



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:40 PM UTC

PDB ID : 3HYW / pdb_00003hyw
Title : 3-D X-Ray structure of the sulfide:quinone oxidoreductase of the hyperthermophilic bacterium Aquifex aeolicus in complex with decylubiquinone
Authors : Marcia, M.; Ermler, U.; Peng, G.H.; Michel, H.
Deposited on : 2009-06-23
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

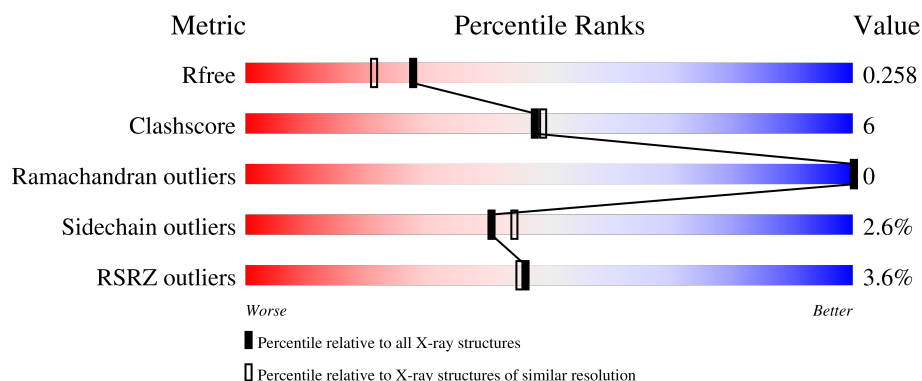
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	430	4% 88% 10% .
1	B	430	3% 87% 12% .
1	C	430	4% 89% 10% .
1	D	430	3% 84% 15% .
1	E	430	4% 85% 14% .

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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
6	PS9	B	800	-	-	-	X
6	PS9	B	802[A]	-	-	-	X
6	PS9	B	802[B]	-	-	-	X
6	PS9	C	800	-	-	X	-
6	PS9	D	802	-	-	-	X
6	PS9	E	800	-	-	X	-
7	SO4	D	431	-	-	-	X

2 Entry composition [i](#)

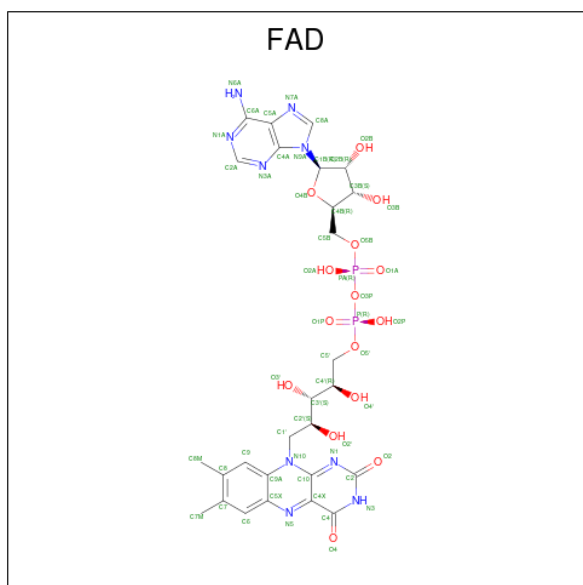
There are 8 unique types of molecules in this entry. The entry contains 22002 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

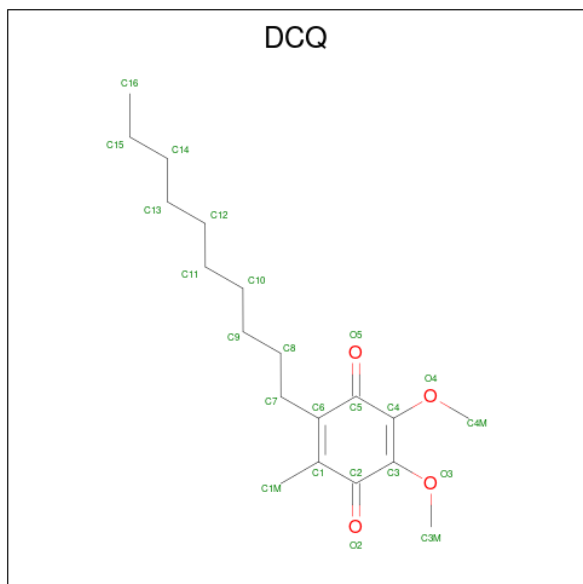
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	3	0
			3339	2161	553	602	23			
1	B	429	Total	C	N	O	S	0	3	0
			3340	2161	553	602	24			
1	C	429	Total	C	N	O	S	0	3	0
			3339	2161	553	602	23			
1	D	429	Total	C	N	O	S	0	3	0
			3340	2161	553	602	24			
1	E	429	Total	C	N	O	S	0	3	0
			3339	2161	553	602	23			
1	F	429	Total	C	N	O	S	0	3	0
			3339	2161	553	602	23			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: C₁₉H₃₀O₄).



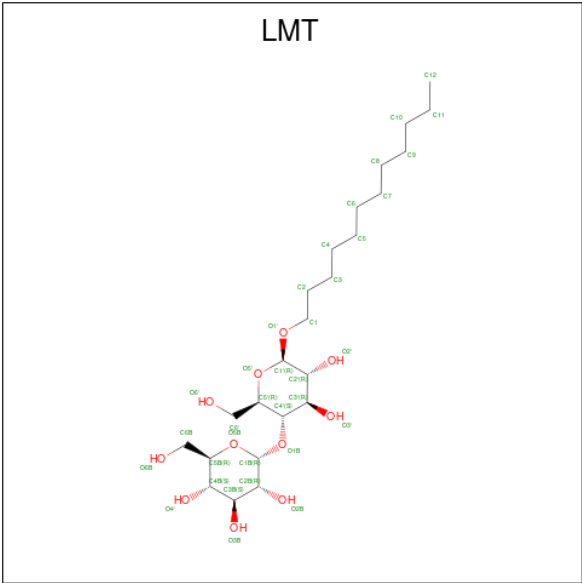
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	19	4		
3	B	1	Total	C	O	0	0
			23	19	4		
3	C	1	Total	C	O	0	0
			23	19	4		
3	D	1	Total	C	O	0	0
			23	19	4		
3	E	1	Total	C	O	0	0
			23	19	4		

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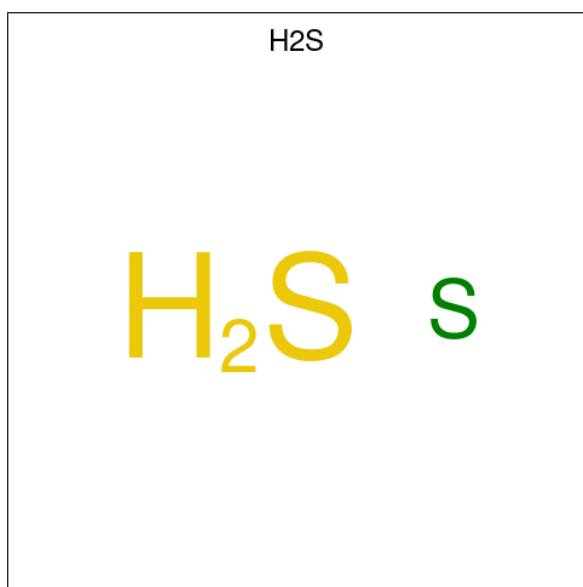
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			23	19	4		

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



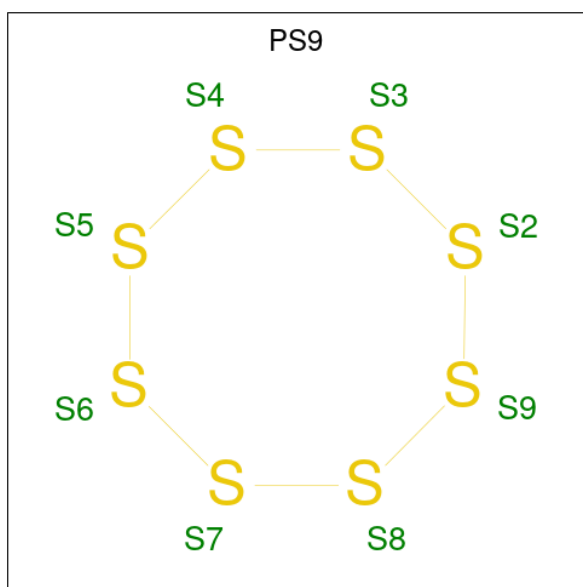
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		
4	B	1	Total	C	O	0	0
			35	24	11		
4	C	1	Total	C	O	0	0
			35	24	11		
4	D	1	Total	C	O	0	0
			35	24	11		
4	E	1	Total	C	O	0	0
			35	24	11		
4	F	1	Total	C	O	0	0
			35	24	11		

- Molecule 5 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S).



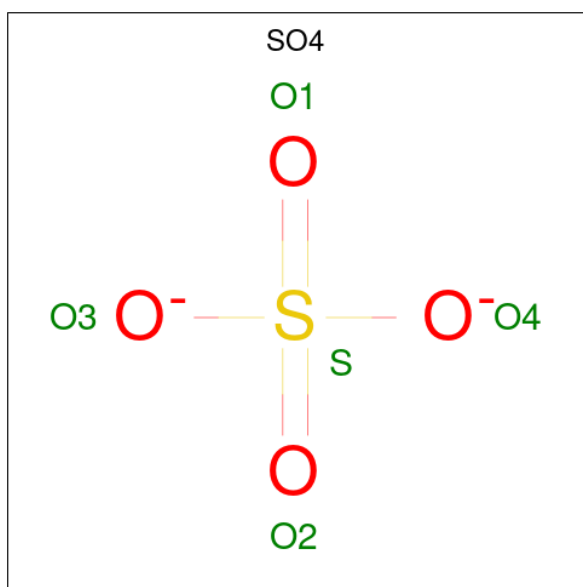
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total S 1 1	0	0
5	B	1	Total S 1 1	0	0
5	C	1	Total S 1 1	0	0
5	D	1	Total S 1 1	0	0
5	E	1	Total S 1 1	0	0
5	F	1	Total S 1 1	0	0

- Molecule 6 is octathiocane (CCD ID: PS9) (formula: S₈).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total S 8 8	0	0
6	B	1	Total S 1 1	0	0
6	B	1	Total S 3 3	0	1
6	C	1	Total S 6 6	0	0
6	D	1	Total S 2 2	0	0
6	D	1	Total S 1 1	0	0
6	E	1	Total S 8 8	0	0
6	F	1	Total S 8 8	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

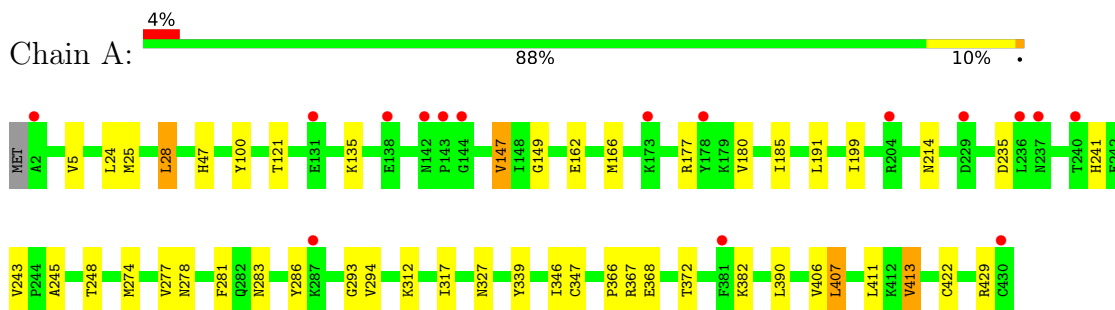
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	214	Total	O	0	0
			214	214		
8	B	197	Total	O	0	0
			197	197		
8	C	189	Total	O	0	0
			189	189		
8	D	160	Total	O	0	0
			160	160		
8	E	179	Total	O	0	0
			179	179		
8	F	198	Total	O	0	0
			198	198		

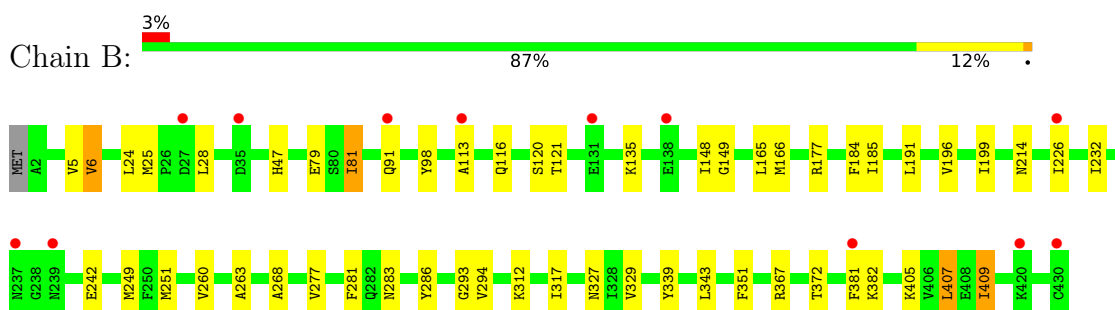
3 Residue-property plots [i](#)

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.

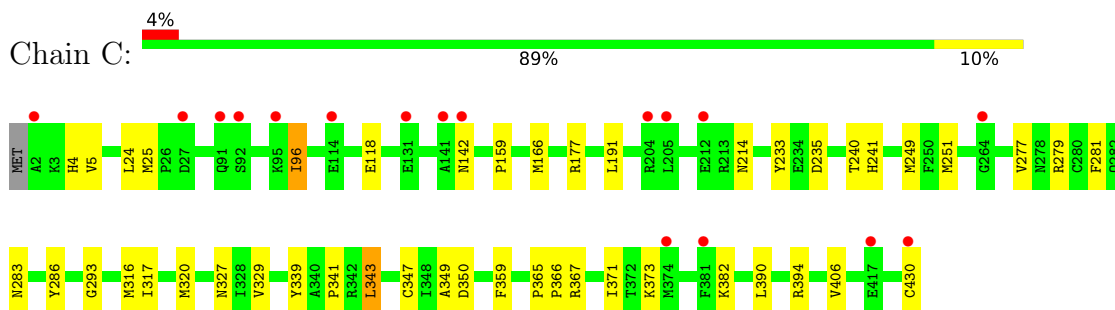
- Molecule 1: Sulfide-quinone reductase



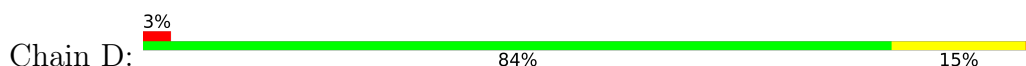
- Molecule 1: Sulfide-quinone reductase

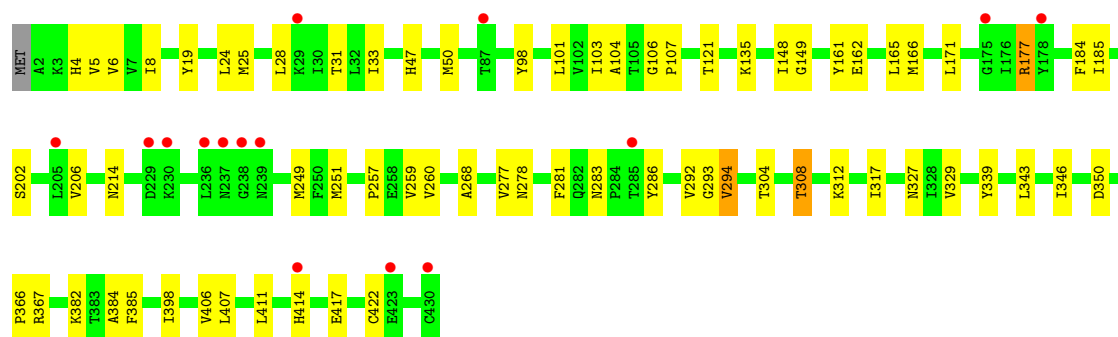


- Molecule 1: Sulfide-quinone reductase

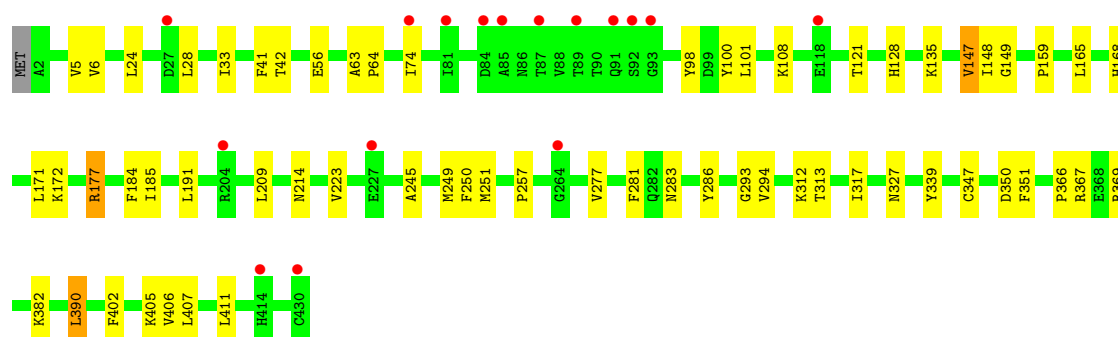
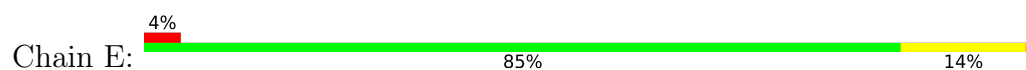


- Molecule 1: Sulfide-quinone reductase

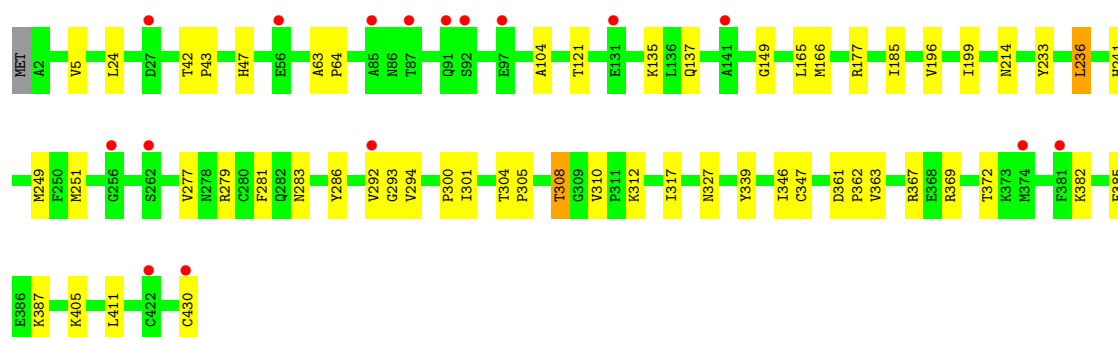
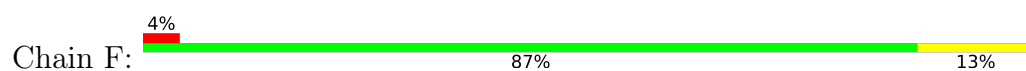




• Molecule 1: Sulfide-quinone reductase



• Molecule 1: Sulfide-quinone reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.78Å 154.01Å 175.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.45 – 2.00 20.45 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (20.45-2.00) 96.1 (20.45-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.236 0.228 , 0.258	Depositor DCC
R_{free} test set	9757 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22002	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0/3417	0.77	1/4637 (0.0%)
1	B	0.52	0/3417	0.78	0/4637
1	C	0.51	0/3417	0.78	0/4637
1	D	0.51	0/3417	0.79	0/4637
1	E	0.50	0/3417	0.79	0/4637
1	F	0.51	0/3417	0.77	0/4637
All	All	0.51	0/20502	0.78	1/27822 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	180	VAL	N-CA-C	5.06	113.16	108.15

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	3339	0	3338	32	0
1	B	3340	0	3338	34	0
1	C	3339	0	3338	32	0
1	D	3340	0	3338	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3339	0	3338	45	0
1	F	3339	0	3338	49	0
2	A	53	0	29	2	0
2	B	53	0	29	1	0
2	C	53	0	29	1	0
2	D	53	0	29	6	0
2	E	53	0	29	1	0
2	F	53	0	29	7	0
3	A	23	0	30	1	0
3	B	23	0	30	1	0
3	C	23	0	30	0	0
3	D	23	0	29	3	0
3	E	23	0	30	2	0
3	F	23	0	30	3	0
4	A	35	0	46	0	0
4	B	35	0	46	1	0
4	C	35	0	46	1	0
4	D	35	0	44	0	0
4	E	35	0	46	0	0
4	F	35	0	46	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	8	0	0	0	0
6	B	4	0	0	0	0
6	C	6	0	0	2	0
6	D	3	0	0	0	0
6	E	8	0	0	2	0
6	F	8	0	0	0	0
7	A	25	0	0	0	0
7	B	20	0	0	0	0
7	C	20	0	0	2	0
7	D	20	0	0	0	0
7	E	15	0	0	0	0
7	F	20	0	0	1	0
8	A	214	0	0	1	0
8	B	197	0	0	0	0
8	C	189	0	0	1	0
8	D	160	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	179	0	0	1	0
8	F	198	0	0	2	0
All	All	22002	0	20655	232	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 6.

