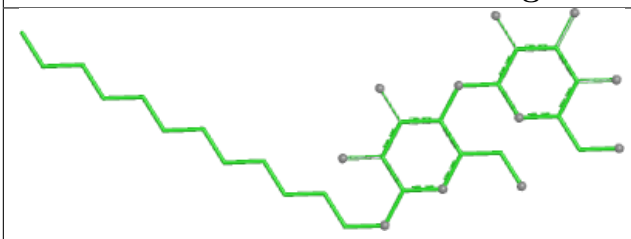


Rings

Ligand LMT E 600



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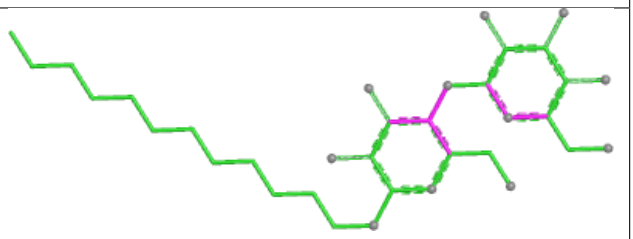

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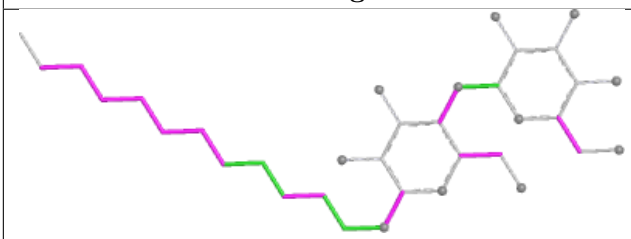

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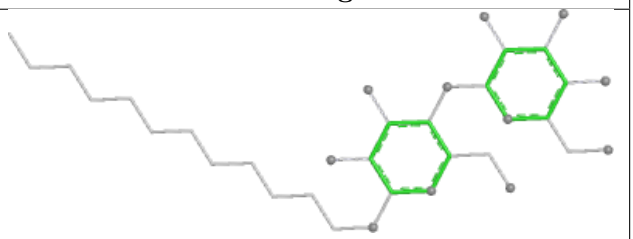
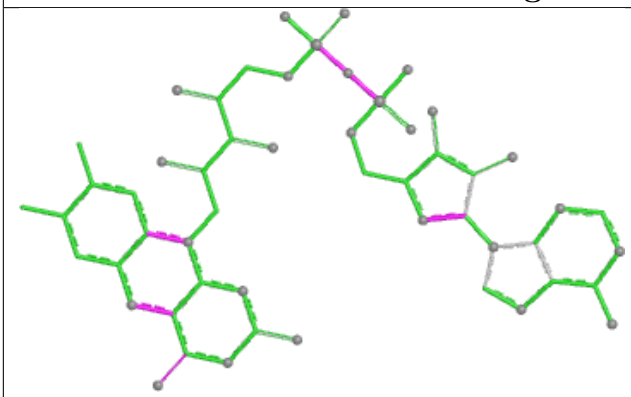


Rings

Ligand FAD D 441



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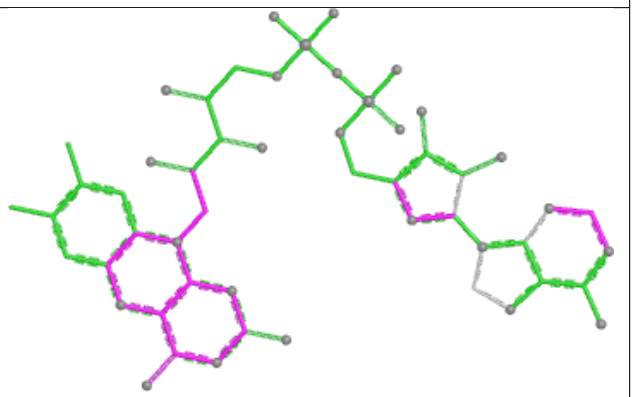

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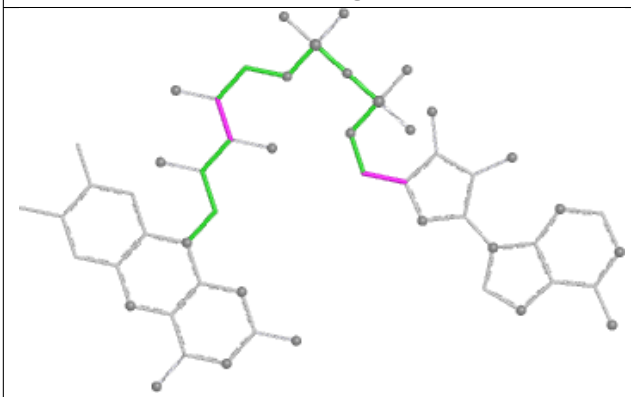

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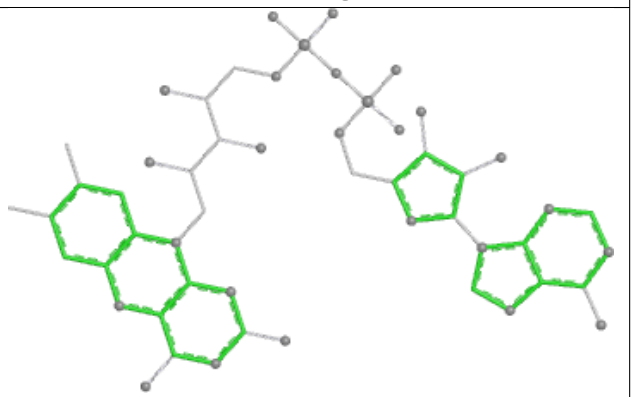
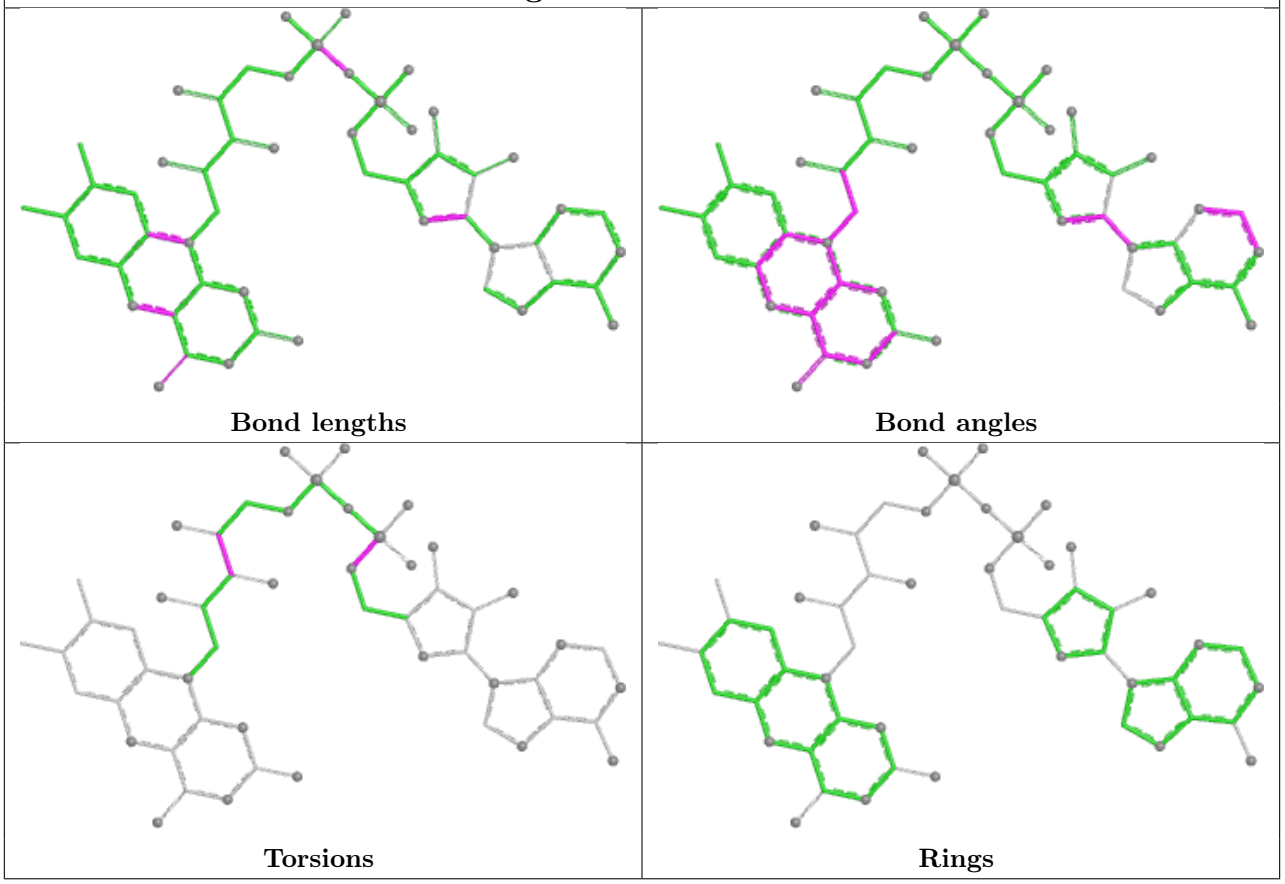
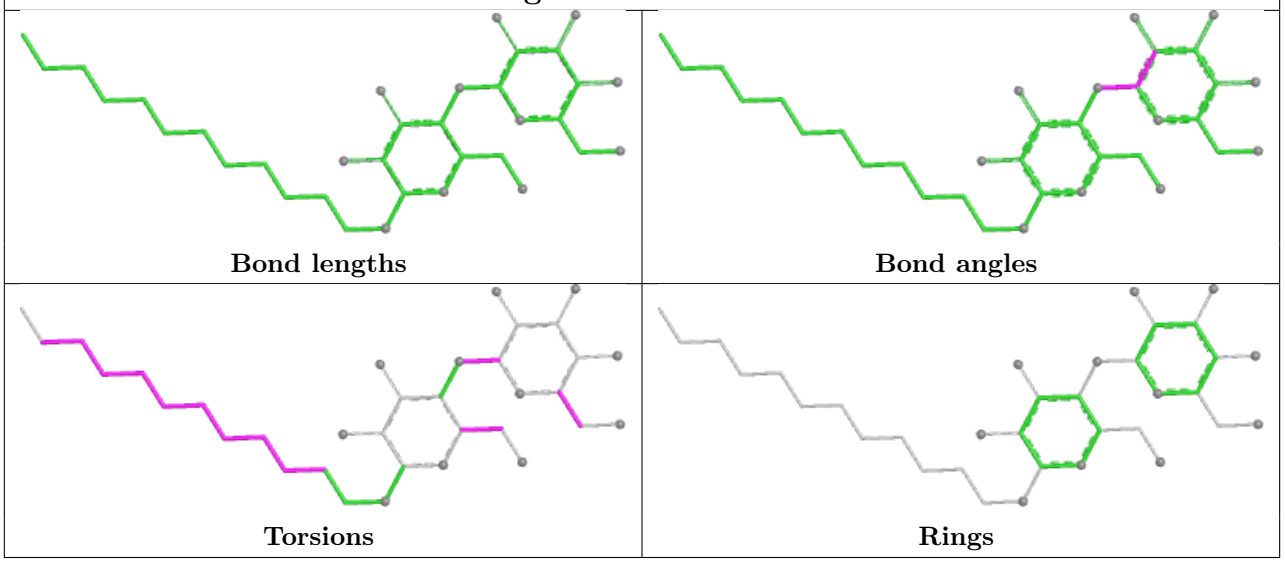


