



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:30 AM UTC

PDB ID : 5C2T / pdb_00005c2t
Title : Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from *Ascaris suum* with rhodoquinone-2
Authors : Harada, S.; Shiba, T.; Sato, D.; Yamamoto, A.; Nagahama, M.; Yone, A.; Inaoka, D.K.; Sakamoto, K.; Inoue, M.; Honma, T.; Kita, K.
Deposited on : 2015-06-16
Resolution : 2.75 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:

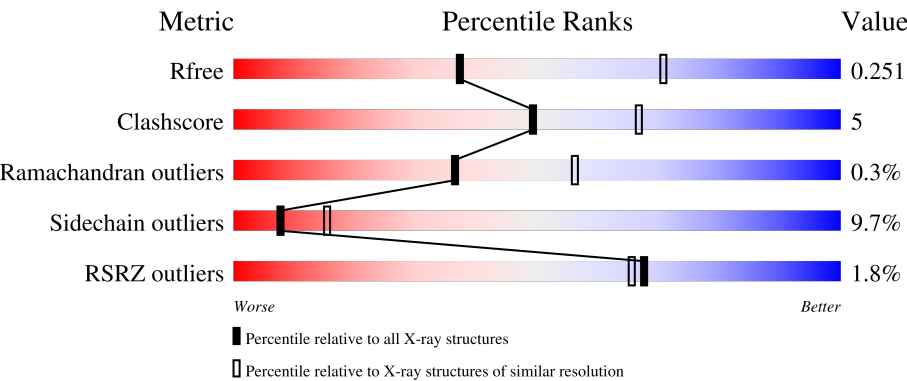
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	645	76%18% . .
1	E	645	2% 74%20% . .
2	B	282	76%12% . 11%
2	F	282	% 75%11% . 11%

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Mol	Chain	Length	Quality of chain
3	C	188	% 66% 13% •• 19%
3	G	188	9% 66% 14% • 19%
4	D	156	2% 63% 17% • 17%
4	H	156	4% 68% 14% • 17%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18467 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 Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	616	Total	C	N	O	S	0	0	0
			4787	3004	855	900	28			
1	E	616	Total	C	N	O	S	0	0	0
			4787	3004	855	900	28			

- Molecule 2 is a protein called Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	250	Total	C	N	O	S	0	0	0
			1985	1263	338	361	23			
2	F	250	Total	C	N	O	S	0	0	0
			1985	1263	338	361	23			

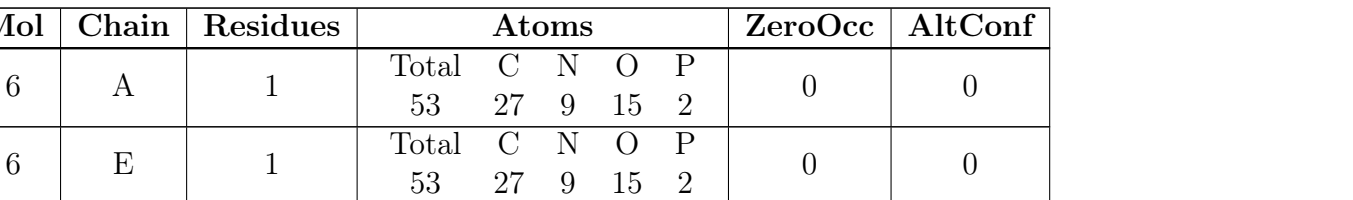
- Molecule 3 is a protein called Cytochrome b-large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	153	Total	C	N	O	S	0	0	0
			1217	813	204	194	6			
3	G	153	Total	C	N	O	S	0	0	0
			1217	813	204	194	6			

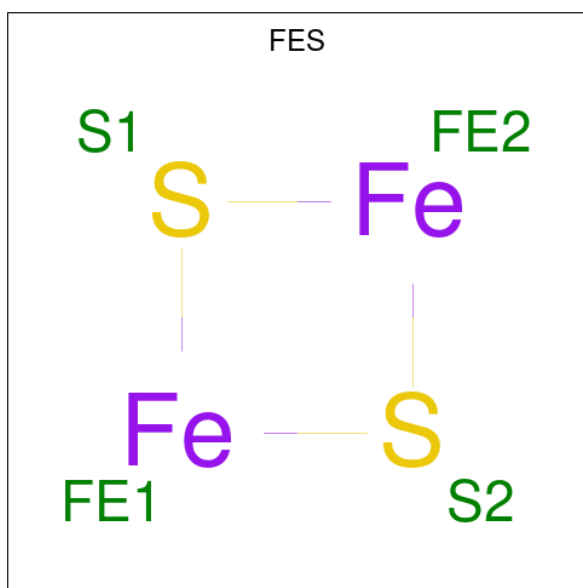
- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	1	0
			1009	665	169	170	5			
4	H	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			

- Molecule 5 is MALONATE ION (CCD ID: MLI) (formula: C₃H₂O₄).

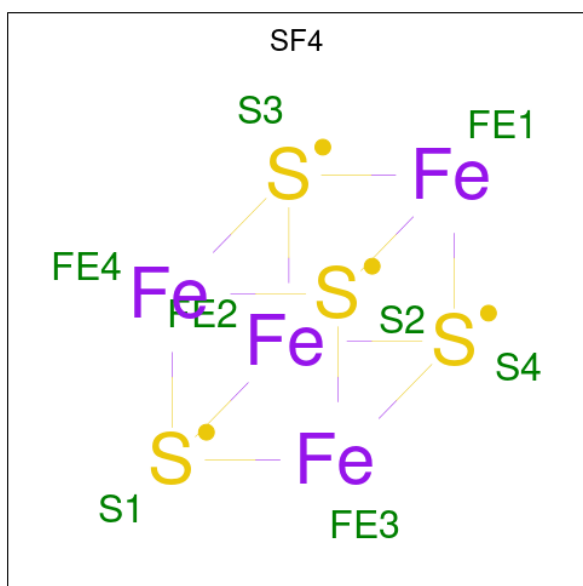


- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



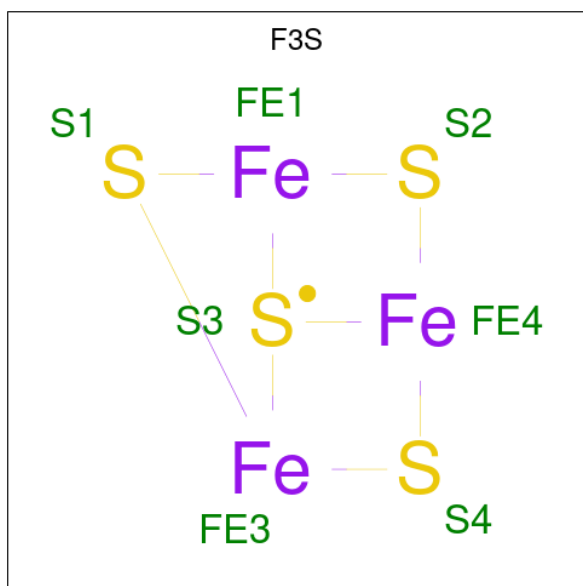
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		

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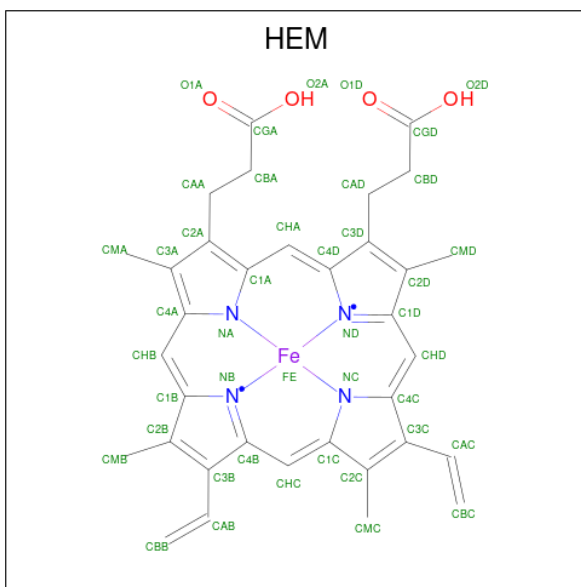
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