All (232) 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:C:327:ASN:HD21	1:C:339:TYR:H	1.05	1.03
1:A:327:ASN:HD21	1:A:339:TYR:H	1.09	0.97
1:D:8:ILE:HD11	2:D:441:FAD:C2A	1.95	0.97
1:E:283:ASN:HD22	1:E:286:TYR:H	1.13	0.95
1:E:327:ASN:HD21	1:E:339:TYR:H	1.13	0.94
1:B:327:ASN:HD21	1:B:339:TYR:H	1.11	0.93
1:D:327:ASN:HD21	1:D:339:TYR:H	1.12	0.92
1:F:249:MET:HE1	1:F:251:MET:HE2	1.49	0.91
1:F:327:ASN:HD21	1:F:339:TYR:H	1.14	0.90
1:D:283:ASN:HD22	1:D:286:TYR:H	1.22	0.87
1:C:249:MET:HE1	1:C:251:MET:HE2	1.56	0.85
1:B:196:VAL:HG22	1:B:367:ARG:NH1	1.92	0.85
1:E:293:GLY:HA2	1:E:317:ILE:HD12	1.57	0.85
1:D:367:ARG:H	1:F:214:ASN:HD22	1.26	0.83
1:B:249:MET:HE1	1:B:251:MET:HE2	1.62	0.81
1:D:50:MET:HG3	1:D:166:MET:HE2	1.60	0.80
1:F:283:ASN:HD22	1:F:286:TYR:H	1.27	0.80
1:A:283:ASN:HD22	1:A:286:TYR:H	1.28	0.79
1:C:283:ASN:HD22	1:C:286:TYR:H	1.31	0.78
1:A:274:MET:SD	8:A:1113:HOH:O	2.42	0.77
1:B:196:VAL:HG22	1:B:367:ARG:HH11	1.50	0.77
1:E:313:THR:O	1:E:317:ILE:HG12	1.85	0.75
1:F:346:ILE:HG22	3:F:500:DCQ:H4MA	1.69	0.74
1:D:249:MET:HE1	1:D:251:MET:HE3	1.69	0.74
1:E:283:ASN:ND2	1:E:286:TYR:H	1.87	0.73
1:B:283:ASN:HD22	1:B:286:TYR:H	1.34	0.72
1:F:42:THR:HG21	2:F:441:FAD:O4'	1.90	0.71
1:B:327:ASN:HD21	1:B:339:TYR:N	1.87	0.71
1:A:147:VAL:HG13	1:A:248:THR:HG22	1.74	0.69
1:B:367:ARG:H	1:D:214:ASN:HD22	1.39	0.68
1:E:327:ASN:HD21	1:E:339:TYR:N	1.89	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:ARG:H	1:F:214:ASN:ND2	1.92	0.68
1:F:42:THR:HG21	2:F:441:FAD:H3'	1.75	0.67
1:C:249:MET:HE1	1:C:251:MET:CE	2.24	0.67
1:F:300:PRO:HA	1:F:310:VAL:HG23	1.76	0.66
1:D:50:MET:CG	1:D:166:MET:HE2	2.26	0.66
1:C:214:ASN:HD22	1:E:367:ARG:H	1.45	0.65
1:F:137:GLN:NE2	8:F:572:HOH:O	2.29	0.65
1:E:350:ASP:HB2	1:E:382:LYS:HD3	1.79	0.65
1:F:385:PHE:CE2	3:F:500:DCQ:H3MB	2.32	0.64
1:F:293:GLY:HA2	1:F:317:ILE:HG12	1.79	0.64
1:A:346:ILE:HD11	1:A:411:LEU:CD1	2.28	0.64
1:C:327:ASN:HD21	1:C:339:TYR:N	1.87	0.64
1:D:106:GLY:HA2	1:D:294:VAL:HG13	1.79	0.64
1:C:214:ASN:ND2	1:E:367:ARG:H	1.96	0.63
1:D:294:VAL:HA	1:D:312:LYS:HD3	1.80	0.63
1:E:121:THR:CG2	1:E:135:LYS:HD3	2.29	0.63
1:B:327:ASN:ND2	1:B:339:TYR:H	1.91	0.62
1:B:232:ILE:HG12	1:B:242:GLU:HG2	1.81	0.62
1:D:162:GLU:HG3	1:D:350:ASP:O	2.00	0.61
1:C:327:ASN:ND2	1:C:339:TYR:H	1.88	0.61
1:F:196:VAL:HG22	1:F:367:ARG:HH11	1.66	0.61
1:E:249:MET:HE1	1:E:251:MET:CE	2.30	0.61
1:C:235:ASP:OD2	1:C:241:HIS:HE1	1.84	0.60
1:A:283:ASN:ND2	1:A:286:TYR:H	2.00	0.60
1:D:414:HIS:HE1	1:D:417:GLU:OE2	1.84	0.60
1:C:25:MET:HE3	1:C:329:VAL:HG13	1.84	0.59
1:E:121:THR:HG22	1:E:135:LYS:HD3	1.85	0.59
1:A:367:ARG:H	1:E:214:ASN:HD22	1.48	0.59
1:F:327:ASN:HD21	1:F:339:TYR:N	1.93	0.59
1:B:79:GLU:HG3	1:B:91:GLN:HA	1.84	0.59
1:F:196:VAL:HG22	1:F:367:ARG:NH1	2.18	0.58
1:E:293:GLY:HA2	1:E:317:ILE:CD1	2.31	0.58
1:E:327:ASN:ND2	1:E:339:TYR:H	1.94	0.58
1:F:283:ASN:ND2	1:F:286:TYR:H	2.00	0.58
1:D:4:HIS:NE2	1:D:31:THR:HG22	2.17	0.58
1:A:199:ILE:O	1:A:372:THR:HG21	2.03	0.58
1:A:214:ASN:HD22	1:C:367:ARG:H	1.50	0.58
1:E:6:VAL:HG12	1:E:98:TYR:HB3	1.86	0.57
1:C:4:HIS:HE1	1:C:96:ILE:HD11	1.69	0.57
1:B:367:ARG:H	1:D:214:ASN:ND2	2.02	0.56
1:F:279:ARG:HD3	1:F:430:CYS:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:GLY:HA3	1:D:185:ILE:O	2.06	0.56
1:A:293:GLY:HA2	1:A:317:ILE:HG12	1.87	0.55
1:D:8:ILE:HD11	2:D:441:FAD:H2A	1.83	0.55
1:D:249:MET:HE1	1:D:251:MET:CE	2.36	0.55
1:D:107:PRO:HD3	1:D:294:VAL:HG11	1.89	0.54
1:D:346:ILE:HD11	1:D:411:LEU:CD1	2.37	0.54
1:B:214:ASN:HD22	1:F:367:ARG:H	1.56	0.54
1:B:199:ILE:O	1:B:372:THR:HG21	2.07	0.54
1:D:304:THR:OG1	1:D:308:THR:HB	2.08	0.54
1:F:104:ALA:HB2	1:F:292:VAL:CG1	2.38	0.54
1:D:293:GLY:HA2	1:D:317:ILE:HG12	1.90	0.53
1:E:405:LYS:HD3	1:F:387:LYS:HD2	1.90	0.53
1:C:279:ARG:HD3	1:C:430:CYS:HB3	1.90	0.53
1:F:249:MET:HE1	1:F:251:MET:CE	2.31	0.53
1:F:304:THR:OG1	1:F:308:THR:HB	2.07	0.53
1:F:42:THR:CG2	1:F:43:PRO:HD3	2.38	0.53
1:D:177:ARG:NH2	8:D:1251:HOH:O	2.43	0.52
1:E:5:VAL:HG22	1:E:100:TYR:HB2	1.90	0.52
1:F:42:THR:HG23	1:F:43:PRO:HD3	1.92	0.52
1:B:293:GLY:HA2	1:B:317:ILE:HG12	1.92	0.52
1:A:367:ARG:H	1:E:214:ASN:ND2	2.07	0.51
1:D:104:ALA:HB2	1:D:292:VAL:CG2	2.39	0.51
1:D:283:ASN:ND2	1:D:286:TYR:H	2.01	0.51
1:E:41:PHE:HB2	1:E:390:LEU:HD11	1.92	0.51
1:E:6:VAL:HG12	1:E:98:TYR:CB	2.41	0.51
1:E:159:PRO:HD3	6:E:800:PS9:S3	2.51	0.51
1:B:277:VAL:HB	1:B:281:PHE:HA	1.92	0.51
1:F:346:ILE:HD11	1:F:411:LEU:CD1	2.41	0.51
1:C:283:ASN:ND2	1:C:286:TYR:H	2.04	0.50
1:F:382:LYS:NZ	2:F:441:FAD:O4	2.44	0.50
1:D:8:ILE:HD12	1:D:33:ILE:O	2.11	0.50
1:B:121:THR:CG2	1:B:135:LYS:HD3	2.42	0.50
1:B:149:GLY:HA3	1:B:185:ILE:O	2.12	0.50
1:C:214:ASN:HD21	1:E:366:PRO:HA	1.76	0.49
1:F:121:THR:CG2	1:F:135:LYS:HD3	2.42	0.49
1:F:327:ASN:ND2	1:F:339:TYR:H	1.96	0.49
1:B:6:VAL:HG13	1:B:98:TYR:HB3	1.94	0.49
1:E:149:GLY:HA3	1:E:185:ILE:O	2.12	0.49
1:F:405:LYS:HE2	8:F:481:HOH:O	2.13	0.49
1:B:283:ASN:ND2	1:B:286:TYR:H	2.09	0.49
1:F:104:ALA:HB2	1:F:292:VAL:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:PRO:HA	1:F:214:ASN:HD21	1.78	0.48
1:D:385:PHE:CE2	3:D:500:DCQ:H3MB	2.48	0.48
1:F:149:GLY:HA3	1:F:185:ILE:O	2.14	0.48
1:A:406:VAL:HG21	3:A:500:DCQ:H14A	1.95	0.48
1:B:294:VAL:HA	1:B:312:LYS:HD3	1.96	0.48
1:D:25:MET:HE3	1:D:329:VAL:HG13	1.96	0.48
1:D:327:ASN:ND2	1:D:339:TYR:H	1.94	0.47
1:B:249:MET:HE1	1:B:251:MET:CE	2.40	0.47
1:D:327:ASN:HD21	1:D:339:TYR:N	1.95	0.47
1:C:394:ARG:NH2	8:C:858:HOH:O	2.47	0.47
1:F:277:VAL:HB	1:F:281:PHE:HA	1.96	0.47
1:A:407:LEU:HB3	1:A:413:VAL:HG13	1.97	0.47
1:D:202:SER:O	1:D:206:VAL:HG23	2.15	0.47
1:C:293:GLY:HA2	1:C:317:ILE:HG12	1.96	0.46
1:E:128:HIS:HE1	8:E:469:HOH:O	1.96	0.46
1:C:277:VAL:HB	1:C:281:PHE:HA	1.97	0.46
1:E:147:VAL:CG1	1:E:245:ALA:HB2	2.46	0.46
1:D:260:VAL:HG12	1:D:268:ALA:HB2	1.96	0.46
1:A:47:HIS:CE1	1:A:166:MET:HE1	2.50	0.46
1:D:6:VAL:HG13	1:D:101:LEU:HD12	1.98	0.46
1:D:8:ILE:HG22	1:D:103:ILE:HA	1.98	0.46
1:E:406:VAL:HG11	3:E:500:DCQ:H13A	1.97	0.46
1:F:385:PHE:HE2	3:F:500:DCQ:H3MB	1.79	0.46
2:A:441:FAD:H9	2:A:441:FAD:H1'1	1.80	0.45
1:D:47:HIS:HA	1:D:166:MET:HE1	1.98	0.45
1:F:42:THR:CG2	2:F:441:FAD:H3'	2.45	0.45
1:F:47:HIS:CE1	1:F:166:MET:HE1	2.51	0.45
1:D:6:VAL:HG13	1:D:101:LEU:CD1	2.46	0.45
1:A:121:THR:CG2	1:A:135:LYS:HD3	2.46	0.45
1:A:366:PRO:O	1:A:429:ARG:NH1	2.50	0.45
1:B:381:PHE:HE1	4:B:600:LMT:H61	1.82	0.45
1:C:394:ARG:NH1	7:C:432:SO4:O1	2.49	0.45
1:D:148:ILE:O	1:D:184:PHE:HA	2.17	0.45
1:F:196:VAL:HG21	1:F:363:VAL:HG13	1.99	0.45
1:A:149:GLY:HA3	1:A:185:ILE:O	2.17	0.44
1:B:25:MET:HE3	1:B:329:VAL:HG13	1.98	0.44
1:B:47:HIS:CE1	1:B:166:MET:HE1	2.53	0.44
1:D:19:TYR:CD2	1:D:398:ILE:HG12	2.53	0.44
1:A:214:ASN:HD21	1:C:365:PRO:HB3	1.82	0.44
1:C:316:MET:O	1:C:320:MET:HG3	2.17	0.44
1:A:382:LYS:NZ	2:A:441:FAD:O4	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:HD13	1:B:351:PHE:CD1	2.52	0.44
1:C:406:VAL:HG22	1:D:384:ALA:HB1	1.99	0.44
1:F:233:TYR:CZ	1:F:241:HIS:HB2	2.52	0.44
1:D:161:TYR:CE1	1:D:206:VAL:HG11	2.52	0.44
1:F:294:VAL:HA	1:F:312:LYS:HD3	1.98	0.44
1:D:8:ILE:CD1	2:D:441:FAD:C2A	2.84	0.44
1:D:346:ILE:O	3:D:500:DCQ:H4MB	2.18	0.44
1:A:277:VAL:HB	1:A:281:PHE:HA	1.98	0.44
1:E:6:VAL:HG13	1:E:101:LEU:CD1	2.47	0.44
1:F:199:ILE:O	1:F:372:THR:HG21	2.17	0.44
1:B:148:ILE:O	1:B:184:PHE:HA	2.18	0.44
1:B:113:ALA:HB3	1:B:116:GLN:HB2	1.99	0.44
2:F:441:FAD:H9	2:F:441:FAD:H1'1	1.79	0.44
1:B:407:LEU:HD21	3:B:500:DCQ:H8	1.98	0.43
1:D:8:ILE:HD11	2:D:441:FAD:N1A	2.28	0.43
1:E:209:LEU:HD21	1:E:351:PHE:CE2	2.53	0.43
1:D:6:VAL:HG12	1:D:98:TYR:HB3	1.99	0.43
1:E:108:LYS:HD2	1:E:257:PRO:HA	1.99	0.43
1:E:294:VAL:HA	1:E:312:LYS:HD3	2.00	0.43
1:A:214:ASN:ND2	1:C:366:PRO:HA	2.33	0.43
1:D:6:VAL:HG12	1:D:98:TYR:CB	2.48	0.43
1:F:236:LEU:HD11	1:F:305:PRO:HB3	2.00	0.43
1:B:120:SER:HB2	1:B:226:ILE:HG21	2.01	0.43
1:D:8:ILE:CG2	1:D:103:ILE:HA	2.48	0.43
1:D:19:TYR:HD2	1:D:398:ILE:HG12	1.84	0.43
1:E:402:PHE:HE2	3:E:500:DCQ:H13	1.84	0.43
1:A:346:ILE:HD11	1:A:411:LEU:HD12	1.98	0.43
1:A:278:ASN:HB2	1:A:422:CYS:O	2.19	0.43
1:D:277:VAL:HB	1:D:281:PHE:HA	2.01	0.43
1:A:235:ASP:OD2	1:A:241:HIS:HE1	2.00	0.43
1:A:368:GLU:O	1:E:172:LYS:HE3	2.19	0.43
1:A:147:VAL:HG12	1:A:245:ALA:HB2	2.00	0.42
1:D:382:LYS:NZ	2:D:441:FAD:O4	2.47	0.42
1:F:42:THR:HG21	2:F:441:FAD:C4'	2.48	0.42
1:D:121:THR:CG2	1:D:135:LYS:HD3	2.48	0.42
1:F:196:VAL:HG23	1:F:301:ILE:CD1	2.49	0.42
1:B:81:ILE:HG23	1:B:263:ALA:HB2	2.00	0.42
1:D:278:ASN:HB2	1:D:422:CYS:O	2.19	0.42
1:E:168:HIS:ND1	1:E:177:ARG:HD3	2.35	0.42
1:B:405:LYS:O	1:B:409:ILE:HG23	2.19	0.42
1:E:148:ILE:O	1:E:184:PHE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:MET:HE2	1:C:350:ASP:HB3	2.01	0.42
1:E:56:GLU:H	1:E:56:GLU:CD	2.27	0.42
1:F:42:THR:HG21	2:F:441:FAD:C3'	2.44	0.42
1:C:349:ALA:HB2	6:C:800:PS9:S6	2.59	0.42
1:E:283:ASN:HD22	1:E:286:TYR:N	1.97	0.42
1:E:6:VAL:HG13	1:E:101:LEU:HD13	2.01	0.42
1:F:369:ARG:NH1	7:F:431:SO4:O3	2.52	0.42
1:A:25:MET:SD	1:A:28:LEU:HG	2.60	0.42
1:C:373:LYS:NZ	4:C:600:LMT:H11	2.35	0.42
1:D:257:PRO:HB2	1:D:259:VAL:HG12	2.02	0.41
1:B:214:ASN:ND2	1:F:367:ARG:H	2.16	0.41
1:C:233:TYR:CZ	1:C:241:HIS:HB2	2.56	0.41
1:D:257:PRO:HG2	1:D:260:VAL:HG23	2.01	0.41
1:E:277:VAL:HB	1:E:281:PHE:HA	2.03	0.41
1:B:260:VAL:HG12	1:B:268:ALA:HB2	2.01	0.41
1:E:223:VAL:HG21	1:E:250:PHE:CE1	2.55	0.41
1:A:327:ASN:HD21	1:A:339:TYR:N	1.94	0.41
1:C:249:MET:CE	1:C:251:MET:HE2	2.39	0.41
1:A:162:GLU:O	1:A:166:MET:HG3	2.20	0.41
1:C:159:PRO:HD3	6:C:800:PS9:S2	2.61	0.41
1:D:406:VAL:HG21	3:D:500:DCQ:H15A	2.02	0.41
1:E:159:PRO:HD3	6:E:800:PS9:S4	2.61	0.41
1:D:294:VAL:HG12	2:D:441:FAD:O2P	2.21	0.41
1:D:366:PRO:HA	1:F:214:ASN:ND2	2.35	0.41
1:F:361:ASP:HA	1:F:362:PRO:HA	1.93	0.41
1:E:33:ILE:HG12	1:E:74:ILE:CG2	2.51	0.41
1:E:63:ALA:HB3	1:E:64:PRO:HD3	2.03	0.41
1:B:382:LYS:NZ	2:B:441:FAD:O4	2.54	0.40
1:F:63:ALA:HB3	1:F:64:PRO:HD3	2.03	0.40
1:A:147:VAL:CG1	1:A:245:ALA:HB2	2.52	0.40
1:C:382:LYS:NZ	2:C:441:FAD:O4	2.54	0.40
7:C:431:SO4:O4	1:E:369:ARG:NH1	2.55	0.40
1:A:5:VAL:HG22	1:A:100:TYR:HB2	2.04	0.40
1:E:382:LYS:NZ	2:E:441:FAD:O4	2.53	0.40
1:C:359:PHE:HB3	1:C:371:ILE:HB	2.04	0.40
1:A:294:VAL:HA	1:A:312:LYS:HD3	2.04	0.40
1:C:341:PRO:HB2	1:C:343:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	426/430 (99%)	419 (98%)	7 (2%)	0	100	100
1	B	426/430 (99%)	417 (98%)	9 (2%)	0	100	100
1	C	426/430 (99%)	419 (98%)	7 (2%)	0	100	100
1	D	426/430 (99%)	421 (99%)	5 (1%)	0	100	100
1	E	426/430 (99%)	417 (98%)	9 (2%)	0	100	100
1	F	426/430 (99%)	419 (98%)	7 (2%)	0	100	100
All	All	2556/2580 (99%)	2512 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	355/355 (100%)	346 (98%)	9 (2%)	42	45
1	B	355/355 (100%)	345 (97%)	10 (3%)	38	41
1	C	355/355 (100%)	345 (97%)	10 (3%)	38	41
1	D	355/355 (100%)	345 (97%)	10 (3%)	38	41
1	E	355/355 (100%)	344 (97%)	11 (3%)	35	37
1	F	355/355 (100%)	349 (98%)	6 (2%)	53	60
All	All	2130/2130 (100%)	2074 (97%)	56 (3%)	40	44

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	28	LEU
1	A	147	VAL
1	A	177	ARG
1	A	191	LEU
1	A	243	VAL
1	A	390	LEU
1	A	407	LEU
1	A	413	VAL
1	B	5	VAL
1	B	6	VAL
1	B	24	LEU
1	B	28	LEU
1	B	81	ILE
1	B	177	ARG
1	B	191	LEU
1	B	343	LEU
1	B	407	LEU
1	B	409	ILE
1	C	5	VAL
1	C	24	LEU
1	C	96	ILE
1	C	118	GLU
1	C	142	ASN
1	C	177	ARG
1	C	191	LEU
1	C	240	THR
1	C	343	LEU
1	C	390	LEU
1	D	5	VAL
1	D	24	LEU
1	D	28	LEU
1	D	165	LEU
1	D	171	LEU
1	D	177	ARG
1	D	294	VAL
1	D	308	THR
1	D	343	LEU
1	D	407	LEU
1	E	24	LEU
1	E	28	LEU
1	E	42	THR

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Mol	Chain	Res	Type
1	E	147	VAL
1	E	165	LEU
1	E	171	LEU
1	E	177	ARG
1	E	191	LEU
1	E	390	LEU
1	E	407	LEU
1	E	411	LEU
1	F	5	VAL
1	F	24	LEU
1	F	165	LEU
1	F	177	ARG
1	F	236	LEU
1	F	308	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	70	ASN
1	A	91	GLN
1	A	214	ASN
1	A	237	ASN
1	A	241	HIS
1	A	283	ASN
1	A	327	ASN
1	A	379	HIS
1	A	395	ASN
1	B	23	ASN
1	B	119	ASN
1	B	128	HIS
1	B	214	ASN
1	B	237	ASN
1	B	241	HIS
1	B	255	GLN
1	B	283	ASN
1	B	327	ASN
1	B	334	ASN
1	B	379	HIS
1	B	395	ASN
1	C	23	ASN
1	C	75	ASN

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Mol	Chain	Res	Type
1	C	128	HIS
1	C	214	ASN
1	C	237	ASN
1	C	239	ASN
1	C	241	HIS
1	C	255	GLN
1	C	283	ASN
1	C	327	ASN
1	C	379	HIS
1	C	395	ASN
1	D	23	ASN
1	D	70	ASN
1	D	91	GLN
1	D	128	HIS
1	D	133	GLN
1	D	137	GLN
1	D	214	ASN
1	D	237	ASN
1	D	241	HIS
1	D	283	ASN
1	D	327	ASN
1	D	379	HIS
1	D	395	ASN
1	D	414	HIS
1	E	20	ASN
1	E	75	ASN
1	E	128	HIS
1	E	133	GLN
1	E	137	GLN
1	E	214	ASN
1	E	237	ASN
1	E	241	HIS
1	E	255	GLN
1	E	283	ASN
1	E	327	ASN
1	E	379	HIS
1	E	395	ASN
1	F	23	ASN
1	F	91	GLN
1	F	128	HIS
1	F	133	GLN
1	F	214	ASN

