



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:37 AM UTC

PDB ID : 2BS2 / pdb_00002bs2
Title : QUINOL:FUMARATE REDUCTASE FROM WOLINELLA SUCCINO-
GENES
Authors : Lancaster, C.R.D.
Deposited on : 2005-05-14
Resolution : 1.78 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

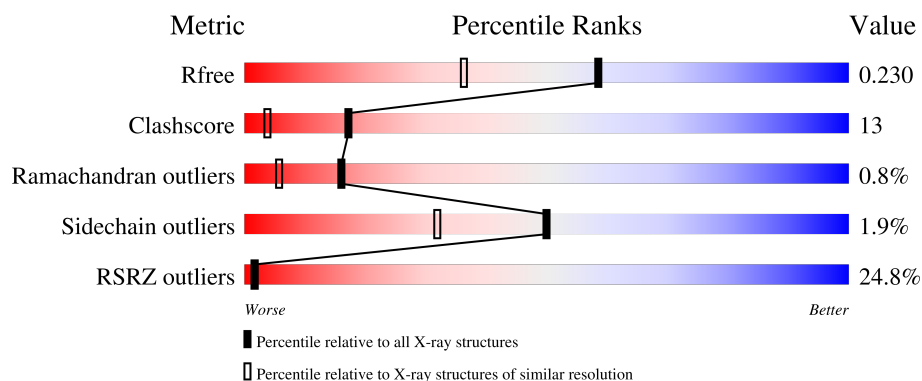
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	660	21% 75% 22% ..
1	D	660	23% 74% 24% ..
2	B	241	10% 78% 19% .
2	E	241	15% 78% 20% .
3	C	256	45% 73% 24% .

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Mol	Chain	Length	Quality of chain
3	F	256	41% 73% 24%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19666 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 QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	27	5	1
			5145	3219	927	967	32			
1	D	656	Total	C	N	O	S	32	3	1
			5125	3207	921	965	32			

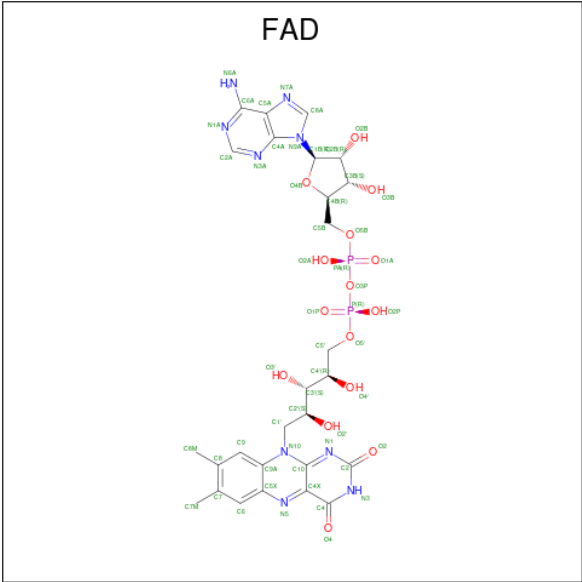
- Molecule 2 is a protein called QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	240	Total	C	N	O	S	6	1	1
			1902	1199	324	355	24			
2	E	240	Total	C	N	O	S	6	1	1
			1902	1199	324	355	24			

- Molecule 3 is a protein called QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C.

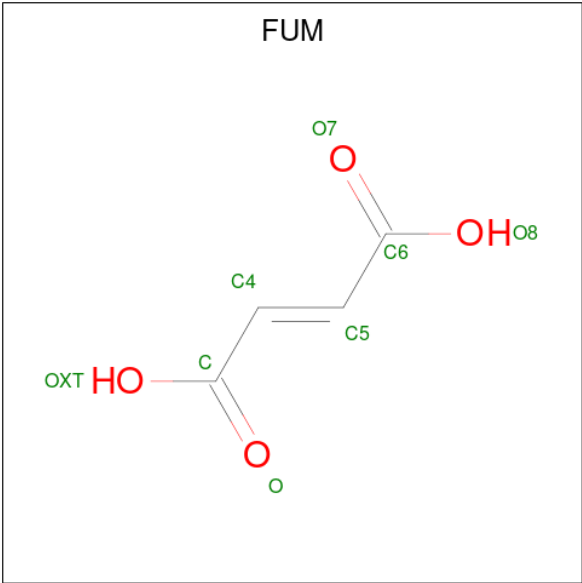
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	255	Total	C	N	O	S	16	2	1
			2099	1398	336	351	14			
3	F	255	Total	C	N	O	S	12	2	1
			2099	1398	336	351	14			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

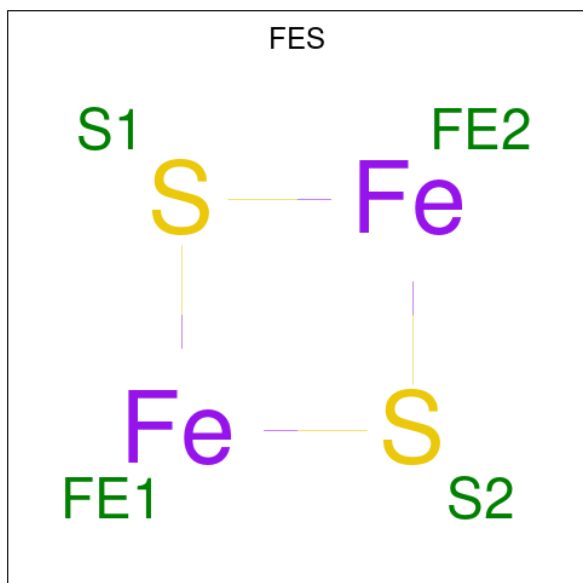
- Molecule 5 is FUMARIC ACID (CCD ID: FUM) (formula: C₄H₄O₄).



- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

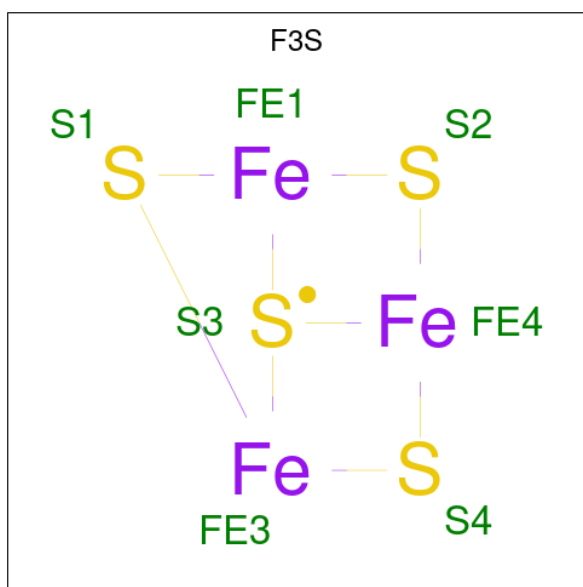
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



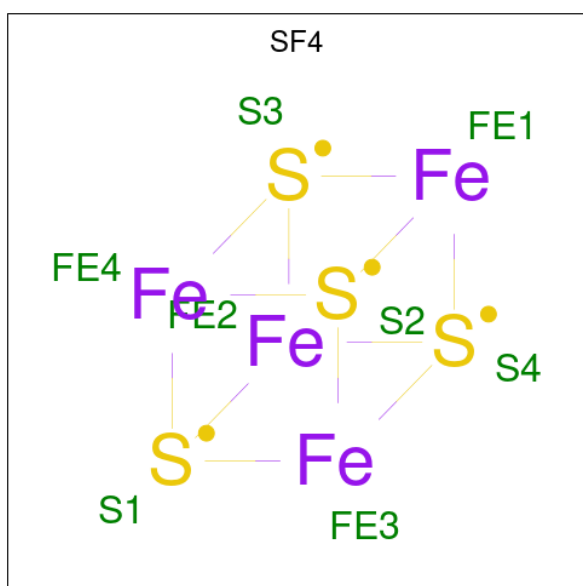
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



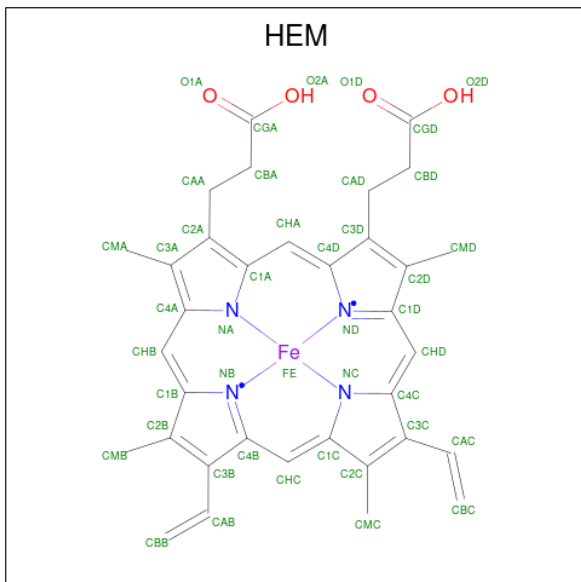
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	E	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



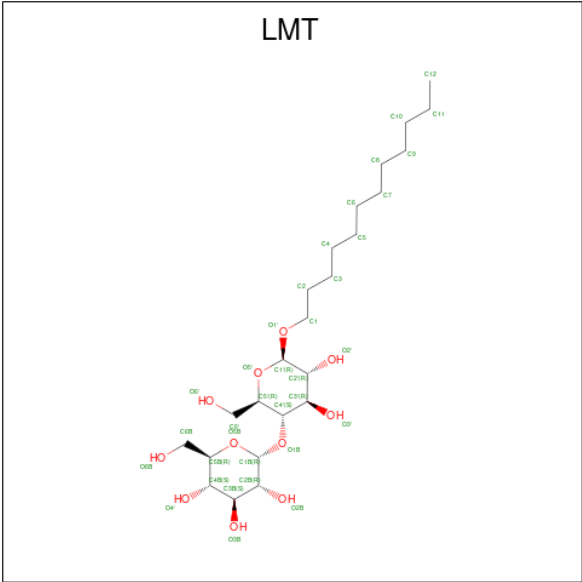
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	E	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 11 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	16	0
			35	24	11		
11	F	1	Total	C	O	16	0
			35	24	11		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	273	Total	O	1	0
			273	273		
12	B	155	Total	O	0	0
			155	155		
12	C	55	Total	O	0	0
			55	55		
12	D	287	Total	O	4	0
			287	287		
12	E	164	Total	O	0	0
			164	164		
12	F	56	Total	O	0	0
			56	56		

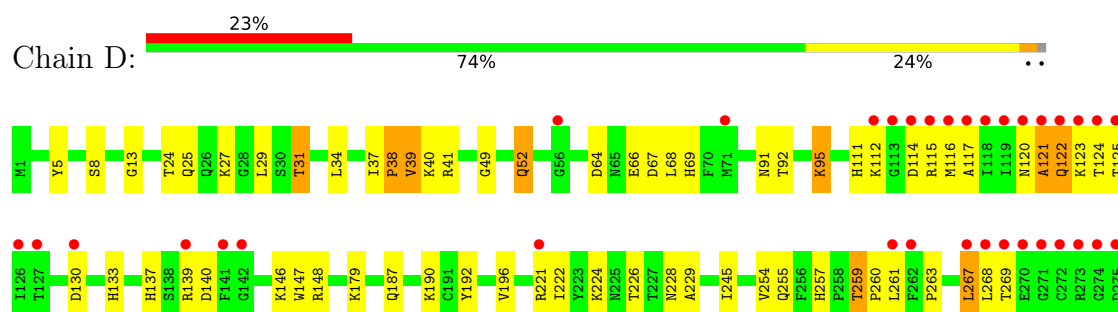
3 Residue-property plots

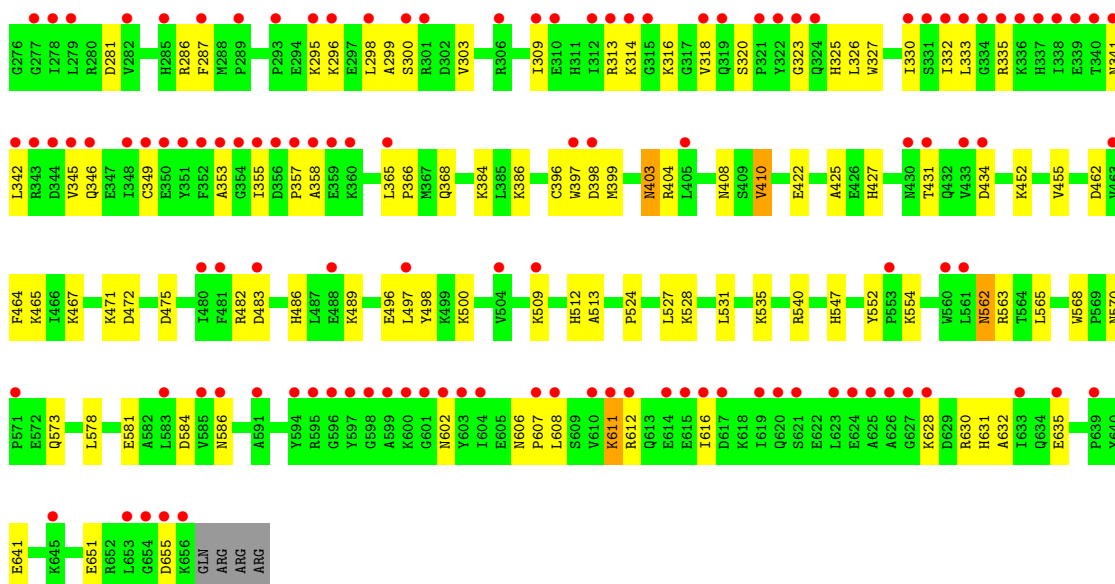
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

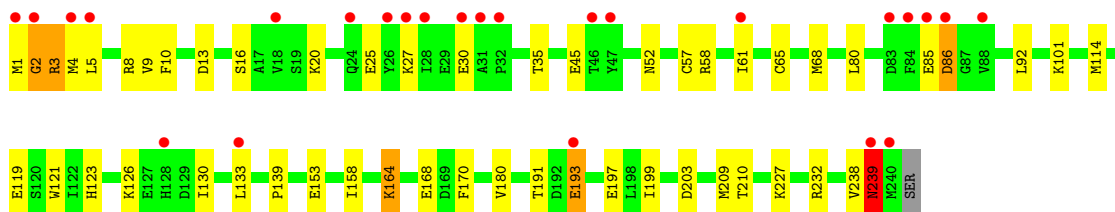
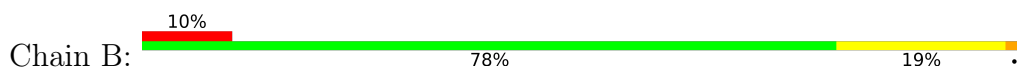


• Molecule 1: QUINOL-FUMARATE REDUCTASE FLAVOPROTEIN SUBUNIT A

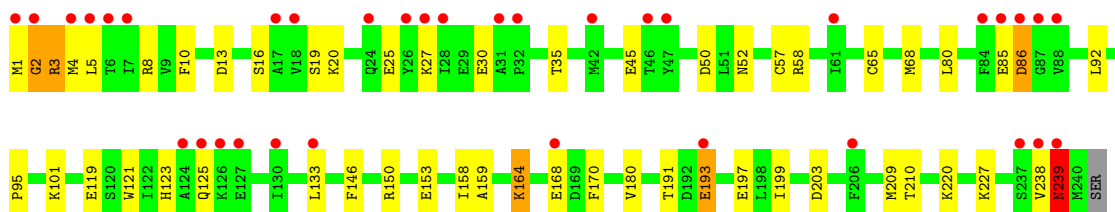
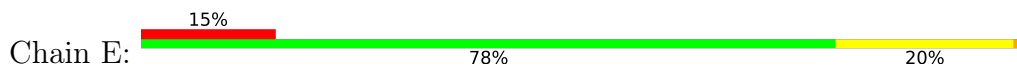




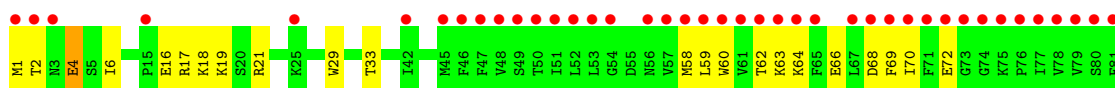
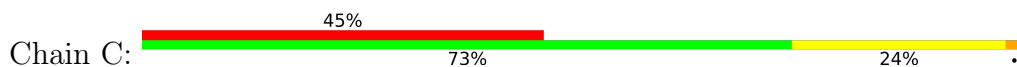
- Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B

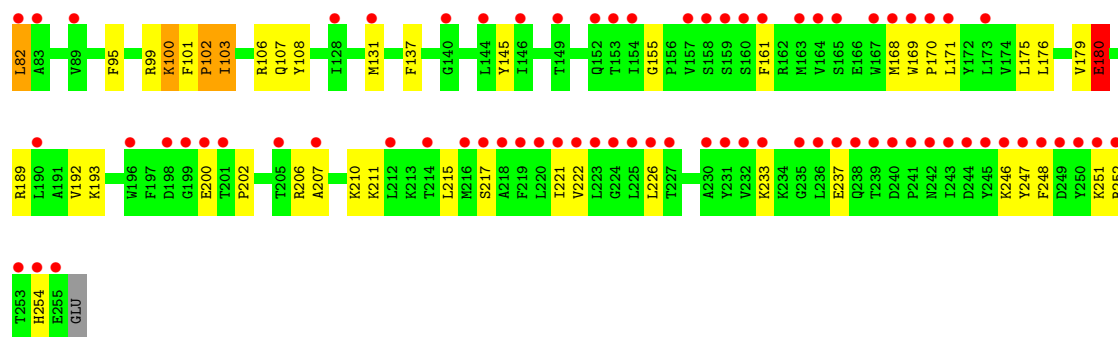


- Molecule 2: QUINOL-FUMARATE REDUCTASE IRON-SULFUR SUBUNIT B

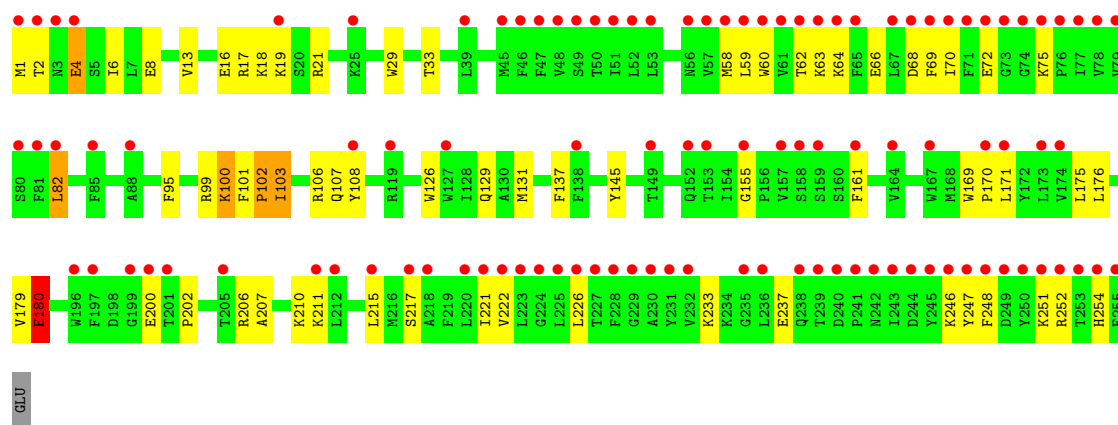
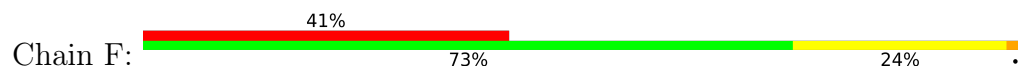


● Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C





• Molecule 3: QUINOL-FUMARATE REDUCTASE DIHEME CYTOCHROME B SUBUNIT C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.10Å 188.77Å 117.82Å 90.00° 104.47° 90.00°	Depositor
Resolution (Å)	28.70 – 1.78 28.70 – 1.78	Depositor EDS
% Data completeness (in resolution range)	92.5 (28.70-1.78) 92.6 (28.70-1.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.78Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.237 0.224 , 0.230	Depositor DCC
R_{free} test set	4488 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19666	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 12.55% 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: SF4, F3S, FES, FAD, HEM, LMT, FUM, NA

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	1.69	3/5241 (0.1%)	0.90	15/7063 (0.2%)
1	D	0.38	1/5221 (0.0%)	0.89	14/7038 (0.2%)
2	B	0.42	1/1939 (0.1%)	0.86	4/2616 (0.2%)
2	E	0.42	1/1939 (0.1%)	0.87	3/2616 (0.1%)
3	C	1.40	3/2165 (0.1%)	0.98	5/2930 (0.2%)
3	F	2.13	7/2165 (0.3%)	1.55	9/2930 (0.3%)
All	All	1.28	16/18670 (0.1%)	1.00	50/25193 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	F	0	1
All	All	0	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2[A]	LYS	CE-NZ	84.19	4.01	1.49
1	A	2[B]	LYS	CE-NZ	84.19	4.01	1.49
3	F	180[A]	GLU	CD-OE2	63.88	2.46	1.25
3	F	180[B]	GLU	CD-OE2	63.88	2.46	1.25
3	C	180[A]	GLU	CD-OE2	44.56	2.10	1.25
3	C	180[B]	GLU	CD-OE2	44.56	2.10	1.25
3	F	180[A]	GLU	CD-OE1	23.56	1.70	1.25
3	F	180[B]	GLU	CD-OE1	23.56	1.70	1.25
3	F	180[A]	GLU	CG-CD	11.48	1.80	1.52
3	F	180[B]	GLU	CG-CD	11.48	1.80	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	254	HIS	C-N	-5.78	1.25	1.33
1	A	655	ASP	C-N	-5.75	1.25	1.33
1	D	655	ASP	C-N	-5.69	1.25	1.33
3	F	254	HIS	C-N	-5.60	1.25	1.33
2	B	239	ASN	C-N	-5.53	1.25	1.33
2	E	239	ASN	C-N	-5.37	1.25	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	180[A]	GLU	OE1-CD-OE2	-36.76	34.68	122.90
3	F	180[B]	GLU	OE1-CD-OE2	-36.76	34.68	122.90
3	F	180[A]	GLU	CG-CD-OE1	-25.83	58.98	118.40
3	F	180[B]	GLU	CG-CD-OE1	-25.83	58.98	118.40
3	F	180[A]	GLU	CG-CD-OE2	-22.90	65.73	118.40
3	F	180[B]	GLU	CG-CD-OE2	-22.90	65.73	118.40
3	C	180[A]	GLU	OE1-CD-OE2	20.64	172.44	122.90
3	C	180[B]	GLU	OE1-CD-OE2	20.64	172.44	122.90
1	D	397	TRP	N-CA-C	-12.79	96.98	111.82
1	A	397	TRP	N-CA-C	-12.73	97.05	111.82
1	D	399	MET	N-CA-C	-9.77	101.01	113.72
1	A	399	MET	N-CA-C	-9.69	101.13	113.72
3	F	102	PRO	N-CA-C	-8.69	97.55	111.19
3	C	102	PRO	N-CA-C	-8.66	97.60	111.19
2	B	65	CYS	N-CA-C	7.82	121.26	112.97
2	E	65	CYS	N-CA-C	7.62	121.04	112.97
1	A	2[A]	LYS	CD-CE-NZ	-7.29	88.58	111.90
1	A	2[B]	LYS	CD-CE-NZ	-7.29	88.58	111.90
3	C	103	ILE	N-CA-C	7.22	119.84	112.90
3	F	103	ILE	N-CA-C	7.11	119.72	112.90
2	E	203	ASP	N-CA-C	-6.09	105.50	113.17
1	A	552	TYR	CA-C-N	5.99	126.10	119.87
1	A	552	TYR	C-N-CA	5.99	126.10	119.87
1	D	552	TYR	CA-C-N	5.96	126.07	119.87
1	D	552	TYR	C-N-CA	5.96	126.07	119.87
1	A	287	PHE	N-CA-C	5.90	120.63	112.90
1	D	287	PHE	N-CA-C	5.85	120.56	112.90
1	A	410	VAL	N-CA-C	-5.80	103.67	111.44
1	A	222	ILE	N-CA-C	-5.74	105.26	113.07
2	E	168	GLU	N-CA-C	5.73	119.37	112.38
2	B	203	ASP	N-CA-C	-5.69	106.00	113.17
1	D	267	LEU	N-CA-C	5.66	118.53	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	137	PHE	N-CA-C	-5.65	105.12	111.28
3	C	137	PHE	N-CA-C	-5.62	105.16	111.28
1	D	222	ILE	N-CA-C	-5.61	105.45	113.07
1	A	39	VAL	N-CA-C	5.58	118.03	111.05
1	A	267	LEU	N-CA-C	5.55	118.37	110.10
2	B	168	GLU	N-CA-C	5.51	119.10	112.38
1	D	568	TRP	CA-C-N	5.43	124.62	118.97
1	D	568	TRP	C-N-CA	5.43	124.62	118.97
1	A	259	THR	N-CA-C	5.42	121.80	109.81
1	A	38	PRO	N-CA-C	-5.42	102.59	111.15
1	D	259	THR	N-CA-C	5.37	121.68	109.81
1	D	39	VAL	N-CA-C	5.30	117.67	111.05
1	D	410	VAL	N-CA-C	-5.19	104.60	111.09
1	D	396	CYS	N-CA-C	-5.16	99.97	108.49
2	B	9	VAL	N-CA-C	5.13	115.88	108.48
1	A	396	CYS	N-CA-C	-5.13	100.03	108.49
1	A	216	THR	N-CA-C	5.02	119.05	113.02
1	D	38	PRO	N-CA-C	-5.02	103.22	111.15

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	180[A]	GLU	Sidechain
3	F	180[A]	GLU	Sidechain

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	5145	0	5124	132	0
1	D	5125	0	5100	133	0
2	B	1902	0	1869	48	0
2	E	1902	0	1869	51	0
3	C	2099	0	2111	57	0
3	F	2099	0	2111	68	0
4	A	53	0	29	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	53	0	29	3	0
5	A	8	0	1	0	0
5	D	8	0	1	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	B	4	0	0	0	0
7	E	4	0	0	0	0
8	B	7	0	0	0	0
8	E	7	0	0	0	0
9	B	8	0	0	0	0
9	E	8	0	0	0	0
10	C	86	0	60	1	0
10	F	86	0	60	1	0
11	C	35	0	46	8	0
11	F	35	0	46	9	0
12	A	273	0	0	9	0
12	B	155	0	0	3	0
12	C	55	0	0	1	0
12	D	287	0	0	5	0
12	E	164	0	0	2	0
12	F	56	0	0	1	0
All	All	19666	0	18456	462	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 13.