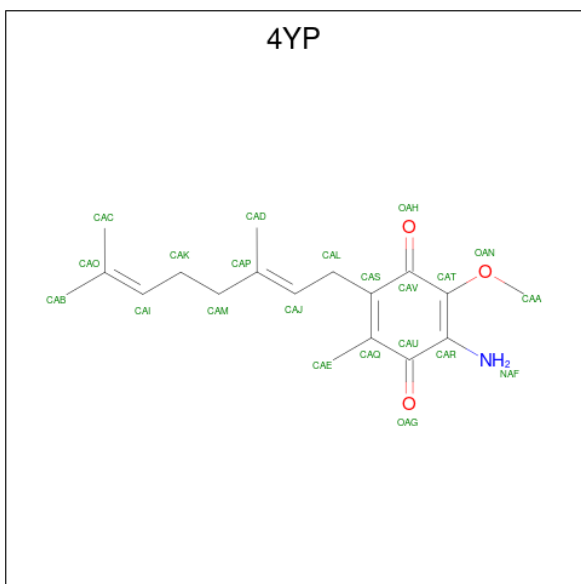
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 11 is 2-amino-5-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]-3-methoxy-6-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: 4YP) (formula: C₁₈H₂₅NO₃).



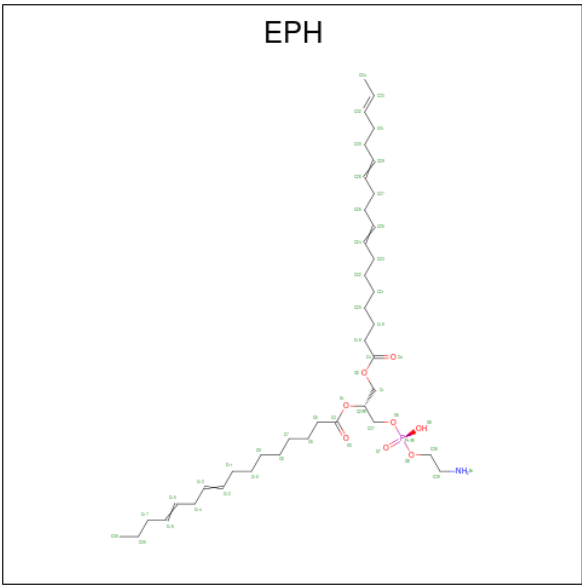
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	N	O	0	0
			22	18	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	G	1	Total	C	N	O	0	0
			22	18	1	3		

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (CCD ID: EPH) (formula: C₃₉H₆₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	54	Total	O	0	0
			54	54		
13	B	13	Total	O	0	0
			13	13		
13	C	6	Total	O	0	0
			6	6		
13	D	7	Total	O	0	0
			7	7		
13	E	10	Total	O	0	0
			10	10		
13	F	10	Total	O	0	0
			10	10		

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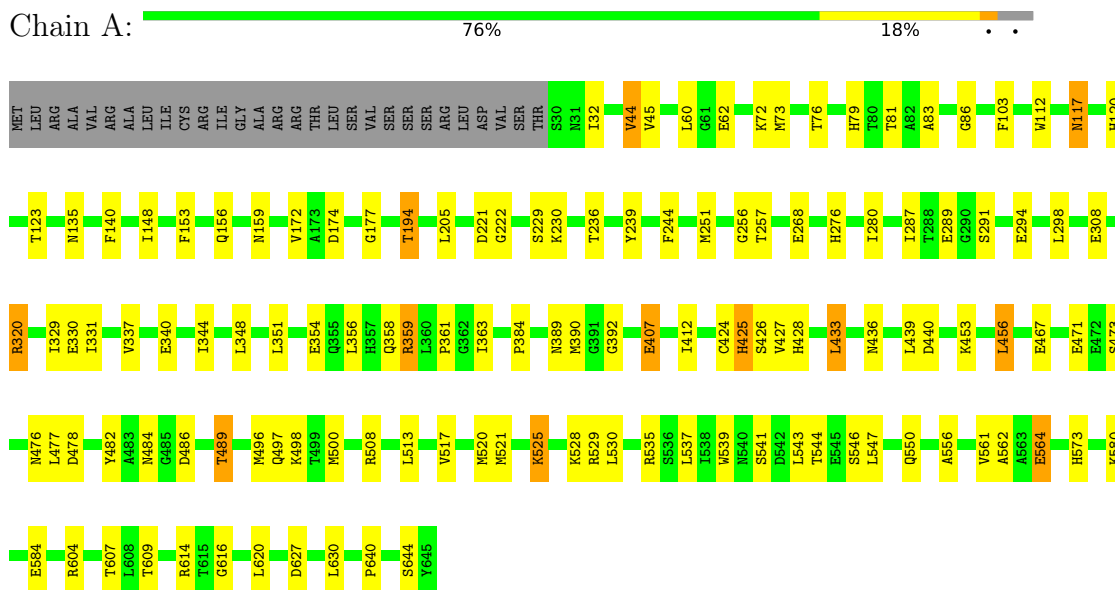
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	G	4	Total	O	0	0
			4	4		
13	H	2	Total	O	0	0
			2	2		

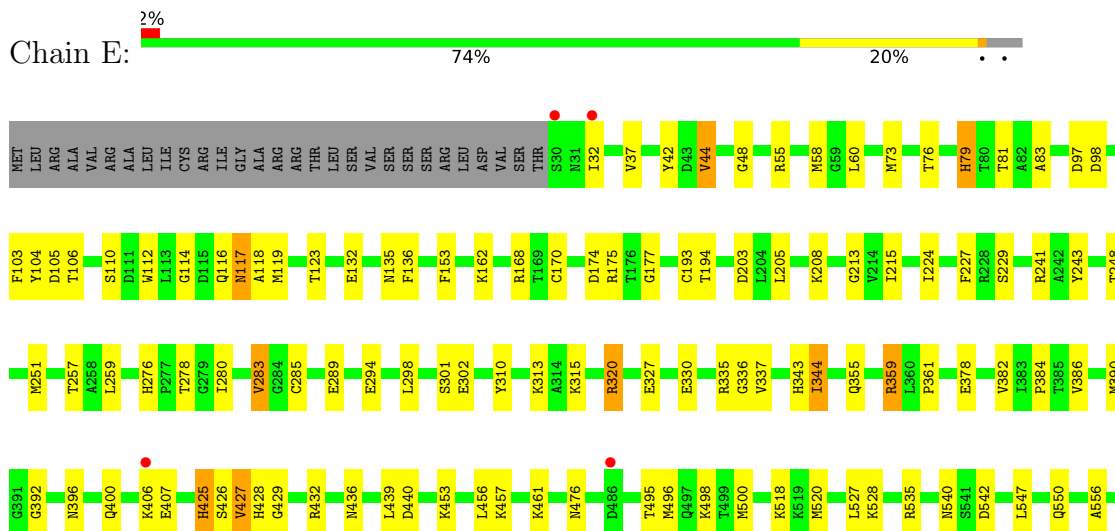
3 Residue-property plots

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: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial



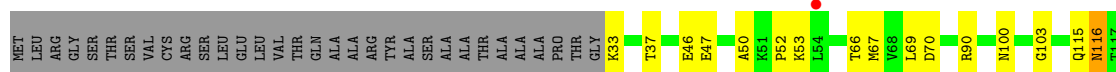
- Molecule 1: Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial





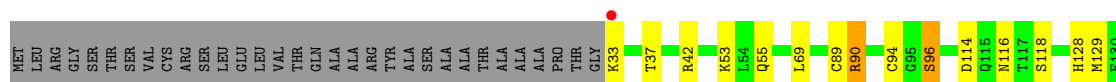
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain B: 76% 12% 11%



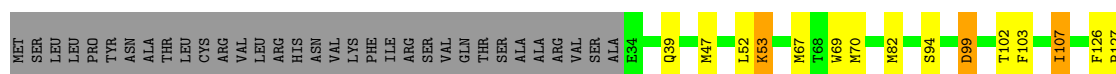
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial

Chain F: 75% 11% 11%



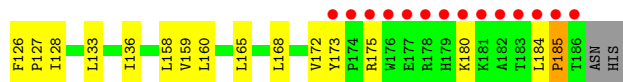
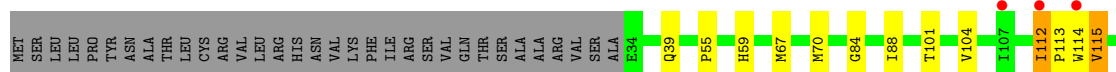
- Molecule 3: Cytochrome b-large subunit

Chain C: 66% 13% 19%

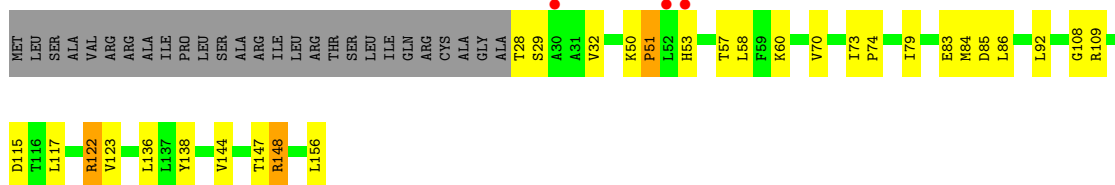


- Molecule 3: Cytochrome b-large subunit

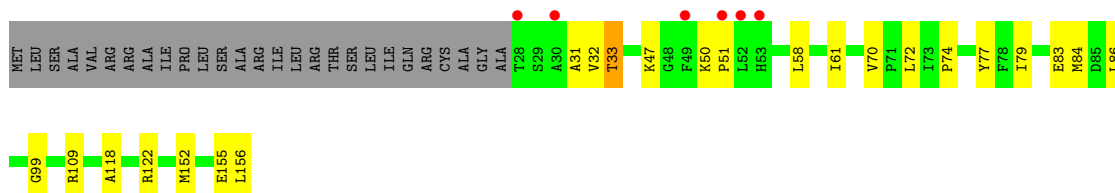
Chain G: 66% 14% 19%



- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial



- Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.81Å 123.63Å 219.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.75 20.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-2.75) 94.0 (20.00-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.196 , 0.252 0.199 , 0.251	Depositor DCC
R_{free} test set	4112 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18467	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: 4YP, FES, F3S, HEM, EPH, MLI, FAD, SF4

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	0.60	0/4889	0.86	4/6605 (0.1%)
1	E	0.54	0/4889	0.87	5/6605 (0.1%)
2	B	0.58	0/2029	0.83	1/2739 (0.0%)
2	F	0.59	0/2029	0.83	1/2739 (0.0%)
3	C	0.56	0/1255	0.86	2/1709 (0.1%)
3	G	0.57	0/1255	0.85	2/1709 (0.1%)
4	D	0.61	0/1041	0.84	1/1420 (0.1%)
4	H	0.54	0/1030	0.76	0/1406
All	All	0.57	0/18417	0.85	16/24932 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	184	LEU	CA-C-N	6.80	128.34	119.84
3	C	184	LEU	C-N-CA	6.80	128.34	119.84
3	G	112	ILE	CA-C-N	6.12	127.49	119.84
3	G	112	ILE	C-N-CA	6.12	127.49	119.84
1	A	86	GLY	N-CA-C	5.80	118.61	110.38
1	E	425	HIS	N-CA-C	5.78	117.66	111.36
1	A	392	GLY	N-CA-C	5.70	117.67	110.38
1	A	425	HIS	N-CA-C	5.59	118.56	111.69
2	B	136	VAL	N-CA-C	5.51	112.57	107.56
1	E	278	THR	N-CA-C	5.24	115.93	108.54
1	E	392	GLY	N-CA-C	5.20	117.45	110.43
1	A	194	THR	CB-CA-C	5.15	118.38	110.14
4	D	115	ASP	N-CA-C	5.08	117.72	111.82
2	F	164	LYS	N-CA-C	5.07	117.39	109.52
1	E	593	GLY	N-CA-C	-5.07	106.14	114.76
1	E	79	HIS	N-CA-C	5.01	118.17	111.75

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	4787	0	4722	66	0
1	E	4787	0	4722	62	0
2	B	1985	0	2001	14	0
2	F	1985	0	2001	21	0
3	C	1217	0	1265	16	0
3	G	1217	0	1265	10	0
4	D	1009	0	997	9	0
4	H	998	0	985	11	0
5	A	7	0	2	1	0
5	E	7	0	2	1	0
6	A	53	0	31	8	0
6	E	53	0	31	6	0
7	B	4	0	0	0	0
7	F	4	0	0	0	0
8	B	8	0	0	0	0
8	F	8	0	0	0	0
9	B	7	0	0	0	0
9	F	7	0	0	0	0
10	C	43	0	30	4	0
10	G	43	0	30	4	0
11	C	22	0	25	1	0
11	G	22	0	25	1	0
12	D	44	0	53	0	0
12	H	44	0	53	2	0
13	A	54	0	0	0	0
13	B	13	0	0	0	0
13	C	6	0	0	0	0
13	D	7	0	0	0	0
13	E	10	0	0	0	0
13	F	10	0	0	0	0
13	G	4	0	0	0	0
13	H	2	0	0	0	0
All	All	18467	0	18240	197	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 5.