Rings

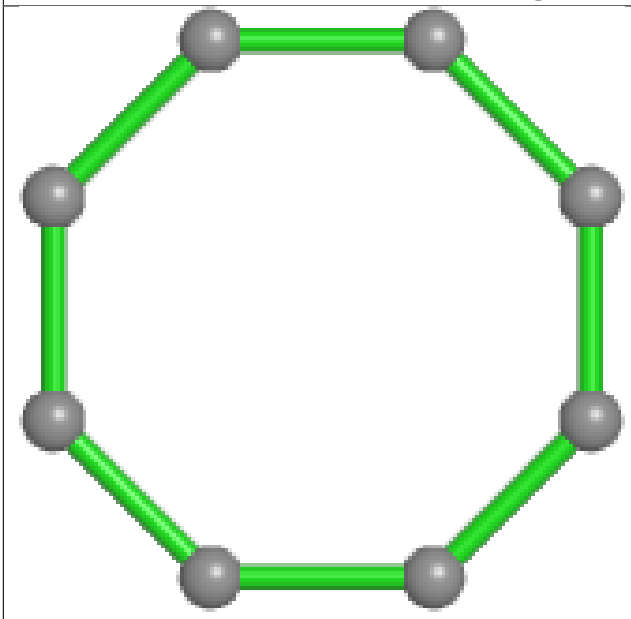
Ligand FAD A 441



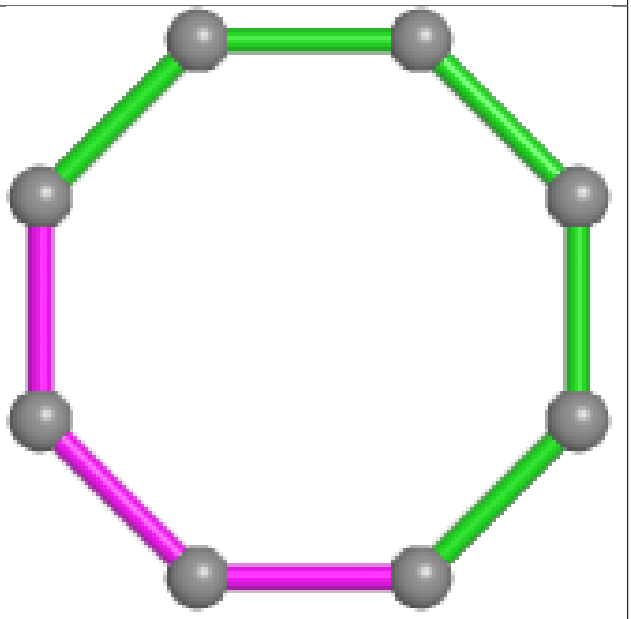
Ligand LMT F 600



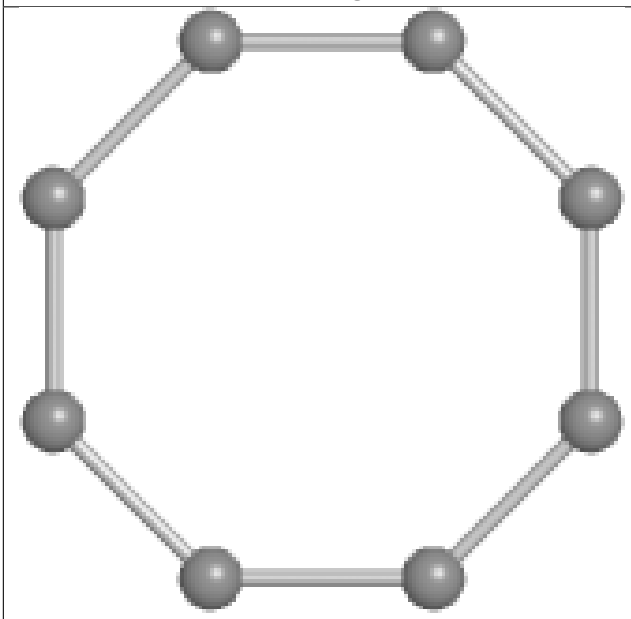
Ligand PS9 A 800



Bond lengths



Bond angles



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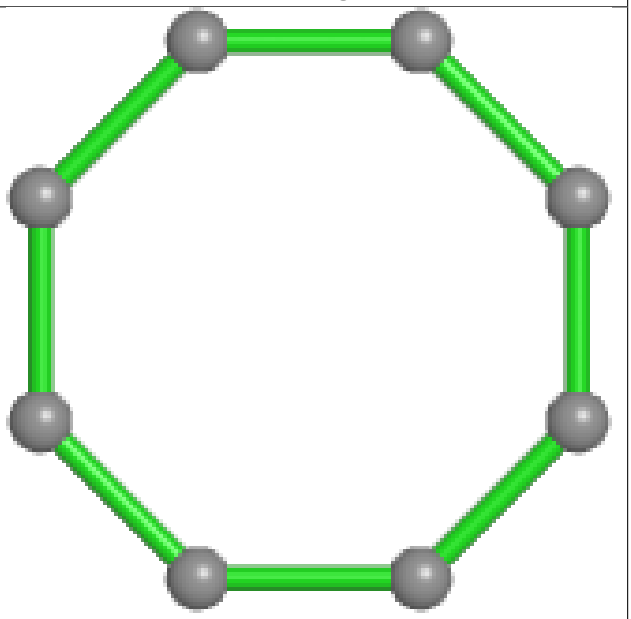
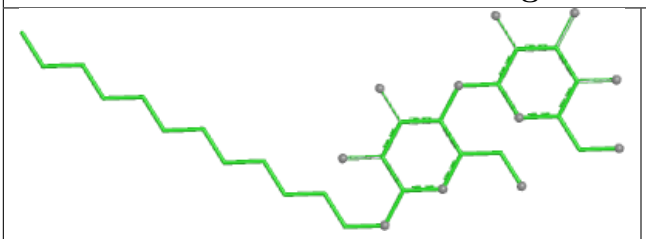


Rings

Ligand LMT C 600



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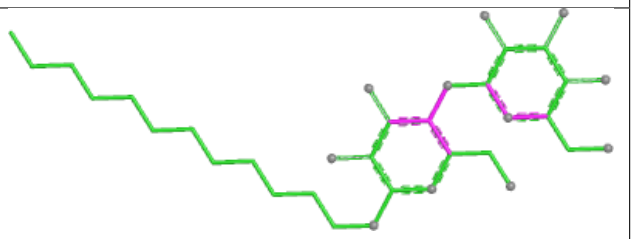
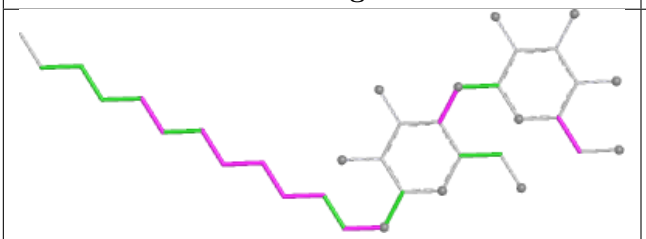
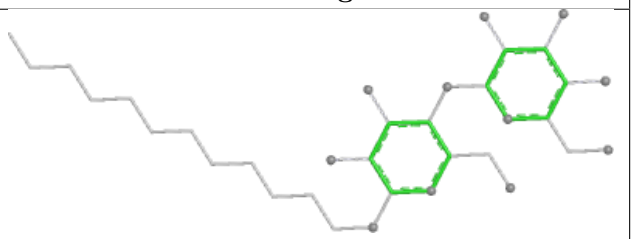