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Mol	Chain	Res	Type
1	F	241	HIS
1	F	283	ASN
1	F	327	ASN
1	F	379	HIS
1	F	395	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 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	E	347[B]	-	4,5,7	1.37	1 (25%)	1,5,8	2.20	1 (100%)
1	CSS	B	347[A]	-	4,5,7	1.18	0	2,5,8	0.61	0
1	CSS	E	156[B]	6	4,6,7	1.05	0	2,6,8	0.78	0
1	CSS	C	156[A]	-	4,5,7	1.02	0	2,5,8	1.06	0
1	CSS	F	156[B]	6	4,6,7	0.98	0	2,6,8	0.51	0
1	CSS	B	156[A]	-	4,5,7	1.04	0	2,5,8	1.08	0
1	CSS	D	156[B]	6	4,6,7	1.07	0	2,6,8	0.68	0
1	CSS	D	347[A]	-	4,5,7	1.06	0	2,5,8	0.81	0
1	CSS	B	347[B]	6	4,6,7	1.12	0	2,6,8	0.98	0
1	CSS	C	347[A]	-	4,5,7	1.51	1 (25%)	1,5,8	2.22	1 (100%)
1	CSS	A	156[A]	-	4,5,7	1.09	0	2,5,8	0.53	0
1	CSS	C	156[B]	6	4,6,7	1.05	0	2,6,8	0.87	0
1	CSS	A	347[A]	-	4,5,7	1.49	1 (25%)	1,5,8	2.42	1 (100%)
1	CSS	B	156[B]	6	4,6,7	1.08	0	2,6,8	0.86	0
1	CSS	F	347[A]	-	4,5,7	1.57	1 (25%)	1,5,8	1.86	0
1	CSS	D	347[B]	6	4,6,7	1.02	0	2,6,8	0.89	0
1	CSS	E	347[A]	-	4,5,7	1.41	1 (25%)	1,5,8	1.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSS	C	347[B]	-	4,5,7	1.36	0	1,5,8	2.16	1 (100%)
1	CSS	E	156[A]	-	4,5,7	1.08	0	2,5,8	0.80	0
1	CSS	A	156[B]	6	4,6,7	1.11	0	2,6,8	0.54	0
1	CSS	A	347[B]	-	4,5,7	1.42	1 (25%)	1,5,8	2.65	1 (100%)
1	CSS	F	347[B]	-	4,5,7	1.36	0	1,5,8	1.76	0
1	CSS	D	156[A]	-	4,5,7	1.05	0	2,5,8	1.05	0
1	CSS	F	156[A]	-	4,5,7	0.99	0	2,5,8	0.93	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	E	347[B]	-	-	1/1/4/7	-
1	CSS	B	347[A]	-	-	0/1/4/7	-
1	CSS	E	156[B]	6	-	0/1/5/7	-
1	CSS	C	156[A]	-	-	1/1/4/7	-
1	CSS	F	156[B]	6	-	0/1/5/7	-
1	CSS	B	156[A]	-	-	1/1/4/7	-
1	CSS	D	156[B]	6	-	0/1/5/7	-
1	CSS	D	347[A]	-	-	0/1/4/7	-
1	CSS	B	347[B]	6	-	1/1/5/7	-
1	CSS	C	347[A]	-	-	0/1/4/7	-
1	CSS	A	156[A]	-	-	1/1/4/7	-
1	CSS	C	156[B]	6	-	0/1/5/7	-
1	CSS	A	347[A]	-	-	0/1/4/7	-
1	CSS	B	156[B]	6	-	0/1/5/7	-
1	CSS	F	347[A]	-	-	0/1/4/7	-
1	CSS	D	347[B]	6	-	1/1/5/7	-
1	CSS	E	347[A]	-	-	0/1/4/7	-
1	CSS	C	347[B]	-	-	1/1/4/7	-
1	CSS	E	156[A]	-	-	1/1/4/7	-
1	CSS	A	156[B]	6	-	0/1/5/7	-
1	CSS	A	347[B]	-	-	1/1/4/7	-
1	CSS	F	347[B]	-	-	1/1/4/7	-
1	CSS	D	156[A]	-	-	1/1/4/7	-
1	CSS	F	156[A]	-	-	1/1/4/7	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	347[A]	CSS	CB-SG	-2.52	1.76	1.81
1	A	347[A]	CSS	CB-SG	-2.37	1.76	1.81
1	C	347[A]	CSS	CB-SG	-2.33	1.76	1.81
1	A	347[B]	CSS	CB-SG	-2.20	1.76	1.81
1	E	347[A]	CSS	CB-SG	-2.16	1.77	1.81
1	E	347[B]	CSS	CB-SG	-2.07	1.77	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347[B]	CSS	CA-CB-SG	-2.65	108.74	114.40
1	A	347[A]	CSS	CA-CB-SG	-2.42	109.22	114.40
1	C	347[A]	CSS	CA-CB-SG	-2.22	109.65	114.40
1	E	347[B]	CSS	CA-CB-SG	-2.20	109.69	114.40
1	C	347[B]	CSS	CA-CB-SG	-2.16	109.78	114.40

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	347[B]	CSS	N-CA-CB-SG
1	B	347[B]	CSS	N-CA-CB-SG
1	C	347[B]	CSS	N-CA-CB-SG
1	D	347[B]	CSS	N-CA-CB-SG
1	E	347[B]	CSS	N-CA-CB-SG
1	F	347[B]	CSS	N-CA-CB-SG
1	A	156[A]	CSS	N-CA-CB-SG
1	B	156[A]	CSS	N-CA-CB-SG
1	C	156[A]	CSS	N-CA-CB-SG
1	D	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.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 57 ligands modelled in this entry, 8 are modelled with single atom - leaving 49 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
6	PS9	D	800	1	0,1,8	-	-	-		
6	PS9	B	802[A]	-	0,1,8	-	-	-		
7	SO4	F	434	-	4,4,4	0.25	0	6,6,6	0.15	0
6	PS9	F	800	1	8,8,8	0.90	0	8,8,8	1.31	0
3	DCQ	C	500	-	23,23,23	2.21	7 (30%)	27,29,29	0.98	1 (3%)
4	LMT	A	600	-	36,36,36	0.49	0	47,47,47	0.71	1 (2%)
4	LMT	D	600	-	36,36,36	0.49	0	47,47,47	0.89	2 (4%)
6	PS9	A	800	1	8,8,8	0.93	0	8,8,8	1.17	0
2	FAD	C	441	5	58,58,58	1.42	7 (12%)	85,89,89	1.65	17 (20%)
7	SO4	E	432	-	4,4,4	0.23	0	6,6,6	0.13	0
7	SO4	B	433	-	4,4,4	0.25	0	6,6,6	0.08	0
7	SO4	A	435	-	4,4,4	0.25	0	6,6,6	0.07	0
3	DCQ	A	500	-	23,23,23	2.21	7 (30%)	27,29,29	0.96	1 (3%)
7	SO4	D	432	-	4,4,4	0.22	0	6,6,6	0.14	0
6	PS9	B	802[B]	-	0,1,8	-	-	-		
7	SO4	B	434	-	4,4,4	0.23	0	6,6,6	0.12	0
7	SO4	C	433	-	4,4,4	0.21	0	6,6,6	0.23	0
7	SO4	C	434	-	4,4,4	0.24	0	6,6,6	0.07	0
2	FAD	D	441	5	58,58,58	1.34	6 (10%)	85,89,89	1.56	16 (18%)
2	FAD	A	441	5	58,58,58	1.37	6 (10%)	85,89,89	1.60	17 (20%)
7	SO4	B	432	-	4,4,4	0.21	0	6,6,6	0.21	0
7	SO4	D	433	-	4,4,4	0.24	0	6,6,6	0.07	0
7	SO4	F	433	-	4,4,4	0.23	0	6,6,6	0.27	0
3	DCQ	E	500	-	23,23,23	2.21	7 (30%)	27,29,29	1.01	1 (3%)
6	PS9	C	800	1	3,5,8	0.84	0	2,4,8	0.92	0
7	SO4	C	432	-	4,4,4	0.24	0	6,6,6	0.14	0
4	LMT	C	600	-	36,36,36	0.55	1 (2%)	47,47,47	0.75	1 (2%)
7	SO4	F	432	-	4,4,4	0.24	0	6,6,6	0.10	0
4	LMT	E	600	-	36,36,36	0.51	0	47,47,47	0.92	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	D	434	-	4,4,4	0.26	0	6,6,6	0.14	0
7	SO4	A	431	-	4,4,4	0.24	0	6,6,6	0.09	0
6	PS9	E	800	1	8,8,8	0.95	0	8,8,8	0.99	0
7	SO4	F	431	-	4,4,4	0.25	0	6,6,6	0.16	0
3	DCQ	B	500	-	23,23,23	2.27	7 (30%)	27,29,29	0.79	0
7	SO4	A	432	-	4,4,4	0.24	0	6,6,6	0.14	0
7	SO4	A	434	-	4,4,4	0.23	0	6,6,6	0.08	0
4	LMT	F	600	-	36,36,36	0.54	0	47,47,47	0.85	1 (2%)
2	FAD	B	441	5	58,58,58	1.31	4 (6%)	85,89,89	1.63	17 (20%)
7	SO4	B	431	-	4,4,4	0.24	0	6,6,6	0.07	0
2	FAD	E	441	5	58,58,58	1.35	5 (8%)	85,89,89	1.58	17 (20%)
4	LMT	B	600	-	36,36,36	0.51	1 (2%)	47,47,47	0.77	1 (2%)
3	DCQ	D	500	-	23,23,23	2.22	7 (30%)	27,29,29	1.03	2 (7%)
3	DCQ	F	500	-	23,23,23	2.36	8 (34%)	27,29,29	1.09	2 (7%)
7	SO4	A	433	-	4,4,4	0.21	0	6,6,6	0.20	0
7	SO4	C	431	-	4,4,4	0.24	0	6,6,6	0.08	0
2	FAD	F	441	5	58,58,58	1.37	6 (10%)	85,89,89	1.65	18 (21%)
7	SO4	E	434	-	4,4,4	0.24	0	6,6,6	0.07	0
7	SO4	D	431	-	4,4,4	0.25	0	6,6,6	0.07	0
7	SO4	E	433	-	4,4,4	0.22	0	6,6,6	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PS9	F	800	1	-	-	0/1/1/1
3	DCQ	C	500	-	-	7/14/38/38	0/1/1/1
4	LMT	A	600	-	-	8/21/61/61	0/2/2/2
4	LMT	D	600	-	-	10/21/61/61	0/2/2/2
6	PS9	A	800	1	-	-	0/1/1/1
2	FAD	C	441	5	-	3/34/50/50	0/6/6/6
3	DCQ	A	500	-	-	5/14/38/38	0/1/1/1
2	FAD	D	441	5	-	4/34/50/50	0/6/6/6
2	FAD	A	441	5	-	0/34/50/50	0/6/6/6
3	DCQ	E	500	-	-	3/14/38/38	0/1/1/1
6	PS9	C	800	1	-	1/3/3/8	-
4	LMT	C	600	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMT	E	600	-	-	18/21/61/61	0/2/2/2
6	PS9	E	800	1	-	-	0/1/1/1
3	DCQ	B	500	-	-	11/14/38/38	0/1/1/1
4	LMT	F	600	-	-	11/21/61/61	0/2/2/2
2	FAD	B	441	5	-	2/34/50/50	0/6/6/6
2	FAD	E	441	5	-	3/34/50/50	0/6/6/6
4	LMT	B	600	-	-	10/21/61/61	0/2/2/2
3	DCQ	D	500	-	-	6/14/38/38	0/1/1/1
3	DCQ	F	500	-	-	7/14/38/38	0/1/1/1
2	FAD	F	441	5	-	4/34/50/50	0/6/6/6

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	441	FAD	O4-C4	7.10	1.37	1.23
2	E	441	FAD	O4-C4	6.70	1.36	1.23
2	F	441	FAD	O4-C4	6.66	1.36	1.23
2	B	441	FAD	O4-C4	6.57	1.36	1.23
2	D	441	FAD	O4-C4	6.46	1.35	1.23
2	C	441	FAD	O4-C4	6.30	1.35	1.23
3	B	500	DCQ	O5-C5	6.14	1.37	1.23
3	F	500	DCQ	O5-C5	6.03	1.36	1.23
3	D	500	DCQ	O5-C5	6.03	1.36	1.23
3	C	500	DCQ	O5-C5	6.02	1.36	1.23
3	B	500	DCQ	O2-C2	5.97	1.36	1.23
3	A	500	DCQ	O5-C5	5.97	1.36	1.23
3	E	500	DCQ	O2-C2	5.87	1.36	1.23
3	E	500	DCQ	O5-C5	5.87	1.36	1.23
3	C	500	DCQ	O2-C2	5.86	1.36	1.23
3	A	500	DCQ	O2-C2	5.84	1.36	1.23
3	F	500	DCQ	O2-C2	5.82	1.36	1.23
3	D	500	DCQ	O2-C2	5.81	1.36	1.23
2	C	441	FAD	P-O3P	4.07	1.63	1.59
3	B	500	DCQ	C3-C2	-3.36	1.39	1.48
3	C	500	DCQ	C3-C2	-3.33	1.39	1.48
3	D	500	DCQ	C3-C2	-3.32	1.39	1.48
3	F	500	DCQ	C3-C2	-3.28	1.39	1.48
3	E	500	DCQ	C3-C2	-3.27	1.39	1.48
3	F	500	DCQ	C4-C5	-3.26	1.39	1.48
3	B	500	DCQ	C4-C5	-3.25	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	DCQ	C3-C2	-3.25	1.39	1.48
3	A	500	DCQ	C4-C5	-3.22	1.39	1.48
3	E	500	DCQ	C4-C5	-3.20	1.39	1.48
3	C	500	DCQ	C4-C5	-3.15	1.39	1.48
3	F	500	DCQ	C16-C15	3.11	1.72	1.50
3	D	500	DCQ	C4-C5	-3.08	1.40	1.48
3	B	500	DCQ	C6-C1	3.07	1.40	1.35
2	C	441	FAD	PA-O3P	2.94	1.62	1.59
3	F	500	DCQ	C6-C1	2.85	1.40	1.35
3	E	500	DCQ	C6-C1	2.80	1.40	1.35
3	D	500	DCQ	C6-C1	2.79	1.40	1.35
2	E	441	FAD	C5X-N5	-2.70	1.34	1.39
3	C	500	DCQ	C6-C1	2.68	1.40	1.35
3	A	500	DCQ	C6-C1	2.67	1.40	1.35
2	F	441	FAD	C9A-N10	-2.67	1.36	1.41
2	B	441	FAD	C9A-N10	-2.66	1.36	1.41
2	F	441	FAD	C4X-N5	2.57	1.36	1.30
2	C	441	FAD	C9A-N10	-2.49	1.36	1.41
2	D	441	FAD	C9A-N10	-2.49	1.36	1.41
2	D	441	FAD	P-O3P	2.46	1.62	1.59
3	A	500	DCQ	C6-C5	-2.43	1.39	1.46
2	E	441	FAD	C9A-N10	-2.42	1.37	1.41
3	B	500	DCQ	C1-C2	-2.41	1.39	1.47
3	E	500	DCQ	C6-C5	-2.40	1.39	1.46
3	F	500	DCQ	C6-C5	-2.39	1.39	1.46
2	D	441	FAD	C4X-N5	2.36	1.35	1.30
2	A	441	FAD	C9A-N10	-2.35	1.37	1.41
3	D	500	DCQ	C6-C5	-2.32	1.39	1.46
2	A	441	FAD	C8A-N7A	2.31	1.36	1.31
3	C	500	DCQ	C6-C5	-2.30	1.40	1.46
2	A	441	FAD	C4X-N5	2.27	1.35	1.30
3	B	500	DCQ	C6-C5	-2.27	1.40	1.46
3	C	500	DCQ	C1-C2	-2.25	1.39	1.47
3	F	500	DCQ	C1-C2	-2.24	1.39	1.47
3	E	500	DCQ	C1-C2	-2.23	1.39	1.47
2	F	441	FAD	P-O3P	2.23	1.61	1.59
3	A	500	DCQ	C1-C2	-2.22	1.39	1.47
3	D	500	DCQ	C1-C2	-2.22	1.39	1.47
2	F	441	FAD	PA-O3P	2.19	1.61	1.59
2	E	441	FAD	C8A-N7A	2.17	1.35	1.31
4	C	600	LMT	O1'-C1'	2.16	1.43	1.40
2	B	441	FAD	C4X-N5	2.16	1.35	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	441	FAD	C5X-N5	-2.15	1.35	1.39
2	D	441	FAD	C5A-N7A	-2.14	1.35	1.39
2	C	441	FAD	C4X-N5	2.13	1.35	1.30
2	D	441	FAD	C8A-N7A	2.11	1.35	1.31
2	A	441	FAD	C5X-N5	-2.10	1.35	1.39
2	C	441	FAD	C8A-N7A	2.07	1.35	1.31
2	F	441	FAD	C5X-N5	-2.05	1.35	1.39
4	B	600	LMT	O1'-C1'	2.02	1.43	1.40
2	A	441	FAD	P-O3P	2.01	1.61	1.59
2	E	441	FAD	C4X-N5	2.01	1.35	1.30
2	B	441	FAD	C5A-N7A	-2.00	1.35	1.39

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	441	FAD	N3A-C2A-N1A	-5.47	120.31	128.58
2	E	441	FAD	N3A-C2A-N1A	-5.33	120.51	128.58
2	A	441	FAD	N3A-C2A-N1A	-5.19	120.72	128.58
2	C	441	FAD	C5A-C4A-N3A	-5.17	119.60	126.72
2	F	441	FAD	N3A-C2A-N1A	-5.16	120.78	128.58
2	B	441	FAD	N3A-C2A-N1A	-5.07	120.91	128.58
2	A	441	FAD	C5A-C4A-N3A	-5.02	119.81	126.72
2	D	441	FAD	C5A-C4A-N3A	-4.95	119.90	126.72
2	E	441	FAD	C5A-C4A-N3A	-4.94	119.92	126.72
2	B	441	FAD	C5A-C4A-N3A	-4.93	119.93	126.72
2	F	441	FAD	C5A-C4A-N3A	-4.93	119.93	126.72
2	D	441	FAD	N3A-C2A-N1A	-4.89	121.18	128.58
2	C	441	FAD	C2A-N3A-C4A	3.79	121.08	111.83
2	C	441	FAD	N9A-C8A-N7A	-3.68	108.71	113.94
2	A	441	FAD	N9A-C8A-N7A	-3.67	108.74	113.94
2	A	441	FAD	C2A-N3A-C4A	3.59	120.60	111.83
2	E	441	FAD	C2A-N3A-C4A	3.50	120.38	111.83
2	B	441	FAD	N9A-C8A-N7A	-3.49	108.98	113.94
2	F	441	FAD	C2A-N3A-C4A	3.46	120.29	111.83
2	F	441	FAD	N9A-C8A-N7A	-3.44	109.06	113.94
2	B	441	FAD	C2A-N3A-C4A	3.43	120.21	111.83
2	B	441	FAD	C4-N3-C2	-3.43	119.55	125.64
2	D	441	FAD	N9A-C8A-N7A	-3.36	109.17	113.94
2	E	441	FAD	N9A-C8A-N7A	-3.33	109.21	113.94
2	F	441	FAD	N3A-C4A-N9A	3.29	132.76	127.17
2	D	441	FAD	C2A-N3A-C4A	3.27	119.83	111.83
2	F	441	FAD	C4-N3-C2	-3.24	119.89	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	441	FAD	N3A-C4A-N9A	3.23	132.66	127.17
2	B	441	FAD	N3A-C4A-N9A	3.23	132.66	127.17
2	D	441	FAD	N3A-C4A-N9A	3.19	132.60	127.17
2	E	441	FAD	N3A-C4A-N9A	3.18	132.57	127.17
2	A	441	FAD	C4-N3-C2	-3.16	120.02	125.64
2	C	441	FAD	C4A-C5A-N7A	-3.14	107.00	110.58
4	C	600	LMT	O1B-C4'-C3'	3.11	115.13	107.23
2	C	441	FAD	N3A-C4A-N9A	3.08	132.40	127.17
2	C	441	FAD	C4-N3-C2	-2.99	120.34	125.64
2	F	441	FAD	C5X-C9A-N10	2.98	120.66	117.97
2	E	441	FAD	C4-N3-C2	-2.96	120.39	125.64
2	D	441	FAD	C4-N3-C2	-2.85	120.58	125.64
2	B	441	FAD	C5X-C9A-N10	2.85	120.54	117.97
2	C	441	FAD	C5A-N7A-C8A	2.81	107.87	103.45
2	B	441	FAD	O4-C4-C4X	-2.81	119.11	126.53
2	F	441	FAD	C2'-C1'-N10	2.81	123.48	110.20
2	B	441	FAD	C4A-C5A-N7A	-2.81	107.37	110.58
2	F	441	FAD	C4A-N9A-C8A	2.80	108.68	105.74
2	C	441	FAD	C4X-C10-N10	2.78	120.46	116.48
2	D	441	FAD	C4X-C10-N10	2.78	120.46	116.48
2	F	441	FAD	C4X-C4-N3	2.76	120.29	113.25
4	E	600	LMT	O1B-C4'-C3'	2.76	114.25	107.23
2	A	441	FAD	C9A-C5X-N5	-2.75	119.54	122.45
2	D	441	FAD	C4X-C4-N3	2.75	120.25	113.25
2	B	441	FAD	C4X-C4-N3	2.75	120.24	113.25
2	B	441	FAD	C4A-N9A-C8A	2.74	108.61	105.74
4	F	600	LMT	O1B-C1B-C2B	2.74	114.82	108.09
2	B	441	FAD	C4X-C10-N1	-2.72	117.93	124.59
2	E	441	FAD	C4X-C4-N3	2.71	120.16	113.25
2	A	441	FAD	C4A-N9A-C8A	2.70	108.58	105.74
2	A	441	FAD	C5X-C9A-N10	2.70	120.41	117.97
2	B	441	FAD	C4X-C10-N10	2.68	120.32	116.48
2	A	441	FAD	O4-C4-C4X	-2.67	119.47	126.53
2	F	441	FAD	C4X-C10-N10	2.67	120.31	116.48
2	C	441	FAD	C4X-C4-N3	2.66	120.03	113.25
2	E	441	FAD	C5X-C9A-N10	2.66	120.37	117.97
2	B	441	FAD	C5A-N7A-C8A	2.66	107.62	103.45
2	E	441	FAD	C4A-C5A-N7A	-2.65	107.55	110.58
2	D	441	FAD	C5X-C9A-N10	2.65	120.36	117.97
2	E	441	FAD	C4X-C10-N1	-2.62	118.16	124.59
2	D	441	FAD	C4A-C5A-N7A	-2.62	107.58	110.58
2	A	441	FAD	C5A-N7A-C8A	2.62	107.57	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	441	FAD	C4A-C5A-N7A	-2.62	107.59	110.58
2	E	441	FAD	C2'-C1'-N10	2.61	122.52	110.20
2	F	441	FAD	C9A-C5X-N5	-2.60	119.70	122.45
2	E	441	FAD	C9A-C5X-N5	-2.59	119.71	122.45
4	E	600	LMT	O1B-C4'-C5'	2.57	116.21	109.48
2	D	441	FAD	C5A-N7A-C8A	2.55	107.46	103.45
2	C	441	FAD	C4A-N9A-C8A	2.55	108.42	105.74
2	A	441	FAD	C4X-C10-N1	-2.54	118.36	124.59
2	F	441	FAD	C4A-C5A-N7A	-2.53	107.69	110.58
2	E	441	FAD	C5A-N7A-C8A	2.51	107.39	103.45
2	D	441	FAD	O4-C4-C4X	-2.50	119.94	126.53
2	B	441	FAD	C2'-C1'-N10	2.49	121.95	110.20
2	A	441	FAD	C4X-C4-N3	2.48	119.58	113.25
4	D	600	LMT	C1B-O5B-C5B	2.48	118.57	113.72
2	E	441	FAD	C4A-N9A-C8A	2.47	108.33	105.74
2	C	441	FAD	O4-C4-C4X	-2.47	120.01	126.53
2	E	441	FAD	O4-C4-C4X	-2.47	120.01	126.53
2	F	441	FAD	C4X-C10-N1	-2.46	118.55	124.59
2	D	441	FAD	C4X-C10-N1	-2.44	118.61	124.59
2	F	441	FAD	C5A-N7A-C8A	2.42	107.26	103.45
2	D	441	FAD	C4A-N9A-C8A	2.42	108.28	105.74
2	C	441	FAD	C5X-C9A-N10	2.41	120.15	117.97
2	E	441	FAD	C4X-C10-N10	2.40	119.92	116.48
4	B	600	LMT	C1B-O1B-C4'	-2.40	112.29	117.98
2	C	441	FAD	C2'-C1'-N10	2.39	121.49	110.20
3	F	500	DCQ	C3M-O3-C3	2.39	124.86	116.47
4	A	600	LMT	C1B-O1B-C4'	-2.35	112.40	117.98
2	C	441	FAD	C4X-C10-N1	-2.28	119.01	124.59
3	F	500	DCQ	C16-C15-C14	-2.27	98.02	113.36
2	A	441	FAD	C2'-C1'-N10	2.23	120.76	110.20
3	D	500	DCQ	C3M-O3-C3	2.20	124.22	116.47
2	F	441	FAD	C10-C4X-N5	-2.19	120.33	124.81
2	B	441	FAD	C9A-C5X-N5	-2.19	120.13	122.45
2	D	441	FAD	C9A-C5X-N5	-2.17	120.15	122.45
2	F	441	FAD	O4-C4-C4X	-2.17	120.81	126.53
3	A	500	DCQ	C1M-C1-C6	-2.16	120.91	124.45
2	D	441	FAD	C10-N1-C2	2.15	121.51	116.85
2	A	441	FAD	C4X-C10-N10	2.14	119.54	116.48
3	C	500	DCQ	C1M-C1-C6	-2.13	120.94	124.45
4	D	600	LMT	C1B-O1B-C4'	-2.11	112.97	117.98
2	A	441	FAD	C10-C4X-N5	-2.09	120.55	124.81
2	C	441	FAD	C9A-C5X-N5	-2.09	120.24	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	441	FAD	C10-N1-C2	2.08	121.35	116.85
2	E	441	FAD	C10-N1-C2	2.07	121.33	116.85
2	F	441	FAD	C10-N1-C2	2.03	121.24	116.85
3	E	500	DCQ	C1M-C1-C6	-2.01	121.14	124.45
3	D	500	DCQ	C4M-O4-C4	2.01	123.55	116.47
2	C	441	FAD	C5A-C4A-N9A	2.00	107.99	105.81