All (197) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:HIS:NE2	6:A:702:FAD:HM82	1.17	1.39
1:E:79:HIS:NE2	6:E:702:FAD:HM82	1.35	1.34
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.11	1.12
1:E:79:HIS:NE2	6:E:702:FAD:C8M	2.22	1.01
2:F:94:CYS:SG	2:F:96:SER:OG	2.22	0.96
1:E:79:HIS:CE1	6:E:702:FAD:HM82	1.99	0.96
1:A:477:LEU:HD11	1:A:543:LEU:HD21	1.53	0.89
1:A:79:HIS:CD2	6:A:702:FAD:HM82	2.18	0.75
1:A:476:ASN:HD21	1:A:550:GLN:HE22	1.38	0.72
4:D:108:GLY:O	4:D:122[A]:ARG:NH2	2.23	0.71
1:E:117:ASN:HD22	1:E:118:ALA:H	1.41	0.69
1:E:604:ARG:NH2	1:E:627:ASP:OD1	2.26	0.69
1:E:289:GLU:OE2	1:E:320:ARG:HD2	1.93	0.68
3:C:107:ILE:HD11	4:D:156:LEU:HD13	1.75	0.67
1:A:79:HIS:CE1	6:A:702:FAD:HM82	2.20	0.67
1:A:44:VAL:HG21	1:A:60:LEU:HD13	1.77	0.66
1:A:289:GLU:OE2	1:A:320:ARG:HD2	1.96	0.66
3:G:180:LYS:HG2	3:G:184:LEU:HD13	1.79	0.64
1:A:477:LEU:CD1	1:A:543:LEU:HD21	2.28	0.63
1:E:174:ASP:HB2	1:E:361:PRO:HD2	1.81	0.63
2:F:197:TRP:NE1	11:G:202:4YP:OAH	2.29	0.62
1:A:425:HIS:N	1:A:426:SER:HA	2.15	0.62
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.81	0.62
2:B:227:LEU:HD22	2:B:266:LEU:HD13	1.82	0.61
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.82	0.61
1:A:103:PHE:HA	1:A:123:THR:HG21	1.82	0.60
1:E:327:GLU:OE2	1:E:344:ILE:HD11	2.02	0.60
1:A:489:THR:HG21	1:A:546:SER:OG	2.01	0.60
2:B:262:ILE:HG22	2:B:266:LEU:HD22	1.84	0.59
1:E:117:ASN:HD22	1:E:118:ALA:N	2.00	0.58
3:G:104:VAL:HG21	4:H:152:MET:HE3	1.85	0.58
1:A:72:LYS:HD3	6:A:702:FAD:C5A	2.32	0.58
1:E:590:PRO:O	1:E:594:GLN:OE1	2.21	0.58
1:E:566:ARG:O	1:E:575:ARG:NH2	2.37	0.58
1:A:471:GLU:OE2	4:D:28:THR:HA	2.04	0.57
3:G:172:VAL:O	3:G:172:VAL:HG13	2.05	0.56
1:A:83:ALA:HA	6:A:702:FAD:C6	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:201:HEM:HBC2	10:C:201:HEM:HHD	1.87	0.56
2:F:179:LEU:HD23	2:F:216:ILE:HD11	1.86	0.56
1:E:425:HIS:N	1:E:426:SER:HA	2.20	0.56
2:F:262:ILE:HG22	2:F:266:LEU:HD22	1.87	0.56
4:D:50:LYS:N	4:D:51:PRO:CD	2.68	0.56
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.86	0.56
1:E:301:SER:HB3	1:E:336:GLY:O	2.06	0.56
3:G:184:LEU:HB2	3:G:185:PRO:CD	2.36	0.55
2:F:227:LEU:HD22	2:F:266:LEU:HD13	1.88	0.55
4:H:77:TYR:HA	12:H:201:EPH:H11	1.87	0.55
1:A:83:ALA:HA	6:A:702:FAD:C5X	2.37	0.55
1:A:525:LYS:O	1:A:528:LYS:HE2	2.07	0.55
1:A:148:ILE:H	2:B:165:GLN:HE22	1.55	0.55
4:H:77:TYR:HA	12:H:201:EPH:C1	2.37	0.55
1:A:73:MET:SD	1:A:251:MET:HG3	2.46	0.54
1:A:117:ASN:HD22	1:A:117:ASN:N	2.05	0.54
1:A:604:ARG:NH2	1:A:627:ASP:OD2	2.39	0.54
10:G:201:HEM:HAD1	4:H:99:GLY:CA	2.37	0.54
3:C:179:HIS:O	3:C:183:THR:HG22	2.07	0.54
2:F:42:ARG:HG3	2:F:55:GLN:HE21	1.72	0.53
10:G:201:HEM:HBB2	10:G:201:HEM:HHC	1.89	0.53
4:D:144:VAL:HB	4:D:148:ARG:HG2	1.90	0.53
1:E:320:ARG:HH12	5:E:701:MLI:C2	2.21	0.53
1:E:83:ALA:HA	6:E:702:FAD:C6	2.39	0.53
1:A:291:SER:HB2	1:A:348:LEU:HD21	1.89	0.53
4:H:50:LYS:N	4:H:51:PRO:CD	2.72	0.53
3:C:184:LEU:C	3:C:184:LEU:HD12	2.33	0.53
1:E:213:GLY:HA3	1:E:227:PHE:O	2.09	0.52
3:G:114:TRP:CD1	3:G:115:VAL:HG13	2.44	0.52
1:A:222:GLY:HA3	1:A:537:LEU:HB3	1.91	0.52
2:B:67:MET:O	2:B:70:ASP:HB2	2.09	0.52
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.91	0.52
1:A:489:THR:HG22	1:A:530:LEU:HD11	1.91	0.52
1:A:45:VAL:HG23	1:A:229:SER:HB3	1.90	0.52
1:A:508:ARG:HH11	1:A:573:HIS:HD2	1.57	0.52
1:A:609:THR:HG22	1:A:620:LEU:HD23	1.92	0.51
1:A:135:ASN:O	2:B:153:LEU:HD23	2.10	0.51
3:C:70:MET:HA	3:C:70:MET:HE2	1.93	0.51
1:A:276:HIS:O	1:A:384:PRO:HA	2.10	0.51
2:B:47:GLU:HB3	2:B:50:ALA:HB2	1.91	0.51
1:A:562:ALA:HB1	1:A:607:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:131:VAL:HG22	3:G:55:PRO:HG2	1.94	0.50
1:A:156:GLN:HG3	1:A:433:LEU:HD21	1.94	0.50
4:D:70:VAL:O	4:D:74:PRO:HD2	2.12	0.50
1:E:105:ASP:OD2	1:E:168:ARG:NH2	2.45	0.50
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.93	0.50
1:A:239:TYR:H	1:A:389:ASN:ND2	2.10	0.49
1:E:355:GLN:O	1:E:359:ARG:HB2	2.13	0.49
2:F:116:ASN:C	2:F:116:ASN:HD22	2.21	0.49
1:E:114:GLY:C	1:E:119:MET:HE2	2.38	0.49
1:A:32:ILE:HG23	1:A:482:TYR:CD1	2.48	0.48
1:A:120:HIS:HD2	1:A:630:LEU:H	1.61	0.48
1:E:276:HIS:O	1:E:384:PRO:HA	2.12	0.48
1:E:612:ASP:HB3	1:E:615:THR:OG1	2.12	0.48
3:C:69:TRP:HE3	11:C:202:4YP:H20	1.77	0.48
1:E:104:TYR:HA	1:E:638:ILE:CD1	2.43	0.48
4:D:85:ASP:OD2	4:D:147:THR:HG23	2.13	0.48
1:E:215:ILE:HD11	1:E:224:ILE:HG21	1.94	0.48
1:E:55:ARG:NH1	1:E:132:GLU:OE2	2.47	0.48
1:E:396:ASN:HD21	1:E:400:GLN:HB2	1.79	0.48
1:A:32:ILE:HG22	1:A:478:ASP:OD1	2.13	0.47
2:F:212:TYR:OH	2:F:261:GLU:HG2	2.14	0.47
10:C:201:HEM:HBB2	10:C:201:HEM:HHC	1.95	0.47
1:A:244:PHE:HA	1:A:497:GLN:HB3	1.97	0.47
1:E:110:SER:HB2	1:E:429:GLY:HA3	1.97	0.47
2:B:234:PHE:CD1	2:B:238:LYS:HG3	2.49	0.47
1:A:320:ARG:HH12	5:A:701:MLI:C2	2.27	0.47
1:A:500:MET:HE1	1:A:556:ALA:O	2.15	0.47
1:E:106:THR:HG22	1:E:119:MET:SD	2.54	0.47
1:A:140:PHE:HA	1:A:172:VAL:HG22	1.98	0.46
1:E:428:HIS:CE1	1:E:432:ARG:HG3	2.51	0.46
2:F:197:TRP:O	4:H:109:ARG:HD3	2.14	0.46
1:A:174:ASP:HB2	1:A:361:PRO:HD2	1.97	0.46
3:C:126:PHE:HB3	3:C:127:PRO:HD3	1.96	0.46
4:D:50:LYS:N	4:D:51:PRO:HD2	2.30	0.46
1:E:44:VAL:HG11	1:E:60:LEU:HD13	1.97	0.46
3:C:173:TYR:HB3	3:C:174:PRO:HD3	1.98	0.46
1:E:73:MET:SD	1:E:251:MET:HG3	2.56	0.46
1:A:294:GLU:CD	1:A:359:ARG:HG2	2.41	0.45
1:E:58:MET:HE1	1:E:136:PHE:CE2	2.50	0.45
1:A:230:LYS:HE2	1:A:456:LEU:HD11	1.98	0.45
1:E:42:TYR:O	1:E:229:SER:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:GLU:O	1:A:358:GLN:HB2	2.16	0.45
1:E:280:ILE:HD12	1:E:285:CYS:HB2	1.99	0.45
1:E:602:HIS:O	1:E:605:LYS:HE2	2.16	0.45
1:A:117:ASN:HD22	1:A:117:ASN:H	1.64	0.45
1:A:174:ASP:OD2	1:A:363:ILE:N	2.44	0.45
1:A:221:ASP:OD2	1:A:221:ASP:C	2.60	0.45
1:A:329:ILE:O	1:A:330:GLU:C	2.59	0.45
1:E:136:PHE:CE1	2:F:161:LEU:HD11	2.52	0.45
1:A:427:VAL:HG23	1:A:428:HIS:CE1	2.51	0.45
1:A:477:LEU:HD12	1:A:543:LEU:HD11	1.97	0.45
1:A:424:CYS:SG	1:A:426:SER:HB2	2.56	0.44
2:B:52:PRO:C	2:B:53:LYS:HG3	2.42	0.44
2:F:222:SER:O	2:F:223:ALA:C	2.59	0.44
3:G:84:GLY:O	3:G:88:ILE:HG12	2.17	0.44
1:E:310:TYR:OH	1:E:330:GLU:OE1	2.36	0.44
1:A:135:ASN:ND2	2:B:162:GLY:H	2.15	0.44
1:A:280:ILE:HD11	1:A:287:ILE:HD11	2.00	0.44
1:E:103:PHE:HA	1:E:123:THR:HG21	2.00	0.44
2:B:100:ASN:HD21	2:B:103:GLY:HA2	1.82	0.44
1:E:116:GLN:HA	1:E:119:MET:HE3	2.00	0.44
1:E:112:TRP:CE2	1:E:640:PRO:HA	2.53	0.44
10:G:201:HEM:HBC2	10:G:201:HEM:HHD	2.00	0.44
1:A:513:LEU:O	1:A:517:VAL:HG23	2.18	0.43
1:E:135:ASN:ND2	2:F:161:LEU:O	2.48	0.43
2:F:114:ASP:OD2	2:F:114:ASP:C	2.60	0.43
1:E:283:VAL:O	2:F:90:ARG:NH1	2.51	0.43
4:H:32:VAL:HG22	4:H:33:THR:N	2.33	0.43
1:A:407:GLU:H	1:A:407:GLU:CD	2.25	0.43
2:F:89:CYS:HB3	2:F:94:CYS:HB3	2.00	0.43
1:A:236:THR:OG1	1:A:256:GLY:HA3	2.18	0.43
2:F:223:ALA:HB2	2:F:272:LYS:HD2	2.00	0.43
2:B:264:MET:SD	3:C:143:MET:HA	2.59	0.43
1:E:215:ILE:HD11	1:E:224:ILE:CG2	2.48	0.43
3:C:52:LEU:O	3:C:53:LYS:C	2.61	0.43
1:E:294:GLU:CD	1:E:359:ARG:HG2	2.43	0.43
1:E:476:ASN:HD21	1:E:550:GLN:HE22	1.66	0.43
1:A:486:ASP:OD1	1:A:529:ARG:NH2	2.47	0.43
3:C:82:MET:HE3	10:C:201:HEM:CAC	2.48	0.43
1:E:496:MET:HG3	1:E:520:MET:HE1	2.00	0.42
1:E:611:GLN:O	1:E:613:PRO:HD3	2.19	0.42
1:E:119:MET:O	1:E:123:THR:OG1	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:ALA:HA	6:E:702:FAD:C5X	2.48	0.42
1:E:427:VAL:HG23	1:E:428:HIS:CD2	2.54	0.42
1:A:496:MET:HG3	1:A:520:MET:HE1	2.02	0.42
1:E:428:HIS:ND1	1:E:432:ARG:HG3	2.34	0.42
1:E:540:ASN:OD1	1:E:542:ASP:HB3	2.19	0.42
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.55	0.42
1:E:97:ASP:OD2	1:E:98:ASP:N	2.53	0.42
1:E:243:TYR:CG	1:E:386:VAL:HG21	2.55	0.42
2:F:234:PHE:O	2:F:235:SER:C	2.63	0.42
1:A:604:ARG:NH2	1:A:627:ASP:CG	2.78	0.41
1:E:344:ILE:CD1	1:E:382:VAL:HG23	2.50	0.41
4:H:118:ALA:HB1	4:H:122:ARG:HH21	1.85	0.41
4:H:155:GLU:O	4:H:156:LEU:C	2.62	0.41
3:C:103:PHE:O	3:C:107:ILE:HG23	2.20	0.41
1:E:456:LEU:HD23	1:E:457:LYS:N	2.35	0.41
1:A:268:GLU:HA	1:A:607:THR:O	2.21	0.41
1:E:500:MET:HE1	1:E:556:ALA:O	2.20	0.41
3:G:126:PHE:HB3	3:G:127:PRO:HD3	2.02	0.41
2:B:179:LEU:HD23	2:B:216:ILE:HD11	2.03	0.41
3:C:132:THR:HG23	10:C:201:HEM:CAB	2.51	0.41
1:E:241:ARG:NH2	1:E:248:THR:O	2.54	0.41
1:E:343:HIS:HB2	1:E:382:VAL:O	2.20	0.41
1:A:135:ASN:HD22	2:B:162:GLY:H	1.69	0.41
2:F:128:HIS:CD2	2:F:196:TRP:HB3	2.56	0.41
1:E:48:GLY:HA2	6:E:702:FAD:H1B	2.02	0.41
1:A:513:LEU:HD13	1:A:564:GLU:HA	2.03	0.41
3:C:47:MET:HE2	3:C:47:MET:HA	2.02	0.41
1:E:440:ASP:OD1	1:E:440:ASP:C	2.64	0.40
3:C:99:ASP:OD1	3:C:102:THR:HG23	2.20	0.40
1:A:83:ALA:HA	6:A:702:FAD:N5	2.36	0.40
2:F:116:ASN:HD22	2:F:118:SER:H	1.68	0.40
1:A:541:SER:HA	1:A:544:THR:OG1	2.22	0.40
3:C:94:SER:HA	4:D:138:TYR:CE1	2.57	0.40
3:G:184:LEU:HB2	3:G:185:PRO:HD2	2.04	0.40
1:A:521:MET:HE1	1:A:616:GLY:O	2.21	0.40
1:E:37:VAL:HB	4:H:31:ALA:CB	2.51	0.40
4:H:70:VAL:O	4:H:74:PRO:HD2	2.21	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	614/645 (95%)	583 (95%)	31 (5%)	0	100	100
1	E	614/645 (95%)	570 (93%)	44 (7%)	0	100	100
2	B	248/282 (88%)	238 (96%)	9 (4%)	1 (0%)	30	50
2	F	248/282 (88%)	237 (96%)	10 (4%)	1 (0%)	30	50
3	C	151/188 (80%)	148 (98%)	2 (1%)	1 (1%)	18	34
3	G	151/188 (80%)	138 (91%)	10 (7%)	3 (2%)	6	11
4	D	128/156 (82%)	119 (93%)	8 (6%)	1 (1%)	16	30
4	H	127/156 (81%)	118 (93%)	9 (7%)	0	100	100
All	All	2281/2542 (90%)	2151 (94%)	123 (5%)	7 (0%)	36	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	116	ASN
3	C	185	PRO
4	D	51	PRO
3	G	113	PRO
2	F	163	GLU
3	G	173	TYR
3	G	185	PRO