All (462) 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)
3:F:180[B]:GLU:CD	3:F:180[B]:GLU:CG	1.80	1.54
3:F:180[A]:GLU:OE1	3:F:180[A]:GLU:CD	1.70	1.33
3:F:180[B]:GLU:OE1	3:F:180[B]:GLU:HG2	1.47	1.11
3:F:180[A]:GLU:CD	3:F:180[A]:GLU:HB2	1.84	1.03
2:B:1:MET:HG2	2:B:2:GLY:H	1.24	1.01
2:E:1:MET:HG2	2:E:2:GLY:H	1.24	0.98
1:D:64:ASP:HB2	1:D:146:LYS:HG2	1.47	0.96
1:A:64:ASP:HB2	1:A:146:LYS:HG2	1.47	0.95
3:F:180[A]:GLU:OE2	3:F:180[A]:GLU:HG3	1.68	0.93
2:B:8:ARG:HG2	2:B:25:GLU:HG2	1.52	0.90
2:E:8:ARG:HG2	2:E:25:GLU:HG2	1.53	0.89
3:C:1:MET:HE3	3:C:6:ILE:HD11	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1:MET:HE3	3:F:6:ILE:HD11	1.55	0.88
3:F:180[A]:GLU:CD	3:F:180[A]:GLU:CB	2.49	0.86
1:D:27:LYS:HD2	1:D:425:ALA:HB1	1.56	0.86
1:A:27:LYS:HD2	1:A:425:ALA:HB1	1.55	0.86
2:E:209:MET:SD	3:F:100:LYS:HG3	2.17	0.85
1:A:52:GLN:HG2	1:A:69:HIS:NE2	1.92	0.85
3:F:180[B]:GLU:HG2	3:F:180[B]:GLU:OE2	1.76	0.84
2:B:209:MET:SD	3:C:100:LYS:HG3	2.17	0.84
1:D:52:GLN:HG2	1:D:69:HIS:NE2	1.92	0.83
1:A:535:LYS:HG3	1:A:578:LEU:HD11	1.60	0.83
1:D:535:LYS:HG3	1:D:578:LEU:HD11	1.61	0.81
3:F:131:MET:HG2	11:F:1257:LMT:H123	1.63	0.80
1:A:330:ILE:HD11	1:A:357:PRO:HB2	1.63	0.80
3:F:103:ILE:H	3:F:107:GLN:NE2	1.80	0.80
3:C:131:MET:HG2	11:C:1257:LMT:H123	1.63	0.79
1:D:330:ILE:HD11	1:D:357:PRO:HB2	1.63	0.79
1:D:112:LYS:H	1:D:133:HIS:HD2	1.31	0.79
2:E:180:VAL:HG11	2:E:227:LYS:HG3	1.65	0.78
3:C:103:ILE:H	3:C:107:GLN:NE2	1.82	0.78
1:A:611:LYS:NZ	1:A:611:LYS:HB3	2.00	0.76
1:D:611:LYS:NZ	1:D:611:LYS:HB3	2.00	0.76
1:D:628:LYS:HG3	1:D:632:ALA:HB3	1.68	0.76
1:A:628:LYS:HG3	1:A:632:ALA:HB3	1.67	0.76
3:C:4:GLU:CD	3:C:4:GLU:H	1.94	0.75
2:E:238:VAL:O	2:E:239:ASN:HB2	1.85	0.75
1:A:112:LYS:H	1:A:133:HIS:HD2	1.32	0.75
3:F:4:GLU:H	3:F:4:GLU:CD	1.94	0.75
2:B:180:VAL:HG11	2:B:227:LYS:HG3	1.67	0.75
3:C:180[B]:GLU:OE2	3:C:180[B]:GLU:HG3	1.87	0.74
1:D:268:LEU:HD22	1:D:345:VAL:HG23	1.70	0.74
1:A:346:GLN:HA	1:A:357:PRO:HG3	1.70	0.74
2:E:1:MET:HG2	2:E:2:GLY:N	2.02	0.74
2:B:238:VAL:O	2:B:239:ASN:HB2	1.86	0.74
1:D:179:LYS:HG3	1:D:196:VAL:HG11	1.70	0.73
1:D:112:LYS:HG3	1:D:130:ASP:HA	1.70	0.73
1:D:482:ARG:HH11	1:D:547:HIS:HD2	1.36	0.73
1:D:346:GLN:HA	1:D:357:PRO:HG3	1.69	0.73
1:A:179:LYS:HG3	1:A:196:VAL:HG11	1.70	0.72
1:A:268:LEU:HD22	1:A:345:VAL:HG23	1.70	0.72
1:A:112:LYS:HG3	1:A:130:ASP:HA	1.70	0.72
1:A:482:ARG:HH11	1:A:547:HIS:HD2	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:180[B]:GLU:CD	3:F:180[B]:GLU:CB	2.63	0.72
3:F:180[B]:GLU:CG	3:F:180[B]:GLU:OE2	2.38	0.72
1:A:179:LYS:HG3	1:A:196:VAL:CG1	2.20	0.71
1:D:179:LYS:HG3	1:D:196:VAL:CG1	2.20	0.71
3:F:180[A]:GLU:OE1	3:F:180[A]:GLU:CG	2.39	0.70
3:F:180[A]:GLU:OE2	3:F:180[A]:GLU:CG	2.38	0.70
3:C:95:PHE:HE1	11:F:1257:LMT:H101	1.58	0.69
2:B:1:MET:HG2	2:B:2:GLY:N	2.02	0.69
3:F:131:MET:HG2	11:F:1257:LMT:C12	2.23	0.68
3:C:131:MET:HG2	11:C:1257:LMT:C12	2.23	0.67
1:D:320:SER:HB3	1:D:323:GLY:O	1.94	0.67
1:A:386:LYS:HG3	12:A:2164:HOH:O	1.95	0.66
1:D:386:LYS:HG3	12:D:2164:HOH:O	1.95	0.66
1:A:320:SER:HB3	1:A:323:GLY:O	1.94	0.66
1:D:121:ALA:O	1:D:122:GLN:HG3	1.96	0.66
1:A:64:ASP:CB	1:A:146:LYS:HG2	2.25	0.66
2:E:191:THR:OG1	2:E:193:GLU:HG2	1.96	0.65
1:D:64:ASP:CB	1:D:146:LYS:HG2	2.25	0.65
1:D:540:ARG:HH22	1:D:562:ASN:ND2	1.95	0.65
1:A:540:ARG:HH22	1:A:562:ASN:ND2	1.93	0.65
2:B:126:LYS:HG2	12:B:2083:HOH:O	1.96	0.65
1:A:342:LEU:HB3	1:A:345:VAL:HG12	1.79	0.64
3:C:69:PHE:CD1	3:C:70:ILE:HG13	2.32	0.64
3:F:69:PHE:HD1	3:F:70:ILE:HG13	1.62	0.64
2:E:68:MET:HB2	2:E:92:LEU:HB2	1.79	0.64
1:A:121:ALA:O	1:A:122:GLN:HG3	1.97	0.64
2:B:191:THR:OG1	2:B:193:GLU:HG2	1.97	0.64
1:D:562:ASN:C	1:D:562:ASN:HD22	2.06	0.64
2:B:68:MET:HB2	2:B:92:LEU:HB2	1.80	0.64
2:B:119:GLU:OE1	2:B:123:HIS:HE1	1.80	0.64
2:E:119:GLU:OE1	2:E:123:HIS:HE1	1.81	0.64
1:A:342:LEU:HB3	1:A:345:VAL:CG1	2.29	0.63
2:B:4:MET:HE3	2:B:27:LYS:HB3	1.81	0.63
2:E:4:MET:HE3	2:E:27:LYS:HB3	1.80	0.63
3:F:69:PHE:CD1	3:F:70:ILE:HG13	2.32	0.63
1:D:342:LEU:HB3	1:D:345:VAL:CG1	2.28	0.63
1:D:342:LEU:HB3	1:D:345:VAL:HG12	1.79	0.63
1:D:64:ASP:HB2	1:D:146:LYS:CG	2.27	0.63
1:D:115[A]:ARG:HD2	1:D:117:ALA:HB2	1.81	0.63
3:C:69:PHE:HD1	3:C:70:ILE:HG13	1.62	0.63
1:A:540:ARG:HH22	1:A:562:ASN:HD22	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ARG:HD2	1:D:226:THR:HG21	1.81	0.63
1:A:562:ASN:HD22	1:A:562:ASN:C	2.07	0.62
1:D:540:ARG:HH22	1:D:562:ASN:HD22	1.46	0.62
1:A:342:LEU:O	1:A:345:VAL:HG12	2.00	0.62
1:A:27:LYS:HD2	1:A:425:ALA:CB	2.29	0.61
1:A:651:GLU:OE2	2:B:133:LEU:HD23	2.01	0.61
1:D:224:LYS:HB3	1:D:475:ASP:OD2	2.00	0.61
2:B:1:MET:HG2	2:B:3:ARG:H	1.66	0.61
3:C:103:ILE:H	3:C:107:GLN:HE21	1.48	0.61
2:B:2:GLY:O	2:B:30:GLU:HB3	2.01	0.61
1:D:342:LEU:O	1:D:345:VAL:HG12	2.00	0.61
3:F:103:ILE:H	3:F:107:GLN:HE21	1.48	0.61
2:E:2:GLY:O	2:E:30:GLU:HB3	2.01	0.61
1:A:64:ASP:HB2	1:A:146:LYS:CG	2.26	0.61
1:D:295:LYS:HG2	1:D:299:ALA:HA	1.83	0.60
3:F:180[B]:GLU:CG	3:F:180[B]:GLU:OE1	2.38	0.60
1:D:651:GLU:OE2	2:E:133:LEU:HD23	2.00	0.60
2:E:1:MET:HG2	2:E:3:ARG:H	1.66	0.60
1:D:27:LYS:HD2	1:D:425:ALA:CB	2.30	0.60
2:E:180:VAL:HG11	2:E:227:LYS:CG	2.32	0.59
3:F:180[B]:GLU:OE1	3:F:180[B]:GLU:OE2	2.19	0.59
1:A:221:ARG:HD2	1:A:226:THR:HG21	1.84	0.59
3:F:180[A]:GLU:OE1	3:F:180[A]:GLU:OE2	2.20	0.59
2:E:13:ASP:HA	2:E:101:LYS:HG3	1.84	0.59
3:F:233:LYS:O	3:F:237:GLU:HG3	2.03	0.59
3:C:17:ARG:NH1	2:E:16:SER:O	2.35	0.59
1:A:295:LYS:HG2	1:A:299:ALA:HA	1.83	0.59
2:B:13:ASP:HA	2:B:101:LYS:HG3	1.84	0.59
3:C:168:MET:HE2	12:C:2043:HOH:O	2.03	0.59
1:D:257:HIS:HD2	1:D:259:THR:H	1.51	0.59
11:C:1257:LMT:H101	3:F:95:PHE:HE1	1.68	0.59
2:B:180:VAL:HG11	2:B:227:LYS:CG	2.33	0.58
3:F:180[B]:GLU:CD	3:F:180[B]:GLU:OE2	2.46	0.58
1:D:92:THR:O	1:D:95:LYS:HG3	2.03	0.58
3:C:233:LYS:O	3:C:237:GLU:HG3	2.03	0.58
2:E:2:GLY:O	2:E:3:ARG:HG2	2.04	0.58
2:B:2:GLY:O	2:B:3:ARG:HG2	2.03	0.58
1:A:332:ILE:HD12	1:A:333:LEU:N	2.19	0.58
3:F:180[A]:GLU:CD	3:F:180[A]:GLU:CG	2.77	0.58
1:A:92:THR:O	1:A:95:LYS:HG3	2.04	0.58
1:A:224:LYS:HB3	1:A:475:ASP:OD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:HIS:HD2	1:A:259:THR:H	1.51	0.57
1:A:611:LYS:HB3	1:A:611:LYS:HZ3	1.69	0.57
1:A:257:HIS:CE1	1:A:267:LEU:HD11	2.39	0.57
1:D:257:HIS:CE1	1:D:267:LEU:HD11	2.39	0.57
3:F:207:ALA:O	3:F:211:LYS:HG3	2.04	0.57
1:A:498:TYR:HA	1:A:527:LEU:HD13	1.87	0.57
3:C:206:ARG:O	3:C:210:LYS:HG3	2.04	0.57
1:D:464:PHE:CD1	2:E:45:GLU:HG2	2.40	0.57
1:D:570:ASN:O	1:D:573:GLN:HG2	2.05	0.57
1:A:455:VAL:O	1:A:509:LYS:HD2	2.04	0.57
3:C:207:ALA:O	3:C:211:LYS:HG3	2.05	0.57
3:F:206:ARG:O	3:F:210:LYS:HG3	2.04	0.57
1:D:455:VAL:O	1:D:509:LYS:HD2	2.05	0.57
1:D:332:ILE:HD12	1:D:333:LEU:N	2.19	0.56
1:A:8:SER:HB2	1:A:31:THR:HB	1.87	0.56
3:F:102:PRO:O	11:F:1257:LMT:H62	2.05	0.56
3:C:102:PRO:O	11:C:1257:LMT:H62	2.06	0.56
3:C:95:PHE:CE1	11:F:1257:LMT:H51	2.42	0.55
2:E:121:TRP:O	2:E:123:HIS:HD2	1.89	0.55
1:A:306:ARG:HD2	12:A:2241:HOH:O	2.07	0.55
1:D:498:TYR:HA	1:D:527:LEU:HD13	1.87	0.55
2:B:85:GLU:O	2:B:86:ASP:HB2	2.07	0.54
2:E:52:ASN:CG	2:E:101:LYS:HE3	2.33	0.54
2:E:85:GLU:O	2:E:86:ASP:HB2	2.07	0.54
3:F:248:PHE:HE2	3:F:252:ARG:HH21	1.55	0.54
3:C:211:LYS:O	3:C:215:LEU:HD23	2.07	0.54
3:C:217:SER:O	3:C:221:ILE:HG12	2.08	0.54
1:A:570:ASN:O	1:A:573:GLN:HG2	2.06	0.54
2:E:10:PHE:HB2	2:E:92:LEU:HD23	1.90	0.54
3:F:217:SER:O	3:F:221:ILE:HG12	2.07	0.54
1:A:464:PHE:CD1	2:B:45:GLU:HG2	2.42	0.54
1:D:341:ASN:C	1:D:342:LEU:HD12	2.33	0.54
1:A:114:ASP:HB3	1:A:125:THR:HG21	1.89	0.54
2:B:121:TRP:O	2:B:123:HIS:HD2	1.91	0.53
2:B:197:GLU:OE1	3:C:19:LYS:HG3	2.08	0.53
2:B:239:ASN:CG	3:C:21:ARG:HE	2.15	0.53
2:B:52:ASN:CG	2:B:101:LYS:HE3	2.33	0.53
2:E:197:GLU:O	3:F:19:LYS:HD2	2.09	0.53
1:A:260:PRO:HD2	1:A:365:LEU:O	2.07	0.53
3:C:169:TRP:N	3:C:170:PRO:HD2	2.24	0.53
1:D:114:ASP:HB3	1:D:125:THR:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:211:LYS:O	3:F:215:LEU:HD23	2.09	0.53
2:E:239:ASN:CG	3:F:21:ARG:HE	2.15	0.53
1:A:341:ASN:C	1:A:342:LEU:HD12	2.33	0.53
2:B:10:PHE:HB2	2:B:92:LEU:HD23	1.90	0.53
3:C:145:TYR:OH	3:F:170:PRO:HG2	2.09	0.53
3:C:248:PHE:HE2	3:C:252:ARG:HH21	1.56	0.53
2:B:197:GLU:O	3:C:19:LYS:HD2	2.09	0.53
2:B:158:ILE:HG23	2:B:164:LYS:HD3	1.91	0.53
1:D:8:SER:HB2	1:D:31:THR:HB	1.91	0.53
1:A:112:LYS:HG3	1:A:130:ASP:CA	2.40	0.52
1:D:140:ASP:HB2	1:D:147:TRP:CE2	2.45	0.52
1:D:260:PRO:HD2	1:D:365:LEU:O	2.08	0.52
3:F:169:TRP:N	3:F:170:PRO:HD2	2.24	0.52
1:A:140:ASP:HB2	1:A:147:TRP:CE2	2.45	0.52
1:D:482:ARG:NH1	1:D:547:HIS:HD2	2.06	0.52
3:C:170:PRO:HG2	3:F:145:TYR:OH	2.09	0.52
1:D:257:HIS:CD2	1:D:259:THR:H	2.28	0.52
1:A:434:ASP:OD1	1:D:434:ASP:OD1	2.28	0.51
1:D:24:THR:OG1	1:D:31:THR:HG21	2.10	0.51
2:E:158:ILE:HG23	2:E:164:LYS:HD3	1.91	0.51
1:A:24:THR:OG1	1:A:31:THR:HG21	2.11	0.51
1:D:255:GLN:HE21	1:D:403:ASN:ND2	2.08	0.51
2:E:197:GLU:OE1	3:F:19:LYS:HG3	2.10	0.51
1:A:245:ILE:O	1:A:384:LYS:HE2	2.10	0.51
1:A:467:LYS:O	1:A:471:LYS:HG3	2.11	0.51
1:D:122:GLN:O	1:D:124:THR:N	2.36	0.51
1:D:524:PRO:O	1:D:528:LYS:HG3	2.10	0.51
1:A:295:LYS:CG	1:A:299:ALA:HA	2.41	0.51
1:D:384:LYS:NZ	12:D:2165:HOH:O	2.43	0.51
1:A:52:GLN:HG3	1:A:148:ARG:HD2	1.94	0.51
2:B:61:ILE:HG23	12:B:2038:HOH:O	2.10	0.51
1:D:295:LYS:CG	1:D:299:ALA:HA	2.41	0.51
1:A:64:ASP:HA	1:A:68:LEU:HD12	1.94	0.50
1:A:257:HIS:CD2	1:A:259:THR:H	2.28	0.50
1:A:325:HIS:HD2	1:A:326:LEU:O	1.94	0.50
3:C:17:ARG:HD2	2:E:19:SER:O	2.11	0.50
1:A:482:ARG:HH11	1:A:547:HIS:CD2	2.23	0.50
1:D:482:ARG:HH11	1:D:547:HIS:CD2	2.23	0.50
3:F:101:PHE:HB3	11:F:1257:LMT:H71	1.93	0.50
3:F:171:LEU:C	3:F:171:LEU:HD23	2.37	0.50
1:A:270:GLU:HG3	1:A:273[A]:ARG:HH22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16[B]:GLU:HA	2:E:20:LYS:CE	2.42	0.50
3:C:16[B]:GLU:HA	2:E:20:LYS:HE3	1.92	0.50
3:C:175:LEU:O	3:C:179:VAL:HG12	2.12	0.50
2:E:1:MET:CG	2:E:2:GLY:H	2.09	0.50
2:E:52:ASN:OD1	2:E:101:LYS:HE3	2.11	0.50
1:A:255:GLN:HE21	1:A:403:ASN:ND2	2.10	0.50
1:A:297:GLU:CD	1:A:297:GLU:H	2.19	0.50
1:A:482:ARG:NH1	1:A:547:HIS:HD2	2.06	0.50
1:A:5:TYR:CD1	1:A:5:TYR:C	2.89	0.50
1:A:257:HIS:O	1:A:366:PRO:HA	2.12	0.50
3:C:171:LEU:C	3:C:171:LEU:HD23	2.36	0.50
1:D:245:ILE:O	1:D:384:LYS:HE2	2.12	0.50
3:C:62:THR:O	3:C:66:GLU:HG3	2.12	0.50
1:D:452:LYS:NZ	12:D:2200:HOH:O	2.45	0.49
1:D:5:TYR:CD1	1:D:5:TYR:C	2.89	0.49
1:D:64:ASP:HA	1:D:68:LEU:HD12	1.93	0.49
1:D:281:ASP:HB2	1:D:316:LYS:HG3	1.93	0.49
2:B:1:MET:CG	2:B:2:GLY:H	2.09	0.49
1:D:116:MET:HE2	1:D:116:MET:HA	1.94	0.49
1:D:467:LYS:O	1:D:471:LYS:HG3	2.11	0.49
3:F:62:THR:O	3:F:66:GLU:HG3	2.12	0.49
1:A:111:HIS:HA	1:A:133:HIS:CD2	2.48	0.49
1:A:631:HIS:O	1:A:635:GLU:HG3	2.12	0.49
1:D:112:LYS:HG3	1:D:130:ASP:CA	2.40	0.49
1:A:116:MET:HE2	1:A:116:MET:HA	1.94	0.49
1:A:228:ASN:N	1:A:228:ASN:HD22	2.10	0.49
1:A:384:LYS:NZ	12:A:2166:HOH:O	2.44	0.49
1:A:427:HIS:O	1:A:431:THR:HG22	2.13	0.49
2:B:193:GLU:CD	2:B:193:GLU:H	2.21	0.49
1:D:325:HIS:HD2	1:D:326:LEU:O	1.95	0.49
1:A:281:ASP:HB2	1:A:316:LYS:HG3	1.93	0.49
1:D:651:GLU:HG2	2:E:133:LEU:CD2	2.43	0.49
1:A:524:PRO:O	1:A:528:LYS:HG3	2.12	0.49
1:A:651:GLU:HG2	2:B:133:LEU:CD2	2.43	0.49
1:D:111:HIS:HA	1:D:133:HIS:CD2	2.48	0.49
2:E:193:GLU:CD	2:E:193:GLU:H	2.20	0.49
3:C:99:ARG:HG2	11:F:1257:LMT:H32	1.95	0.48
3:C:101:PHE:HB3	11:C:1257:LMT:H71	1.94	0.48
1:D:52:GLN:HG3	1:D:148:ARG:HD2	1.94	0.48
3:F:175:LEU:O	3:F:179:VAL:HG12	2.13	0.48
1:A:462:ASP:HB3	1:A:465:LYS:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:THR:N	1:D:260:PRO:HD3	2.29	0.48
1:D:611:LYS:HB3	1:D:611:LYS:HZ2	1.74	0.48
1:D:427:HIS:O	1:D:431:THR:HG22	2.13	0.48
1:D:462:ASP:HB3	1:D:465:LYS:HD3	1.95	0.48
1:D:631:HIS:O	1:D:635:GLU:HG3	2.12	0.48
1:D:228:ASN:N	1:D:228:ASN:HD22	2.12	0.48
1:D:257:HIS:O	1:D:366:PRO:HA	2.13	0.48
1:D:190:LYS:HE3	12:D:2069:HOH:O	2.14	0.48
1:D:342:LEU:HD12	1:D:342:LEU:N	2.29	0.48
1:A:179:LYS:CG	1:A:196:VAL:HG11	2.42	0.47
1:D:179:LYS:CG	1:D:196:VAL:HG11	2.42	0.47
3:F:2:THR:OG1	3:F:4:GLU:HG2	2.15	0.47
1:A:410:VAL:HG13	4:A:1656:FAD:C2	2.44	0.47
1:D:309:ILE:O	1:D:313:ARG:HG3	2.14	0.47
11:C:1257:LMT:H32	3:F:99:ARG:HG2	1.97	0.47
1:A:342:LEU:HD12	1:A:342:LEU:N	2.30	0.47
1:D:67:ASP:OD2	1:D:630:ARG:HD2	2.14	0.47
1:A:25:GLN:OE1	1:A:31:THR:HG23	2.14	0.47
1:A:120:ASN:HB3	1:A:298:LEU:CD1	2.45	0.47
2:B:130:ILE:HG12	12:B:2087:HOH:O	2.14	0.47
3:C:200:GLU:C	3:C:202:PRO:HD3	2.40	0.47
3:C:16[A]:GLU:HA	2:E:20:LYS:HE3	1.95	0.47
3:C:16[A]:GLU:HA	2:E:20:LYS:CE	2.45	0.47
1:D:120:ASN:HB3	1:D:298:LEU:CD1	2.45	0.47
1:D:410:VAL:HG13	4:D:1656:FAD:C2	2.45	0.47
1:A:259:THR:N	1:A:260:PRO:HD3	2.30	0.47
1:D:66:GLU:HG2	1:D:91:ASN:HD22	1.79	0.47
1:D:120:ASN:HB3	1:D:298:LEU:HD13	1.97	0.47
1:A:120:ASN:HB3	1:A:298:LEU:HD13	1.97	0.47
2:B:2:GLY:O	2:B:3:ARG:CG	2.64	0.47
3:F:108:TYR:CD2	11:F:1257:LMT:H52	2.50	0.47
3:F:200:GLU:C	3:F:202:PRO:HD3	2.40	0.46
1:A:270:GLU:HG3	1:A:273[A]:ARG:NH2	2.30	0.46
1:A:607:PRO:HG2	1:A:608:LEU:HD12	1.97	0.46
3:C:108:TYR:CD2	11:C:1257:LMT:H52	2.50	0.46
3:C:176:LEU:O	3:C:180[B]:GLU:HB2	2.15	0.46
1:D:607:PRO:HG2	1:D:608:LEU:HD12	1.96	0.46
1:A:115[B]:ARG:HB2	12:A:2055:HOH:O	2.15	0.46
1:A:512:HIS:O	1:A:513:ALA:C	2.58	0.46
1:D:512:HIS:O	1:D:513:ALA:C	2.58	0.46
2:E:57:CYS:O	2:E:58:ARG:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:LYS:HG2	1:A:602:ASN:ND2	2.31	0.46
1:A:67:ASP:OD2	1:A:630:ARG:HD2	2.15	0.46
1:A:273[A]:ARG:NH1	1:A:273[A]:ARG:HB2	2.30	0.46
1:D:261:LEU:HD21	1:D:353:ALA:HB2	1.97	0.46
1:D:611:LYS:HB3	1:D:611:LYS:HZ3	1.75	0.46
1:A:410:VAL:HG13	4:A:1656:FAD:N1	2.31	0.46
2:B:52:ASN:OD1	2:B:101:LYS:HE3	2.15	0.46
3:C:2:THR:OG1	3:C:4:GLU:HG2	2.15	0.46
1:A:122:GLN:O	1:A:124:THR:N	2.37	0.46
1:D:187:GLN:HB3	1:D:192:TYR:HE2	1.81	0.46
2:B:57:CYS:O	2:B:58:ARG:HG3	2.16	0.46
3:C:58:MET:HE2	3:C:155:GLY:HA2	1.98	0.46
1:A:13:GLY:HA3	1:A:39:VAL:HG12	1.98	0.45
1:A:540:ARG:NH2	1:A:562:ASN:ND2	2.63	0.45
1:D:40:LYS:HE2	2:E:153:GLU:CD	2.41	0.45
2:E:2:GLY:O	2:E:3:ARG:CG	2.64	0.45
1:A:187:GLN:HB3	1:A:192:TYR:HE2	1.81	0.45
1:A:261:LEU:HD21	1:A:353:ALA:HB2	1.98	0.45
1:A:309:ILE:O	1:A:313:ARG:HG3	2.16	0.45
1:A:483:ASP:CG	1:A:486:HIS:HD1	2.25	0.45
1:A:66:GLU:HG2	1:A:91:ASN:HD22	1.80	0.45
3:C:59:LEU:HD22	3:C:252:ARG:NH1	2.32	0.45
4:D:1656:FAD:H1'1	4:D:1656:FAD:H9	1.61	0.45
3:F:59:LEU:HD22	3:F:252:ARG:NH1	2.32	0.45
1:D:13:GLY:HA3	1:D:39:VAL:HG12	1.98	0.45
1:D:410:VAL:HG13	4:D:1656:FAD:N1	2.32	0.45
2:E:125:GLN:HG2	12:E:2094:HOH:O	2.16	0.45
1:D:554:LYS:HG2	1:D:602:ASN:ND2	2.31	0.45
2:E:52:ASN:OD1	2:E:101:LYS:CE	2.64	0.45
3:F:176:LEU:O	3:F:180[B]:GLU:HB2	2.17	0.45
2:B:35:THR:HG22	2:B:80:LEU:HD23	1.98	0.44
11:C:1257:LMT:H51	3:F:95:PHE:CE1	2.52	0.44
1:D:221:ARG:HD3	1:D:229:ALA:O	2.17	0.44
1:D:540:ARG:NH2	1:D:562:ASN:ND2	2.64	0.44
1:A:455:VAL:CG1	1:A:509:LYS:HG3	2.48	0.44
1:D:122:GLN:C	1:D:124:THR:H	2.22	0.44
1:A:554:LYS:HG2	1:A:602:ASN:HD22	1.83	0.44
1:A:122:GLN:C	1:A:124:THR:H	2.22	0.44
2:E:35:THR:HG22	2:E:80:LEU:HD23	2.00	0.44
1:A:608:LEU:HD12	1:A:608:LEU:N	2.33	0.44
1:D:25:GLN:OE1	1:D:31:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:HE2	2:B:153:GLU:CD	2.42	0.44
1:D:49:GLY:HA2	1:D:139[A]:ARG:HH21	1.82	0.44
1:D:422:GLU:HG2	12:D:2177:HOH:O	2.18	0.44
1:A:2[A]:LYS:HE3	12:A:2108:HOH:O	2.18	0.44
1:A:34:LEU:HD22	1:A:179:LYS:HG2	2.00	0.44
2:B:85:GLU:OE2	2:B:85:GLU:HA	2.18	0.43
3:F:8:GLU:HA	3:F:13:VAL:O	2.18	0.43
3:F:247:TYR:O	3:F:251:LYS:HG3	2.18	0.43
1:D:332:ILE:HD12	1:D:332:ILE:C	2.43	0.43
1:D:483:ASP:CG	1:D:486:HIS:HD1	2.26	0.43
2:E:210:THR:HG22	2:E:210:THR:O	2.18	0.43
3:F:58:MET:HE2	3:F:155:GLY:HA2	2.00	0.43
3:F:82:LEU:HD12	10:F:1256:HEM:CBB	2.49	0.43
1:A:611:LYS:HB3	1:A:611:LYS:HZ2	1.78	0.43
1:A:52:GLN:HE21	1:A:52:GLN:HB2	1.51	0.43
1:A:332:ILE:HD12	1:A:332:ILE:C	2.44	0.43
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.86	0.43
3:C:2:THR:HB	3:C:4:GLU:OE2	2.18	0.43
1:D:554:LYS:HG2	1:D:602:ASN:HD22	1.83	0.43
3:F:2:THR:HB	3:F:4:GLU:OE2	2.19	0.43
2:B:164:LYS:HG2	2:B:170:PHE:HD2	1.84	0.43
2:E:5:LEU:HD11	2:E:30:GLU:HB2	2.01	0.43
1:A:318:VAL:HG21	1:A:327:TRP:NE1	2.33	0.43
1:D:314:LYS:NZ	1:D:314:LYS:HB3	2.34	0.43
2:E:164:LYS:HG2	2:E:170:PHE:HD2	1.83	0.43
2:B:16:SER:O	3:F:17:ARG:NH1	2.45	0.42
1:D:124:THR:OG1	1:D:125:THR:N	2.52	0.42
1:A:584:ASP:OD1	1:A:586:ASN:HB2	2.19	0.42
2:B:114[A]:MET:SD	2:B:114[A]:MET:C	3.02	0.42
3:F:29:TRP:O	3:F:33:THR:HG23	2.19	0.42
1:A:254:VAL:CG1	1:A:368:GLN:HG2	2.49	0.42
2:B:199:ILE:C	2:B:199:ILE:HD12	2.45	0.42
1:D:455:VAL:HG13	1:D:509:LYS:HG3	2.02	0.42
2:E:95:PRO:HD2	2:E:159:ALA:HB1	2.01	0.42
3:F:126:TRP:O	3:F:129:GLN:HB2	2.19	0.42
1:A:335:ARG:NH1	1:A:358:ALA:HB3	2.35	0.42
1:A:422:GLU:OE2	1:A:645:LYS:NZ	2.52	0.42
2:E:85:GLU:OE2	2:E:85:GLU:HA	2.19	0.42
1:A:115[A]:ARG:HB2	12:A:2055:HOH:O	2.20	0.42
1:A:608:LEU:HD12	1:A:608:LEU:H	1.84	0.42
3:C:59:LEU:O	3:C:63:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:ASN:OD1	2:B:101:LYS:CE	2.67	0.42
1:D:286:ARG:NH2	1:D:296:LYS:HE2	2.35	0.42
1:D:254:VAL:CG1	1:D:368:GLN:HG2	2.50	0.42
3:C:63:LYS:HE2	3:C:68:ASP:OD2	2.20	0.42
3:C:247:TYR:O	3:C:251:LYS:HG3	2.19	0.42
1:D:584:ASP:OD1	1:D:586:ASN:HB2	2.19	0.42
2:E:121:TRP:O	2:E:123:HIS:CD2	2.72	0.42
1:A:95:LYS:HB3	1:A:95:LYS:HE3	1.91	0.42
1:D:34:LEU:HD22	1:D:179:LYS:HG2	2.01	0.42
1:D:224:LYS:HD3	1:D:472:ASP:OD1	2.20	0.42
1:D:455:VAL:CG1	1:D:509:LYS:HG3	2.49	0.42
1:A:349:CYS:HB3	1:A:355:ILE:HG13	2.00	0.42
2:B:232:ARG:CZ	3:C:193:LYS:HD2	2.50	0.42
3:C:29:TRP:O	3:C:33:THR:HG23	2.20	0.42
3:C:161:PHE:CD2	3:C:246:LYS:HE3	2.55	0.42
1:D:37:ILE:O	1:D:38:PRO:C	2.63	0.42
1:D:565:LEU:HD11	1:D:581:GLU:HB2	2.01	0.42
1:D:612:ARG:O	1:D:616:ILE:HG13	2.19	0.42
2:E:199:ILE:HD12	2:E:199:ILE:C	2.45	0.42
3:F:59:LEU:O	3:F:63:LYS:HG3	2.20	0.42
1:A:612:ARG:O	1:A:616:ILE:HG13	2.20	0.41
2:B:210:THR:O	2:B:210:THR:HG22	2.19	0.41
1:D:41:ARG:HG2	1:D:41:ARG:HH11	1.85	0.41
2:E:50:ASP:HA	12:E:2035:HOH:O	2.20	0.41
3:F:161:PHE:CD2	3:F:246:LYS:HE3	2.55	0.41
3:C:4:GLU:CD	3:C:4:GLU:N	2.71	0.41
3:C:82:LEU:HD13	3:C:82:LEU:O	2.20	0.41
1:D:349:CYS:HB3	1:D:355:ILE:HG13	2.01	0.41
1:D:455:VAL:HG13	1:D:509:LYS:CD	2.50	0.41
1:D:606:ASN:OD1	1:D:608:LEU:HD13	2.20	0.41
1:D:608:LEU:HD12	1:D:608:LEU:N	2.34	0.41
1:A:111:HIS:HB3	2:B:139:PRO:HG3	2.03	0.41
1:A:224:LYS:HD3	1:A:472:ASP:OD1	2.21	0.41
1:A:455:VAL:HG13	1:A:509:LYS:HG3	2.01	0.41
2:B:5:LEU:HD11	2:B:30:GLU:HB2	2.01	0.41
3:C:82:LEU:HD12	10:C:1256:HEM:CBB	2.49	0.41
3:F:60:TRP:CZ2	3:F:64:LYS:HD2	2.55	0.41
1:A:71:MET:HE2	12:A:2027:HOH:O	2.21	0.41
1:A:455:VAL:HG13	1:A:509:LYS:CD	2.50	0.41
1:A:565:LEU:HD11	1:A:581:GLU:HB2	2.02	0.41
1:D:268:LEU:HD22	1:D:345:VAL:CG2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:SER:HB3	1:D:303:VAL:HG23	2.03	0.41
3:F:180[B]:GLU:CD	3:F:180[B]:GLU:CA	2.93	0.41
1:A:29:LEU:O	1:A:31:THR:HG22	2.19	0.41
1:A:314:LYS:NZ	1:A:314:LYS:HB3	2.35	0.41
1:A:562:ASN:ND2	1:A:562:ASN:C	2.74	0.41
1:D:27:LYS:HE3	1:D:27:LYS:HB3	1.89	0.41
1:D:335:ARG:NH1	1:D:358:ALA:HB3	2.35	0.41
1:D:608:LEU:HD12	1:D:608:LEU:H	1.85	0.41
1:A:221:ARG:HD3	1:A:229:ALA:O	2.21	0.41
1:A:606:ASN:OD1	1:A:608:LEU:HD13	2.20	0.41
1:D:318:VAL:HG21	1:D:327:TRP:NE1	2.35	0.41
3:F:75:LYS:HE2	12:F:2021:HOH:O	2.21	0.41
1:A:224:LYS:NZ	12:A:2207:HOH:O	2.54	0.41
1:A:301:ARG:HH12	1:A:404:ARG:NH1	2.19	0.41
1:A:57:ASN:HB2	12:A:2023:HOH:O	2.20	0.41
4:A:1656:FAD:H1'1	4:A:1656:FAD:H9	1.62	0.41
2:B:227:LYS:HD3	2:B:227:LYS:HA	1.95	0.41
3:C:222:VAL:O	3:C:226:LEU:HG	2.21	0.41
1:D:49:GLY:HA2	1:D:139[A]:ARG:NH2	2.35	0.41
1:D:52:GLN:HG2	1:D:69:HIS:CE1	2.54	0.41
2:E:146:PHE:O	2:E:150:ARG:HG3	2.21	0.41
3:F:17:ARG:O	3:F:17:ARG:HG2	2.21	0.41
3:F:222:VAL:O	3:F:226:LEU:HG	2.21	0.41
3:C:60:TRP:CZ2	3:C:64:LYS:HD2	2.55	0.41
1:D:455:VAL:HG13	1:D:509:LYS:HD3	2.03	0.41
3:F:63:LYS:HE2	3:F:68:ASP:OD2	2.20	0.41
1:D:52:GLN:HB3	1:D:408:ASN:HD22	1.87	0.40
1:D:496:GLU:O	1:D:500:LYS:HG3	2.21	0.40
2:B:20:LYS:HE3	3:F:16[B]:GLU:HA	2.03	0.40
3:C:169:TRP:N	3:C:170:PRO:CD	2.84	0.40
3:C:189:ARG:HA	3:C:192:VAL:HG22	2.02	0.40
1:D:531:LEU:O	1:D:535:LYS:HB3	2.21	0.40
2:E:220:LYS:HE2	2:E:220:LYS:HA	2.03	0.40
1:A:22:VAL:O	1:A:26:GLN:HG2	2.21	0.40
1:D:489:LYS:HE2	1:D:489:LYS:HB3	1.95	0.40
1:A:52:GLN:HG2	1:A:69:HIS:CE1	2.56	0.40
1:D:29:LEU:O	1:D:31:THR:HG22	2.21	0.40
1:D:341:ASN:HB2	1:D:342:LEU:HD12	2.04	0.40
1:D:398:ASP:OD2	1:D:563:ARG:NE	2.47	0.40
3:F:108:TYR:HD2	11:F:1257:LMT:H52	1.87	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	659/660 (100%)	634 (96%)	21 (3%)	4 (1%)	21	9
1	D	657/660 (100%)	631 (96%)	22 (3%)	4 (1%)	21	9
2	B	239/241 (99%)	227 (95%)	8 (3%)	4 (2%)	7	1
2	E	239/241 (99%)	227 (95%)	8 (3%)	4 (2%)	7	1
3	C	255/256 (100%)	247 (97%)	7 (3%)	1 (0%)	30	16
3	F	255/256 (100%)	247 (97%)	7 (3%)	1 (0%)	30	16
All	All	2304/2314 (100%)	2213 (96%)	73 (3%)	18 (1%)	16	6