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	500	DCQ	C5-C6-C7-C8
3	B	500	DCQ	C1-C6-C7-C8
4	A	600	LMT	C2-C1-O1'-C1'
4	C	600	LMT	O5'-C1'-O1'-C1
4	C	600	LMT	C3'-C4'-O1B-C1B
3	F	500	DCQ	C6-C7-C8-C9
4	E	600	LMT	C4'-C5'-C6'-O6'
4	F	600	LMT	C2B-C1B-O1B-C4'
4	B	600	LMT	O5B-C5B-C6B-O6B
4	A	600	LMT	O5'-C5'-C6'-O6'
4	E	600	LMT	O5'-C5'-C6'-O6'
4	A	600	LMT	C4'-C5'-C6'-O6'
4	F	600	LMT	O5B-C1B-O1B-C4'
4	B	600	LMT	C2'-C1'-O1'-C1
4	E	600	LMT	O5B-C5B-C6B-O6B
3	A	500	DCQ	C6-C7-C8-C9
4	B	600	LMT	O5'-C1'-O1'-C1
4	B	600	LMT	C4B-C5B-C6B-O6B
4	B	600	LMT	O1'-C1-C2-C3
4	C	600	LMT	O1'-C1-C2-C3
4	E	600	LMT	C5'-C4'-O1B-C1B
4	D	600	LMT	C2'-C1'-O1'-C1
4	F	600	LMT	C4'-C5'-C6'-O6'
4	D	600	LMT	O1'-C1-C2-C3
4	C	600	LMT	C7-C8-C9-C10
4	E	600	LMT	O1'-C1-C2-C3
3	A	500	DCQ	C11-C10-C9-C8
4	A	600	LMT	C11-C10-C9-C8
4	B	600	LMT	C6-C7-C8-C9
4	D	600	LMT	C11-C10-C9-C8
4	F	600	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	D	500	DCQ	C10-C11-C12-C13
4	A	600	LMT	C5-C6-C7-C8
4	C	600	LMT	C2-C1-O1'-C1'
4	F	600	LMT	C2-C1-O1'-C1'
4	E	600	LMT	C3'-C4'-O1B-C1B
4	C	600	LMT	C11-C10-C9-C8
4	B	600	LMT	C11-C10-C9-C8
3	F	500	DCQ	C7-C8-C9-C10
2	F	441	FAD	C3B-C4B-C5B-O5B
3	F	500	DCQ	C11-C12-C13-C14
3	B	500	DCQ	C6-C7-C8-C9
4	E	600	LMT	C1-C2-C3-C4
3	A	500	DCQ	C10-C11-C12-C13
3	A	500	DCQ	C7-C8-C9-C10
4	D	600	LMT	C2-C3-C4-C5
4	C	600	LMT	C2-C3-C4-C5
4	C	600	LMT	C4'-C5'-C6'-O6'
3	B	500	DCQ	C12-C13-C14-C15
3	C	500	DCQ	C11-C12-C13-C14
3	C	500	DCQ	C12-C13-C14-C15
4	F	600	LMT	C7-C8-C9-C10
4	C	600	LMT	C2'-C1'-O1'-C1
3	D	500	DCQ	C11-C10-C9-C8
2	F	441	FAD	O4B-C4B-C5B-O5B
4	D	600	LMT	C4-C5-C6-C7
4	C	600	LMT	C4-C5-C6-C7
4	A	600	LMT	C6-C7-C8-C9
4	F	600	LMT	C11-C10-C9-C8
4	E	600	LMT	C4-C5-C6-C7
4	D	600	LMT	C1-C2-C3-C4
3	A	500	DCQ	C9-C10-C11-C12
4	D	600	LMT	O5'-C1'-O1'-C1
3	D	500	DCQ	C11-C12-C13-C14
4	D	600	LMT	C7-C8-C9-C10
4	F	600	LMT	O5B-C5B-C6B-O6B
4	F	600	LMT	C2-C3-C4-C5
4	B	600	LMT	C3-C4-C5-C6
4	E	600	LMT	C4B-C5B-C6B-O6B
4	E	600	LMT	C2-C3-C4-C5
3	C	500	DCQ	C11-C10-C9-C8
4	C	600	LMT	O5'-C5'-C6'-O6'
2	D	441	FAD	C2'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
4	B	600	LMT	C1-C2-C3-C4
4	D	600	LMT	C6-C7-C8-C9
4	E	600	LMT	C9-C10-C11-C12
3	B	500	DCQ	C11-C12-C13-C14
3	E	500	DCQ	C13-C14-C15-C16
4	B	600	LMT	C9-C10-C11-C12
3	D	500	DCQ	C13-C14-C15-C16
3	B	500	DCQ	C13-C14-C15-C16
4	F	600	LMT	O5'-C5'-C6'-O6'
2	D	441	FAD	C2'-C3'-C4'-C5'
3	E	500	DCQ	C7-C8-C9-C10
2	E	441	FAD	PA-O3P-P-O5'
3	C	500	DCQ	C9-C10-C11-C12
3	C	500	DCQ	C10-C11-C12-C13
4	D	600	LMT	C3-C4-C5-C6
4	A	600	LMT	C2-C3-C4-C5
3	D	500	DCQ	C12-C13-C14-C15
6	C	800	PS9	S2-S3-S4-S5
4	E	600	LMT	C2'-C1'-O1'-C1
4	F	600	LMT	C6-C7-C8-C9
2	D	441	FAD	O3'-C3'-C4'-O4'
3	F	500	DCQ	C5-C4-O4-C4M
2	C	441	FAD	C2'-C3'-C4'-O4'
3	C	500	DCQ	C6-C7-C8-C9
4	E	600	LMT	C7-C8-C9-C10
2	F	441	FAD	C2'-C3'-C4'-C5'
3	B	500	DCQ	C5-C4-O4-C4M
4	E	600	LMT	C3-C4-C5-C6
3	F	500	DCQ	C11-C10-C9-C8
3	F	500	DCQ	C3-C4-O4-C4M
4	E	600	LMT	C11-C10-C9-C8
3	F	500	DCQ	C9-C10-C11-C12
4	E	600	LMT	C6-C7-C8-C9
4	E	600	LMT	C5-C6-C7-C8
3	B	500	DCQ	C11-C10-C9-C8
4	A	600	LMT	C9-C10-C11-C12
3	B	500	DCQ	C9-C10-C11-C12
3	C	500	DCQ	C13-C14-C15-C16
2	C	441	FAD	O3'-C3'-C4'-O4'
2	F	441	FAD	C2'-C3'-C4'-O4'
3	B	500	DCQ	C10-C11-C12-C13
2	D	441	FAD	O3'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
4	E	600	LMT	O5'-C1'-O1'-C1
4	C	600	LMT	C3-C4-C5-C6
4	C	600	LMT	C9-C10-C11-C12
2	B	441	FAD	O4B-C4B-C5B-O5B
2	E	441	FAD	O3'-C3'-C4'-O4'
2	C	441	FAD	O4B-C4B-C5B-O5B
3	E	500	DCQ	C12-C13-C14-C15
3	D	500	DCQ	C7-C8-C9-C10
3	B	500	DCQ	C3-C4-O4-C4M
2	B	441	FAD	C2B-C1B-N9A-C8A
2	E	441	FAD	O4B-C4B-C5B-O5B

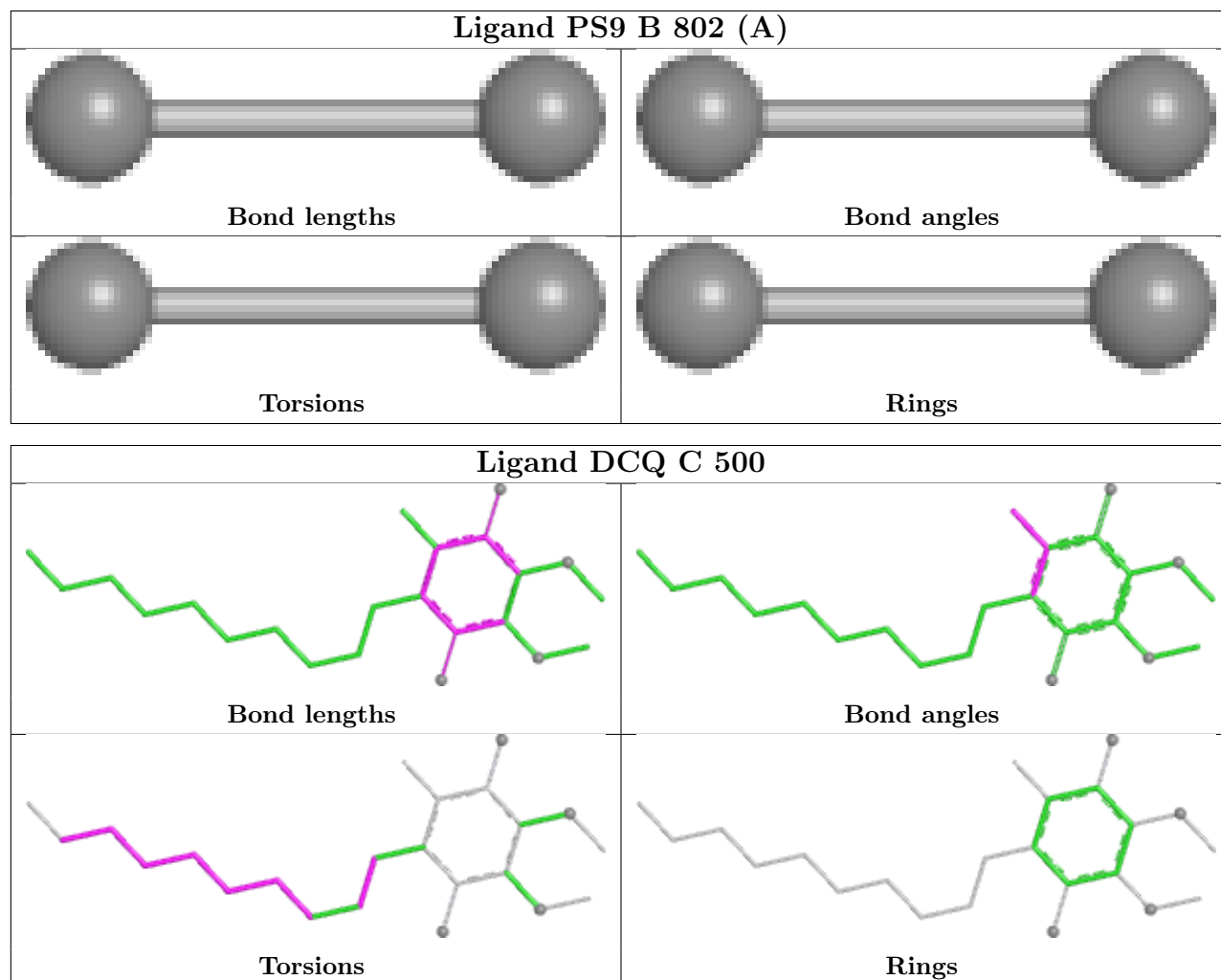
There are no ring outliers.

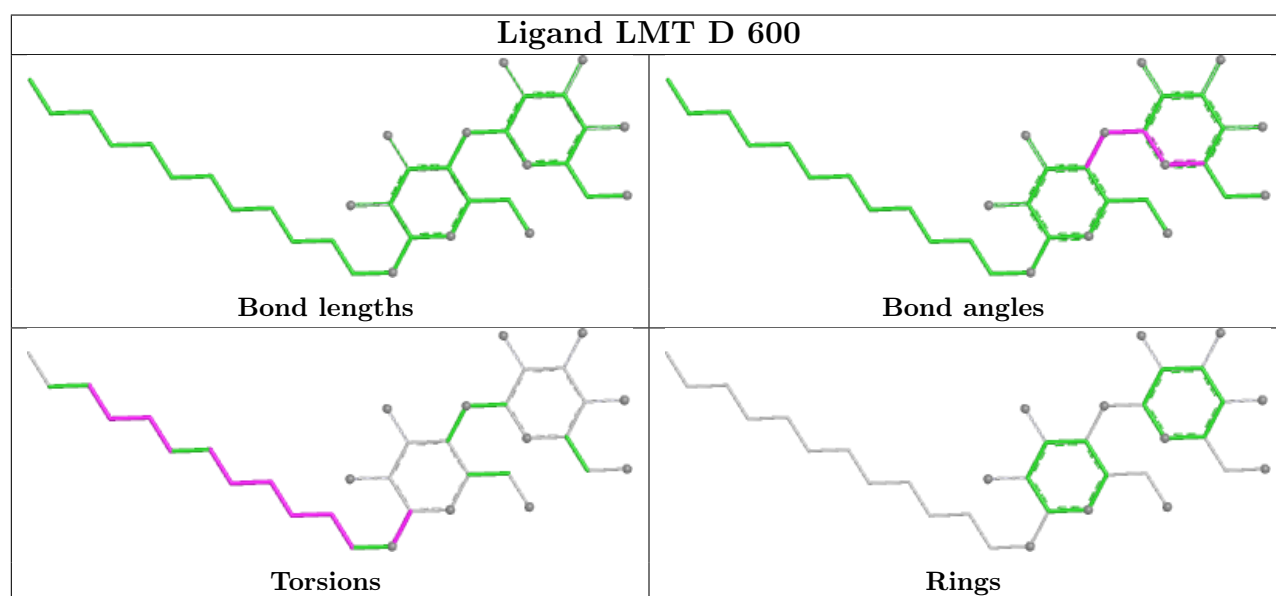
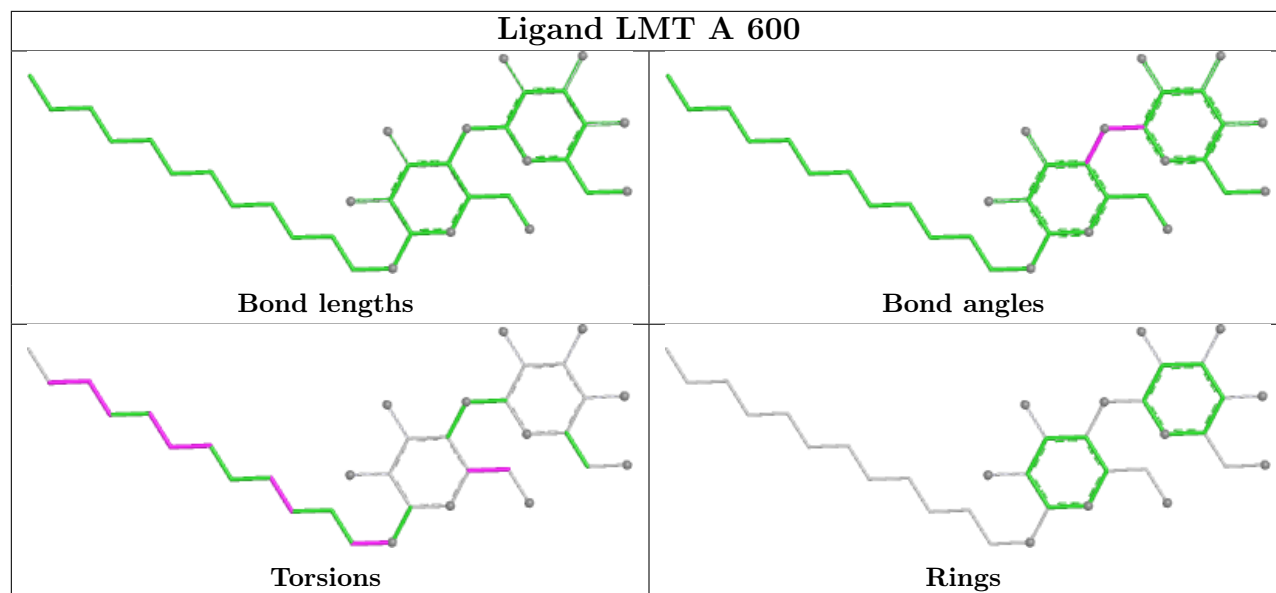
18 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	441	FAD	1	0
3	A	500	DCQ	1	0
2	D	441	FAD	6	0
2	A	441	FAD	2	0
3	E	500	DCQ	2	0
6	C	800	PS9	2	0
7	C	432	SO4	1	0
4	C	600	LMT	1	0
6	E	800	PS9	2	0
7	F	431	SO4	1	0
3	B	500	DCQ	1	0
2	B	441	FAD	1	0
2	E	441	FAD	1	0
4	B	600	LMT	1	0
3	D	500	DCQ	3	0
3	F	500	DCQ	3	0
7	C	431	SO4	1	0
2	F	441	FAD	7	0

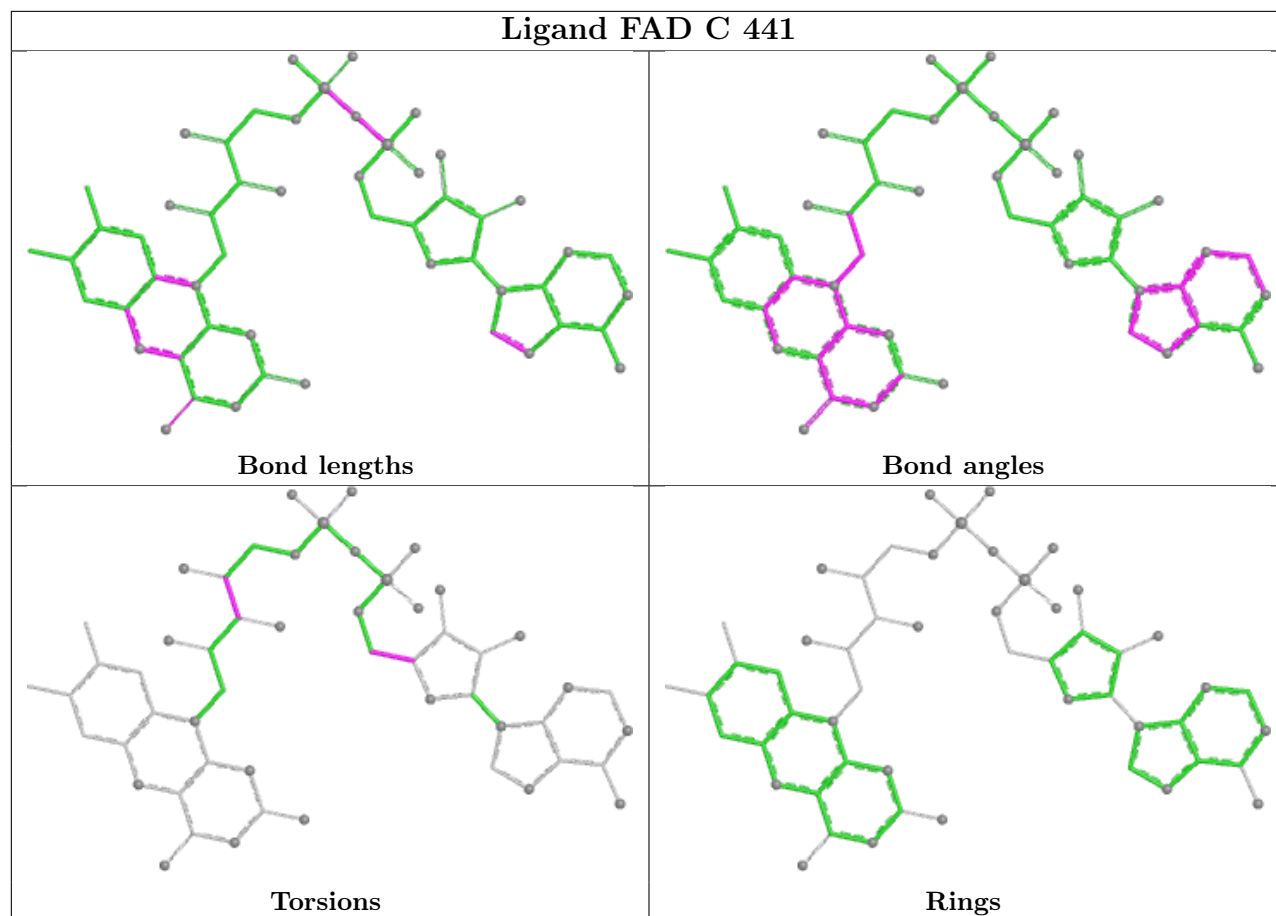
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