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	502/527 (95%)	458 (91%)	44 (9%)	9	18
1	E	502/527 (95%)	451 (90%)	51 (10%)	7	14
2	B	220/242 (91%)	201 (91%)	19 (9%)	10	18
2	F	220/242 (91%)	203 (92%)	17 (8%)	12	22
3	C	127/158 (80%)	117 (92%)	10 (8%)	11	21
3	G	127/158 (80%)	112 (88%)	15 (12%)	5	9
4	D	99/119 (83%)	80 (81%)	19 (19%)	1	2
4	H	98/119 (82%)	89 (91%)	9 (9%)	8	17
All	All	1895/2092 (91%)	1711 (90%)	184 (10%)	8	15

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	62	GLU
1	A	76	THR
1	A	81	THR
1	A	117	ASN
1	A	153	PHE
1	A	159	ASN
1	A	194	THR
1	A	205	LEU
1	A	257	THR
1	A	298	LEU
1	A	308	GLU
1	A	320	ARG
1	A	331	ILE
1	A	337	VAL
1	A	340	GLU
1	A	344	ILE
1	A	351	LEU
1	A	356	LEU
1	A	359	ARG
1	A	390	MET
1	A	407	GLU
1	A	412	ILE
1	A	433	LEU
1	A	436	ASN
1	A	439	LEU
1	A	440	ASP