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
2	B	86	ASP
3	C	72	GLU
1	D	121	ALA
2	E	86	ASP
3	F	72	GLU
1	A	123	LYS
2	B	3	ARG
1	D	123	LYS
2	E	3	ARG
1	A	269	THR
2	B	239	ASN
1	D	269	THR
2	E	2	GLY
2	E	239	ASN
1	A	122	GLN
2	B	2	GLY
1	D	122	GLN

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	537/537 (100%)	524 (98%)	13 (2%)	43	24
1	D	535/537 (100%)	524 (98%)	11 (2%)	47	27
2	B	212/213 (100%)	210 (99%)	2 (1%)	70	59
2	E	212/213 (100%)	210 (99%)	2 (1%)	70	59
3	C	223/223 (100%)	218 (98%)	5 (2%)	45	26
3	F	223/223 (100%)	218 (98%)	5 (2%)	45	26
All	All	1942/1946 (100%)	1904 (98%)	38 (2%)	50	29

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

Mol	Chain	Res	Type
1	A	2[A]	LYS
1	A	2[B]	LYS
1	A	31	THR
1	A	52	GLN
1	A	95	LYS
1	A	137	HIS
1	A	297	GLU
1	A	403	ASN
1	A	404	ARG
1	A	497	LEU
1	A	562	ASN
1	A	611	LYS
1	A	641	GLU
2	B	164	LYS
2	B	193	GLU
3	C	4	GLU
3	C	18	LYS
3	C	82	LEU
3	C	100	LYS
3	C	106	ARG
1	D	31	THR
1	D	52	GLN

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Mol	Chain	Res	Type
1	D	95	LYS
1	D	137	HIS
1	D	263	PRO
1	D	403	ASN
1	D	404	ARG
1	D	497	LEU
1	D	562	ASN
1	D	611	LYS
1	D	641	GLU
2	E	164	LYS
2	E	193	GLU
3	F	4	GLU
3	F	18	LYS
3	F	82	LEU
3	F	100	LYS
3	F	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	48	GLN
1	A	57	ASN
1	A	91	ASN
1	A	120	ASN
1	A	133	HIS
1	A	225	ASN
1	A	228	ASN
1	A	247	GLN
1	A	257	HIS
1	A	319	GLN
1	A	325	HIS
1	A	341	ASN
1	A	403	ASN
1	A	408	ASN
1	A	430	ASN
1	A	468	ASN
1	A	547	HIS
1	A	562	ASN
1	A	586	ASN
1	A	602	ASN
1	A	631	HIS

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Mol	Chain	Res	Type
2	B	24	GLN
2	B	123	HIS
2	B	177	ASN
3	C	107	GLN
1	D	26	GLN
1	D	48	GLN
1	D	57	ASN
1	D	91	ASN
1	D	120	ASN
1	D	133	HIS
1	D	225	ASN
1	D	228	ASN
1	D	247	GLN
1	D	257	HIS
1	D	325	HIS
1	D	341	ASN
1	D	403	ASN
1	D	408	ASN
1	D	430	ASN
1	D	468	ASN
1	D	547	HIS
1	D	562	ASN
1	D	586	ASN
1	D	602	ASN
1	D	631	HIS
2	E	24	GLN
2	E	116	GLN
2	E	123	HIS
2	E	177	ASN
3	F	107	GLN
3	F	150	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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
9	SF4	E	1242	2	0,12,12	-	-	-		
8	F3S	B	1241	2	0,9,9	-	-	-		
7	FES	E	1240	2	0,4,4	-	-	-		
10	HEM	C	1255	3	50,50,50	1.35	7 (14%)	67,82,82	0.74	0
5	FUM	A	1657	-	7,7,7	1.18	1 (14%)	8,8,8	0.71	0
10	HEM	F	1255	3	50,50,50	1.34	8 (16%)	67,82,82	0.76	1 (1%)
8	F3S	E	1241	2	0,9,9	-	-	-		
7	FES	B	1240	2	0,4,4	-	-	-		
4	FAD	A	1656	1	58,58,58	2.02	15 (25%)	85,89,89	1.23	7 (8%)
11	LMT	F	1257	-	36,36,36	1.10	2 (5%)	47,47,47	1.29	4 (8%)
11	LMT	C	1257	-	36,36,36	1.09	2 (5%)	47,47,47	1.28	4 (8%)
10	HEM	F	1256	3	50,50,50	1.33	7 (14%)	67,82,82	0.93	3 (4%)
5	FUM	D	1657	-	7,7,7	1.17	0	8,8,8	0.69	0
4	FAD	D	1656	1	58,58,58	1.98	12 (20%)	85,89,89	1.23	6 (7%)
9	SF4	B	1242	2	0,12,12	-	-	-		
10	HEM	C	1256	3	50,50,50	1.35	7 (14%)	67,82,82	0.93	3 (4%)