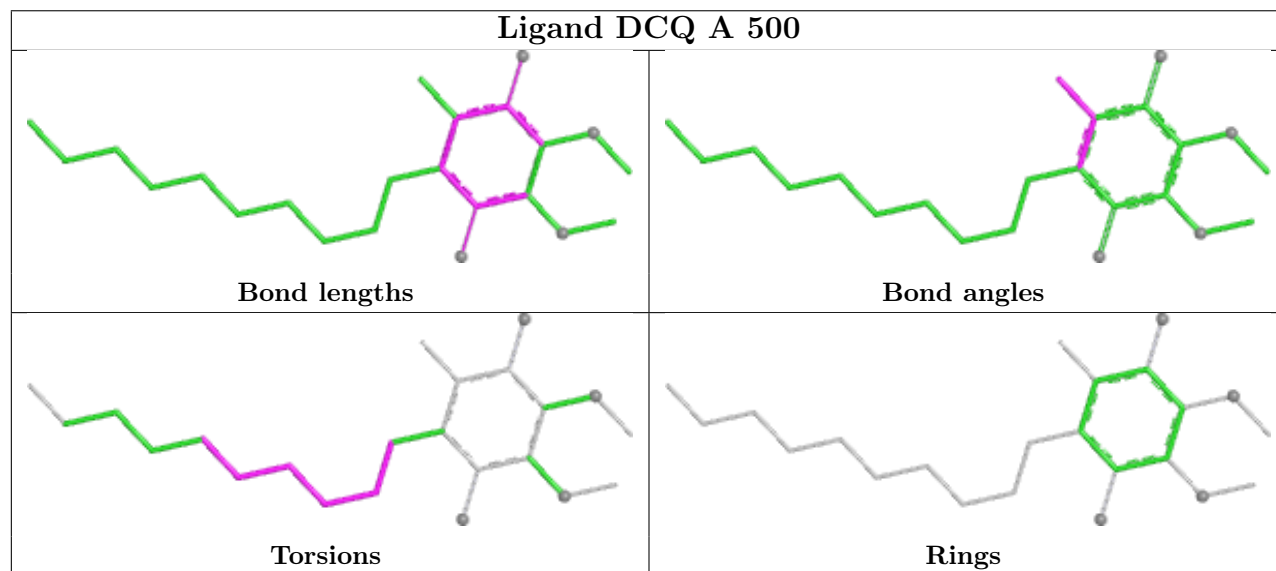


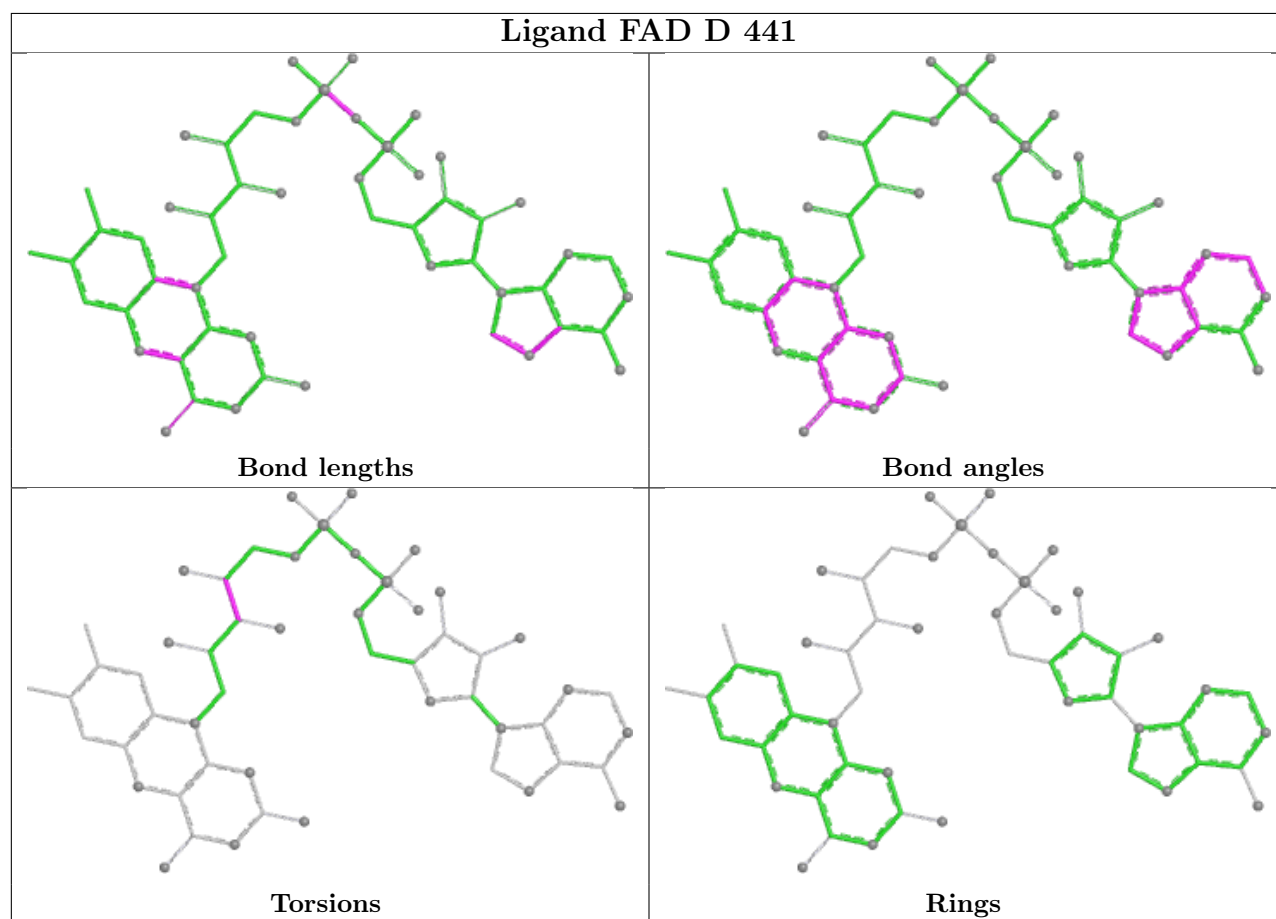
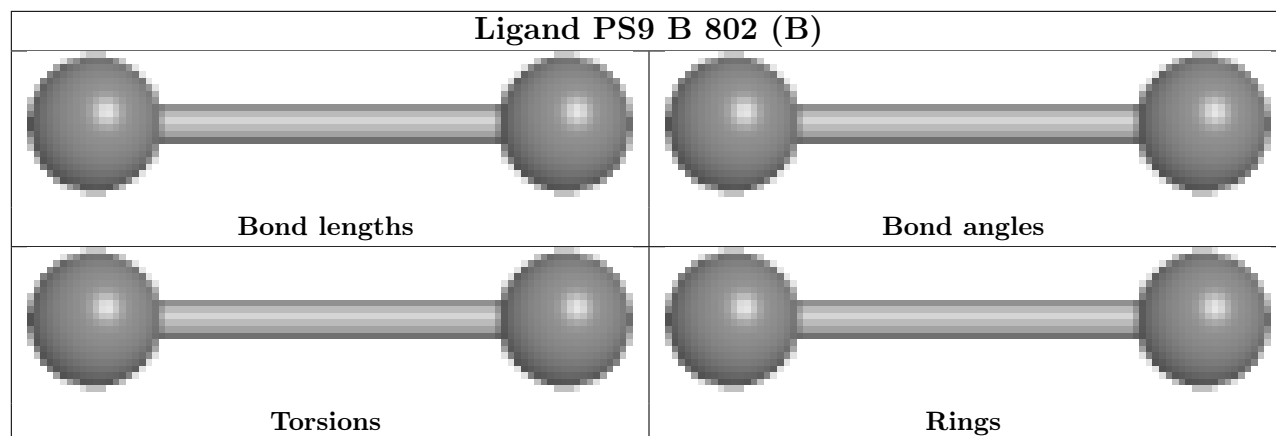


Ligand FAD C 441

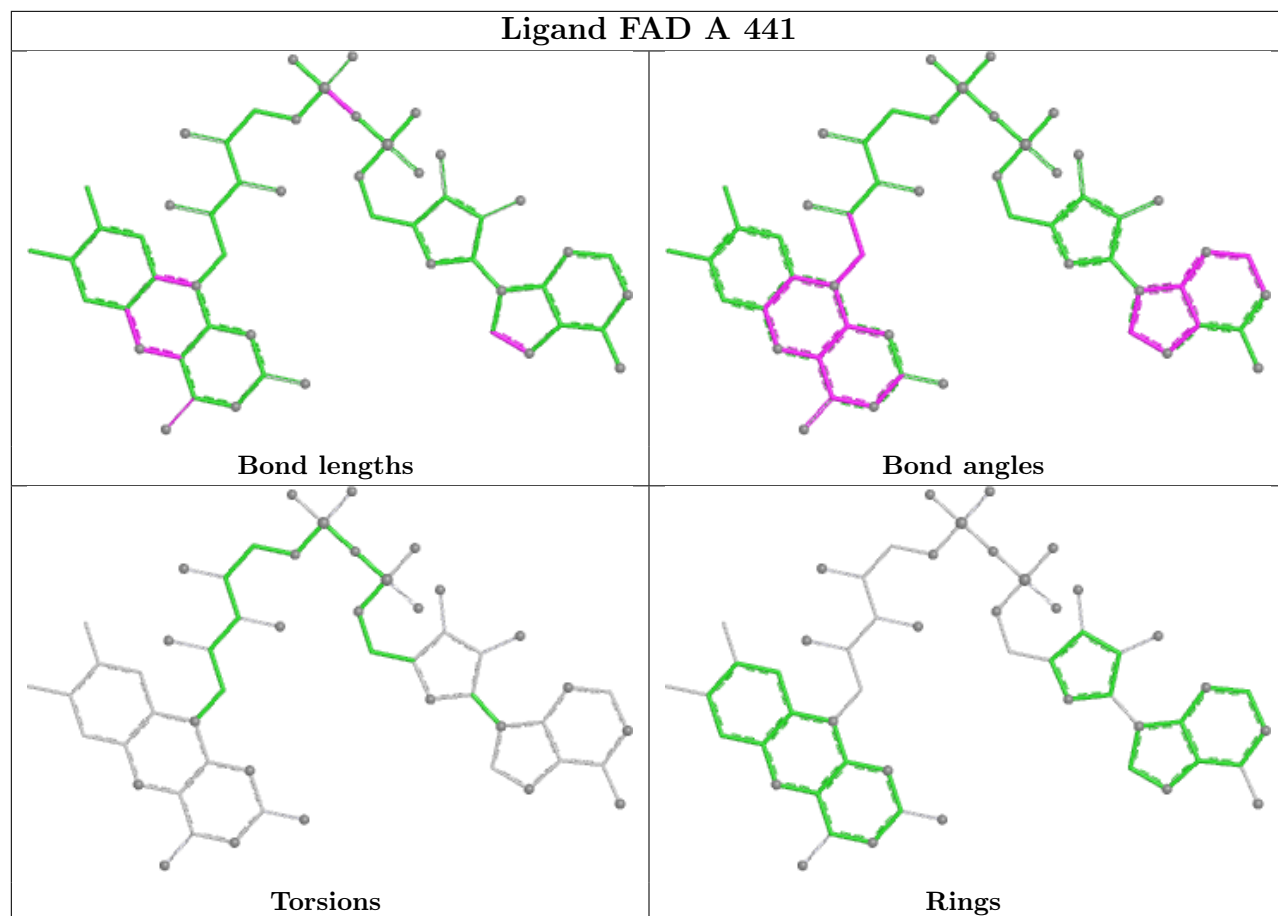


Ligand DCQ A 500

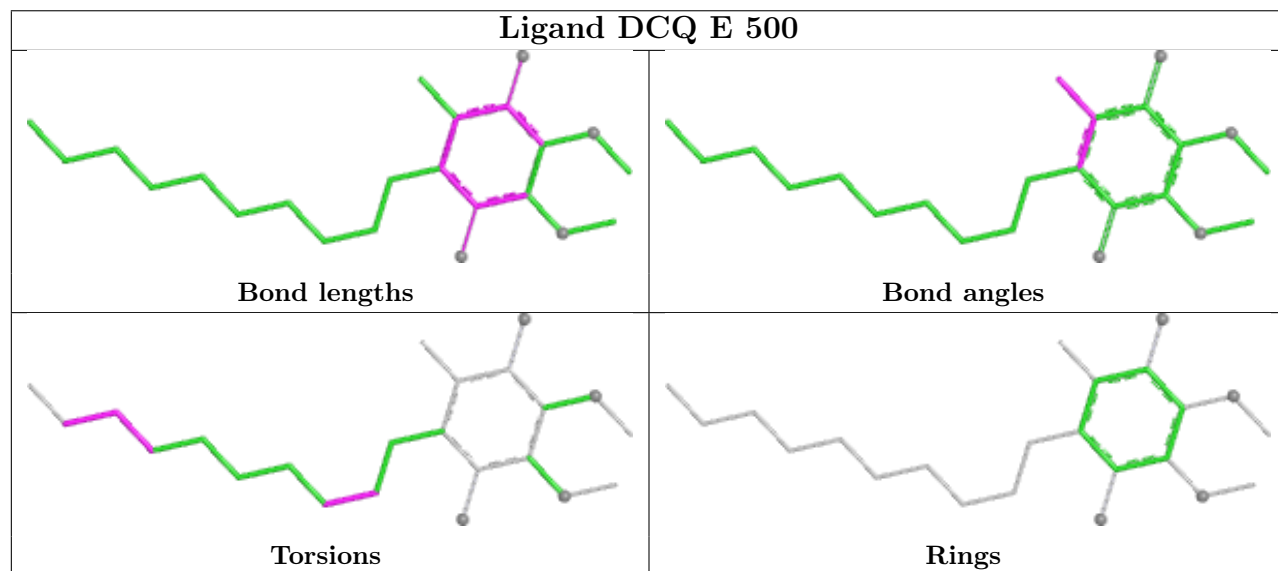


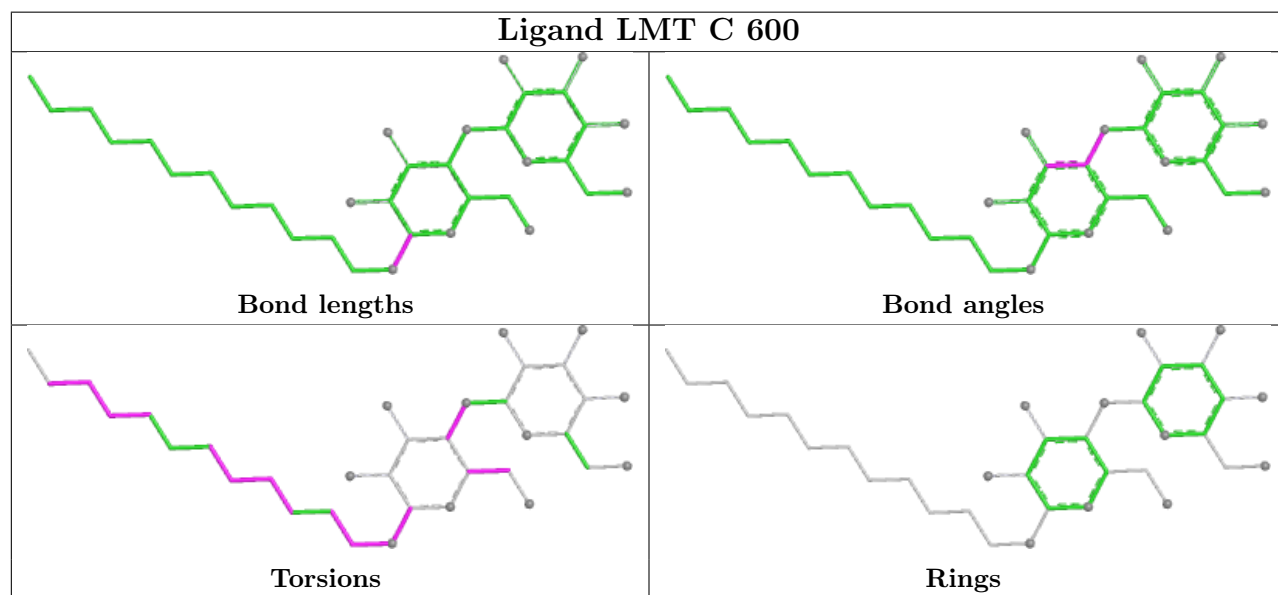
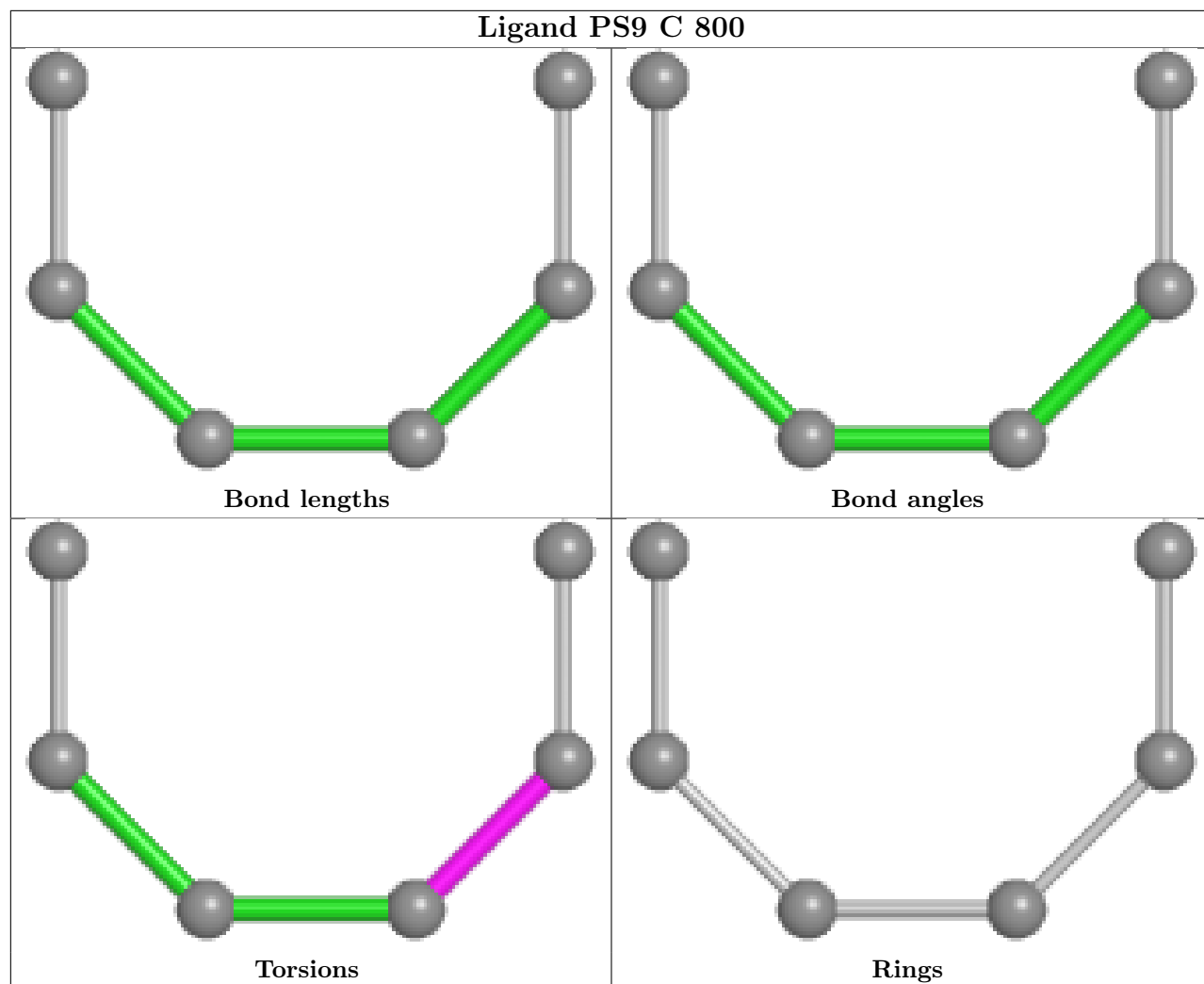