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Mol	Chain	Res	Type
1	A	453	LYS
1	A	456	LEU
1	A	467	GLU
1	A	473	SER
1	A	484	ASN
1	A	489	THR
1	A	498	LYS
1	A	525	LYS
1	A	535	ARG
1	A	539	TRP
1	A	547	LEU
1	A	561	VAL
1	A	564	GLU
1	A	580	LYS
1	A	584	GLU
1	A	614	ARG
1	A	644	SER
2	B	33	LYS
2	B	37	THR
2	B	46	GLU
2	B	66	THR
2	B	69	LEU
2	B	90	ARG
2	B	115	GLN
2	B	116	ASN
2	B	118	SER
2	B	131	VAL
2	B	173	GLN
2	B	176	LEU
2	B	179	LEU
2	B	184	LEU
2	B	216	ILE
2	B	248	THR
2	B	261	GLU
2	B	266	LEU
2	B	278	THR
3	C	53	LYS
3	C	67	MET
3	C	99	ASP
3	C	107	ILE
3	C	133	LEU
3	C	136	ILE

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Mol	Chain	Res	Type
3	C	165	LEU
3	C	170	VAL
3	C	177	GLU
3	C	184	LEU
4	D	29	SER
4	D	32	VAL
4	D	53	HIS
4	D	57	THR
4	D	58	LEU
4	D	60	LYS
4	D	73	ILE
4	D	79	ILE
4	D	83	GLU
4	D	84	MET
4	D	86	LEU
4	D	92	LEU
4	D	109	ARG
4	D	117	LEU
4	D	122[A]	ARG
4	D	122[B]	ARG
4	D	123	VAL
4	D	136	LEU
4	D	148	ARG
1	E	32	ILE
1	E	44	VAL
1	E	76	THR
1	E	81	THR
1	E	117	ASN
1	E	153	PHE
1	E	162	LYS
1	E	170	CYS
1	E	175	ARG
1	E	193	CYS
1	E	194	THR
1	E	203	ASP
1	E	205	LEU
1	E	208	LYS
1	E	257	THR
1	E	259	LEU
1	E	283	VAL
1	E	298	LEU
1	E	302	GLU

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Mol	Chain	Res	Type
1	E	313	LYS
1	E	315	LYS
1	E	320	ARG
1	E	335	ARG
1	E	337	VAL
1	E	344	ILE
1	E	359	ARG
1	E	378	GLU
1	E	390	MET
1	E	406	LYS
1	E	407	GLU
1	E	427	VAL
1	E	436	ASN
1	E	439	LEU
1	E	453	LYS
1	E	461	LYS
1	E	495	THR
1	E	498	LYS
1	E	518	LYS
1	E	527	LEU
1	E	528	LYS
1	E	535	ARG
1	E	547	LEU
1	E	561	VAL
1	E	564	GLU
1	E	584	GLU
1	E	591	ILE
1	E	595	THR
1	E	601	LYS
1	E	610	LYS
1	E	614	ARG
1	E	642	ILE
2	F	33	LYS
2	F	37	THR
2	F	53	LYS
2	F	69	LEU
2	F	90	ARG
2	F	96	SER
2	F	129	MET
2	F	131	VAL
2	F	156	LYS
2	F	158	LYS

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Mol	Chain	Res	Type
2	F	173	GLN
2	F	179	LEU
2	F	184	LEU
2	F	201	LYS
2	F	216	ILE
2	F	266	LEU
2	F	278	THR
3	G	59	HIS
3	G	67	MET
3	G	70	MET
3	G	101	THR
3	G	112	ILE
3	G	115	VAL
3	G	128	ILE
3	G	133	LEU
3	G	136	ILE
3	G	158	LEU
3	G	159	VAL
3	G	160	LEU
3	G	165	LEU
3	G	168	LEU
3	G	175	ARG
4	H	33	THR
4	H	47	LYS
4	H	58	LEU
4	H	61	ILE
4	H	72	LEU
4	H	79	ILE
4	H	83	GLU
4	H	84	MET
4	H	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	117	ASN
1	A	120	HIS
1	A	125	ASN
1	A	135	ASN
1	A	150	GLN
1	A	159	ASN

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Mol	Chain	Res	Type
1	A	182	HIS
1	A	250	HIS
1	A	252	ASN
1	A	349	HIS
1	A	389	ASN
1	A	431	ASN
1	A	436	ASN
1	A	451	ASN
1	A	476	ASN
1	A	484	ASN
1	A	551	ASN
1	A	573	HIS
2	B	77	ASN
2	B	100	ASN
2	B	105	ASN
2	B	116	ASN
2	B	154	GLN
2	B	160	ASN
2	B	165	GLN
4	D	105	ASN
4	D	140	ASN
1	E	88	ASN
1	E	117	ASN
1	E	125	ASN
1	E	156	GLN
1	E	252	ASN
1	E	355	GLN
1	E	428	HIS
1	E	436	ASN
1	E	451	ASN
1	E	476	ASN
1	E	484	ASN
1	E	497	GLN
1	E	503	HIS
1	E	551	ASN
1	E	573	HIS
2	F	55	GLN
2	F	100	ASN
2	F	105	ASN
2	F	116	ASN
2	F	145	GLN
3	G	59	HIS

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Mol	Chain	Res	Type
3	G	66	GLN
4	H	140	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	EPH	D	201	-	43,43,48	1.10	2 (4%)	46,48,53	1.03	4 (8%)
7	FES	B	301	2	0,4,4	-	-	-	-	-
10	HEM	C	201	4,3	50,50,50	1.61	7 (14%)	67,82,82	1.78	19 (28%)
9	F3S	B	303	2	0,9,9	-	-	-	-	-
7	FES	F	301	2	0,4,4	-	-	-	-	-
5	MLI	A	701	-	6,6,6	1.15	0	7,7,7	1.28	0
10	HEM	G	201	4,3	50,50,50	1.56	8 (16%)	67,82,82	1.91	17 (25%)
8	SF4	B	302	2	0,12,12	-	-	-	-	-
11	4YP	C	202	-	22,22,22	3.34	9 (40%)	24,30,30	1.64	8 (33%)
8	SF4	F	302	2	0,12,12	-	-	-	-	-
11	4YP	G	202	-	22,22,22	3.45	8 (36%)	24,30,30	1.23	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	EPH	H	201	-	43,43,48	1.09	2 (4%)	46,48,53	1.23	4 (8%)
9	F3S	F	303	2	0,9,9	-	-	-		
5	MLI	E	701	-	6,6,6	1.08	0	7,7,7	0.96	0
6	FAD	A	702	-	58,58,58	1.50	12 (20%)	85,89,89	1.82	20 (23%)
6	FAD	E	702	-	58,58,58	1.46	10 (17%)	85,89,89	1.73	21 (24%)

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
12	EPH	D	201	-	-	21/47/47/52	-
7	FES	B	301	2	-	-	0/1/1/1
10	HEM	C	201	4,3	-	2/14/54/54	-
9	F3S	B	303	2	-	-	0/3/3/3
7	FES	F	301	2	-	-	0/1/1/1
5	MLI	A	701	-	-	0/4/4/4	-
10	HEM	G	201	4,3	-	4/14/54/54	-
11	4YP	C	202	-	-	3/13/37/37	0/1/1/1
11	4YP	G	202	-	-	2/13/37/37	0/1/1/1
8	SF4	B	302	2	-	-	0/6/5/5
8	SF4	F	302	2	-	-	0/6/5/5
12	EPH	H	201	-	-	27/47/47/52	-
9	F3S	F	303	2	-	-	0/3/3/3
5	MLI	E	701	-	-	0/4/4/4	-
6	FAD	A	702	-	-	10/34/50/50	0/6/6/6
6	FAD	E	702	-	-	5/34/50/50	0/6/6/6