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
9	SF4	E	1242	2	-	-	0/6/5/5
8	F3S	B	1241	2	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEM	F	1255	3	-	0/14/54/54	-
10	HEM	C	1255	3	-	0/14/54/54	-
5	FUM	A	1657	-	-	0/5/5/5	-
7	FES	E	1240	2	-	-	0/1/1/1
8	F3S	E	1241	2	-	-	0/3/3/3
7	FES	B	1240	2	-	-	0/1/1/1
4	FAD	A	1656	1	-	3/34/50/50	0/6/6/6
11	LMT	F	1257	-	-	12/21/61/61	0/2/2/2
11	LMT	C	1257	-	-	12/21/61/61	0/2/2/2
10	HEM	F	1256	3	-	4/14/54/54	-
5	FUM	D	1657	-	-	0/5/5/5	-
4	FAD	D	1656	1	-	3/34/50/50	0/6/6/6
9	SF4	B	1242	2	-	-	0/6/5/5
10	HEM	C	1256	3	-	4/14/54/54	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1656	FAD	P-O3P	-9.22	1.49	1.59
4	A	1656	FAD	P-O3P	-8.86	1.49	1.59
4	D	1656	FAD	C1'-C2'	4.01	1.58	1.52
4	A	1656	FAD	PA-O2A	-3.89	1.37	1.55
4	A	1656	FAD	C1'-C2'	3.87	1.58	1.52
4	D	1656	FAD	PA-O2A	-3.85	1.37	1.55
4	A	1656	FAD	O5'-C5'	3.79	1.59	1.44
4	D	1656	FAD	O5'-C5'	3.71	1.58	1.44
10	C	1256	HEM	FE-NB	3.60	2.06	1.94
10	F	1255	HEM	FE-NB	3.56	2.05	1.94
10	F	1256	HEM	FE-NA	3.45	2.06	1.95
4	A	1656	FAD	P-O2P	-3.41	1.39	1.55
10	C	1255	HEM	FE-NC	3.38	2.06	1.95
11	F	1257	LMT	O5B-C1B	3.31	1.50	1.41
11	C	1257	LMT	O5B-C1B	3.27	1.50	1.41
10	F	1255	HEM	CBC-CAC	3.24	1.46	1.30
10	C	1256	HEM	CBC-CAC	3.24	1.46	1.30
10	C	1256	HEM	FE-NC	3.18	2.05	1.95
10	C	1255	HEM	CBC-CAC	3.17	1.45	1.30
10	F	1256	HEM	CBB-CAB	3.14	1.45	1.30
10	C	1255	HEM	FE-ND	3.13	2.04	1.94
10	F	1255	HEM	CBB-CAB	3.11	1.45	1.30
10	F	1256	HEM	CBC-CAC	3.10	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	1256	HEM	CBB-CAB	3.07	1.45	1.30
10	F	1256	HEM	FE-ND	3.04	2.04	1.94
4	D	1656	FAD	P-O2P	-3.04	1.41	1.55
10	C	1255	HEM	CBB-CAB	3.03	1.44	1.30
10	F	1255	HEM	FE-NA	3.03	2.05	1.95
10	C	1255	HEM	FE-NB	2.97	2.04	1.94
10	F	1256	HEM	CAB-C3B	-2.93	1.39	1.47
11	F	1257	LMT	C3'-C4'	2.92	1.60	1.52
4	A	1656	FAD	O2-C2	-2.90	1.18	1.24
11	C	1257	LMT	C3'-C4'	2.88	1.60	1.52
4	D	1656	FAD	O2-C2	-2.85	1.18	1.24
10	C	1256	HEM	CAB-C3B	-2.84	1.39	1.47
10	C	1256	HEM	FE-NA	2.81	2.04	1.95
4	D	1656	FAD	C4X-N5	2.67	1.36	1.30
10	F	1255	HEM	FE-ND	2.66	2.03	1.94
10	C	1256	HEM	CAC-C3C	-2.62	1.40	1.47
10	F	1256	HEM	CAC-C3C	-2.59	1.40	1.47
10	C	1255	HEM	CAC-C3C	-2.57	1.40	1.47
10	F	1255	HEM	CAC-C3C	-2.56	1.40	1.47
10	F	1256	HEM	FE-NC	2.54	2.03	1.95
10	C	1255	HEM	CAB-C3B	-2.54	1.40	1.47
4	A	1656	FAD	C4A-N3A	2.48	1.39	1.34
4	A	1656	FAD	C4X-N5	2.44	1.36	1.30
4	A	1656	FAD	C5A-C6A	2.36	1.47	1.41
4	A	1656	FAD	O4B-C1B	2.35	1.47	1.42
4	A	1656	FAD	C6-C5X	2.34	1.43	1.40
4	D	1656	FAD	C4A-N3A	2.31	1.38	1.34
4	D	1656	FAD	C5A-C6A	2.30	1.47	1.41
4	A	1656	FAD	C8-C7	2.25	1.46	1.40
4	D	1656	FAD	C6-C5X	2.25	1.43	1.40
4	D	1656	FAD	O4B-C1B	2.24	1.47	1.42
4	A	1656	FAD	C9A-N10	2.22	1.45	1.41
10	F	1255	HEM	CAB-C3B	-2.21	1.41	1.47
4	A	1656	FAD	C2A-N1A	2.20	1.37	1.33
10	F	1255	HEM	CMB-C2B	2.10	1.55	1.50
4	D	1656	FAD	C8-C7	2.03	1.45	1.40
4	A	1656	FAD	C2-N3	2.02	1.43	1.39
5	A	1657	FUM	C5-C4	2.02	1.39	1.33

All (28) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	1257	LMT	C1-O1'-C1'	4.94	122.11	113.68
11	C	1257	LMT	C1-O1'-C1'	4.88	122.02	113.68
4	D	1656	FAD	C1'-N10-C9A	-4.32	112.23	120.63
4	A	1656	FAD	C1'-N10-C9A	-4.30	112.27	120.63
10	F	1256	HEM	CAD-C3D-C4D	3.71	131.16	124.70
10	C	1256	HEM	CAD-C3D-C4D	3.58	130.93	124.70
11	C	1257	LMT	C3'-C4'-C5'	-3.39	103.41	110.93
11	F	1257	LMT	C3'-C4'-C5'	-3.38	103.43	110.93
10	F	1256	HEM	CAD-C3D-C2D	-3.33	121.64	127.87
10	C	1256	HEM	CAD-C3D-C2D	-3.28	121.72	127.87
4	A	1656	FAD	C5'-C4'-C3'	-3.26	106.06	112.22
4	D	1656	FAD	O4B-C1B-N9A	-3.26	101.83	108.09
4	A	1656	FAD	O4B-C1B-N9A	-3.24	101.87	108.09
4	D	1656	FAD	C5'-C4'-C3'	-3.17	106.24	112.22
11	C	1257	LMT	O1'-C1'-C2'	-2.67	104.21	108.27
11	F	1257	LMT	O1'-C1'-C2'	-2.66	104.23	108.27
4	D	1656	FAD	C2A-N1A-C6A	2.58	122.96	118.73
4	A	1656	FAD	C2A-N1A-C6A	2.51	122.86	118.73
10	C	1256	HEM	CBA-CAA-C2A	2.34	119.01	112.53
4	A	1656	FAD	C4'-C3'-C2'	-2.23	109.87	113.57
10	F	1255	HEM	CAC-C3C-C4C	2.17	130.01	124.82
4	A	1656	FAD	C4-N3-C2	-2.17	121.80	125.64
10	F	1256	HEM	CBA-CAA-C2A	2.16	118.51	112.53
11	C	1257	LMT	O1B-C4'-C3'	2.16	112.72	107.23
11	F	1257	LMT	O1B-C4'-C3'	2.15	112.69	107.23
4	A	1656	FAD	O3'-C3'-C2'	2.10	113.71	108.93
4	D	1656	FAD	C4-N3-C2	-2.10	121.91	125.64
4	D	1656	FAD	C4'-C3'-C2'	-2.02	110.21	113.57

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1656	FAD	PA-O3P-P-O5'
4	D	1656	FAD	PA-O3P-P-O5'
11	C	1257	LMT	C2'-C1'-O1'-C1
11	F	1257	LMT	C2'-C1'-O1'-C1
11	C	1257	LMT	C4'-C5'-C6'-O6'
11	F	1257	LMT	C4'-C5'-C6'-O6'
11	C	1257	LMT	O5'-C5'-C6'-O6'

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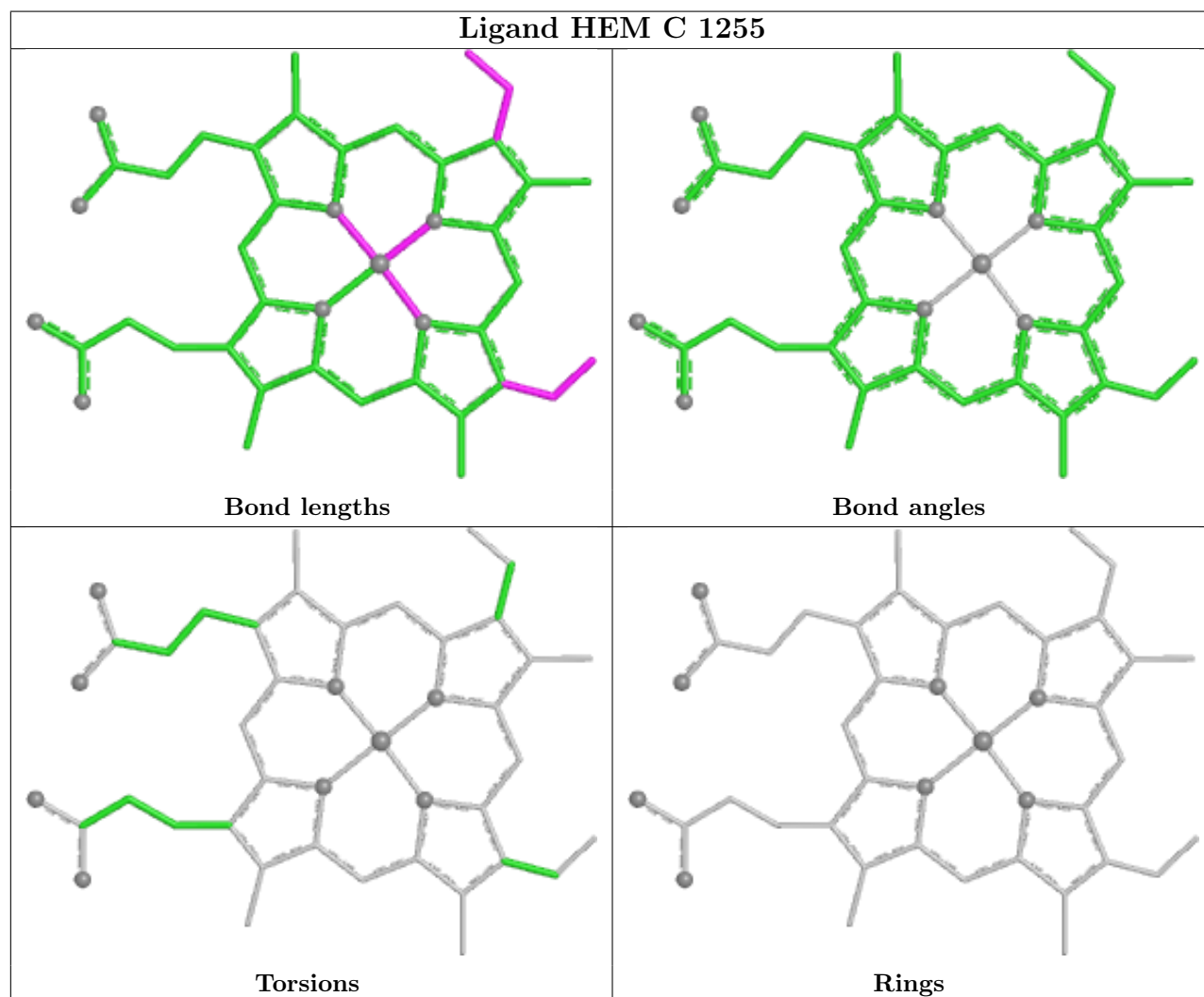
Mol	Chain	Res	Type	Atoms
11	F	1257	LMT	O5'-C5'-C6'-O6'
11	C	1257	LMT	O5'-C1'-O1'-C1
11	F	1257	LMT	O5'-C1'-O1'-C1
11	C	1257	LMT	O1'-C1-C2-C3
11	F	1257	LMT	O1'-C1-C2-C3
11	C	1257	LMT	C7-C8-C9-C10
11	F	1257	LMT	C7-C8-C9-C10
11	F	1257	LMT	C11-C10-C9-C8
11	C	1257	LMT	C11-C10-C9-C8
10	C	1256	HEM	C2B-C3B-CAB-CBB
10	C	1256	HEM	C2C-C3C-CAC-CBC
10	F	1256	HEM	C2B-C3B-CAB-CBB
10	F	1256	HEM	C2C-C3C-CAC-CBC
4	A	1656	FAD	P-O3P-PA-O2A
4	D	1656	FAD	P-O3P-PA-O2A
11	F	1257	LMT	C5'-C4'-O1B-C1B
11	C	1257	LMT	C5'-C4'-O1B-C1B
11	C	1257	LMT	C2B-C1B-O1B-C4'
11	F	1257	LMT	C2B-C1B-O1B-C4'
4	D	1656	FAD	P-O3P-PA-O1A
11	C	1257	LMT	O5B-C1B-O1B-C4'
11	F	1257	LMT	O5B-C1B-O1B-C4'
11	F	1257	LMT	C9-C10-C11-C12
11	C	1257	LMT	C9-C10-C11-C12
4	A	1656	FAD	P-O3P-PA-O1A
10	C	1256	HEM	C4B-C3B-CAB-CBB
10	C	1256	HEM	C4C-C3C-CAC-CBC
10	F	1256	HEM	C4B-C3B-CAB-CBB
10	F	1256	HEM	C4C-C3C-CAC-CBC
11	F	1257	LMT	C3'-C4'-O1B-C1B
11	C	1257	LMT	C3'-C4'-O1B-C1B

There are no ring outliers.

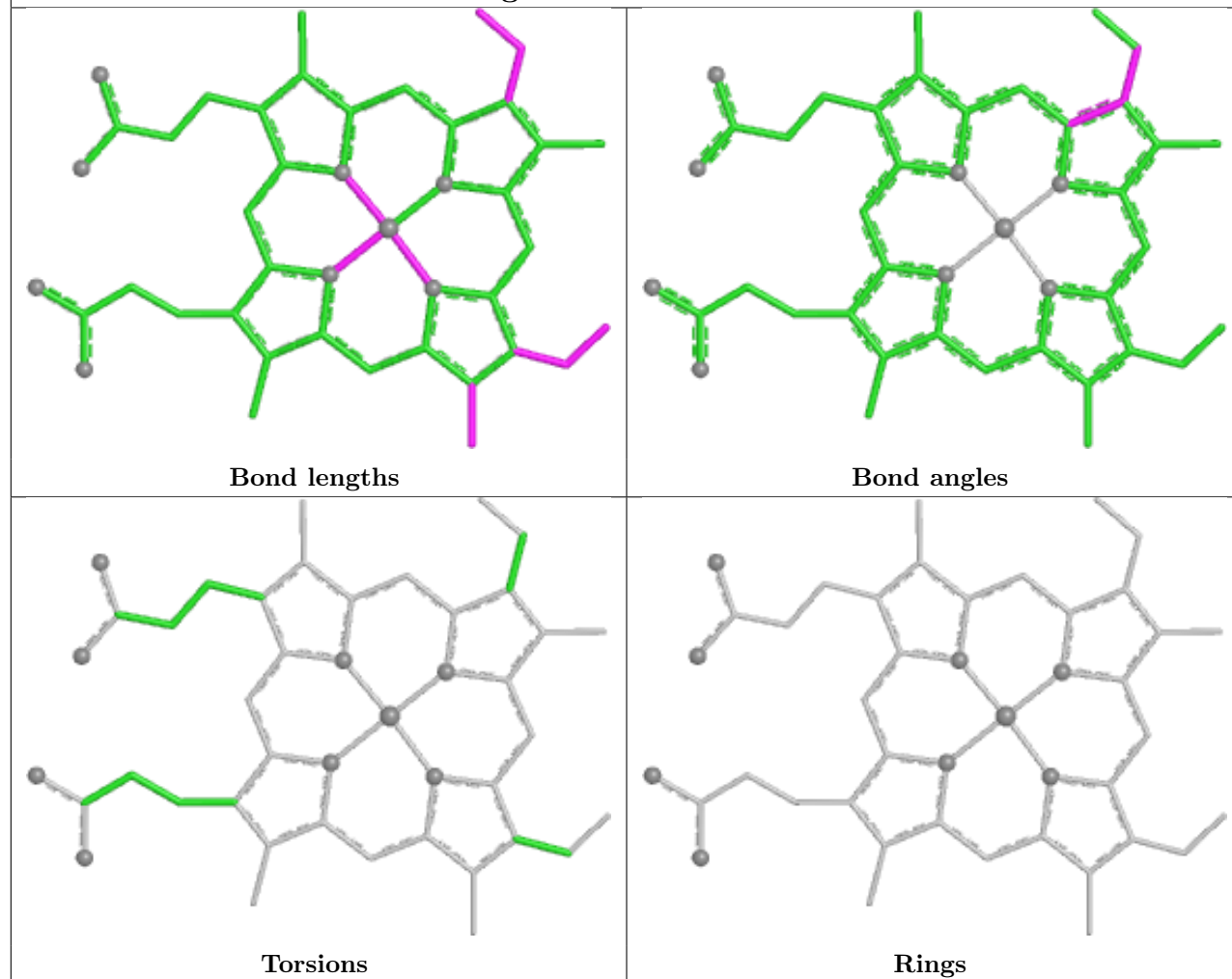
6 monomers are involved in 25 short contacts:

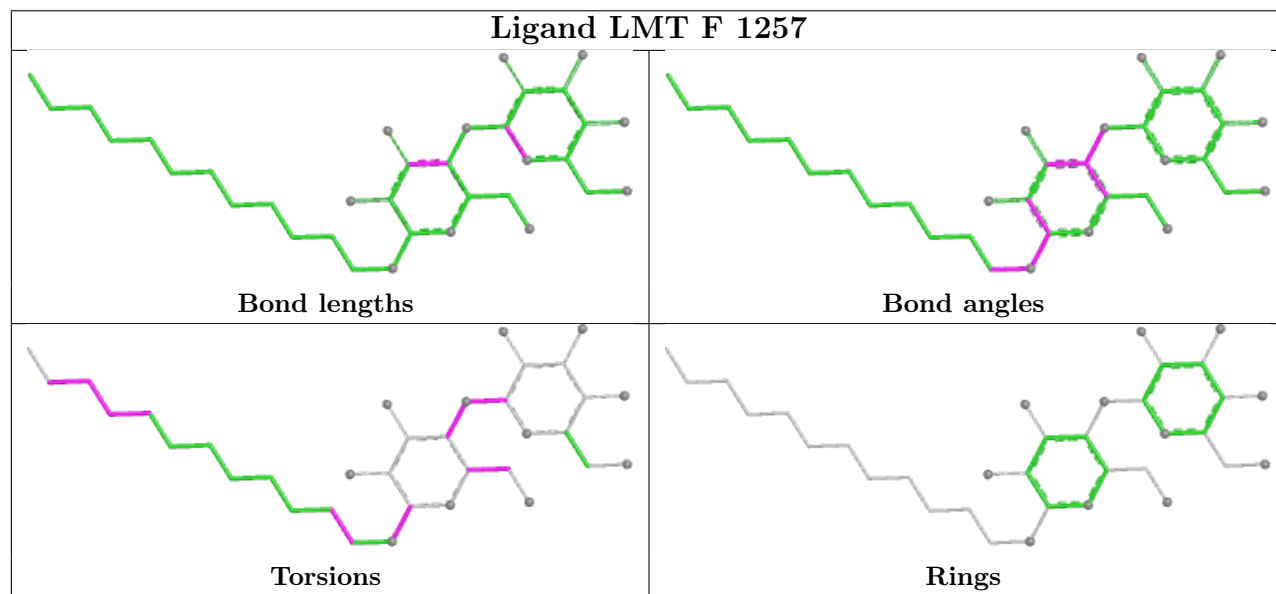
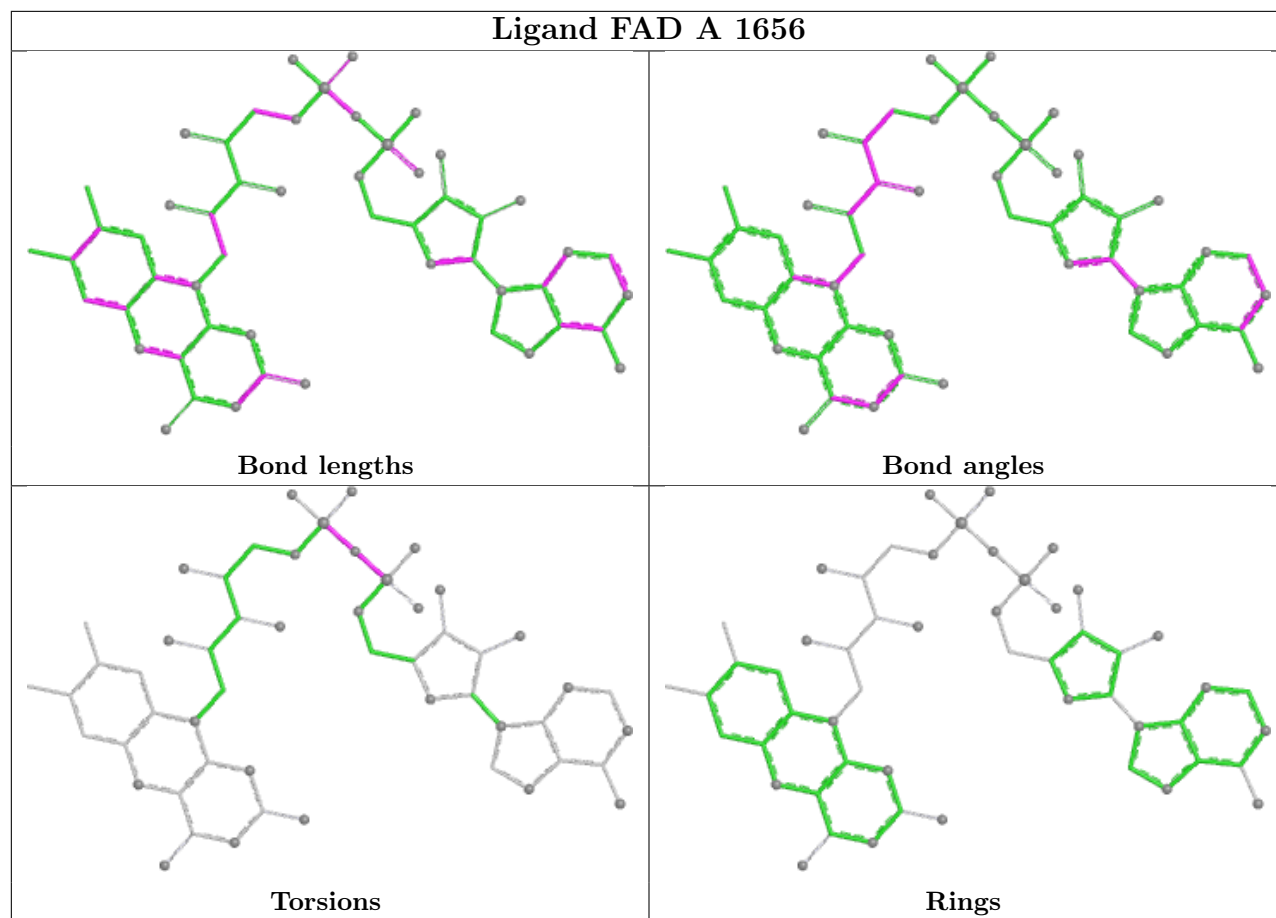
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1656	FAD	3	0
11	F	1257	LMT	9	0
11	C	1257	LMT	8	0
10	F	1256	HEM	1	0
4	D	1656	FAD	3	0
10	C	1256	HEM	1	0

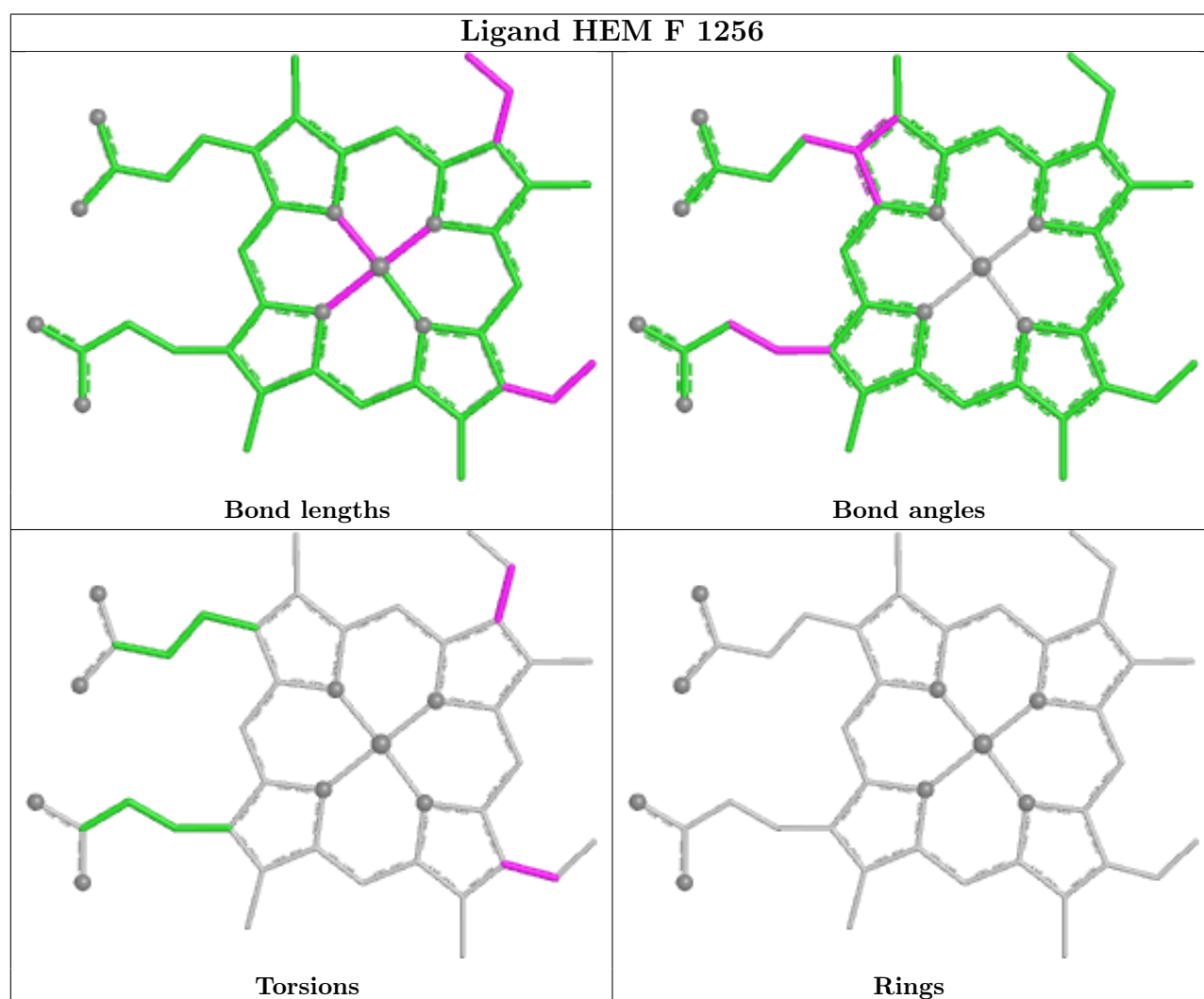
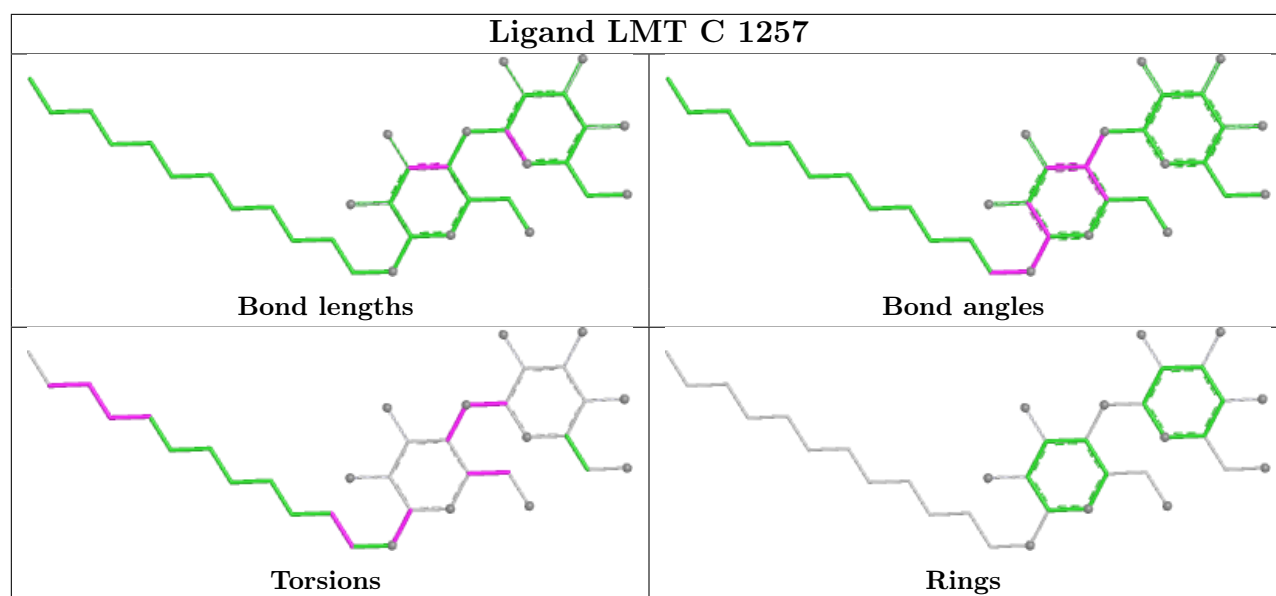
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

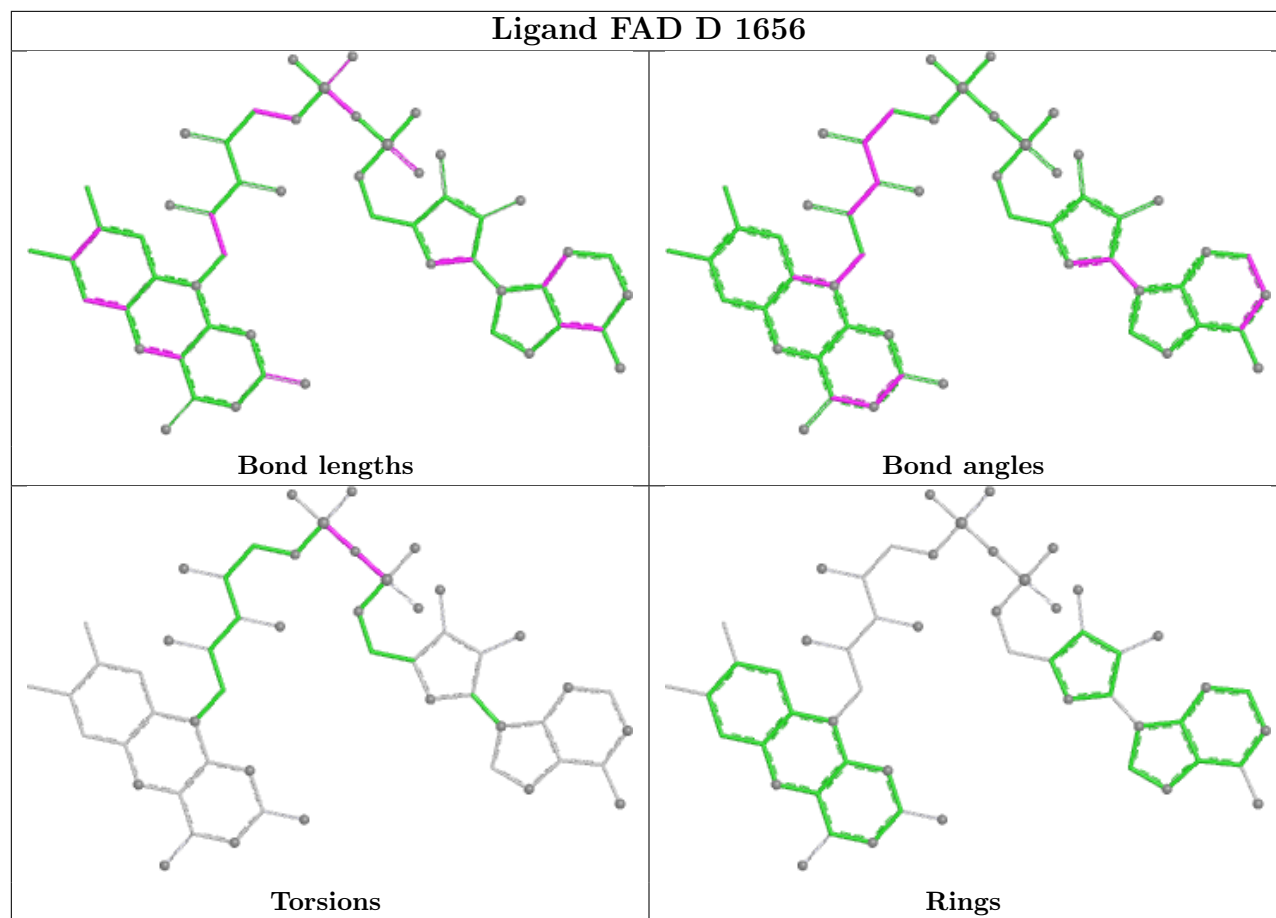


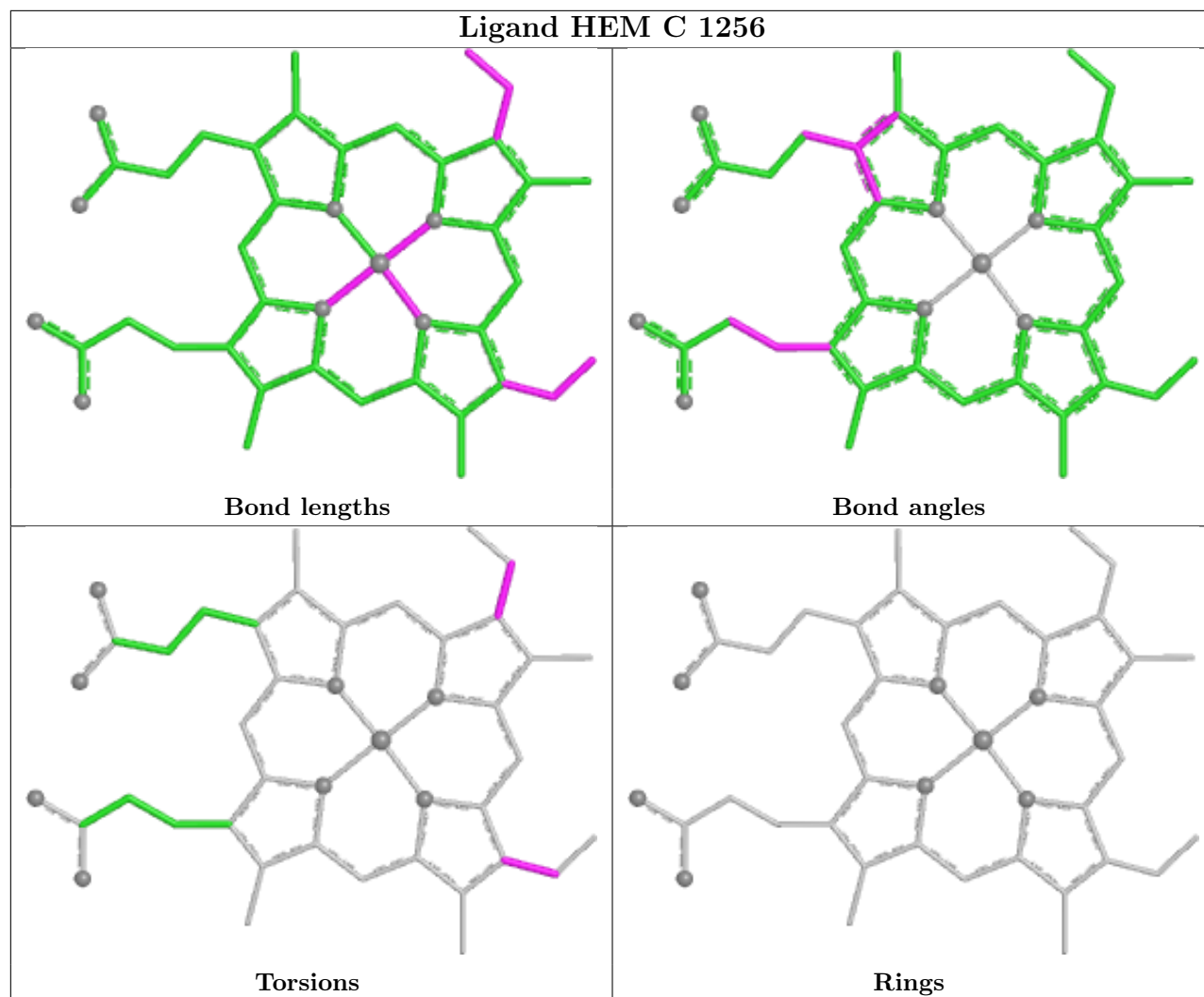
Ligand HEM F 1255











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	656/660 (99%)	1.18	141 (21%)	2 2	16, 33, 68, 80	19 (2%)
1	D	656/660 (99%)	1.27	151 (23%)	2 2	16, 33, 68, 80	19 (2%)
2	B	240/241 (99%)	0.76	25 (10%)	11 13	11, 29, 50, 74	3 (1%)
2	E	240/241 (99%)	0.78	35 (14%)	6 6	11, 28, 50, 74	3 (1%)
3	C	255/256 (99%)	2.07	114 (44%)	0 0	20, 43, 75, 91	13 (5%)
3	F	255/256 (99%)	2.00	106 (41%)	0 0	19, 42, 75, 90	12 (4%)
All	All	2302/2314 (99%)	1.31	572 (24%)	2 2	11, 33, 68, 91	69 (2%)