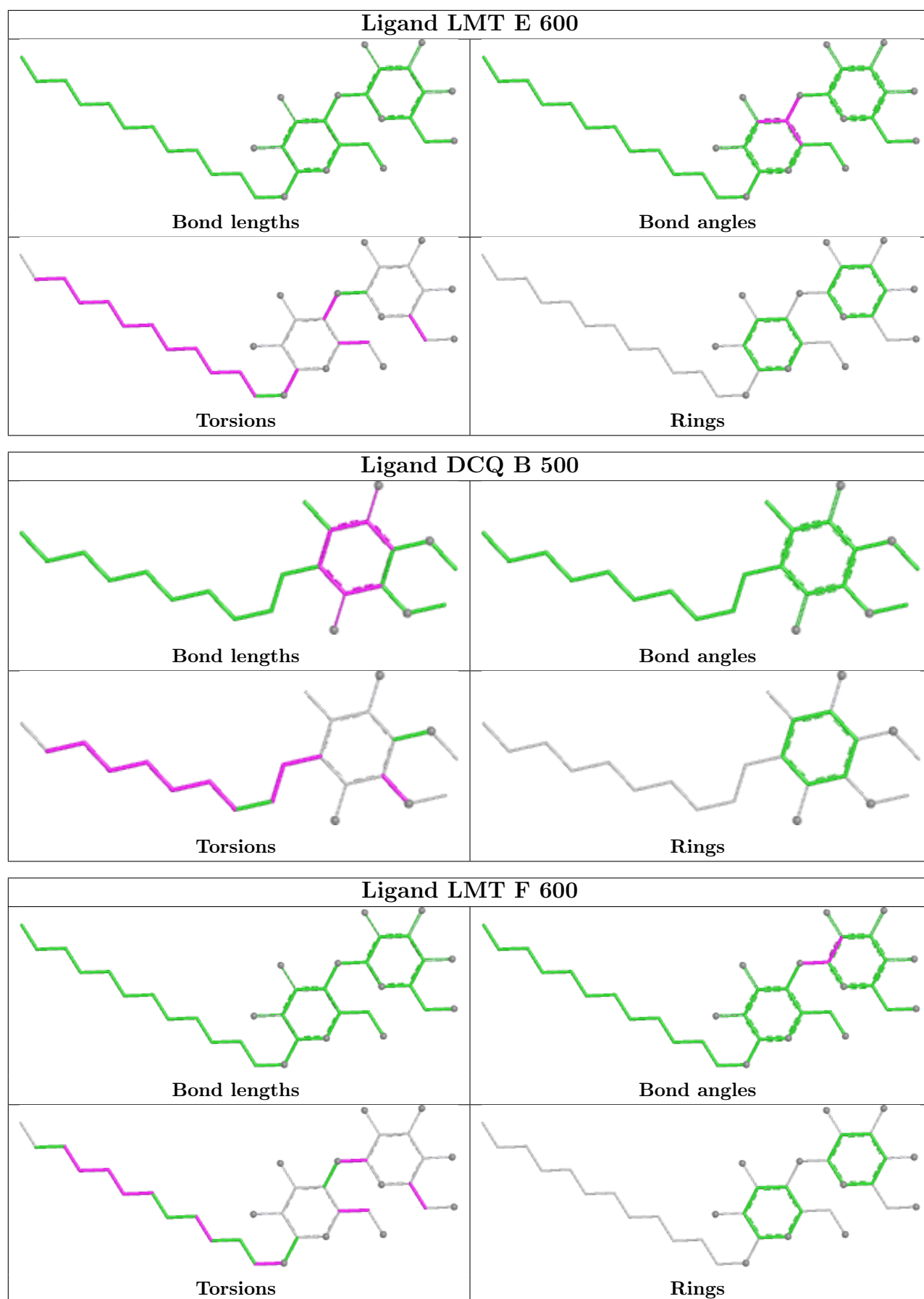
Ligand FAD A 441

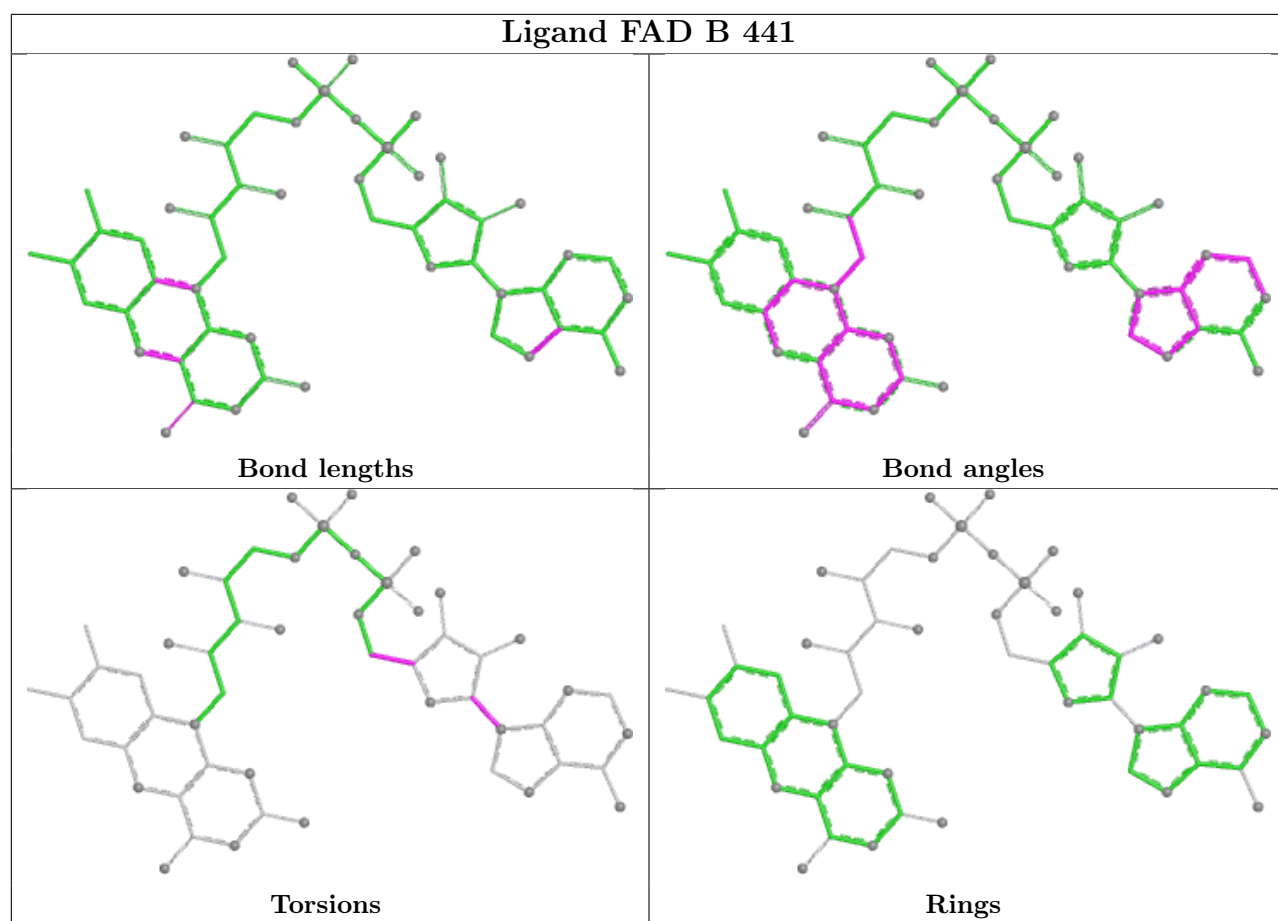


Ligand DCQ E 500

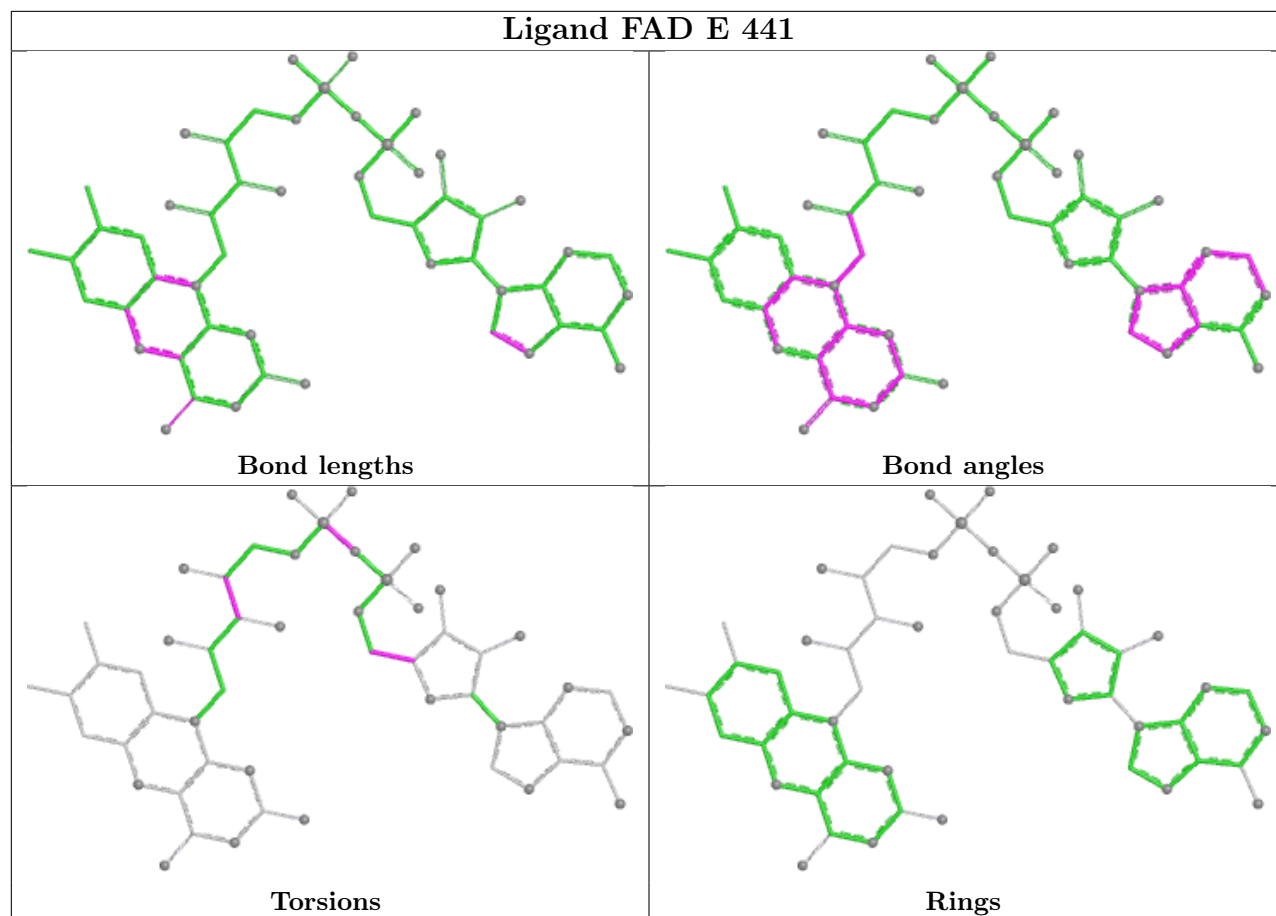




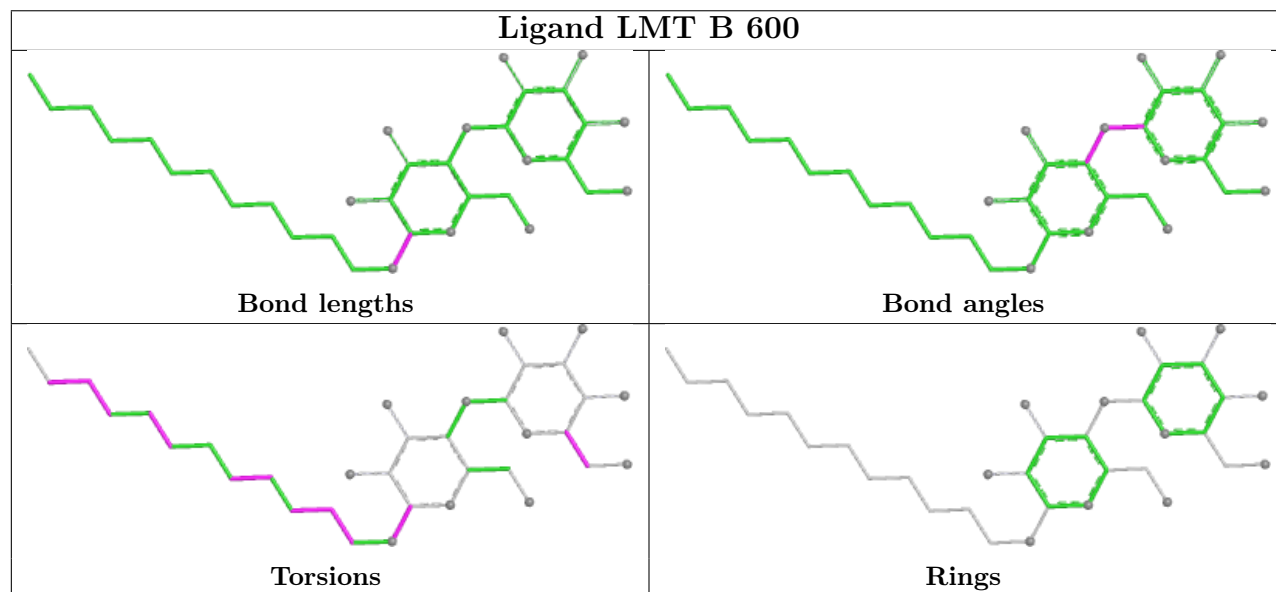


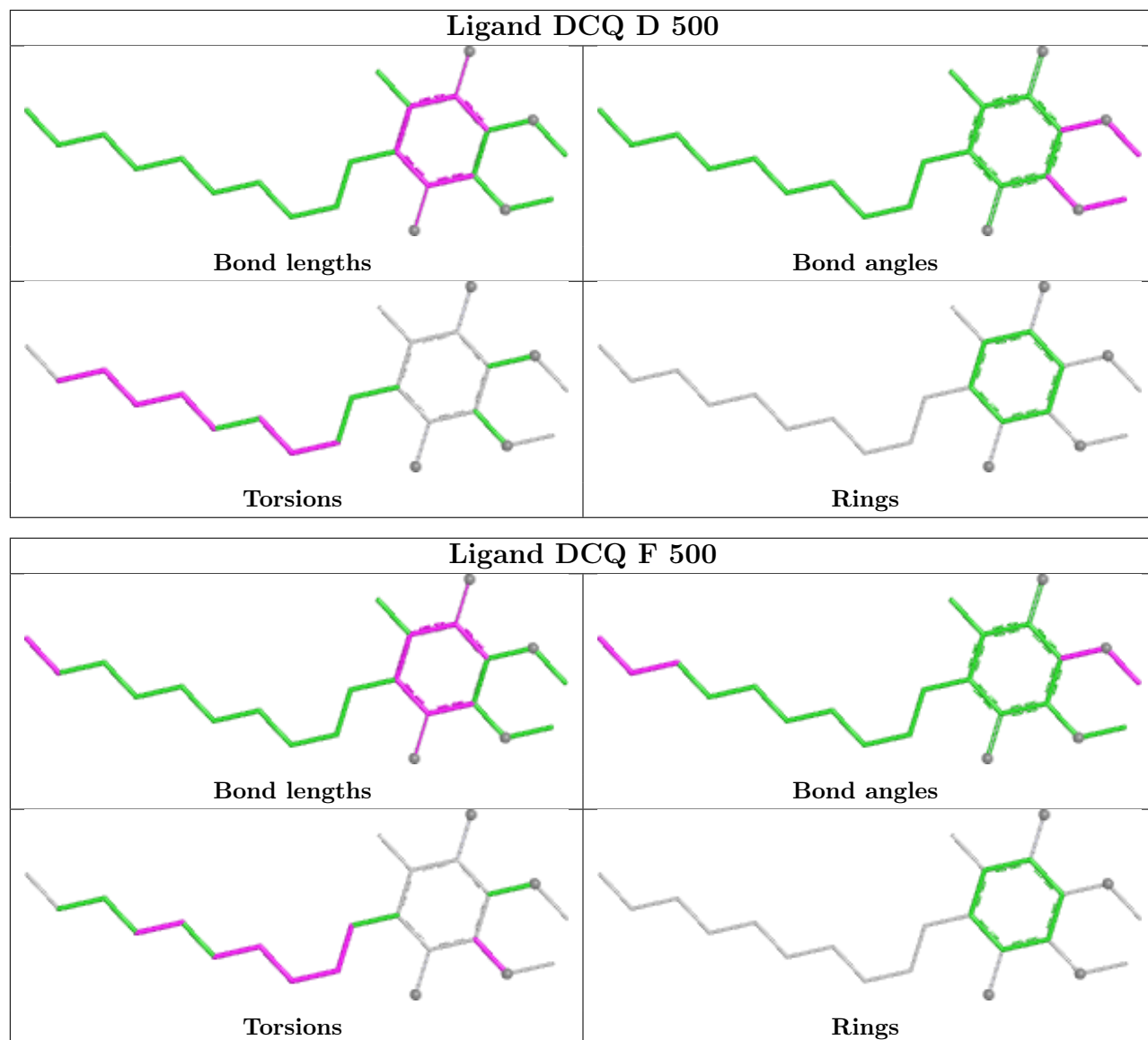


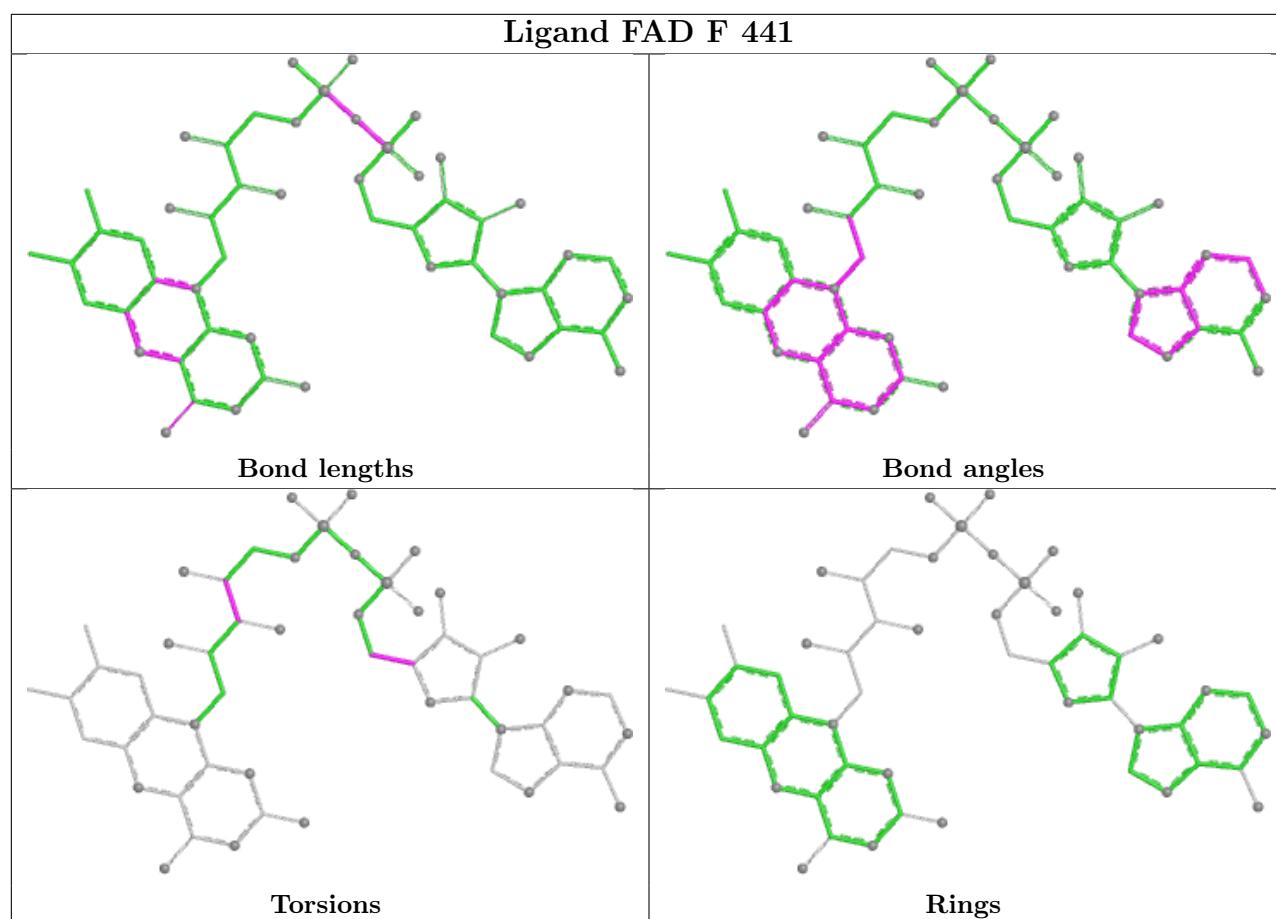
Ligand FAD E 441



Ligand LMT B 600







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	427/430 (99%)	0.50	16 (3%)	45 44	29, 35, 41, 46	1 (0%)
1	B	427/430 (99%)	0.47	12 (2%)	55 54	29, 35, 41, 47	1 (0%)
1	C	427/430 (99%)	0.50	17 (3%)	42 41	29, 35, 42, 49	1 (0%)
1	D	427/430 (99%)	0.57	15 (3%)	47 46	29, 35, 41, 44	1 (0%)
1	E	427/430 (99%)	0.46	16 (3%)	45 44	29, 35, 42, 45	1 (0%)
1	F	427/430 (99%)	0.45	16 (3%)	45 44	29, 35, 41, 48	1 (0%)
All	All	2562/2580 (99%)	0.49	92 (3%)	46 45	29, 35, 42, 49	6 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	430	CYS	6.3
1	F	430	CYS	4.9
1	A	430	CYS	4.4
1	B	430	CYS	4.4
1	A	229	ASP	4.0
1	C	27	ASP	4.0
1	E	430	CYS	3.9
1	C	2	ALA	3.9
1	D	238	GLY	3.8
1	E	74	ILE	3.5
1	D	430	CYS	3.3
1	C	141	ALA	3.2
1	A	138	GLU	3.2
1	A	237	ASN	3.2
1	E	93	GLY	3.1
1	E	27	ASP	3.1
1	D	175	GLY	3.1
1	C	114	GLU	3.0
1	C	264	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	141	ALA	2.9
1	B	27	ASP	2.8
1	A	178	TYR	2.8
1	C	142	ASN	2.7
1	C	92	SER	2.7
1	D	87	THR	2.7
1	D	236	LEU	2.7
1	E	92	SER	2.7
1	A	2	ALA	2.7
1	A	143	PRO	2.7
1	D	178	TYR	2.7
1	A	204	ARG	2.7
1	B	91	GLN	2.6
1	E	91	GLN	2.6
1	F	85	ALA	2.6
1	F	262	SER	2.6
1	D	230	LYS	2.6
1	A	381	PHE	2.5
1	B	381	PHE	2.5
1	B	420	LYS	2.5
1	A	144	GLY	2.5
1	F	97	GLU	2.5
1	C	381	PHE	2.4
1	A	142	ASN	2.4
1	C	374	MET	2.4
1	E	204	ARG	2.4
1	B	113	ALA	2.4
1	E	87	THR	2.4
1	E	118	GLU	2.3
1	A	236	LEU	2.3
1	E	227	GLU	2.3
1	E	85	ALA	2.3
1	B	237	ASN	2.3
1	C	205	LEU	2.3
1	B	226	ILE	2.3
1	A	131	GLU	2.3
1	B	131	GLU	2.3
1	C	204	ARG	2.3
1	B	239	ASN	2.3
1	C	417	GLU	2.2
1	F	91	GLN	2.2
1	D	239	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	229	ASP	2.2
1	F	256	GLY	2.2
1	E	414	HIS	2.2
1	F	92	SER	2.2
1	D	285	THR	2.2
1	F	374	MET	2.2
1	F	422	CYS	2.2
1	B	35	ASP	2.2
1	E	81	ILE	2.2
1	C	131	GLU	2.2
1	D	414	HIS	2.2
1	D	237	ASN	2.2
1	F	292	VAL	2.1
1	B	138	GLU	2.1
1	F	87	THR	2.1
1	D	423	GLU	2.1
1	C	91	GLN	2.1
1	F	381	PHE	2.1
1	F	56	GLU	2.1
1	E	84	ASP	2.1
1	E	89	THR	2.1
1	A	173	LYS	2.1
1	C	212	GLU	2.0
1	F	131	GLU	2.0
1	D	205	LEU	2.0
1	F	27	ASP	2.0
1	A	287	LYS	2.0
1	C	95	LYS	2.0
1	D	29	LYS	2.0
1	A	240	THR	2.0
1	E	264	GLY	2.0