Bond angles

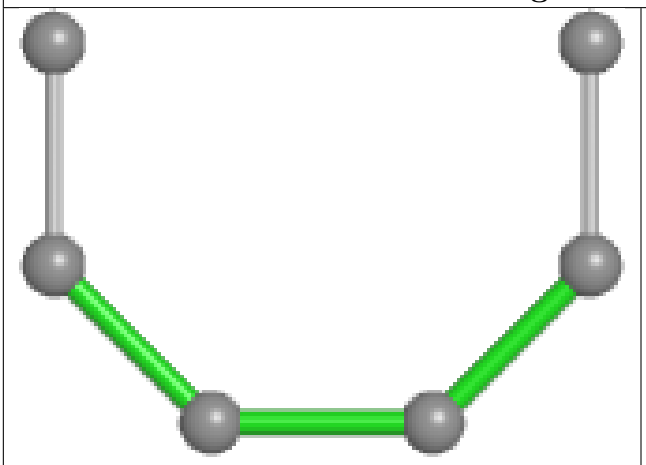


Torsions

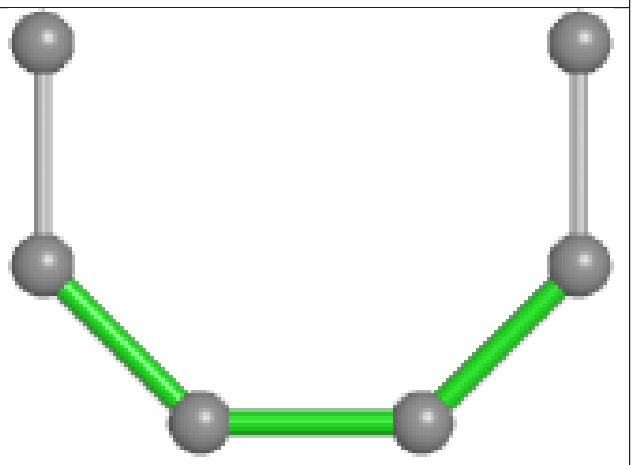


Rings

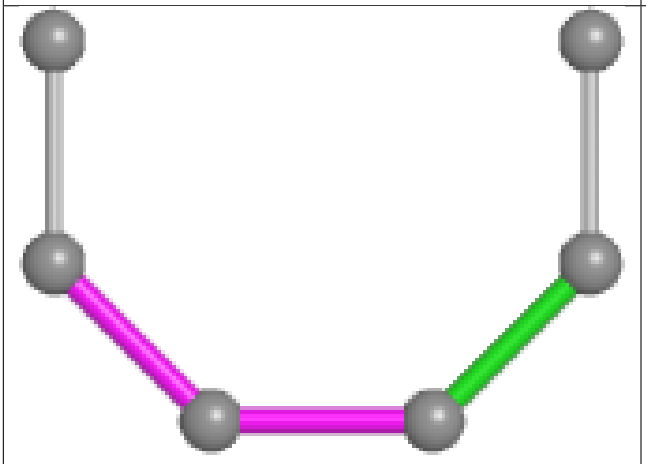
Ligand PS9 B 800



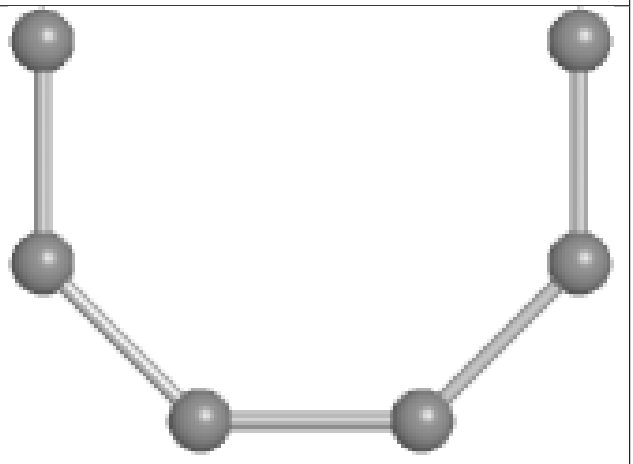
Bond lengths



Bond angles

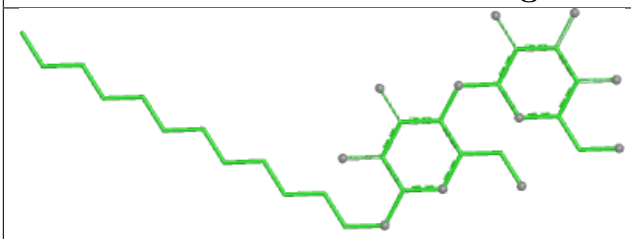


Torsions

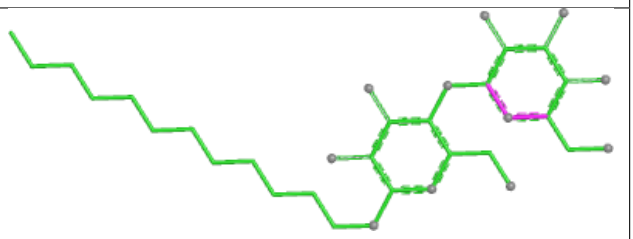


Rings

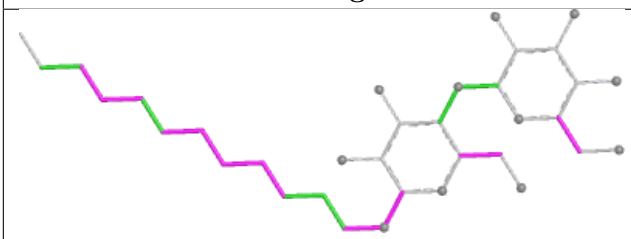
Ligand LMT D 600



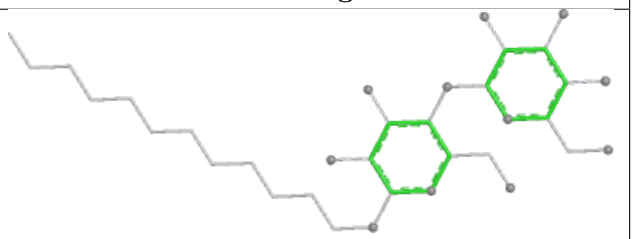
Bond lengths



Bond angles

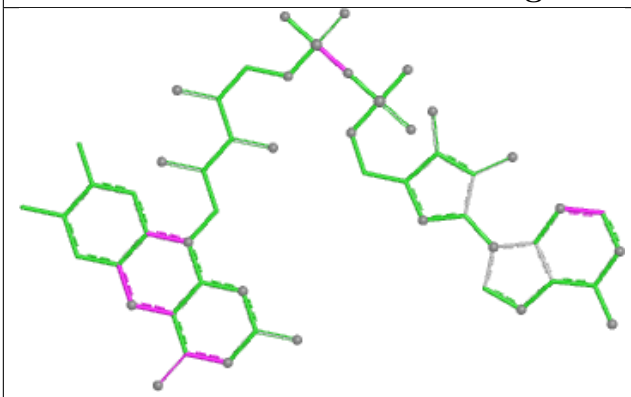


Torsions

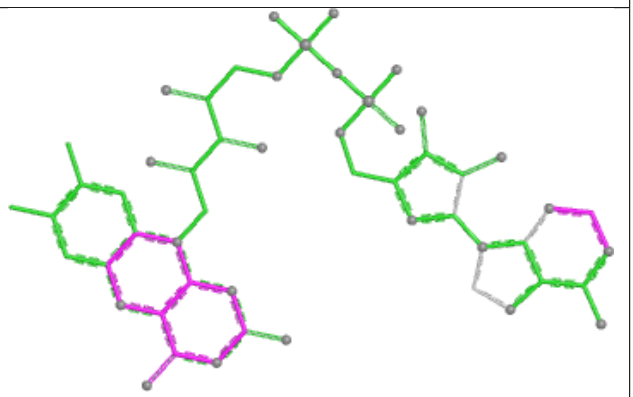


Rings

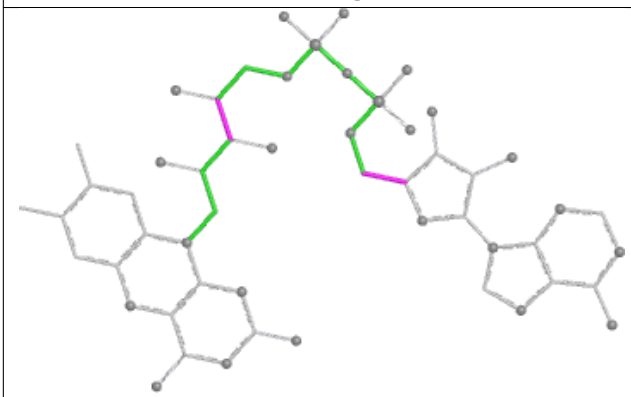
Ligand FAD C 441



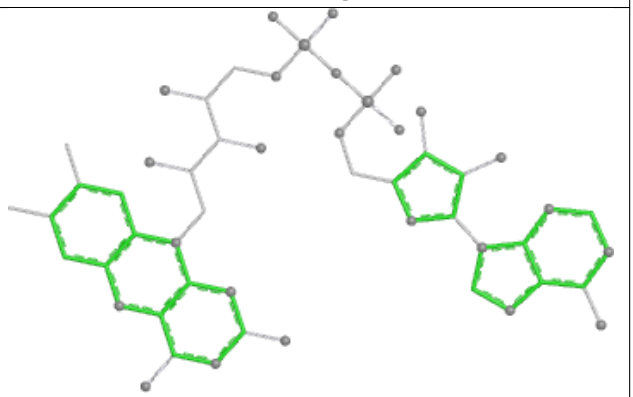
Bond lengths



Bond angles

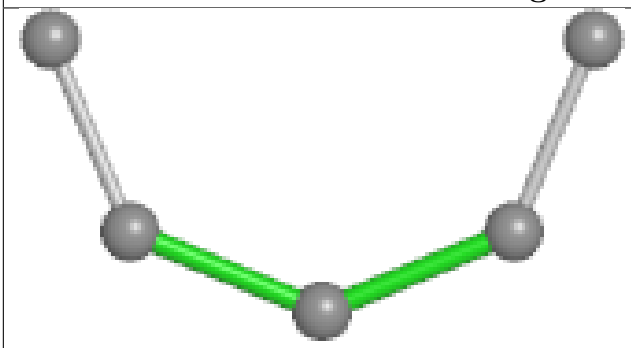


Torsions

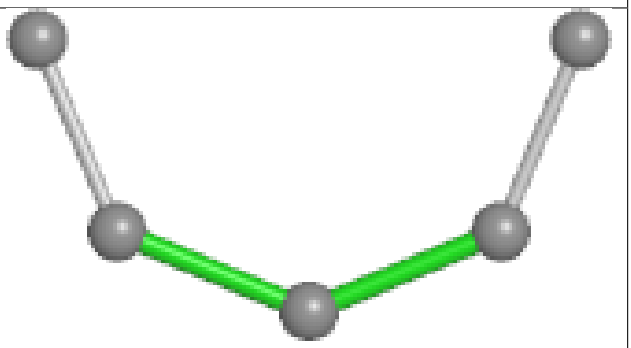


Rings

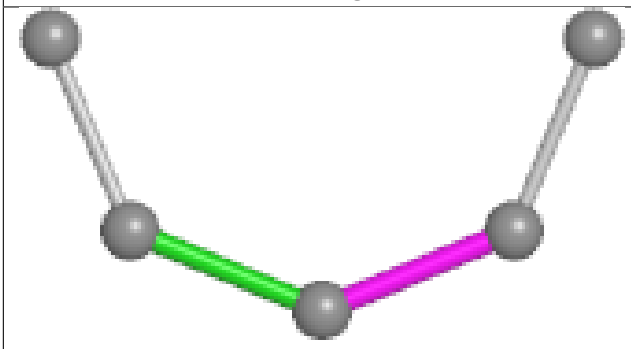
Ligand PS9 D 802



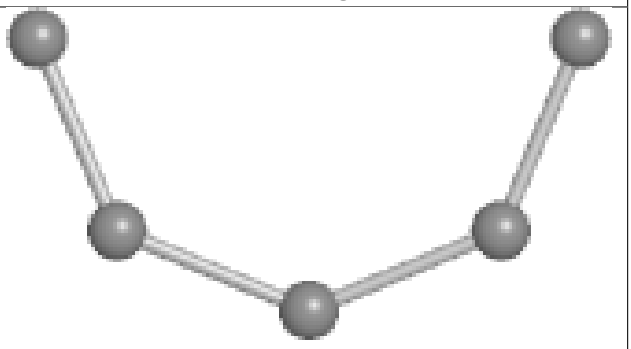
Bond lengths



Bond angles

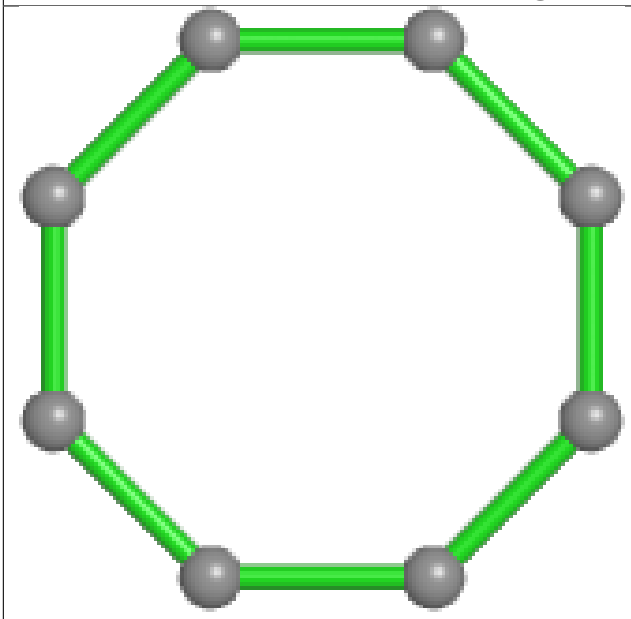


Torsions

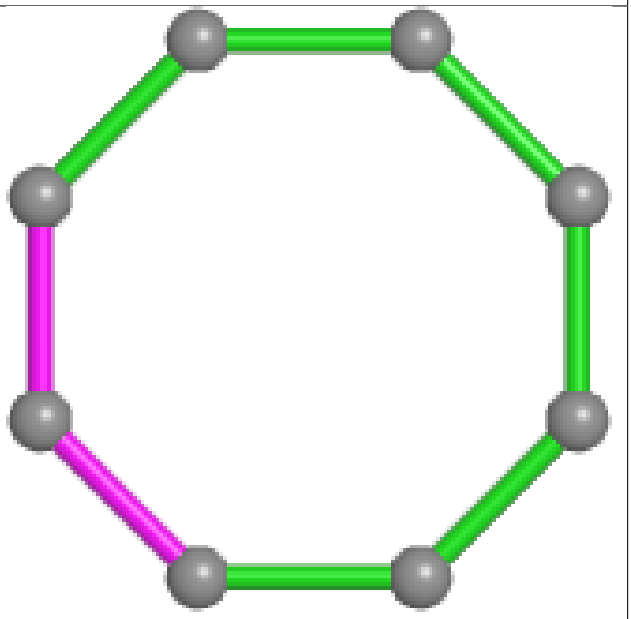


Rings

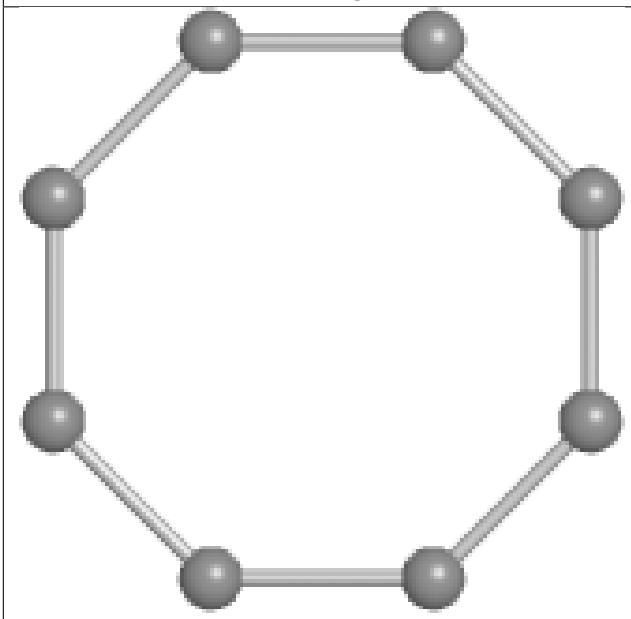
Ligand PS9 E 800



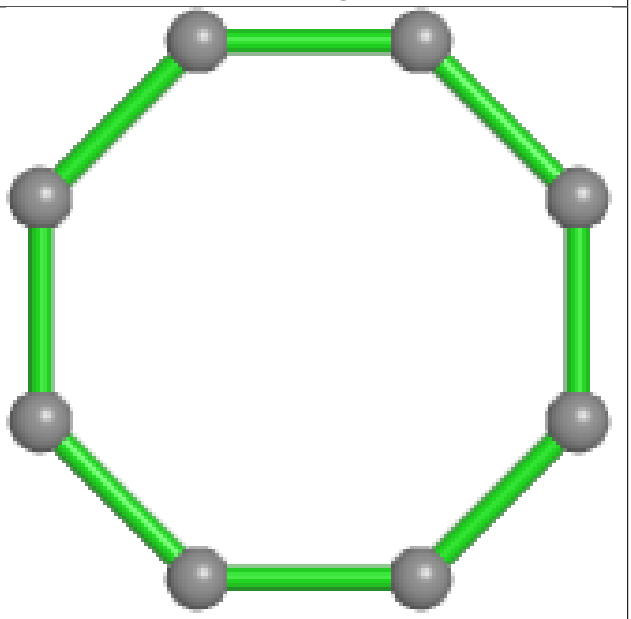
Bond lengths



Bond angles

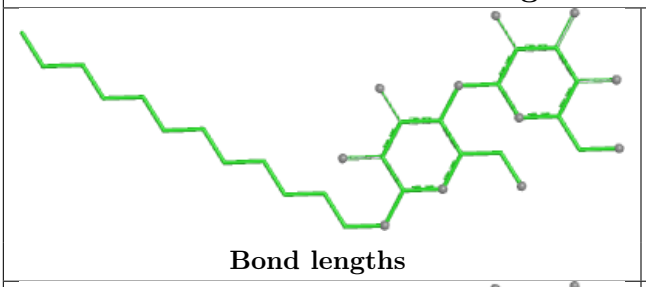


Torsions

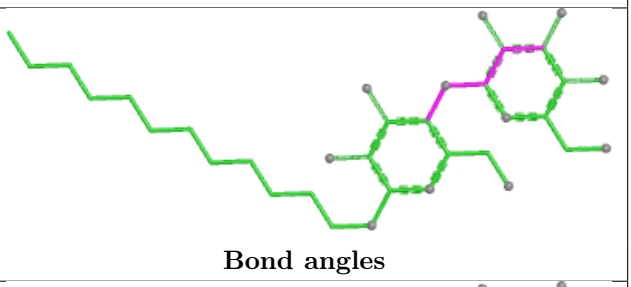


Rings

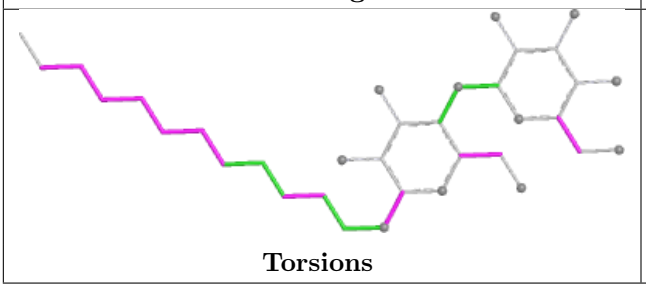
Ligand LMT A 600



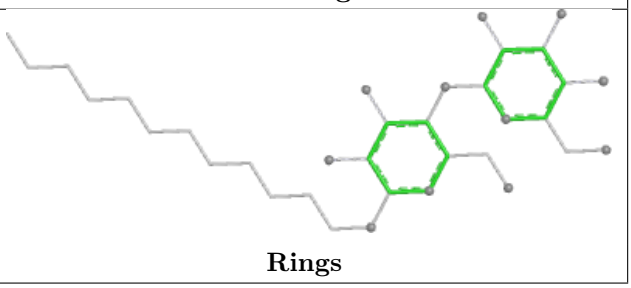
Bond lengths



Bond angles

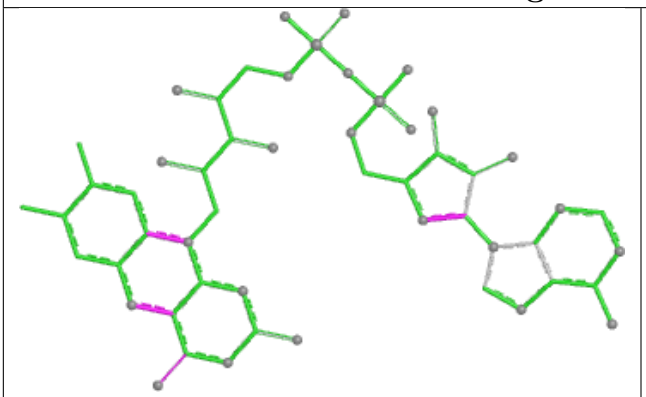


Torsions

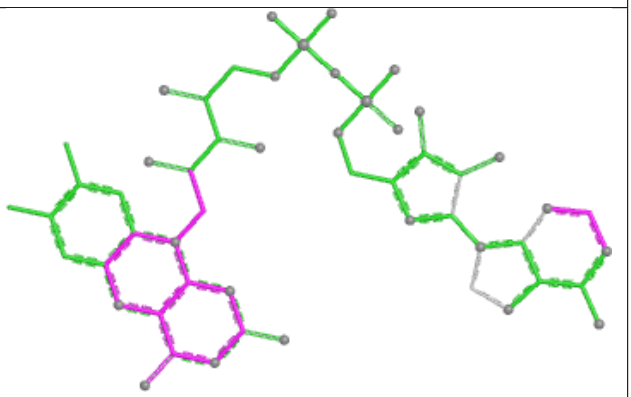


Rings

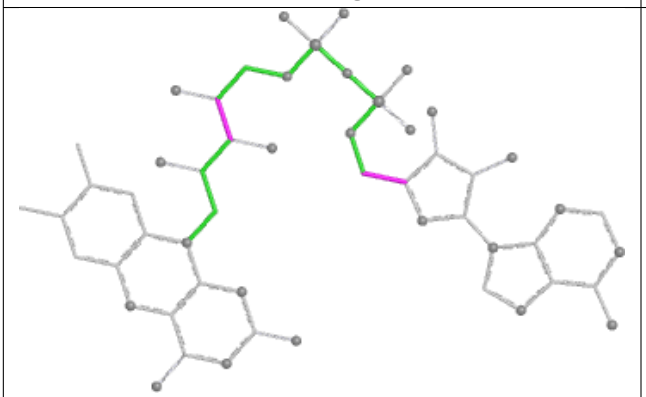
Ligand FAD F 441



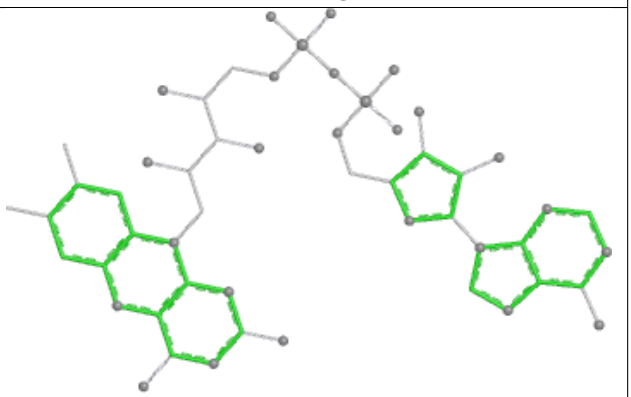
Bond lengths



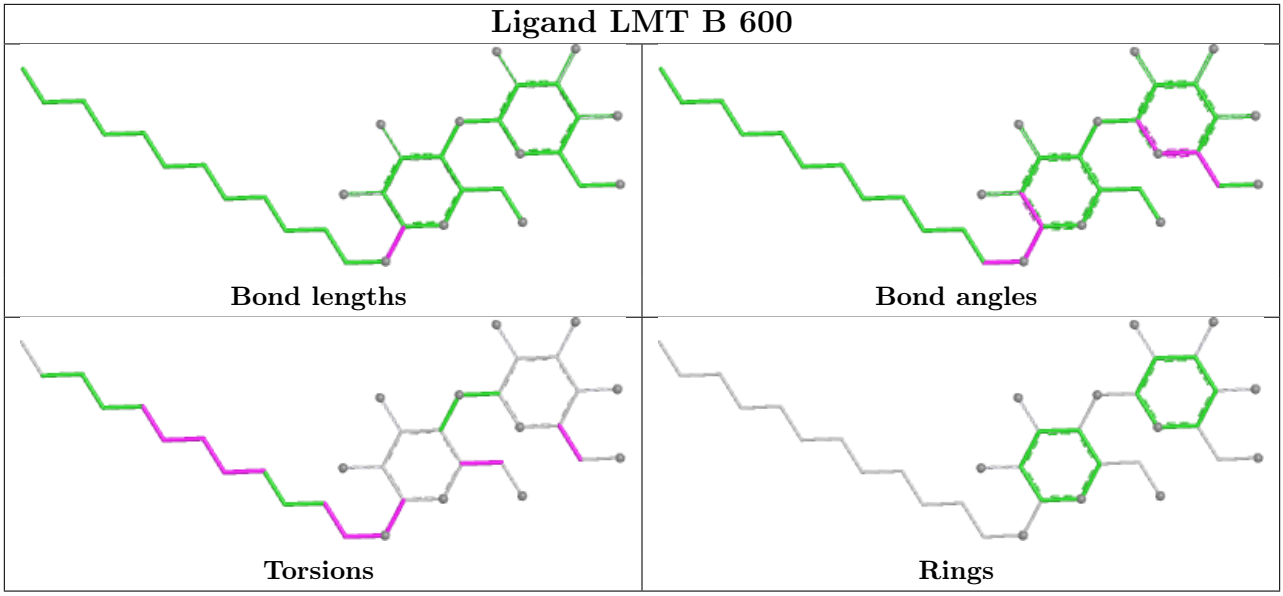
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	428/430 (99%)	-0.06	3 (0%)	84	84	23, 38, 45, 51	7 (1%)
1	B	428/430 (99%)	-0.04	2 (0%)	87	88	22, 38, 45, 54	6 (1%)
1	C	428/430 (99%)	-0.02	5 (1%)	76	76	24, 38, 44, 49	5 (1%)
1	D	428/430 (99%)	0.29	6 (1%)	73	74	22, 38, 44, 47	5 (1%)