All (572) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	338	ILE	10.7
1	D	342	LEU	9.7
2	B	2	GLY	9.0
3	F	253	THR	8.6
1	D	121	ALA	7.9
3	F	243	ILE	7.7
1	D	599	ALA	7.5
1	A	597	TYR	7.5
3	C	69	PHE	7.5
3	F	69	PHE	7.1
3	C	255	GLU	7.0
1	A	124	THR	7.0
2	E	2	GLY	6.8
1	A	351	TYR	6.5
1	A	123	LYS	6.4
1	A	121	ALA	6.4
1	A	342	LEU	6.3
3	C	59	LEU	6.3
3	C	67	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	119	ILE	6.2
1	A	338	ILE	6.2
3	C	77	ILE	6.1
1	D	340	THR	6.0
1	A	333	LEU	5.9
1	D	123	LYS	5.9
3	F	60	TRP	5.8
3	C	236	LEU	5.8
3	F	47	PHE	5.8
3	C	254	HIS	5.8
1	D	597	TYR	5.8
1	D	117	ALA	5.7
1	D	355	ILE	5.7
1	A	332	ILE	5.6
1	D	124	THR	5.6
1	D	118	ILE	5.6
1	D	358	ALA	5.5
1	D	598	GLY	5.5
3	C	250	TYR	5.5
1	A	619	ILE	5.5
3	C	56	ASN	5.4
1	A	118	ILE	5.4
3	F	68	ASP	5.4
3	C	60	TRP	5.4
1	D	341	ASN	5.4
3	C	247	TYR	5.4
3	F	250	TYR	5.4
3	F	67	LEU	5.3
1	A	117	ALA	5.3
3	C	72	GLU	5.3
2	B	240	MET	5.3
3	C	243	ILE	5.2
3	F	251	LYS	5.2
2	B	85	GLU	5.2
1	D	126	ILE	5.1
3	C	53	LEU	5.1
1	A	353	ALA	5.1
1	A	116	MET	5.1
1	D	611	LYS	5.1
1	A	122	GLN	5.1
3	C	253	THR	5.1
3	F	59	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	1	MET	5.0
1	D	337	HIS	5.0
3	F	70	ILE	5.0
3	F	77	ILE	5.0
3	F	236	LEU	5.0
3	C	161	PHE	4.9
3	F	76	PRO	4.9
1	D	626	ALA	4.9
1	A	616	ILE	4.9
3	C	70	ILE	4.9
3	C	157	VAL	4.9
3	C	252	ARG	4.9
3	F	252	ARG	4.9
3	C	63	LYS	4.8
1	D	344	ASP	4.8
3	F	74	GLY	4.8
1	A	348	ILE	4.8
1	D	271	GLY	4.8
3	F	249	ASP	4.7
3	F	157	VAL	4.7
3	F	71	PHE	4.7
1	A	623	LEU	4.7
3	F	246	LYS	4.6
1	A	344	ASP	4.6
3	C	245	TYR	4.6
1	A	355	ILE	4.6
1	A	621	SER	4.6
1	D	351	TYR	4.5
1	D	623	LEU	4.5
3	C	239	THR	4.5
3	C	81	PHE	4.5
1	A	345	VAL	4.5
1	D	348	ILE	4.5
3	C	251	LYS	4.5
1	D	357	PRO	4.5
3	C	61	VAL	4.5
3	F	48	VAL	4.5
2	E	31	ALA	4.5
3	C	1	MET	4.5
1	D	115[A]	ARG	4.4
1	D	330	ILE	4.4
3	F	1	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	271	GLY	4.4
1	D	585	VAL	4.4
1	D	125	THR	4.3
3	C	248	PHE	4.3
1	A	268	LEU	4.3
3	F	79	VAL	4.3
1	D	119	ILE	4.3
3	C	51	ILE	4.3
3	F	254	HIS	4.3
3	C	201	THR	4.3
1	A	340	THR	4.2
1	A	620	GLN	4.2
3	F	53	LEU	4.2
1	D	352	PHE	4.2
3	F	72	GLU	4.2
1	D	619	ILE	4.2
3	C	74	GLY	4.2
2	E	1	MET	4.2
1	D	122	GLN	4.2
1	D	343	ARG	4.2
1	D	345	VAL	4.1
1	D	346	GLN	4.1
3	C	242	ASN	4.1
1	A	120	ASN	4.1
3	F	58	MET	4.1
1	D	336	LYS	4.0
1	D	315	GLY	4.0
1	A	316	LYS	4.0
1	D	653	LEU	4.0
2	E	4	MET	4.0
3	F	56	ASN	4.0
1	A	335	ARG	4.0
3	F	248	PHE	4.0
3	C	49	SER	4.0
1	A	599	ALA	4.0
1	A	618	LYS	4.0
3	C	48	VAL	4.0
1	A	113	GLY	4.0
3	F	52	LEU	3.9
3	C	47	PHE	3.9
3	F	65	PHE	3.9
1	D	332	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	269	THR	3.9
1	D	322	TYR	3.9
1	A	358	ALA	3.9
3	F	235	GLY	3.9
2	B	47	TYR	3.9
3	F	57	VAL	3.8
1	D	627	GLY	3.8
1	D	654	GLY	3.8
3	C	52	LEU	3.8
3	C	246	LYS	3.8
3	C	170	PRO	3.8
3	C	65	PHE	3.8
1	A	334	GLY	3.8
1	A	337	HIS	3.8
1	D	116	MET	3.8
3	C	57	VAL	3.8
3	F	224	GLY	3.8
3	C	238	GLN	3.8
1	A	625	ALA	3.8
3	F	231	TYR	3.8
1	D	277	GLY	3.7
2	B	61	ILE	3.7
3	F	61	VAL	3.7
1	A	324	GLN	3.7
3	C	68	ASP	3.7
3	F	244	ASP	3.7
3	F	215	LEU	3.7
3	C	214	THR	3.7
1	A	594	TYR	3.7
3	C	235	GLY	3.7
1	D	312	ILE	3.7
3	F	217	SER	3.7
1	D	604	ILE	3.7
1	D	616	ILE	3.7
3	C	71	PHE	3.6
3	C	222	VAL	3.6
3	F	164	VAL	3.6
3	F	62	THR	3.6
1	A	302	ASP	3.6
3	C	249	ASP	3.6
3	F	247	TYR	3.6
1	A	330	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	625	ALA	3.6
1	A	301	ARG	3.6
3	C	54	GLY	3.6
3	F	75	LYS	3.6
1	A	603	TYR	3.6
1	D	314	LYS	3.6
3	F	63	LYS	3.6
1	A	433	VAL	3.6
1	D	601	GLY	3.6
3	C	232	VAL	3.6
3	C	226	LEU	3.6
3	C	62	THR	3.5
1	A	593	GLY	3.5
1	A	318	VAL	3.5
1	D	635	GLU	3.5
3	C	200	GLU	3.5
3	F	173	LEU	3.5
1	D	120	ASN	3.5
1	D	324	GLN	3.5
1	D	603	TYR	3.5
3	C	241	PRO	3.5
1	D	301	ARG	3.5
3	C	154	ILE	3.4
3	F	51	ILE	3.4
2	E	87	GLY	3.4
1	D	289	PRO	3.4
2	B	31	ALA	3.4
3	C	218	ALA	3.4
3	F	82	LEU	3.4
1	D	610	VAL	3.4
1	A	596	GLY	3.4
3	C	244	ASP	3.4
2	B	239	ASN	3.4
1	A	359	GLU	3.4
1	A	624	GLU	3.4
3	C	58	MET	3.4
3	F	245	TYR	3.3
1	D	114	ASP	3.3
1	A	278	ILE	3.3
3	F	2	THR	3.3
3	F	212	LEU	3.3
3	C	237	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
3	F	255	GLU	3.3
3	F	223	LEU	3.3
3	F	81	PHE	3.3
3	F	228	PHE	3.3
1	A	611	LYS	3.3
3	C	79	VAL	3.3
2	B	86	ASP	3.3
1	D	430	ASN	3.3
1	D	596	GLY	3.3
3	C	158	SER	3.3
1	D	313	ARG	3.3
3	C	83	ALA	3.3
3	F	4	GLU	3.2
3	C	231	TYR	3.2
1	A	269	THR	3.2
1	A	608	LEU	3.2
3	C	164	VAL	3.2
1	A	125	THR	3.2
1	A	322	TYR	3.2
1	D	335	ARG	3.2
3	C	223	LEU	3.2
1	A	341	ASN	3.2
1	D	278	ILE	3.2
3	C	221	ILE	3.2
1	D	333	LEU	3.2
1	A	349	CYS	3.2
1	A	595	ARG	3.2
1	D	56	GLY	3.2
1	D	130	ASP	3.2
1	A	488	GLU	3.2
3	F	205	THR	3.2
1	D	296	LYS	3.1
1	D	621	SER	3.1
1	D	142	GLY	3.1
3	C	219	PHE	3.1
1	D	334	GLY	3.1
1	D	354	GLY	3.1
1	A	626	ALA	3.1
1	D	620	GLN	3.1
1	A	115[A]	ARG	3.1
3	C	167	TRP	3.1
1	D	433	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
3	F	78	VAL	3.1
1	D	615	GLU	3.1
2	B	28	ILE	3.1
1	A	267	LEU	3.1
1	D	112	LYS	3.1
1	D	602	ASN	3.1
3	C	230	ALA	3.1
3	F	218	ALA	3.0
3	F	230	ALA	3.0
3	F	80	SER	3.0
3	C	45	MET	3.0
1	A	343	ARG	3.0
1	A	610	VAL	3.0
1	A	339	GLU	3.0
2	E	85	GLU	3.0
1	A	405	LEU	3.0
3	C	190	LEU	3.0
1	D	398	ASP	3.0
1	D	273	ARG	3.0
1	A	604	ILE	3.0
1	D	306	ARG	3.0
1	A	570	ASN	3.0
3	C	233	LYS	2.9
1	A	653	LEU	2.9
2	B	5	LEU	2.9
2	B	84	PHE	2.9
3	C	240	ASP	2.9
2	B	128	HIS	2.9
1	D	624	GLU	2.9
1	D	594	TYR	2.9
3	F	220	LEU	2.9
1	A	354	GLY	2.9
1	D	321	PRO	2.9
2	E	32	PRO	2.9
3	F	45	MET	2.9
3	F	200	GLU	2.9
3	C	220	LEU	2.9
2	E	130	ILE	2.9
1	D	339	GLU	2.9
3	F	138	PHE	2.8
1	A	504	VAL	2.8
2	B	88	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	655	ASP	2.8
1	D	656	LYS	2.8
3	C	165	SER	2.8
2	E	7	ILE	2.8
1	A	273[A]	ARG	2.8
1	D	397	TRP	2.8
3	C	50	THR	2.8
1	D	356	ASP	2.8
1	D	268	LEU	2.8
1	A	590	ILE	2.8
3	C	168	MET	2.8
1	A	323	GLY	2.8
2	E	84	PHE	2.8
2	E	47	TYR	2.8
1	A	356	ASP	2.8
1	A	274	GLY	2.8
1	A	654	GLY	2.8
1	D	287	PHE	2.7
3	F	46	PHE	2.7
3	F	64	LYS	2.7
2	E	5	LEU	2.7
1	A	434	ASP	2.7
1	A	309	ILE	2.7
3	C	153	THR	2.7
1	A	112	LYS	2.7
3	C	25	LYS	2.7
3	C	76	PRO	2.7
2	E	86	ASP	2.7
1	D	261	LEU	2.7
1	D	267	LEU	2.7
1	D	583	LEU	2.7
3	C	144	LEU	2.7
3	C	212	LEU	2.7
1	A	320	SER	2.7
3	C	2	THR	2.7
3	C	217	SER	2.7
3	C	227	THR	2.7
1	A	294	GLU	2.7
1	A	276	GLY	2.7
3	F	73	GLY	2.7
3	F	242	ASN	2.7
1	A	2[A]	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	83	ASP	2.7
3	F	240	ASP	2.7
3	F	238	GLN	2.7
3	F	222	VAL	2.7
1	A	336	LYS	2.7
3	C	64	LYS	2.7
1	D	293	PRO	2.6
1	D	628	LYS	2.6
3	F	227	THR	2.6
3	F	39	LEU	2.6
1	A	126	ILE	2.6
1	A	285	HIS	2.6
1	A	484	GLY	2.6
1	D	323	GLY	2.6
3	F	155	GLY	2.6
1	D	139[A]	ARG	2.6
1	A	655	ASP	2.6
1	D	298	LEU	2.6
2	B	18	VAL	2.6
3	F	232	VAL	2.6
2	E	124	ALA	2.6
3	C	80	SER	2.6
3	F	158	SER	2.6
1	A	627	GLY	2.6
1	D	113	GLY	2.6
2	E	46	THR	2.6
3	F	239	THR	2.6
1	A	352	PHE	2.6
3	F	197	PHE	2.6
3	C	173	LEU	2.6
1	A	296	LYS	2.6
3	C	146	ILE	2.6
3	C	159	SER	2.6
1	D	488	GLU	2.6
3	C	152	GLN	2.5
3	F	225	LEU	2.5
3	F	226	LEU	2.5
1	A	321	PRO	2.5
1	D	607	PRO	2.5
1	A	277	GLY	2.5
3	C	160	SER	2.5
1	A	503	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	239	ASN	2.5
3	F	119	ARG	2.5
3	F	161	PHE	2.5
1	A	578	LEU	2.5
1	A	346	GLN	2.5
1	A	591	ALA	2.5
1	D	318	VAL	2.5
2	B	32	PRO	2.5
2	E	28	ILE	2.5
1	A	601	GLY	2.5
1	D	270	GLU	2.5
2	B	193	GLU	2.5
3	F	3	ASN	2.5
1	D	481	PHE	2.5
3	C	171	LEU	2.5
1	A	315	GLY	2.5
3	C	75	LYS	2.5
3	C	224	GLY	2.5
3	F	221	ILE	2.5
1	A	139[A]	ARG	2.5
1	A	572	GLU	2.5
3	C	205	THR	2.5
2	E	237	SER	2.5
1	A	586	ASN	2.4
1	A	272	CYS	2.4
3	F	171	LEU	2.4
1	A	306	ARG	2.4
1	D	359	GLU	2.4
2	B	30	GLU	2.4
1	D	480	ILE	2.4
3	F	174	VAL	2.4
1	A	602	ASN	2.4
1	D	350	GLU	2.4
1	D	614	GLU	2.4
1	D	272	CYS	2.4
1	A	261	LEU	2.4
1	A	598	GLY	2.4
1	A	642	LEU	2.4
1	D	274	GLY	2.4
3	C	196	TRP	2.4
3	F	199	GLY	2.4
1	A	141	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	46	PHE	2.4
1	D	300	SER	2.4
3	F	153	THR	2.4
2	E	133	LEU	2.4
3	F	196	TRP	2.4
1	D	310	GLU	2.4
2	E	61	ILE	2.4
2	E	125	GLN	2.3
3	F	49	SER	2.3
1	A	289	PRO	2.3
1	A	635	GLU	2.3
1	D	349	CYS	2.3
1	D	608	LEU	2.3
3	C	225	LEU	2.3
3	F	50	THR	2.3
3	F	149	THR	2.3
1	A	131	PHE	2.3
1	D	319	GLN	2.3
2	B	24	GLN	2.3
1	A	56	GLY	2.3
2	E	193	GLU	2.3
1	D	295	LYS	2.3
1	D	509	LYS	2.3
3	C	131	MET	2.3
1	D	405	LEU	2.3
1	D	497	LEU	2.3
3	C	3	ASN	2.3
2	E	238	VAL	2.3
3	F	152	GLN	2.3
1	A	614	GLU	2.3
1	D	262	PHE	2.3
1	A	647	LYS	2.3
1	D	504	VAL	2.3
3	C	169	TRP	2.2
1	D	553	PRO	2.2
3	C	15	PRO	2.2
3	F	170	PRO	2.2
2	B	46	THR	2.2
2	E	6	THR	2.2
1	D	353	ALA	2.2
2	E	42	MET	2.2
3	C	73	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	285	HIS	2.2
1	A	622	GLU	2.2
3	F	201	THR	2.2
3	F	167	TRP	2.2
3	C	207	ALA	2.2
1	A	489	LYS	2.2
1	D	600	LYS	2.2
3	C	199	GLY	2.2
2	E	168	GLU	2.2
1	D	141	PHE	2.2
3	F	108	TYR	2.2
1	D	309	ILE	2.2
1	D	571	PRO	2.2
1	D	331	SER	2.2
1	A	283	ASP	2.2
2	B	4	MET	2.2
1	D	560	TRP	2.2
1	A	319	GLN	2.2
1	D	279	LEU	2.2
1	D	561	LEU	2.2
1	D	612	ARG	2.2
1	A	291	TYR	2.2
1	A	360	LYS	2.2
2	B	26	TYR	2.2
2	E	126	LYS	2.2
3	F	19	LYS	2.2
1	D	633	ILE	2.2
1	D	639	PRO	2.2
1	A	609	SER	2.2
1	D	71	MET	2.1
3	C	216	MET	2.1
2	E	127	GLU	2.1
1	A	63	GLY	2.1
3	C	140	GLY	2.1
3	F	127	TRP	2.1
1	A	314	LYS	2.1
3	F	25	LYS	2.1
1	D	617	ASP	2.1
3	F	159	SER	2.1
2	E	88	VAL	2.1
3	C	89	VAL	2.1
1	A	27	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	628	LYS	2.1
1	D	360	LYS	2.1
2	E	27	LYS	2.1
1	D	365	LEU	2.1
2	B	133	LEU	2.1
3	C	163	MET	2.1
1	A	398	ASP	2.1
1	A	476	ASP	2.1
1	D	275	ASP	2.1
2	E	24	GLN	2.1
1	D	595	ARG	2.1
1	A	143	GLY	2.1
1	A	295	LYS	2.1
1	A	632	ALA	2.1
2	E	17	ALA	2.1
3	F	88	ALA	2.1
1	D	282	VAL	2.1
2	E	18	VAL	2.1
3	C	78	VAL	2.1
1	D	586	ASN	2.1
3	C	198	ASP	2.1
1	A	431	THR	2.1
3	F	241	PRO	2.1
1	A	147	TRP	2.1
1	D	645	LYS	2.1
3	F	211	LYS	2.1
2	E	26	TYR	2.1
3	C	42	ILE	2.1
3	C	128	ILE	2.1
1	A	430	ASN	2.0
1	A	491	VAL	2.0
3	C	82	LEU	2.0
1	D	127	THR	2.0
1	D	431	THR	2.0
3	C	149	THR	2.0
1	A	59	LYS	2.0
1	A	600	LYS	2.0
3	F	229	GLY	2.0
1	A	361	TRP	2.0
1	D	221	ARG	2.0
2	E	206	PHE	2.0
3	F	85	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	636	ALA	2.0
1	D	434	ASP	2.0
1	D	483	ASP	2.0
1	D	591	ALA	2.0
1	A	331	SER	2.0
1	D	463	VAL	2.0
2	B	27	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
11	LMT	C	1257	35/35	0.68	0.30	59,63,68,69	16
11	LMT	F	1257	35/35	0.74	0.26	59,63,69,69	16
5	FUM	A	1657	8/8	0.75	0.18	42,46,48,50	0
5	FUM	D	1657	8/8	0.81	0.16	43,46,47,48	0
10	HEM	C	1256	43/43	0.94	0.12	38,40,43,45	0
6	NA	D	1658	1/1	0.95	0.07	26,26,26,26	0
10	HEM	F	1256	43/43	0.95	0.10	36,40,43,45	0
4	FAD	D	1656	53/53	0.96	0.07	18,22,25,25	0
10	HEM	C	1255	43/43	0.96	0.09	26,31,34,38	0
10	HEM	F	1255	43/43	0.97	0.09	26,32,35,38	0
4	FAD	A	1656	53/53	0.98	0.05	16,22,25,27	0
8	F3S	E	1241	7/7	0.98	0.04	23,24,25,25	0
7	FES	B	1240	4/4	0.99	0.04	22,22,23,24	0
7	FES	E	1240	4/4	0.99	0.03	21,21,21,23	0
8	F3S	B	1241	7/7	0.99	0.04	24,25,26,27	0
6	NA	A	1658	1/1	0.99	0.04	26,26,26,26	0