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

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
1	CSS	D	347[A]	6/8	0.80	0.14	44,44,44,47	1
1	CSS	D	347[B]	7/8	0.80	0.14	44,44,44,45	2

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSS	E	347[A]	6/8	0.80	0.13	44,44,44,47	1
1	CSS	E	347[B]	6/8	0.80	0.13	44,44,44,45	1
1	CSS	A	347[A]	6/8	0.82	0.12	45,45,46,49	1
1	CSS	A	347[B]	6/8	0.82	0.12	45,45,46,47	1
1	CSS	F	347[A]	6/8	0.84	0.10	44,44,45,48	1
1	CSS	F	347[B]	6/8	0.84	0.10	44,44,45,45	1
1	CSS	C	347[A]	6/8	0.87	0.10	43,43,44,47	1
1	CSS	C	347[B]	6/8	0.87	0.10	43,43,43,44	1
1	CSS	E	156[A]	6/8	0.90	0.09	35,36,37,39	1
1	CSS	E	156[B]	7/8	0.90	0.09	35,36,38,38	2
1	CSS	B	347[A]	6/8	0.90	0.09	43,44,44,47	1
1	CSS	B	347[B]	7/8	0.90	0.09	43,44,44,45	2
1	CSS	C	156[A]	6/8	0.90	0.09	35,36,36,40	1
1	CSS	C	156[B]	7/8	0.90	0.09	35,35,36,37	2
1	CSS	F	156[A]	6/8	0.92	0.08	35,36,37,39	1
1	CSS	F	156[B]	7/8	0.92	0.08	35,36,37,37	2
1	CSS	B	156[A]	6/8	0.92	0.08	35,35,36,39	1
1	CSS	B	156[B]	7/8	0.92	0.08	33,35,36,36	2
1	CSS	A	156[A]	6/8	0.93	0.10	36,36,37,40	1
1	CSS	A	156[B]	7/8	0.93	0.10	36,36,38,38	2
1	CSS	D	156[A]	6/8	0.95	0.07	35,35,36,37	1
1	CSS	D	156[B]	7/8	0.95	0.07	35,35,36,36	2

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PS9	B	802[A]	2/8	0.30	0.49	41,41,41,41	2
6	PS9	B	802[B]	2/8	0.30	0.49	39,39,39,41	2
7	SO4	A	435	5/5	0.44	0.28	38,39,39,39	5
7	SO4	C	431	5/5	0.46	0.38	39,39,39,39	5
7	SO4	D	434	5/5	0.49	0.24	54,54,54,55	5
7	SO4	D	431	5/5	0.52	0.43	38,38,38,38	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	PS9	E	800	8/8	0.52	0.24	42,43,43,43	8
6	PS9	A	800	8/8	0.56	0.22	40,41,41,42	8
6	PS9	C	800	6/8	0.58	0.26	39,40,42,42	6
6	PS9	F	800	8/8	0.59	0.24	39,40,41,41	8
6	PS9	D	800	2/8	0.59	0.22	33,33,33,34	2
7	SO4	B	433	5/5	0.59	0.29	51,51,52,52	5
4	LMT	E	600	35/35	0.60	0.31	53,55,58,58	35
4	LMT	C	600	35/35	0.61	0.29	53,57,59,60	35
7	SO4	B	431	5/5	0.63	0.38	37,37,38,38	5
7	SO4	E	433	5/5	0.63	0.23	56,56,56,56	5
4	LMT	D	600	35/35	0.64	0.29	47,51,53,54	35
7	SO4	D	433	5/5	0.65	0.29	57,57,57,58	5
4	LMT	B	600	35/35	0.65	0.27	49,50,52,53	35
3	DCQ	B	500	23/23	0.65	0.25	43,48,48,48	23
3	DCQ	D	500	23/23	0.67	0.25	49,50,51,51	23
3	DCQ	A	500	23/23	0.67	0.28	46,51,51,51	23
4	LMT	A	600	35/35	0.68	0.26	50,55,57,58	35
7	SO4	F	434	5/5	0.69	0.17	54,54,55,55	5
7	SO4	A	434	5/5	0.71	0.16	47,47,48,48	5
4	LMT	F	600	35/35	0.71	0.24	44,50,54,55	35
7	SO4	C	434	5/5	0.71	0.16	60,60,61,61	5
6	PS9	B	800	1/8	0.72	0.42	32,32,32,32	1
3	DCQ	F	500	23/23	0.72	0.21	52,53,53,54	23
6	PS9	D	802	1/8	0.72	0.45	44,44,44,44	1
7	SO4	F	431	5/5	0.72	0.24	33,34,34,34	5
3	DCQ	C	500	23/23	0.72	0.20	43,46,47,47	23
7	SO4	F	433	5/5	0.74	0.23	39,41,41,41	5
3	DCQ	E	500	23/23	0.74	0.25	47,48,48,48	23
7	SO4	E	434	5/5	0.77	0.14	42,43,43,43	5
7	SO4	B	434	5/5	0.78	0.17	44,45,45,46	5
7	SO4	A	431	5/5	0.79	0.27	39,39,39,39	5
7	SO4	C	433	5/5	0.80	0.23	36,37,37,38	5
7	SO4	F	432	5/5	0.82	0.18	41,42,42,42	5
7	SO4	D	432	5/5	0.85	0.17	34,34,34,35	5
7	SO4	A	433	5/5	0.85	0.22	29,31,32,32	5
7	SO4	C	432	5/5	0.85	0.20	35,35,36,36	5
5	H2S	F	700	1/1	0.93	0.09	31,31,31,31	1
7	SO4	A	432	5/5	0.93	0.11	30,31,31,31	5
7	SO4	E	432	5/5	0.93	0.14	36,36,36,37	5
5	H2S	B	700	1/1	0.94	0.06	28,28,28,28	1
5	H2S	C	700	1/1	0.94	0.07	31,31,31,31	1
5	H2S	E	700	1/1	0.94	0.06	32,32,32,32	1

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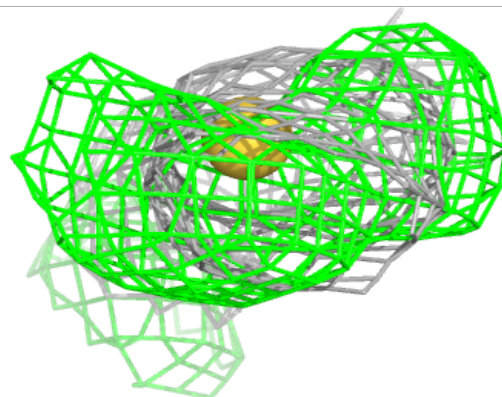
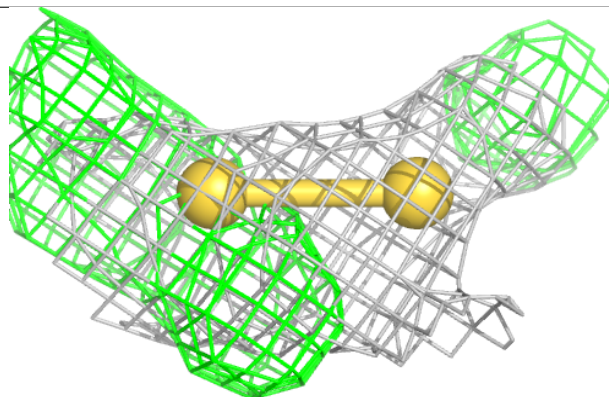
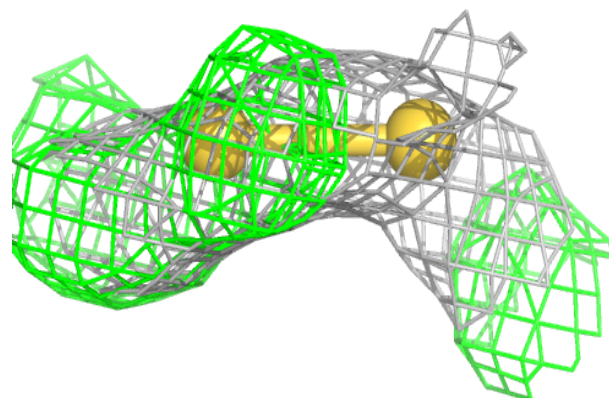
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	C	441	53/53	0.94	0.07	21,27,30,31	0
2	FAD	F	441	53/53	0.95	0.07	24,28,34,34	0
2	FAD	D	441	53/53	0.95	0.07	23,32,33,33	0
7	SO4	B	432	5/5	0.95	0.14	25,26,26,27	5
2	FAD	E	441	53/53	0.95	0.07	26,29,37,37	0
5	H2S	D	700	1/1	0.96	0.05	33,33,33,33	1
2	FAD	A	441	53/53	0.96	0.06	20,23,26,26	0
2	FAD	B	441	53/53	0.96	0.06	22,26,28,29	0
5	H2S	A	700	1/1	0.98	0.04	28,28,28,28	1

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.

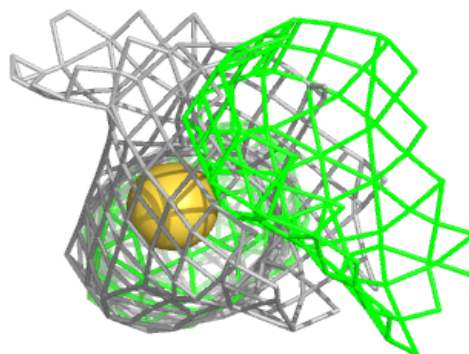
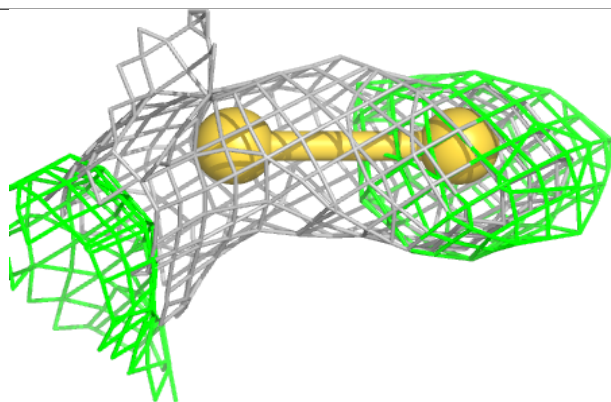
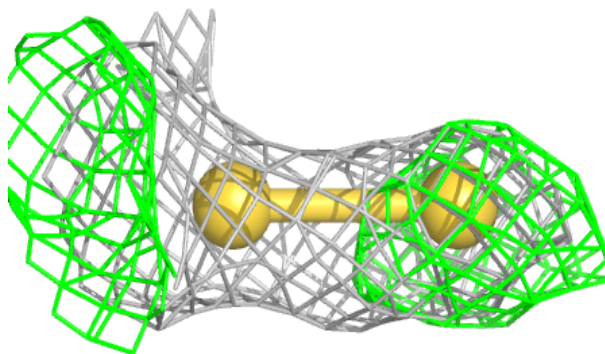
Electron density around PS9 B 802 (A):

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



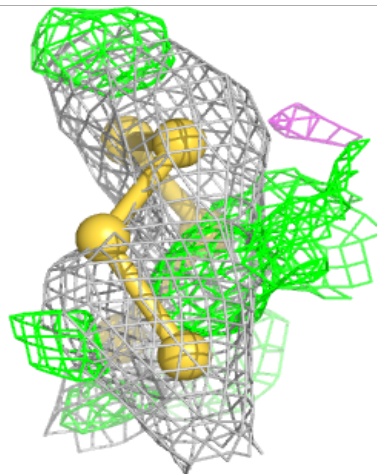
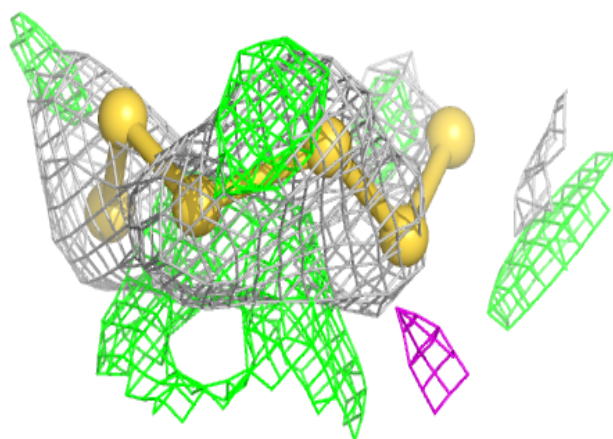
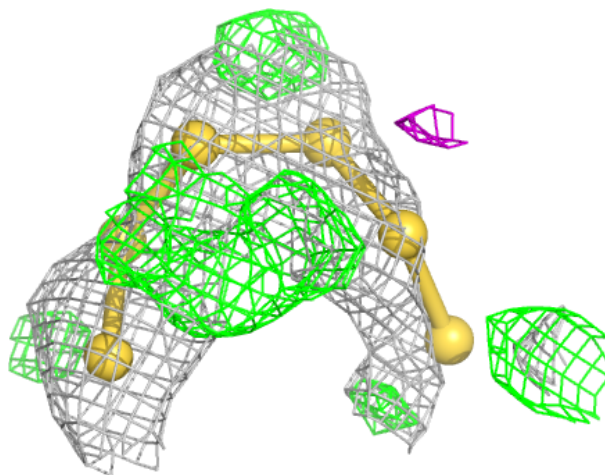
Electron density around PS9 B 802 (B):

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



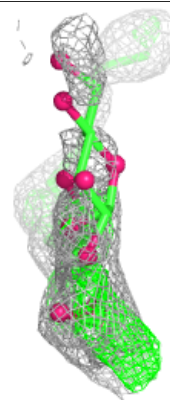
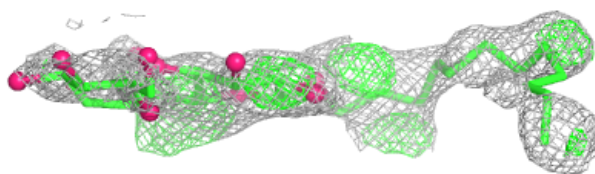
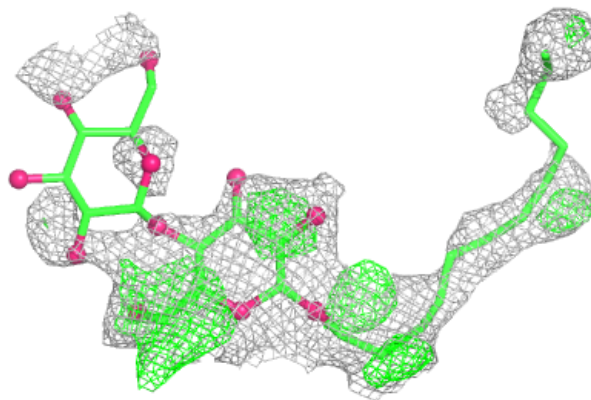
Electron density around PS9 C 800:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

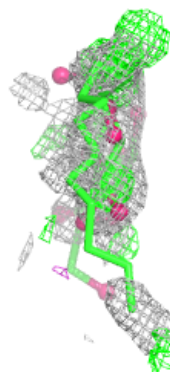
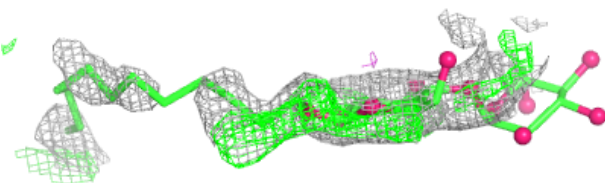
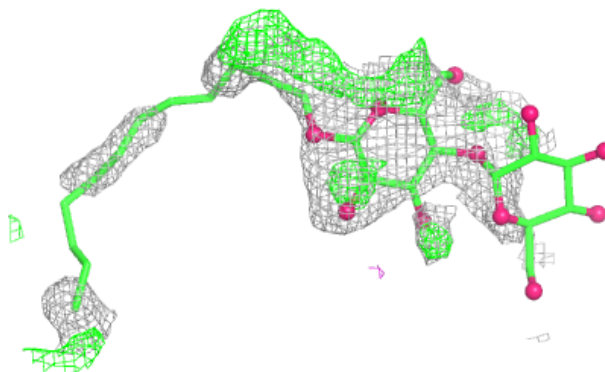


Electron density around LMT E 600:

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

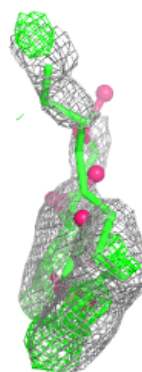
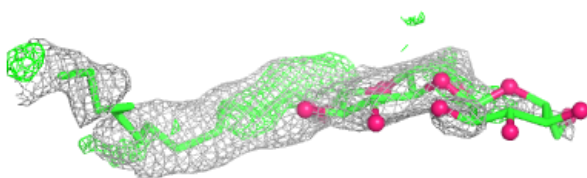
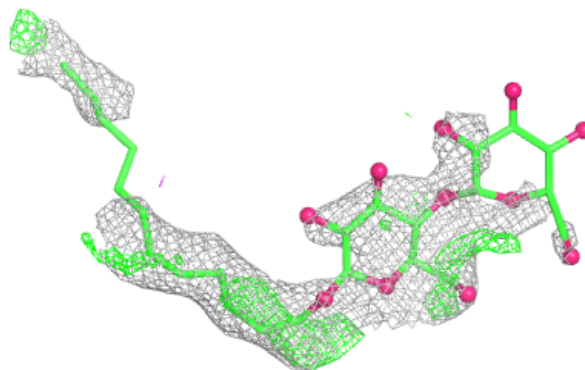
**Electron density around LMT C 600:**

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

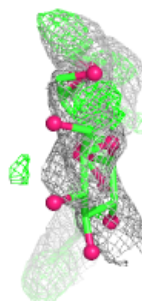
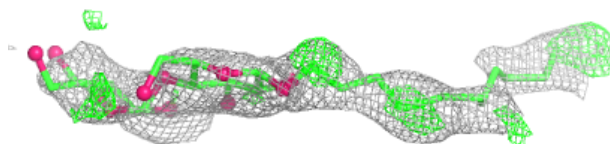
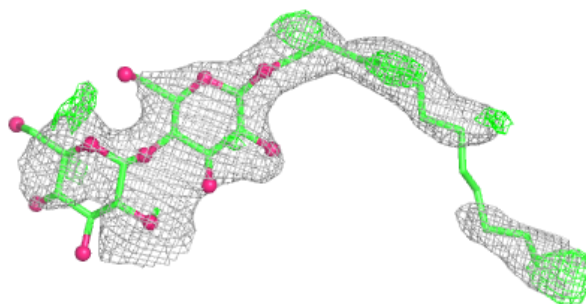


Electron density around LMT D 600:

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

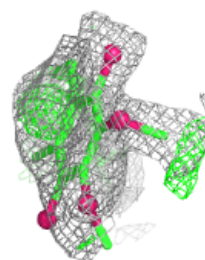
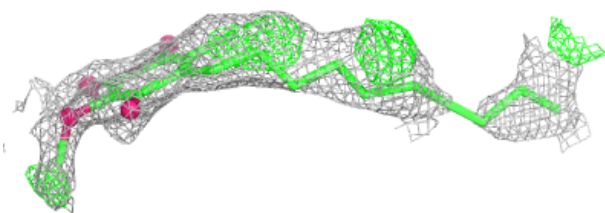
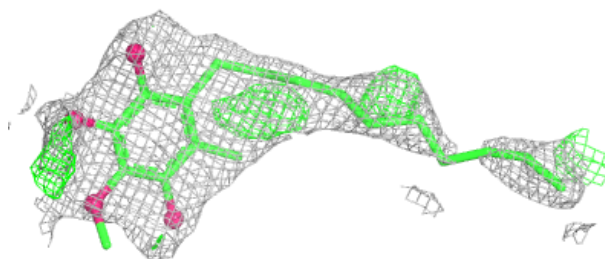
**Electron density around LMT B 600:**

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

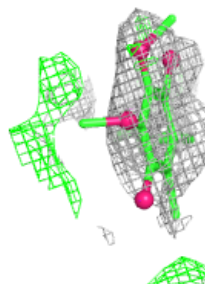
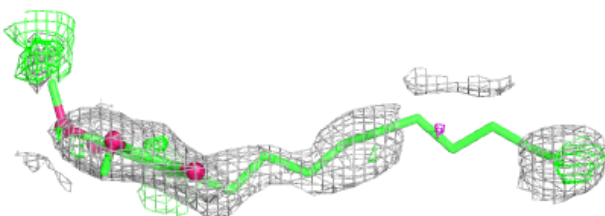
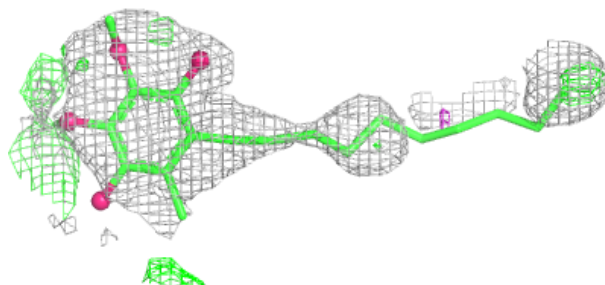


Electron density around DCQ B 500:

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

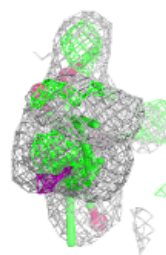
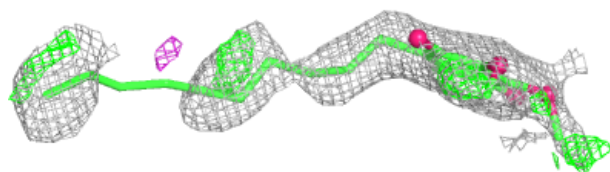
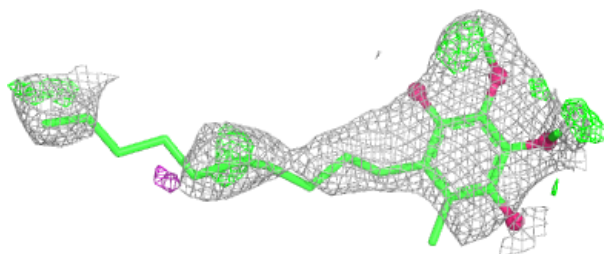
**Electron density around DCQ D 500:**

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

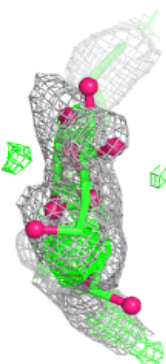
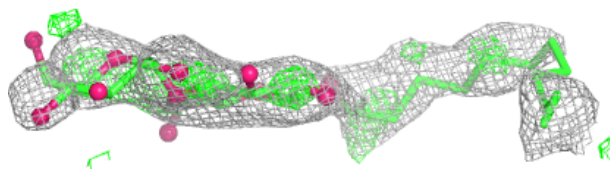
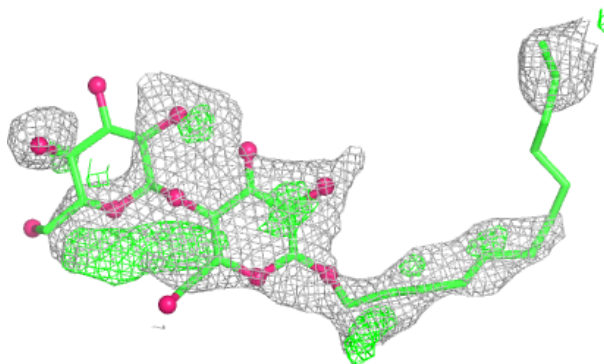


Electron density around DCQ A 500:

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

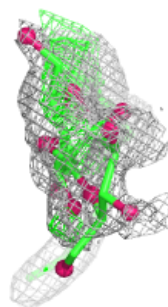
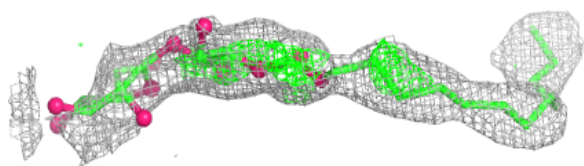
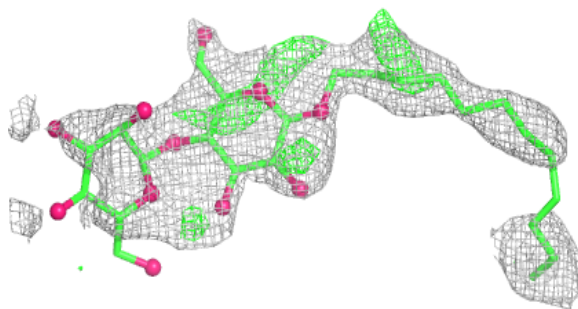
**Electron density around LMT A 600:**

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



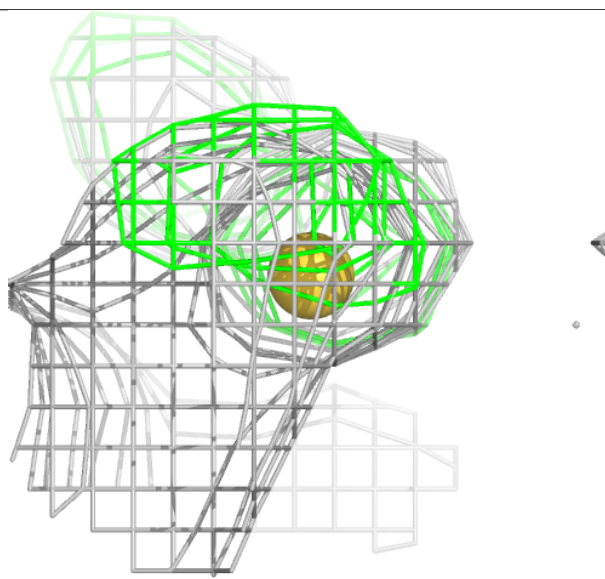
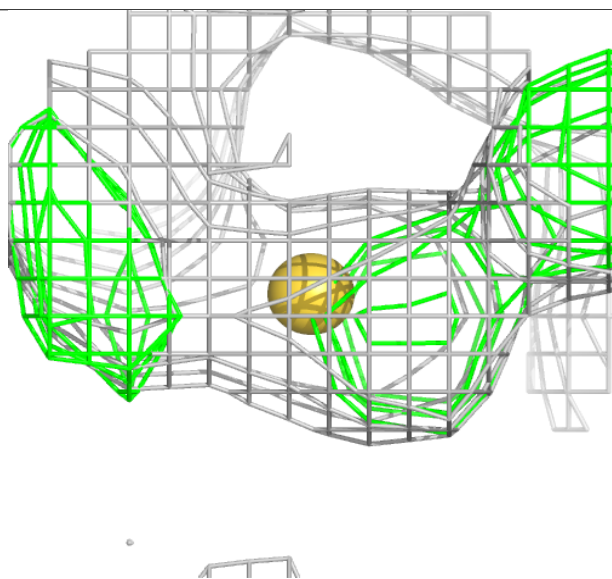
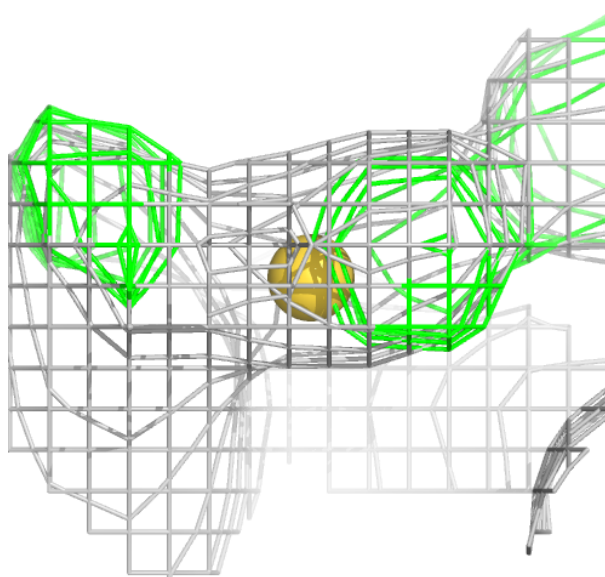
Electron density around LMT F 600:

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



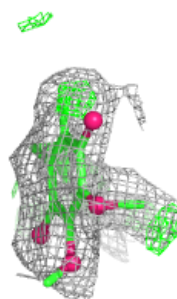
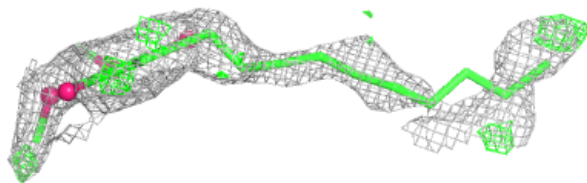
Electron density around PS9 B 800:

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



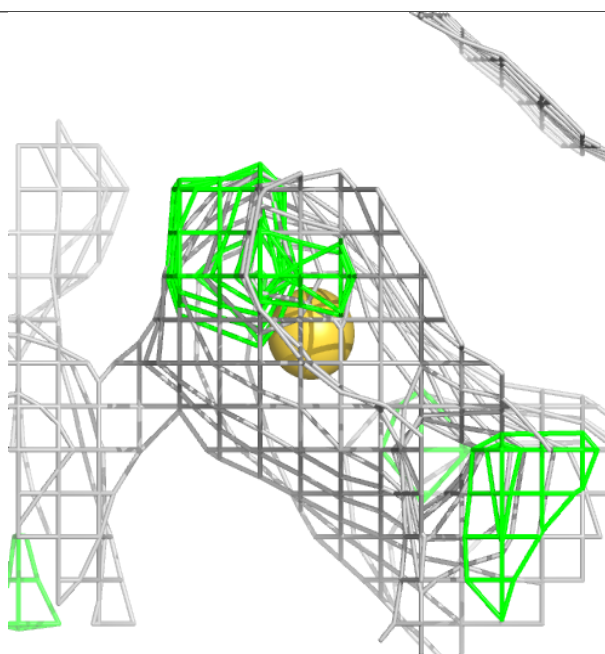
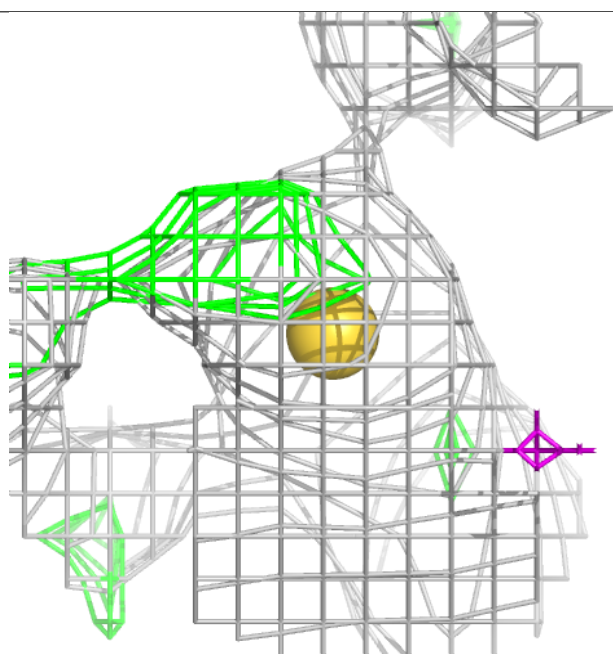
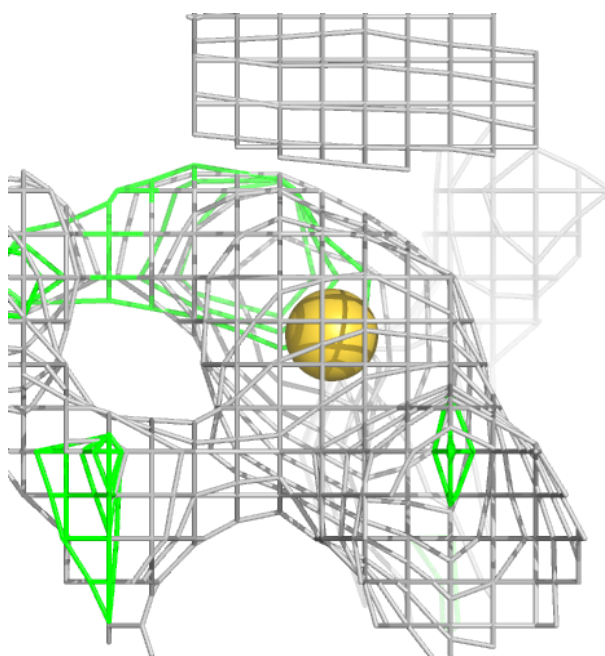
Electron density around DCQ F 500:

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



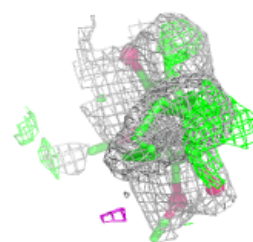
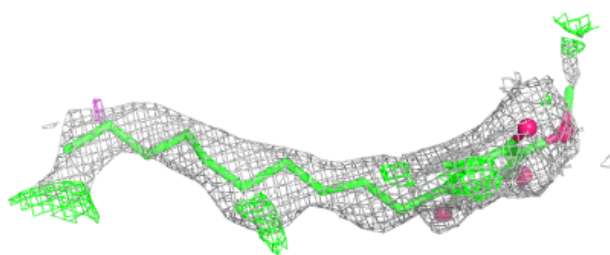
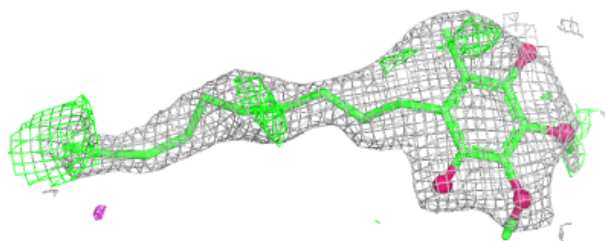
Electron density around PS9 D 802:

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

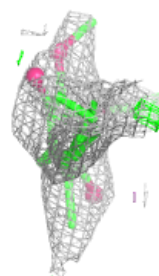
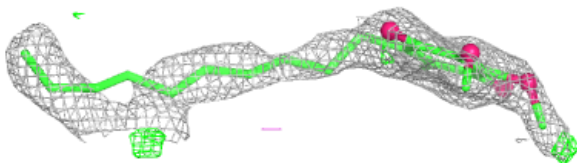
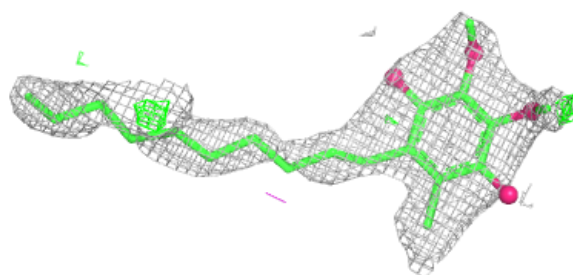


Electron density around DCQ C 500:

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

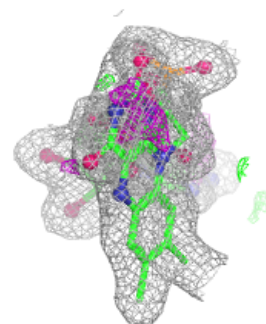
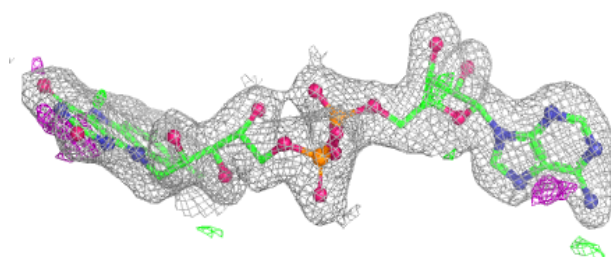
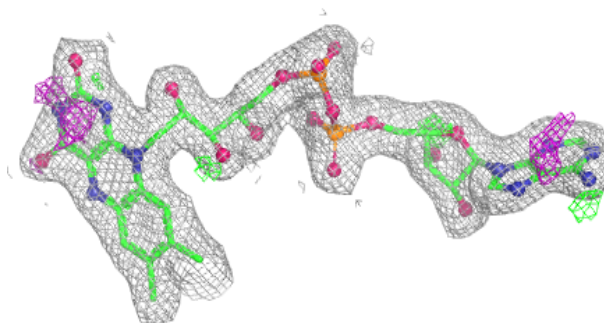
**Electron density around DCQ E 500:**

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

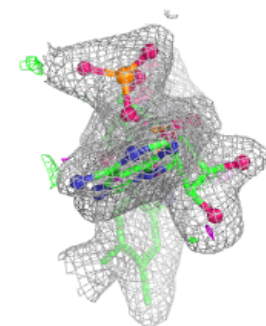
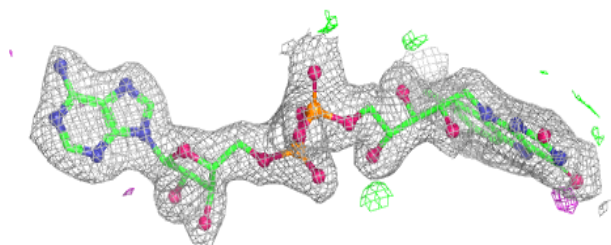
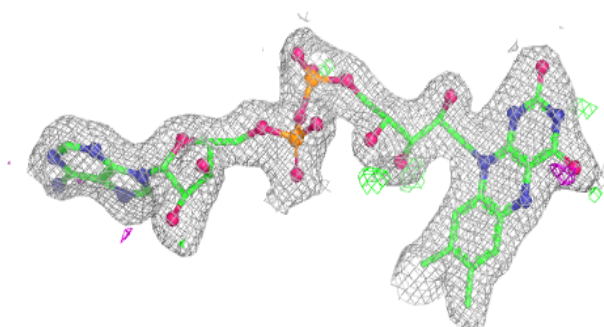


Electron density around FAD C 441:

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

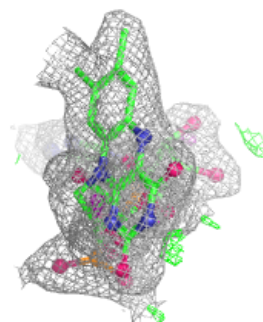
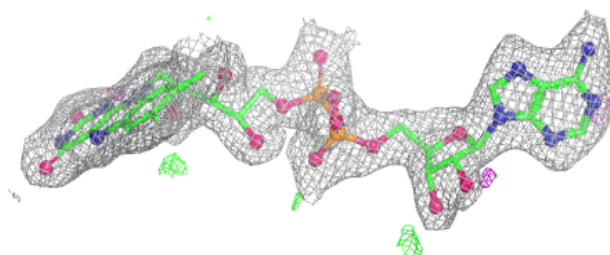
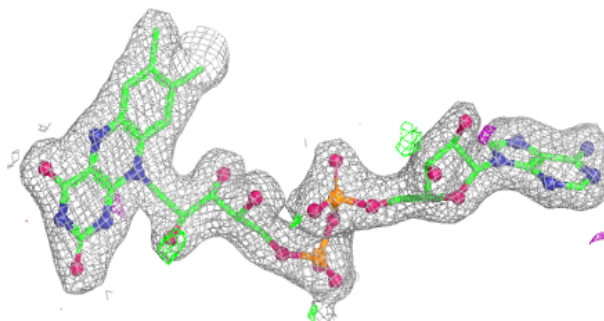
**Electron density around FAD F 441:**

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

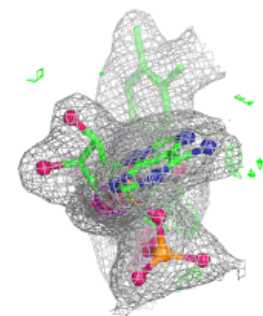
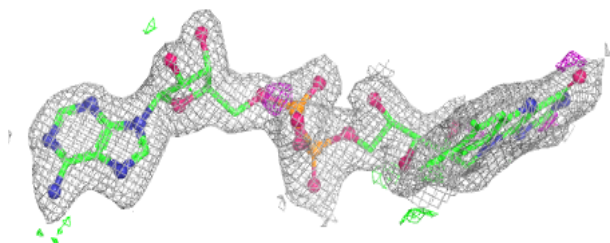
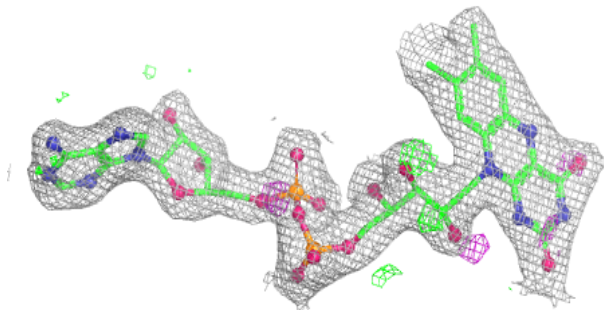


Electron density around FAD D 441:

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

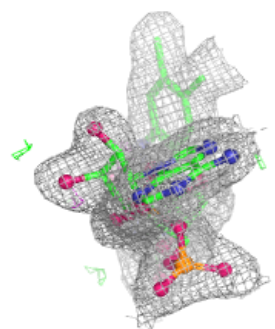
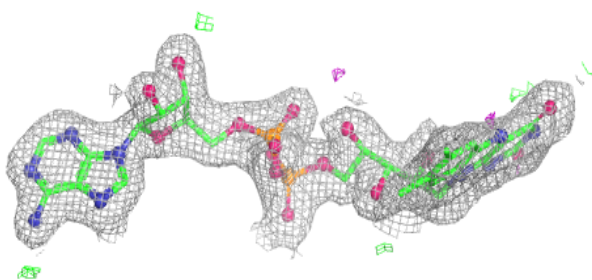
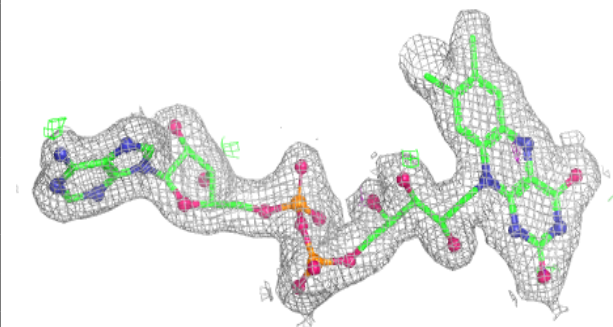
**Electron density around FAD E 441:**

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

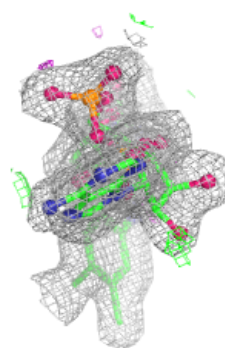
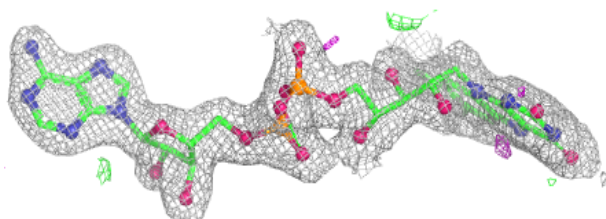
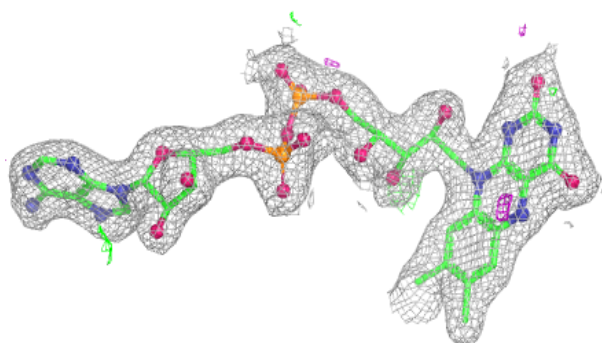


Electron density around FAD A 441:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.