1	E	428/430 (99%)	-0.02	2 (0%)	87	88	24, 38, 45, 47	3 (0%)
1	F	428/430 (99%)	-0.05	4 (0%)	81	81	25, 38, 44, 54	3 (0%)
All	All	2568/2580 (99%)	0.02	22 (0%)	81	81	22, 38, 44, 54	29 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	430	CYS	5.6
1	A	430	CYS	4.7
1	B	430	CYS	3.8
1	C	430	CYS	3.8
1	E	430	CYS	3.2
1	F	237	ASN	3.0
1	D	89	THR	2.9
1	C	141	ALA	2.6
1	A	423	GLU	2.6
1	C	264	GLY	2.6
1	A	2	ALA	2.5
1	C	142	ASN	2.5
1	D	82	ASP	2.4
1	D	430	CYS	2.4
1	B	91	GLN	2.3
1	F	56	GLU	2.3
1	C	27	ASP	2.3
1	D	79	GLU	2.2
1	E	35	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	285	THR	2.1
1	D	88	VAL	2.1
1	F	423	GLU	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, 95^{th} 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
1	CSS	C	156[A]	6/8	0.89	0.09	39,39,40,43	1
1	CSS	C	156[B]	7/8	0.89	0.09	38,39,40,40	2
1	CSS	E	156[A]	6/8	0.90	0.09	37,38,38,40	1
1	CSS	E	156[B]	7/8	0.90	0.09	37,38,38,38	2
1	CSS	F	156[A]	6/8	0.90	0.10	37,37,37,38	1
1	CSS	F	156[B]	7/8	0.90	0.10	35,37,37,37	2
1	CSS	A	156[A]	6/8	0.91	0.11	37,38,39,42	1
1	CSS	A	156[B]	7/8	0.91	0.11	35,38,38,39	2
1	CSS	B	156[A]	6/8	0.92	0.08	36,36,36,36	1
1	CSS	B	156[B]	7/8	0.92	0.08	35,36,36,36	2
1	CSS	D	156[A]	6/8	0.93	0.08	35,35,35,37	1
1	CSS	D	156[B]	7/8	0.93	0.08	34,35,35,35	2

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, 95^{th} 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
5	PS9	D	802	5/8	0.49	0.34	48,48,48,49	5
5	PS9	E	800	8/8	0.57	0.28	39,39,40,40	8
5	PS9	C	800	6/8	0.59	0.24	37,38,38,39	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PS9	B	800	6/8	0.60	0.27	36,37,37,37	6
3	LMT	B	600	35/35	0.62	0.29	41,47,51,52	35
3	LMT	D	600	35/35	0.67	0.28	43,49,50,51	35
3	LMT	C	600	35/35	0.68	0.23	34,46,51,52	35
3	LMT	A	600	35/35	0.70	0.25	40,44,49,50	35
5	PS9	F	800	8/8	0.70	0.28	35,35,36,37	8
3	LMT	F	600	35/35	0.71	0.25	36,45,52,53	35
7	SO4	B	433	5/5	0.72	0.15	65,66,66,67	0
7	SO4	D	433	5/5	0.73	0.17	101,101,101,101	0
5	PS9	A	800	8/8	0.74	0.22	34,35,35,35	8
7	SO4	D	432	5/5	0.74	0.15	71,72,72,72	0