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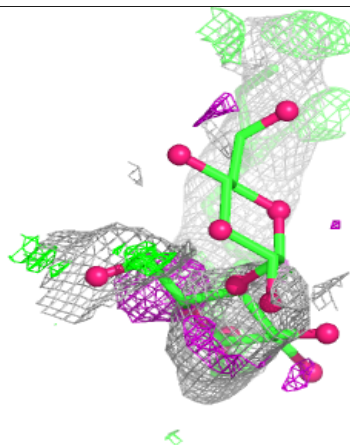
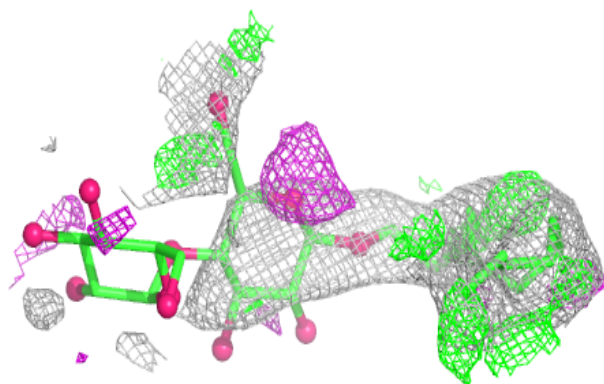
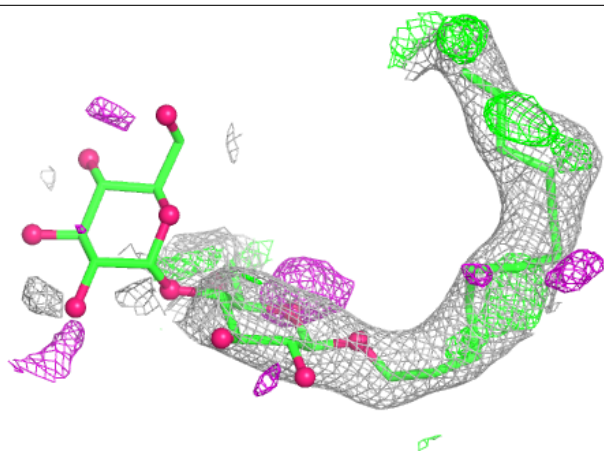
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SF4	B	1242	8/8	0.99	0.03	22,24,25,25	0
9	SF4	E	1242	8/8	0.99	0.03	21,23,23,24	0

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.

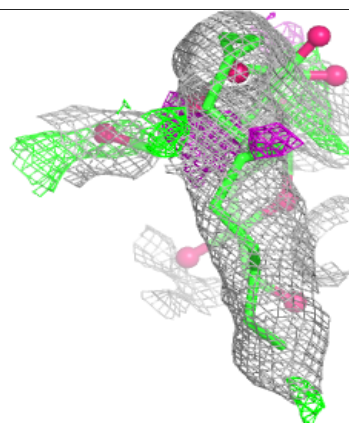
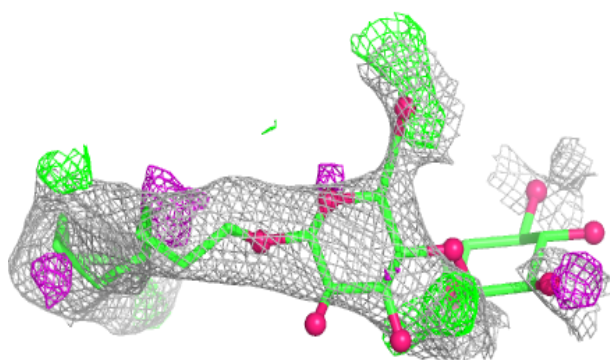
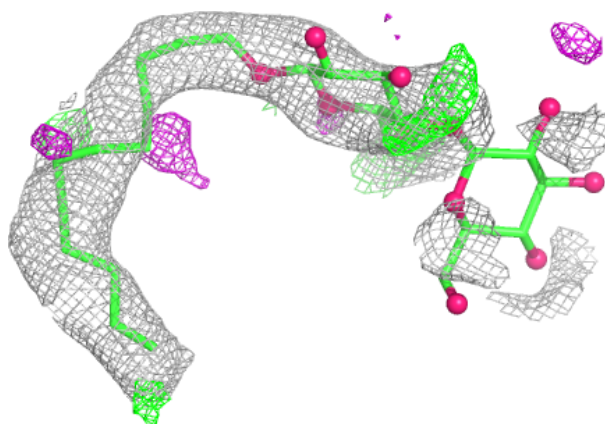
Electron density around LMT C 1257:

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



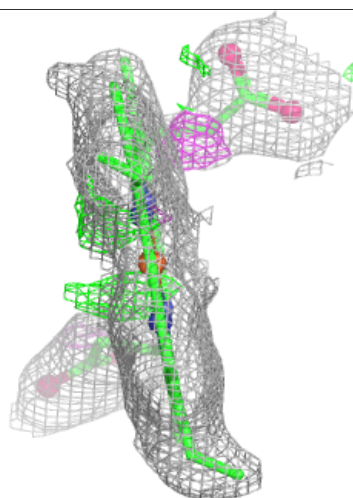
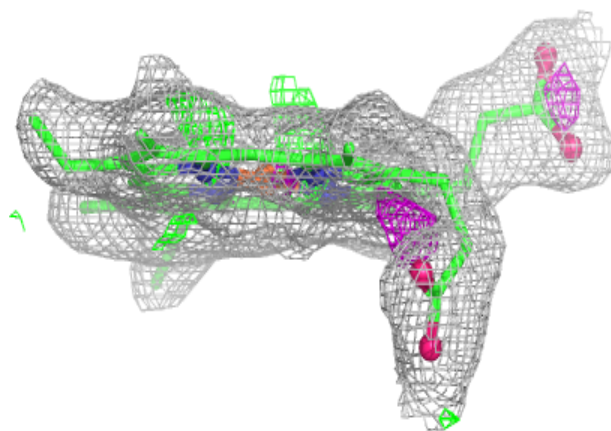
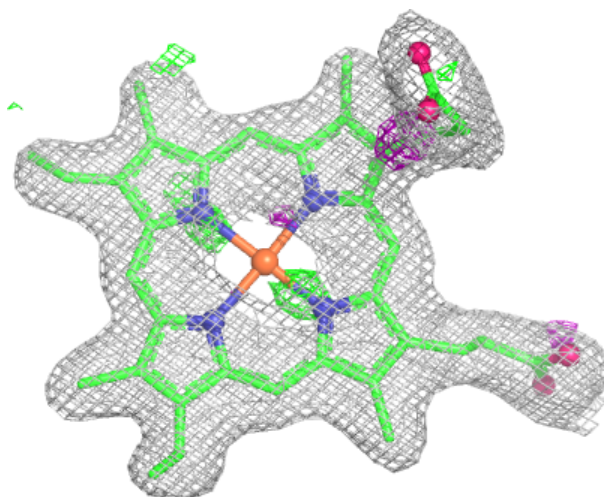
Electron density around LMT F 1257:

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



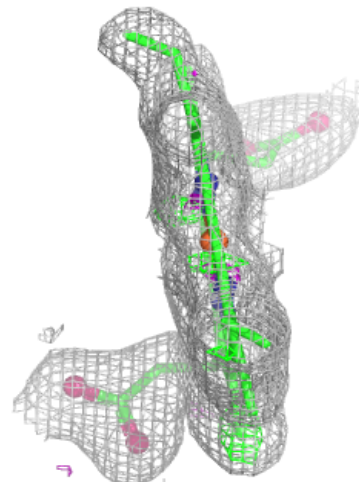
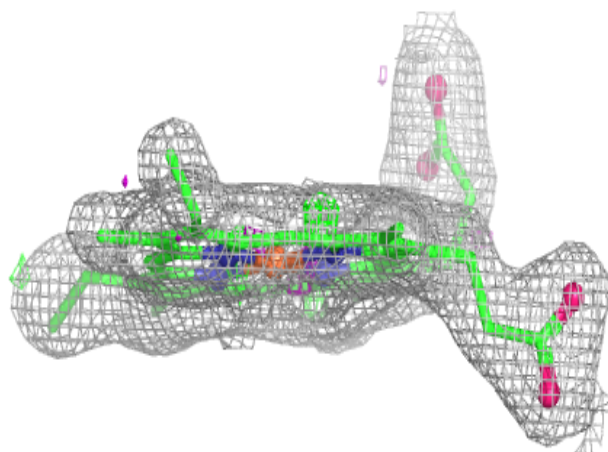
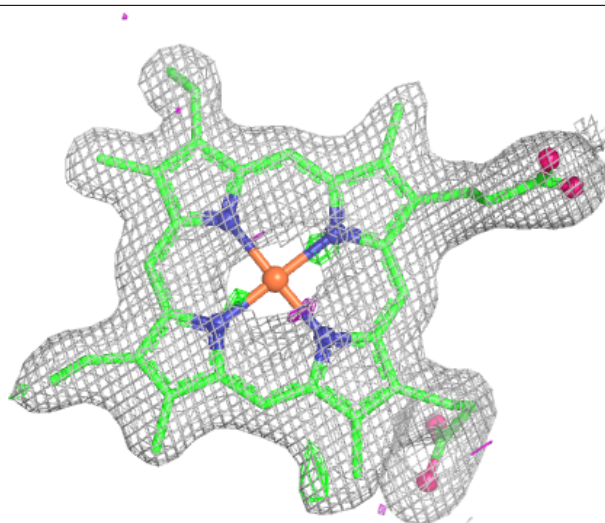
Electron density around HEM C 1256:

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



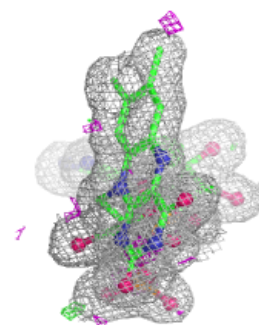
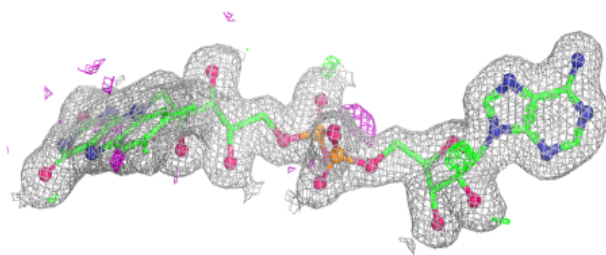
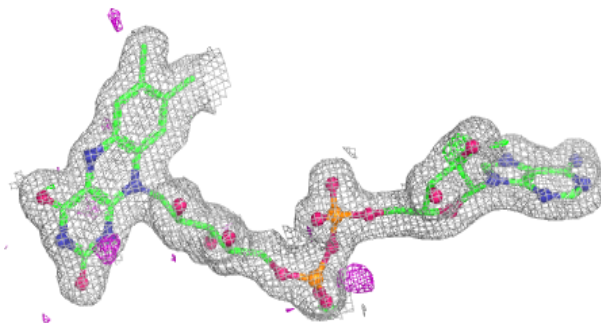
Electron density around HEM F 1256:

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



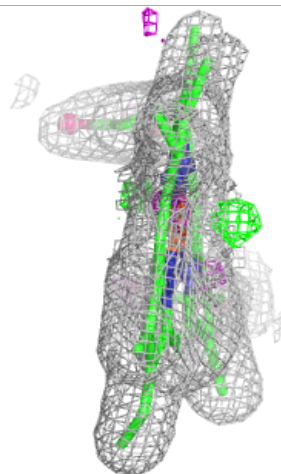
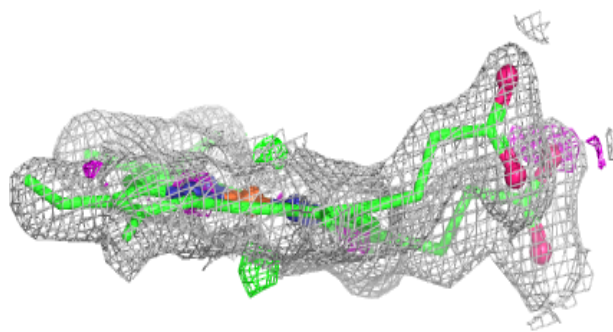
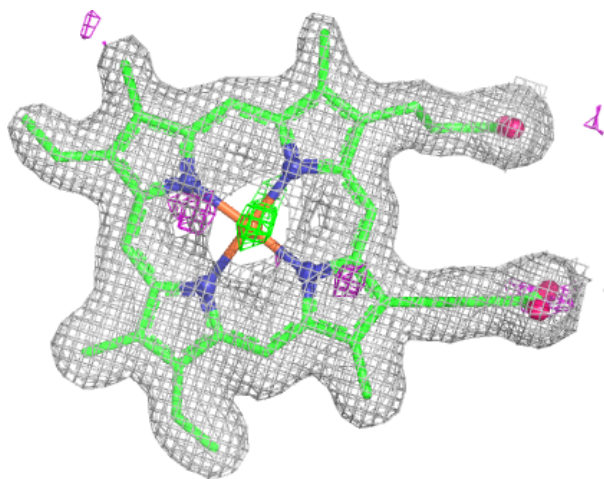
Electron density around FAD D 1656:

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



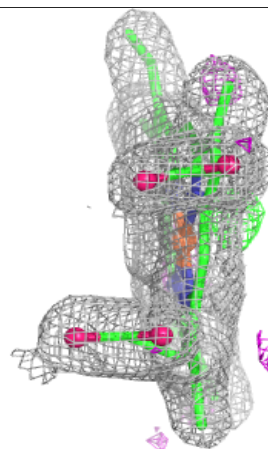
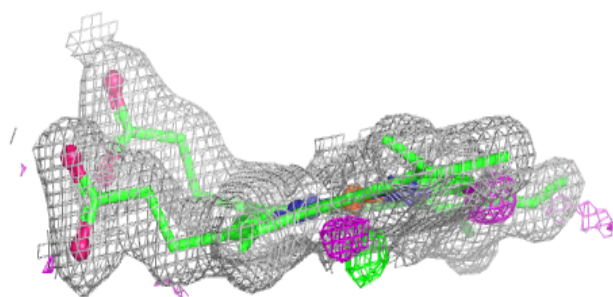
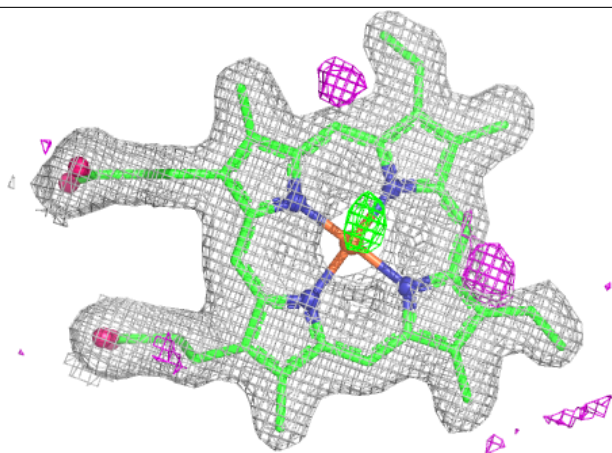
Electron density around HEM C 1255:

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

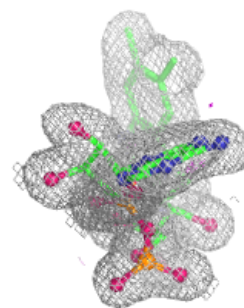
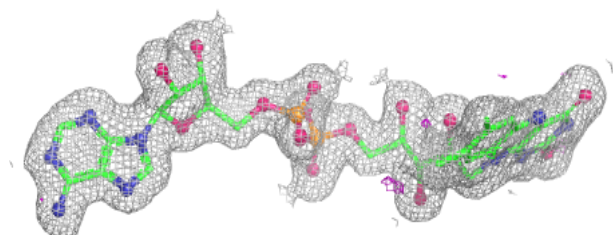
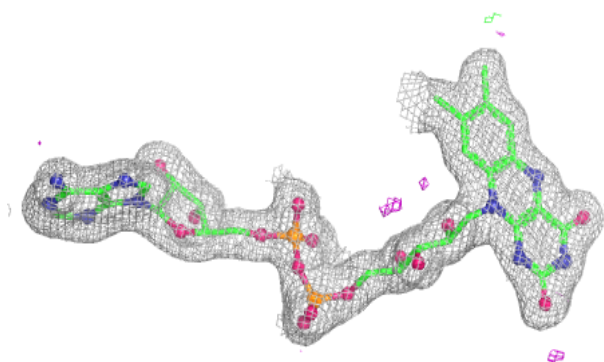


Electron density around HEM F 1255:

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

**Electron density around FAD A 1656:**

$2mF_o-DF_c$ (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.