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	202	4YP	CAJ-CAP	9.76	1.55	1.33
11	C	202	4YP	CAJ-CAP	9.43	1.54	1.33
11	G	202	4YP	CAI-CAO	7.94	1.56	1.32
11	C	202	4YP	CAI-CAO	7.50	1.54	1.32
11	C	202	4YP	CAE-CAQ	-5.69	1.39	1.50
11	G	202	4YP	CAE-CAQ	-5.69	1.39	1.50
10	C	201	HEM	FE-NB	5.05	2.10	1.94
12	H	201	EPH	O2-C4	4.59	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	201	HEM	FE-NB	4.55	2.08	1.94
6	E	702	FAD	C9A-C5X	4.55	1.48	1.41
12	D	201	EPH	O2-C4	4.54	1.46	1.33
6	A	702	FAD	C9A-C5X	4.53	1.48	1.41
12	D	201	EPH	O1-C3	4.51	1.47	1.34
12	H	201	EPH	O1-C3	4.42	1.46	1.34
11	G	202	4YP	CAL-CAS	-4.26	1.43	1.51
10	G	201	HEM	C1B-NB	-4.12	1.33	1.40
10	G	201	HEM	FE-NC	4.08	2.08	1.95
10	C	201	HEM	FE-NC	3.96	2.08	1.95
11	C	202	4YP	CAL-CAS	-3.88	1.44	1.51
6	A	702	FAD	C5A-C4A	3.67	1.45	1.39
11	G	202	4YP	CAS-CAQ	3.67	1.41	1.35
11	C	202	4YP	CAL-CAJ	3.57	1.56	1.50
10	C	201	HEM	C1B-NB	-3.57	1.34	1.40
6	E	702	FAD	C5A-C4A	3.51	1.45	1.39
11	G	202	4YP	CAS-CAV	3.25	1.55	1.46
6	A	702	FAD	C8-C7	3.14	1.48	1.40
6	A	702	FAD	C5X-N5	-3.08	1.33	1.39
11	C	202	4YP	CAS-CAV	3.07	1.55	1.46
11	C	202	4YP	CAS-CAQ	3.01	1.40	1.35
10	C	201	HEM	C3B-C4B	2.89	1.50	1.44
6	E	702	FAD	C5A-N7A	-2.86	1.33	1.39
11	G	202	4YP	CAL-CAJ	2.84	1.55	1.50
6	A	702	FAD	C4A-N9A	-2.80	1.31	1.37
10	C	201	HEM	C1C-C2C	-2.71	1.40	1.45
10	C	201	HEM	C4D-ND	-2.68	1.35	1.40
10	G	201	HEM	C3B-C4B	2.68	1.50	1.44
10	G	201	HEM	C4B-NB	-2.61	1.33	1.38
6	E	702	FAD	C4A-N9A	-2.58	1.32	1.37
6	E	702	FAD	C8A-N7A	2.56	1.36	1.31
6	E	702	FAD	C8-C7	2.55	1.47	1.40
6	E	702	FAD	P-O3P	2.55	1.62	1.59
6	A	702	FAD	C5A-N7A	-2.55	1.34	1.39
6	A	702	FAD	P-O3P	2.47	1.62	1.59
6	E	702	FAD	C8M-C8	-2.45	1.46	1.51
6	A	702	FAD	C5A-C6A	2.41	1.47	1.41
10	C	201	HEM	C4B-NB	-2.40	1.34	1.38
10	G	201	HEM	C1C-C2C	-2.34	1.40	1.45
6	A	702	FAD	C8M-C8	-2.31	1.46	1.51
11	C	202	4YP	CAM-CAP	2.28	1.56	1.51
11	G	202	4YP	CAQ-CAU	2.27	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	702	FAD	C1'-C2'	2.20	1.55	1.52
6	A	702	FAD	C8A-N7A	2.20	1.35	1.31
6	A	702	FAD	O4-C4	2.14	1.27	1.23
11	C	202	4YP	CAQ-CAU	2.07	1.54	1.47
10	G	201	HEM	C4D-C3D	2.05	1.48	1.45
6	E	702	FAD	C4-N3	-2.04	1.35	1.38
10	G	201	HEM	C1D-ND	-2.00	1.34	1.38
6	A	702	FAD	C9-C8	-2.00	1.36	1.39

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	201	HEM	CAD-C3D-C4D	5.61	134.47	124.70
12	H	201	EPH	O1-C3-C5	5.48	123.33	111.48
6	E	702	FAD	C5A-C4A-N3A	-5.44	119.22	126.72
6	A	702	FAD	C5A-C4A-N3A	-5.33	119.37	126.72
6	A	702	FAD	O2-C2-N1	-5.32	112.96	121.80
10	C	201	HEM	CHA-C4D-ND	4.60	130.05	124.37
10	G	201	HEM	CHD-C1D-ND	4.57	129.34	124.42
6	E	702	FAD	N3A-C2A-N1A	-4.32	122.05	128.58
10	G	201	HEM	C1B-NB-C4B	4.09	110.05	105.21
6	E	702	FAD	N3A-C4A-N9A	4.08	134.10	127.17
10	C	201	HEM	CHA-C4D-C3D	-4.06	117.75	125.23
10	C	201	HEM	C1B-NB-C4B	4.02	109.97	105.21
6	E	702	FAD	C2A-N3A-C4A	3.96	121.51	111.83
10	G	201	HEM	CAC-C3C-C4C	3.96	134.28	124.82
6	A	702	FAD	N3A-C4A-N9A	3.95	133.88	127.17
12	D	201	EPH	O1-C3-C5	3.80	119.70	111.48
6	A	702	FAD	C2A-N3A-C4A	3.79	121.09	111.83
10	G	201	HEM	CBD-CAD-C3D	3.55	122.34	112.53
10	G	201	HEM	CAD-C3D-C2D	-3.52	121.28	127.87
6	A	702	FAD	O4-C4-C4X	-3.51	117.25	126.53
6	A	702	FAD	C4A-C5A-N7A	-3.41	106.68	110.58
6	A	702	FAD	N3A-C2A-N1A	-3.39	123.45	128.58
10	G	201	HEM	CHD-C1D-C2D	-3.36	119.73	125.03
6	A	702	FAD	O4-C4-N3	3.35	126.40	120.11
12	D	201	EPH	O2-C4-C18	3.31	121.92	111.83
6	E	702	FAD	C4A-C5A-N7A	-3.22	106.90	110.58
10	C	201	HEM	CHC-C1C-NC	3.22	127.96	124.45
10	C	201	HEM	CHD-C1D-ND	3.14	127.80	124.42
10	C	201	HEM	C3B-C4B-NB	-3.14	107.22	109.47
12	H	201	EPH	O2-C4-C18	3.10	121.29	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	201	HEM	C3B-C4B-NB	-3.10	107.24	109.47
6	E	702	FAD	C1'-C2'-C3'	3.08	118.00	109.66
6	A	702	FAD	O2-C2-N3	3.01	124.35	118.58
6	E	702	FAD	C4A-N9A-C8A	3.00	108.89	105.74
11	C	202	4YP	CAE-CAQ-CAS	-2.94	119.62	124.45
6	A	702	FAD	C4A-N9A-C8A	2.91	108.79	105.74
6	E	702	FAD	O4-C4-C4X	-2.91	118.85	126.53
10	G	201	HEM	CAC-C3C-C2C	-2.89	119.05	128.43
10	C	201	HEM	CMD-C2D-C1D	2.87	129.52	125.03
6	E	702	FAD	O2-C2-N1	-2.85	117.06	121.80
12	H	201	EPH	O1-C3-O3	-2.84	117.06	123.70
10	C	201	HEM	C4C-NC-C1C	2.83	110.43	105.82
10	C	201	HEM	CAC-C3C-C4C	2.82	131.56	124.82
6	A	702	FAD	C9-C8-C7	2.80	123.80	119.69
10	C	201	HEM	CBD-CAD-C3D	-2.78	104.84	112.53
6	E	702	FAD	C9-C8-C7	2.78	123.77	119.69
11	C	202	4YP	CAS-CAQ-CAU	2.76	121.35	119.17
11	C	202	4YP	CAL-CAS-CAV	2.75	121.71	118.52
10	C	201	HEM	CHB-C1B-NB	2.73	127.74	124.37
10	G	201	HEM	CHB-C1B-NB	2.66	127.66	124.37
6	E	702	FAD	N9A-C8A-N7A	-2.62	110.21	113.94
10	G	201	HEM	CHA-C4D-ND	2.56	127.53	124.37
11	C	202	4YP	CAU-CAR-NAF	2.56	120.85	114.40
12	D	201	EPH	O2-C4-O4	-2.55	117.24	123.63
6	E	702	FAD	C5X-C9A-N10	2.51	120.24	117.97
11	C	202	4YP	CAD-CAP-CAM	2.48	119.53	115.23
6	E	702	FAD	C5A-N7A-C8A	2.46	107.31	103.45
10	G	201	HEM	CHA-C4D-C3D	-2.45	120.72	125.23
6	A	702	FAD	C4'-C3'-C2'	-2.43	109.53	113.57
6	A	702	FAD	C1'-C2'-C3'	2.43	116.24	109.66
6	A	702	FAD	C6A-C5A-N7A	2.42	136.75	132.09
10	G	201	HEM	CHC-C4B-NB	2.41	127.02	124.42
6	E	702	FAD	C6A-C5A-N7A	2.41	136.74	132.09
6	E	702	FAD	C4'-C3'-C2'	-2.38	109.61	113.57
10	G	201	HEM	O2D-CGD-CBD	2.37	121.50	114.00
10	C	201	HEM	CHD-C1D-C2D	-2.37	121.29	125.03
6	E	702	FAD	O2'-C2'-C3'	-2.36	103.72	109.25
11	C	202	4YP	CAL-CAS-CAQ	-2.34	120.88	124.89
6	A	702	FAD	C5A-N7A-C8A	2.32	107.09	103.45
10	C	201	HEM	CAB-C3B-C2B	-2.31	120.93	128.43
6	A	702	FAD	N9A-C8A-N7A	-2.30	110.67	113.94
11	G	202	4YP	CAD-CAP-CAJ	-2.29	117.74	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	702	FAD	C4X-C10-N10	2.28	119.75	116.48
11	C	202	4YP	CAQ-CAS-CAV	-2.27	117.41	119.62
10	C	201	HEM	CAC-C3C-C2C	-2.25	121.11	128.43
6	A	702	FAD	C10-N1-C2	2.25	121.72	116.85
6	A	702	FAD	C8M-C8-C9	-2.25	115.61	119.57
10	C	201	HEM	C1A-CHA-C4D	-2.24	120.98	126.25
6	A	702	FAD	C4X-C10-N1	-2.23	119.13	124.59
10	C	201	HEM	CMB-C2B-C1B	2.16	128.41	125.03
6	E	702	FAD	C4X-C10-N1	-2.15	119.31	124.59
12	D	201	EPH	O1-C3-O3	-2.15	118.68	123.70
6	E	702	FAD	O2A-PA-O3P	2.14	113.05	107.27
10	C	201	HEM	O2D-CGD-O1D	-2.14	117.84	123.33
10	G	201	HEM	CAB-C3B-C2B	-2.10	121.62	128.43
10	G	201	HEM	CHC-C1C-NC	2.09	126.73	124.45
10	C	201	HEM	CAB-C3B-C4B	2.09	133.64	124.39
11	C	202	4YP	CAK-CAI-CAO	-2.08	120.69	127.64
12	H	201	EPH	O2-C4-O4	-2.07	118.44	123.63
6	E	702	FAD	O2P-P-O1P	2.07	122.06	112.44
6	E	702	FAD	C4X-C10-N10	2.04	119.41	116.48
10	G	201	HEM	CMC-C2C-C1C	2.02	128.29	124.73
10	C	201	HEM	C4B-C3B-C2B	-2.02	105.42	107.28
6	E	702	FAD	C4-N3-C2	-2.01	122.07	125.64