3	LMT	E	600	35/35	0.74	0.25	40,43,47,47	35
5	PS9	D	800	1/8	0.78	0.27	33,33,33,33	1
7	SO4	E	431	5/5	0.79	0.13	69,69,70,70	0
7	SO4	A	431	5/5	0.82	0.15	75,76,76,76	0
7	SO4	C	434	5/5	0.83	0.14	62,62,63,63	0
7	SO4	A	432	5/5	0.84	0.13	61,61,62,62	0
7	SO4	C	432	5/5	0.84	0.13	66,66,66,66	0
7	SO4	F	431	5/5	0.84	0.11	72,72,73,73	0
7	SO4	C	433	5/5	0.85	0.12	60,61,61,62	0
7	SO4	E	433	5/5	0.85	0.11	72,72,73,73	0
7	SO4	F	433	5/5	0.85	0.13	62,63,63,64	0
7	SO4	D	434	5/5	0.87	0.17	69,69,70,70	0
7	SO4	E	434	5/5	0.88	0.12	68,68,68,69	0
7	SO4	E	432	5/5	0.89	0.17	66,66,67,67	0
7	SO4	B	432	5/5	0.89	0.10	54,54,55,55	0
7	SO4	B	435	5/5	0.89	0.12	70,70,70,71	0
7	SO4	F	434	5/5	0.89	0.15	63,64,64,65	0
7	SO4	E	435	5/5	0.90	0.11	75,75,76,76	0
6	MES	E	900	12/12	0.90	0.11	55,59,63,63	0
7	SO4	B	431	5/5	0.90	0.09	77,77,78,78	0
4	H2S	D	700	1/1	0.90	0.14	37,37,37,37	1
4	H2S	C	700	1/1	0.91	0.21	34,34,34,34	1
7	SO4	C	431	5/5	0.91	0.11	71,71,71,71	0
4	H2S	A	700	1/1	0.91	0.19	31,31,31,31	1
4	H2S	B	700	1/1	0.91	0.16	32,32,32,32	1
4	H2S	E	700	1/1	0.92	0.18	32,32,32,32	1
6	MES	C	900	12/12	0.92	0.11	50,57,61,62	0
6	MES	D	900	12/12	0.92	0.11	48,53,57,58	0
7	SO4	B	434	5/5	0.92	0.18	64,64,64,65	0
7	SO4	A	434	5/5	0.93	0.10	61,62,62,63	0
6	MES	A	900	12/12	0.93	0.11	56,60,63,63	0

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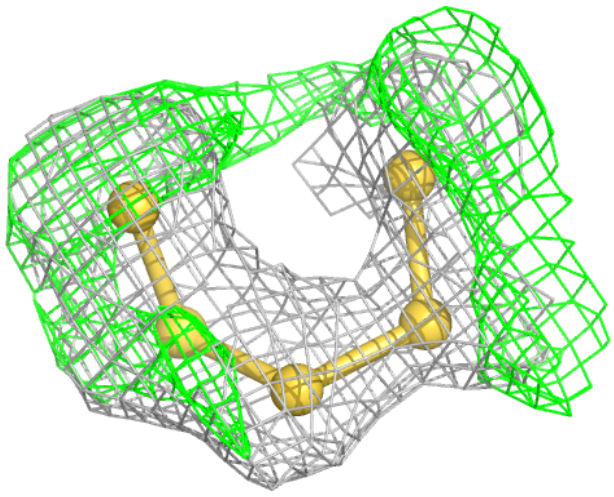
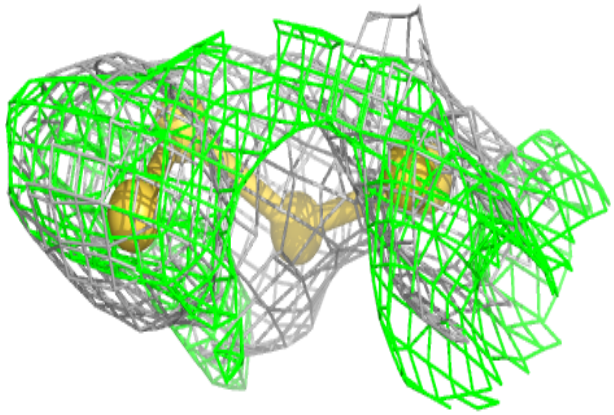
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	D	441	53/53	0.93	0.07	31,36,38,40	0
2	FAD	E	441	53/53	0.95	0.07	26,29,42,43	0
6	MES	B	900	12/12	0.95	0.09	47,52,55,55	0
4	H2S	F	700	1/1	0.96	0.16	30,30,30,30	1
6	MES	F	900	12/12	0.96	0.09	47,51,55,55	0
2	FAD	F	441	53/53	0.96	0.06	25,30,34,35	0
2	FAD	B	441	53/53	0.96	0.06	23,30,30,32	0
2	FAD	C	441	53/53	0.96	0.06	22,30,32,32	0
2	FAD	A	441	53/53	0.97	0.06	23,28,30,32	0
7	SO4	A	433	5/5	0.98	0.05	42,42,43,43	0

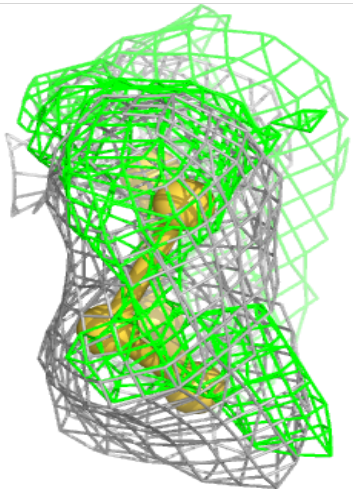
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PS9 D 802:

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

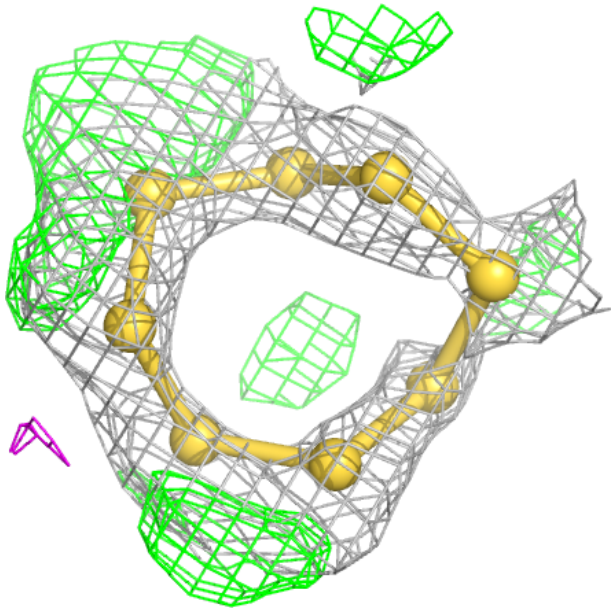


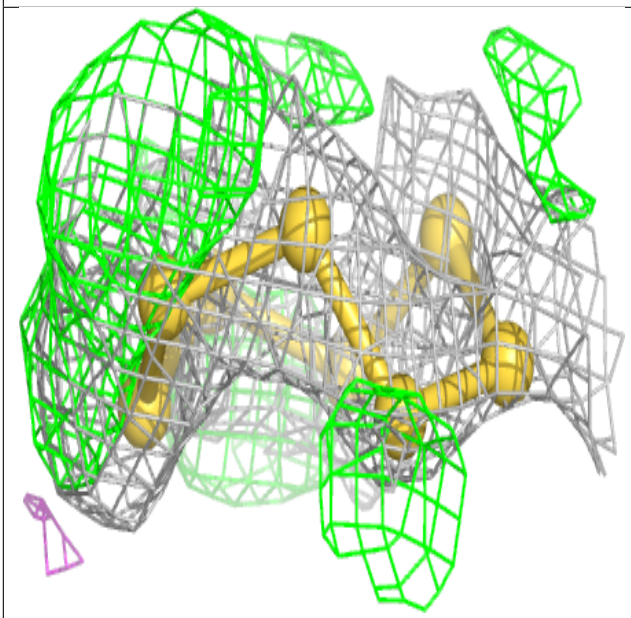


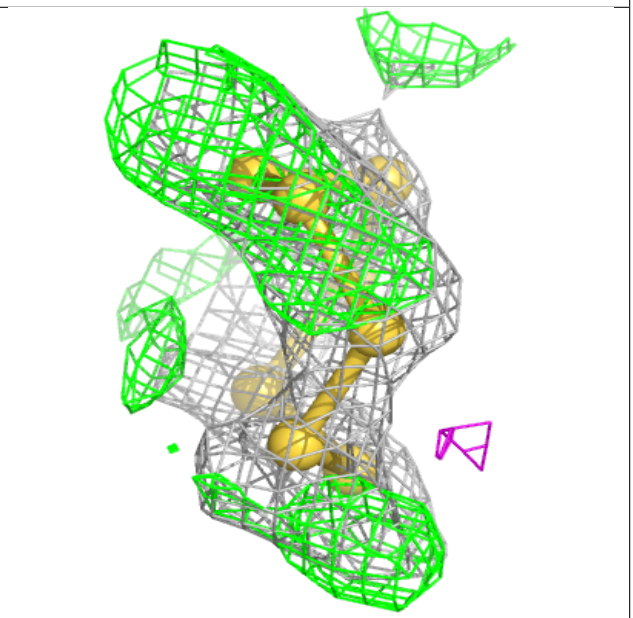


Electron density around PS9 E 800:

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

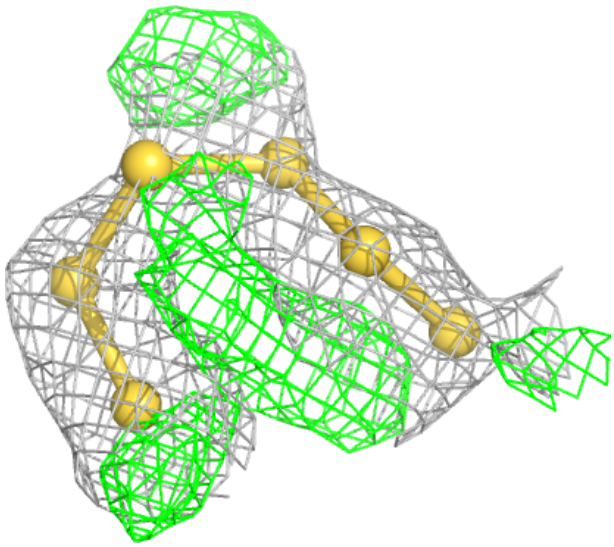


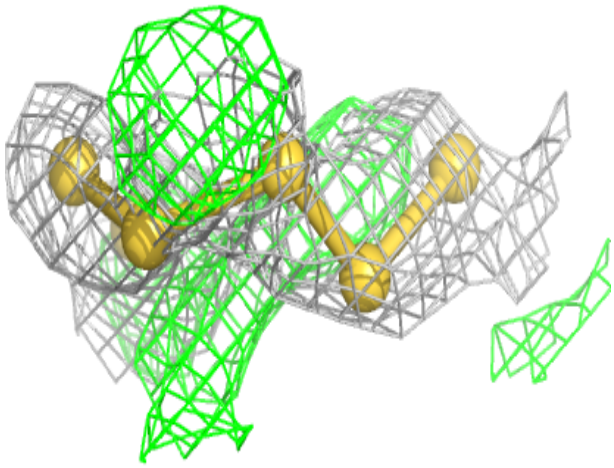


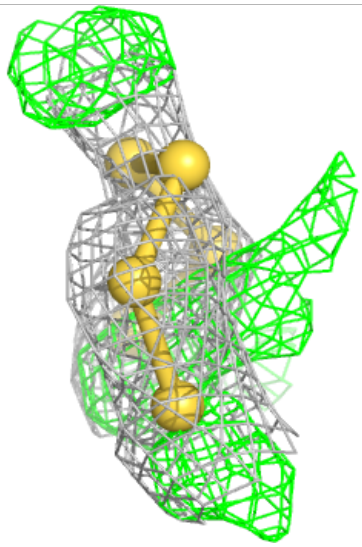


Electron density around PS9 C 800:

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

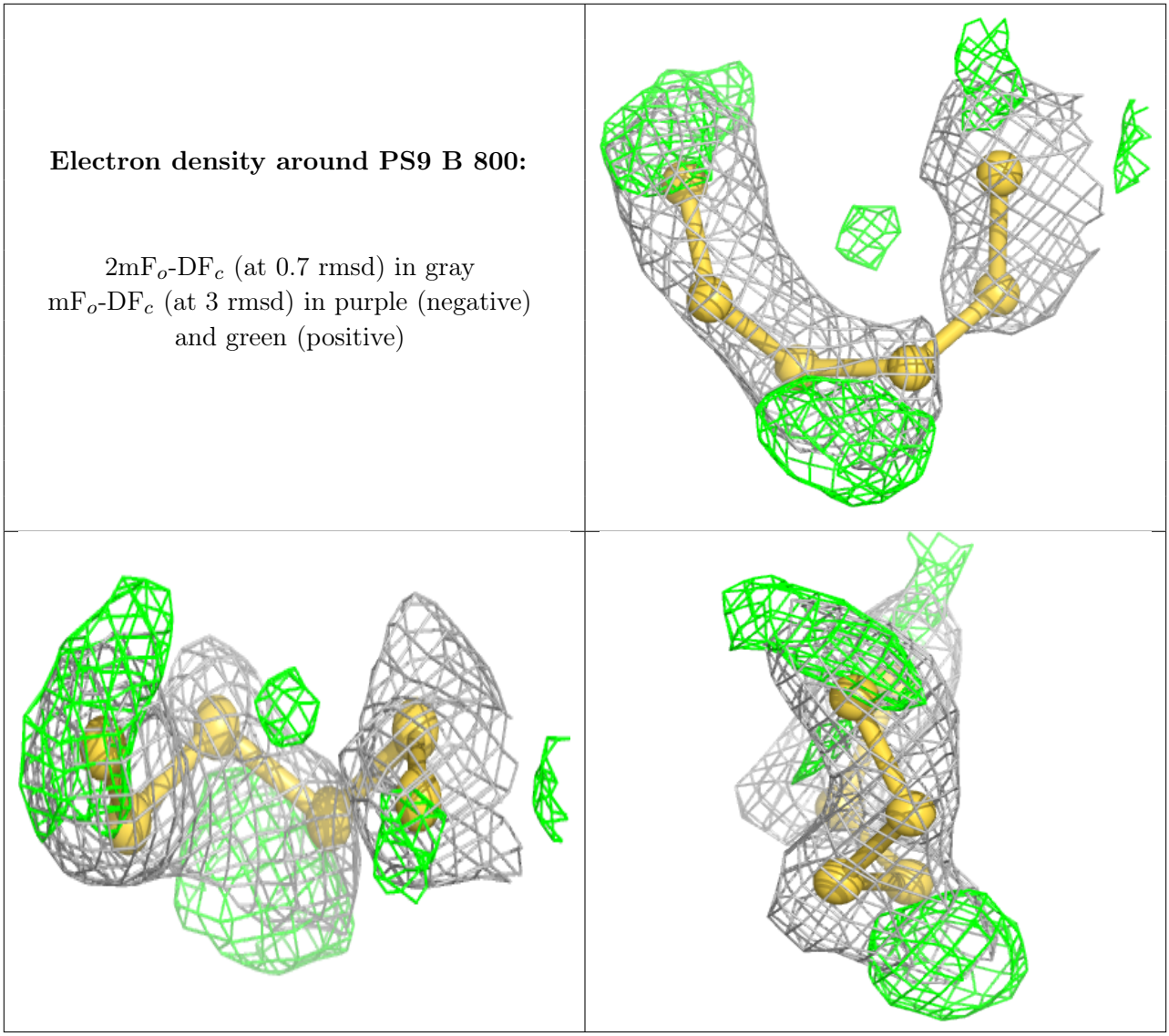






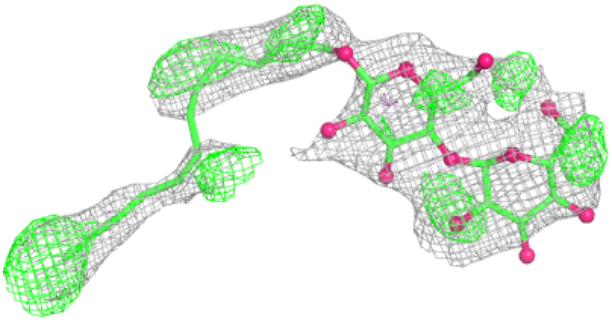
Electron density around PS9 B 800:

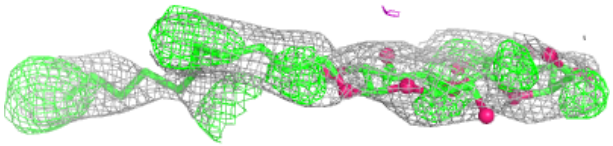
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

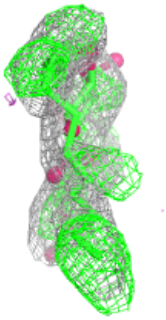


Electron density around LMT B 600:

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

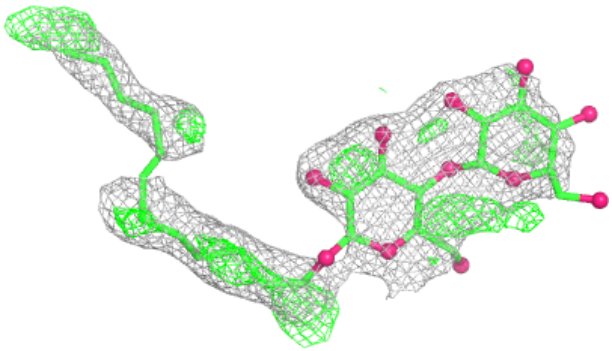


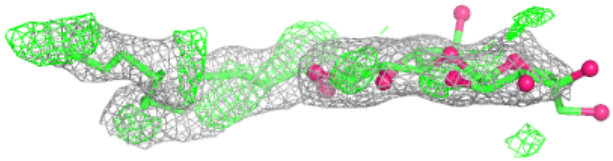


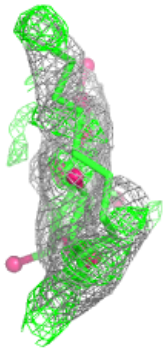


Electron density around LMT D 600:

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

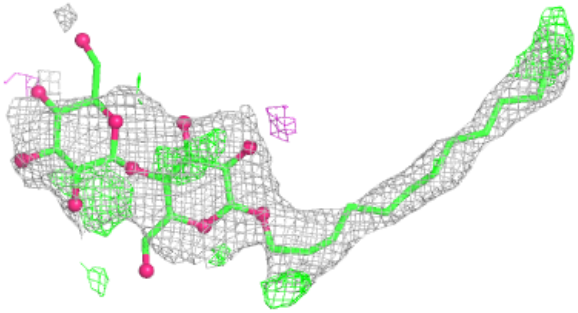


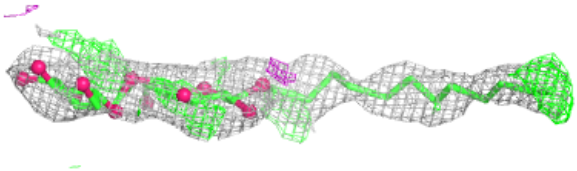


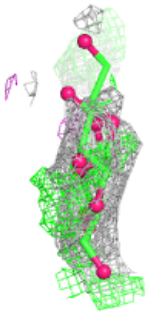


Electron density around LMT C 600:

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

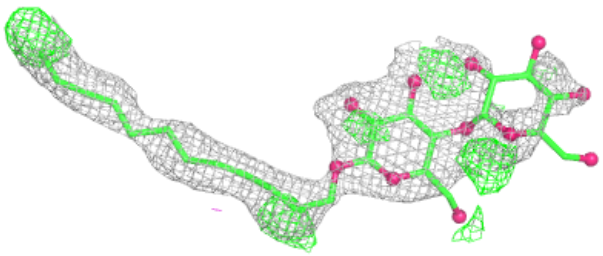


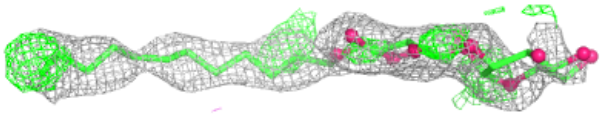


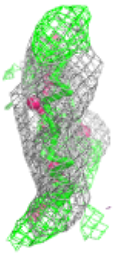


Electron density around LMT A 600:

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

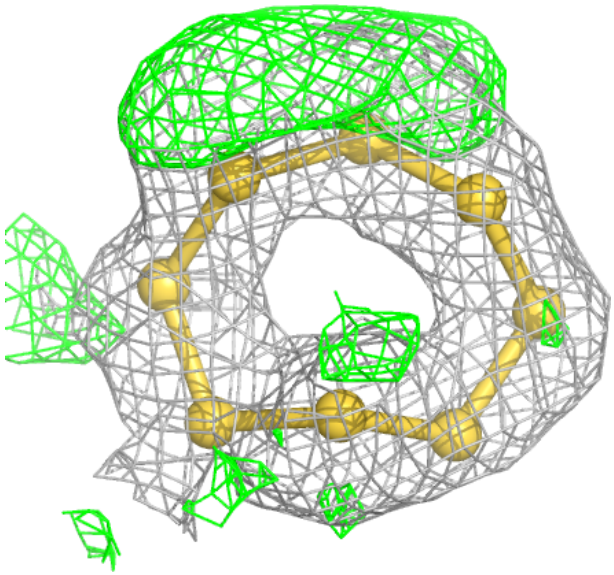


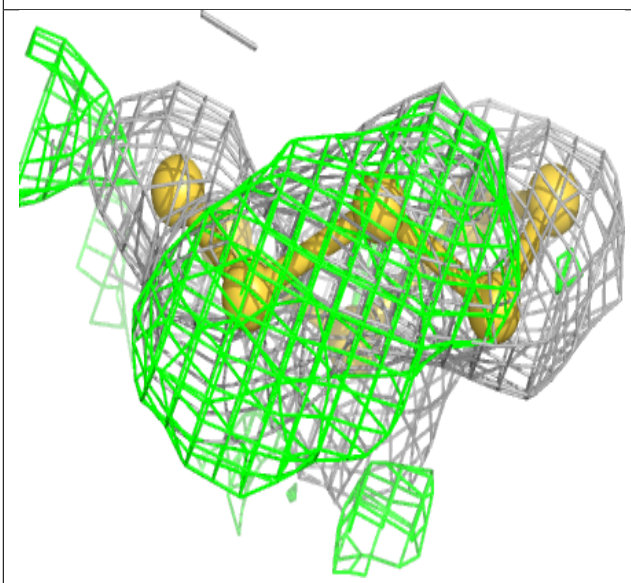


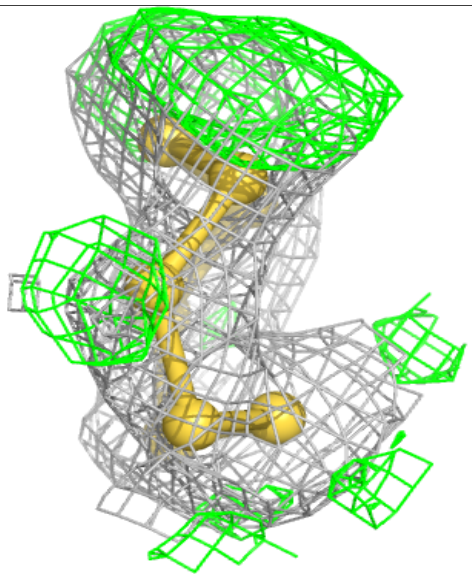


Electron density around PS9 F 800:

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

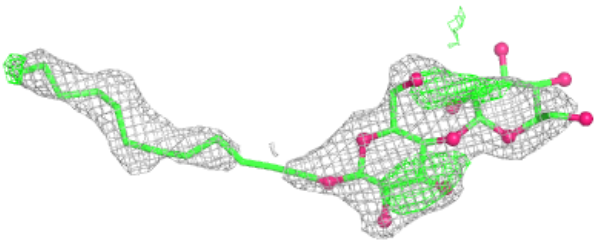


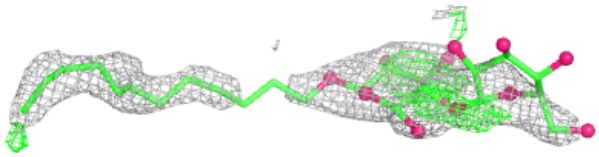


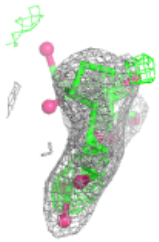


Electron density around LMT F 600:

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

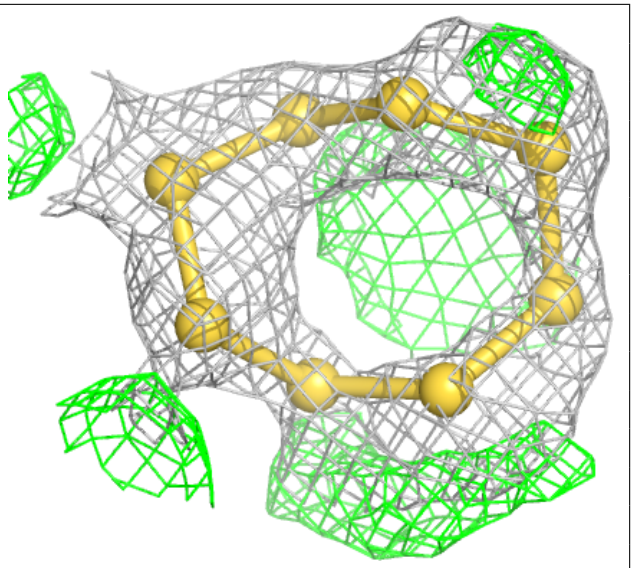


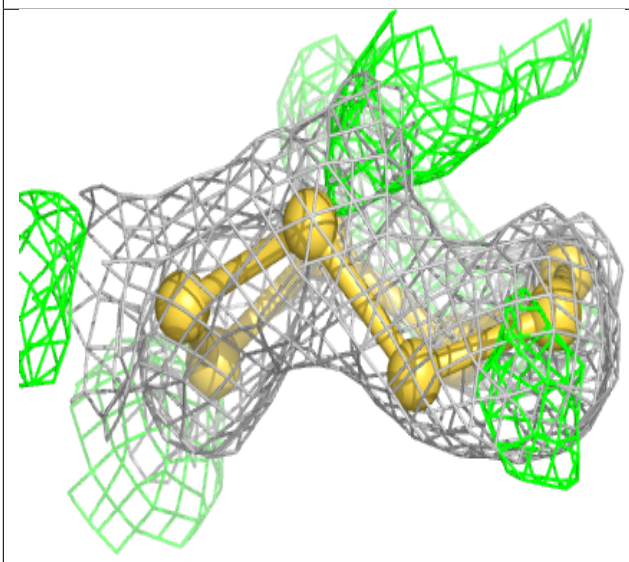


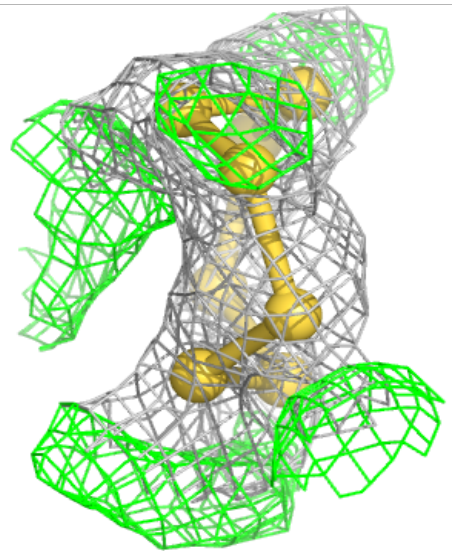


Electron density around PS9 A 800:

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

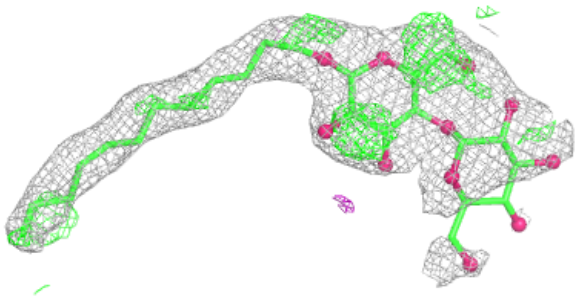


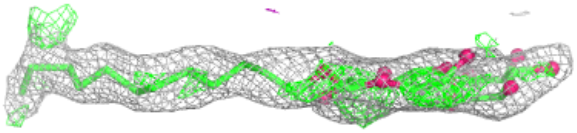


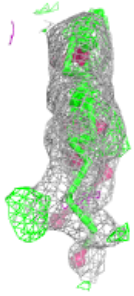


Electron density around LMT E 600:

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

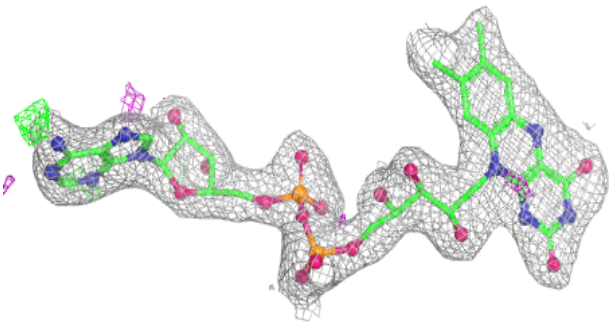


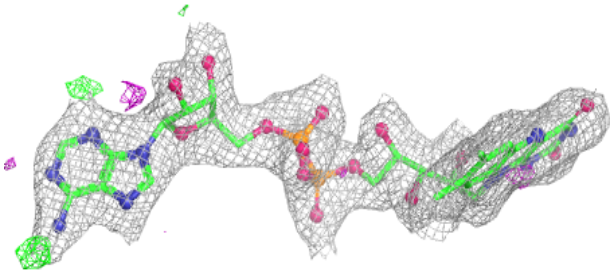


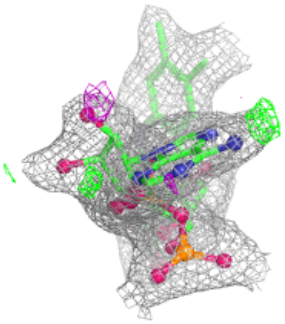


Electron density around FAD D 441:

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

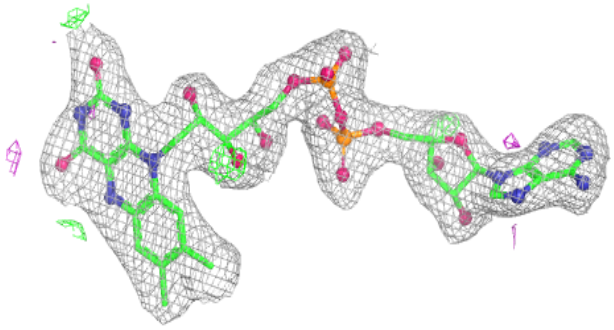


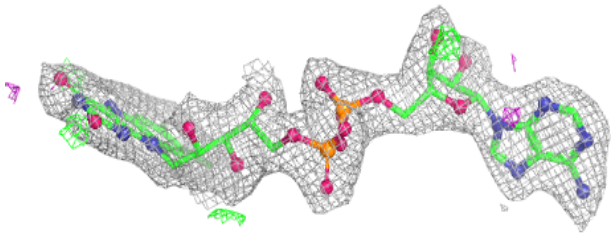


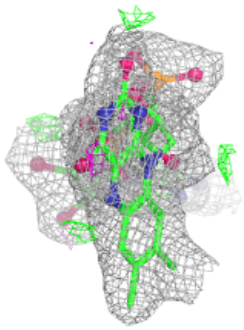


Electron density around FAD E 441:

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

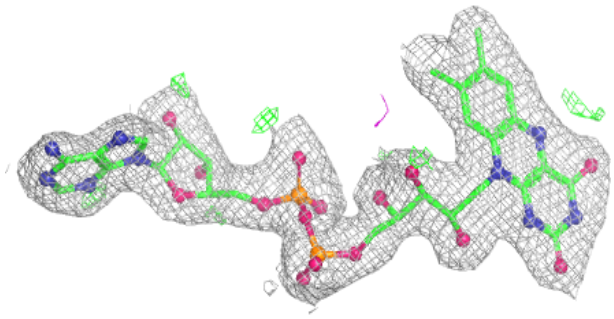


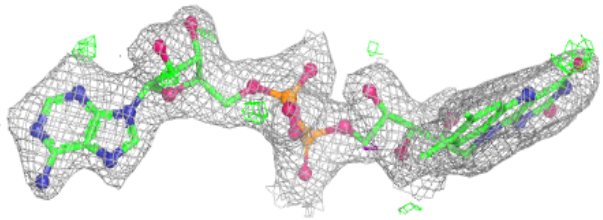


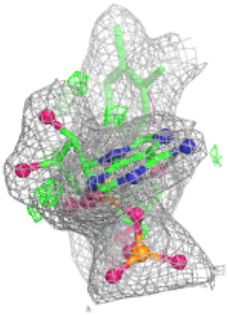


Electron density around FAD F 441:

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

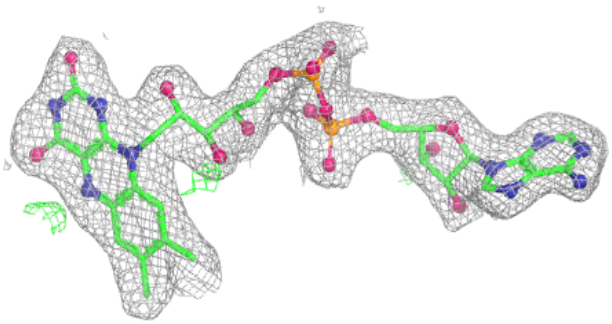


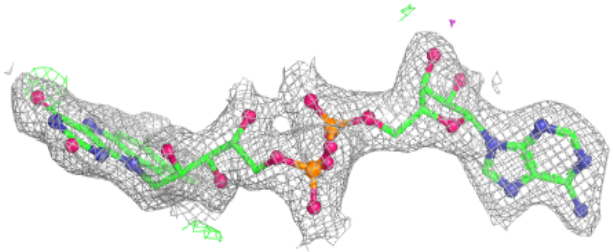




Electron density around FAD B 441:

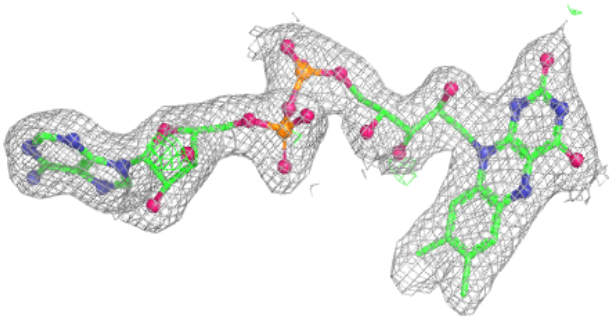
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

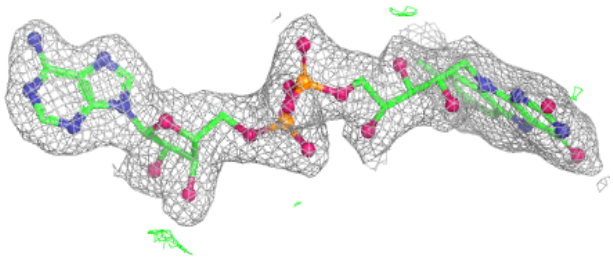


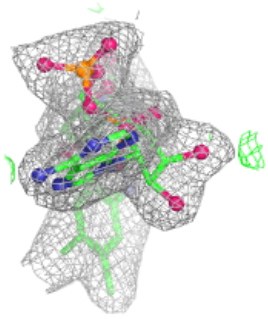


Electron density around FAD C 441:

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

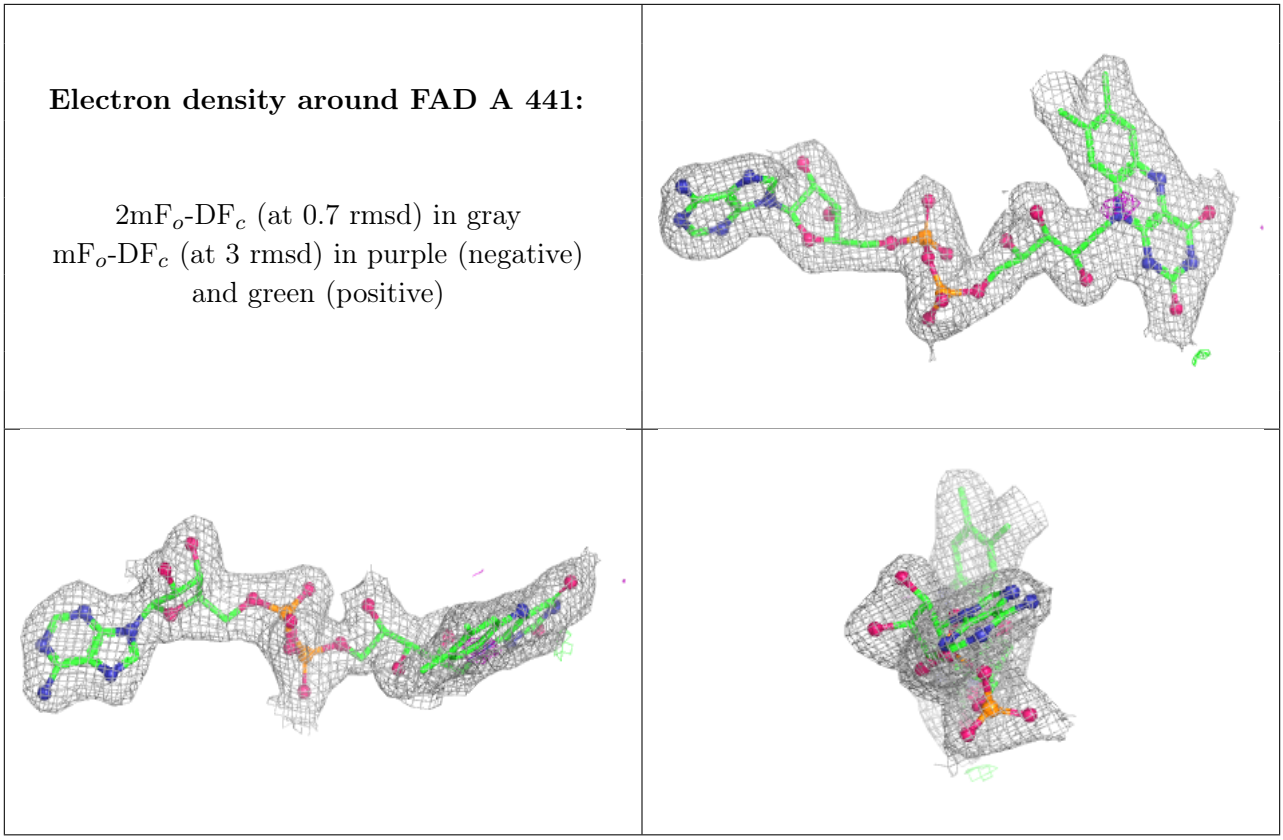






Electron density around FAD A 441:

$2mF_o$-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.