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	FAD	N10-C1'-C2'-O2'
6	A	702	FAD	C3'-C4'-C5'-O5'
6	A	702	FAD	O4'-C4'-C5'-O5'
6	A	702	FAD	C5'-O5'-P-O1P
6	A	702	FAD	C5'-O5'-P-O2P
6	A	702	FAD	C5'-O5'-P-O3P
6	E	702	FAD	N10-C1'-C2'-O2'
6	E	702	FAD	N10-C1'-C2'-C3'
6	E	702	FAD	PA-O3P-P-O5'
10	G	201	HEM	C2D-C3D-CAD-CBD
10	G	201	HEM	C4D-C3D-CAD-CBD
11	C	202	4YP	CAJ-CAL-CAS-CAV
11	C	202	4YP	CAJ-CAL-CAS-CAQ
12	D	201	EPH	C37-O5-P1-O7
12	D	201	EPH	O3-C3-O1-C2

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Mol	Chain	Res	Type	Atoms
12	D	201	EPH	C5-C3-O1-C2
12	D	201	EPH	C38-O8-P1-O5
12	D	201	EPH	C38-O8-P1-O7
12	H	201	EPH	C25-C26-C27-C28
12	H	201	EPH	C37-O5-P1-O6
12	H	201	EPH	C37-O5-P1-O8
12	H	201	EPH	C38-O8-P1-O5
12	H	201	EPH	C38-O8-P1-O7
12	H	201	EPH	O8-C38-C39-N1
12	D	201	EPH	O4-C4-O2-C1
12	D	201	EPH	C18-C4-O2-C1
12	H	201	EPH	C18-C4-O2-C1
12	H	201	EPH	O4-C4-O2-C1
11	C	202	4YP	CAI-CAK-CAM-CAP
11	G	202	4YP	CAI-CAK-CAM-CAP
12	H	201	EPH	C5-C3-O1-C2
12	H	201	EPH	O3-C3-O1-C2
12	H	201	EPH	C11-C10-C9-C8
12	H	201	EPH	C7-C8-C9-C10
12	D	201	EPH	O2-C1-C2-C37
12	D	201	EPH	C7-C8-C9-C10
12	D	201	EPH	C6-C7-C8-C9
12	H	201	EPH	C6-C7-C8-C9
12	H	201	EPH	C5-C6-C7-C8
12	H	201	EPH	C2-C1-O2-C4
12	H	201	EPH	C20-C21-C22-C23
12	D	201	EPH	C19-C20-C21-C22
12	D	201	EPH	C11-C10-C9-C8
12	H	201	EPH	C12-C13-C14-C15
12	H	201	EPH	C13-C14-C15-C16
6	A	702	FAD	PA-O3P-P-O5'
12	H	201	EPH	C28-C29-C30-C31
12	H	201	EPH	O1-C3-C5-C6
12	H	201	EPH	O2-C1-C2-C37
10	C	201	HEM	C4B-C3B-CAB-CBB
10	C	201	HEM	C4C-C3C-CAC-CBC
10	G	201	HEM	C4B-C3B-CAB-CBB
10	G	201	HEM	C4C-C3C-CAC-CBC
11	G	202	4YP	CAJ-CAL-CAS-CAV
12	D	201	EPH	O2-C1-C2-O1
6	E	702	FAD	P-O3P-PA-O1A
12	H	201	EPH	O2-C1-C2-O1

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Mol	Chain	Res	Type	Atoms
12	D	201	EPH	C37-O5-P1-O8
12	D	201	EPH	O8-C38-C39-N1
6	A	702	FAD	P-O3P-PA-O2A
6	E	702	FAD	P-O3P-PA-O2A
12	H	201	EPH	C9-C10-C11-C12
12	D	201	EPH	C1-C2-O1-C3
12	D	201	EPH	C25-C26-C27-C28
12	D	201	EPH	C22-C23-C24-C25
12	D	201	EPH	C13-C14-C15-C16
12	D	201	EPH	C28-C29-C30-C31
12	H	201	EPH	C10-C11-C12-C13
12	D	201	EPH	C24-C25-C26-C27
12	H	201	EPH	O3-C3-C5-C6
6	A	702	FAD	O4B-C4B-C5B-O5B
6	A	702	FAD	P-O3P-PA-O1A
12	H	201	EPH	C18-C19-C20-C21
12	H	201	EPH	C19-C20-C21-C22

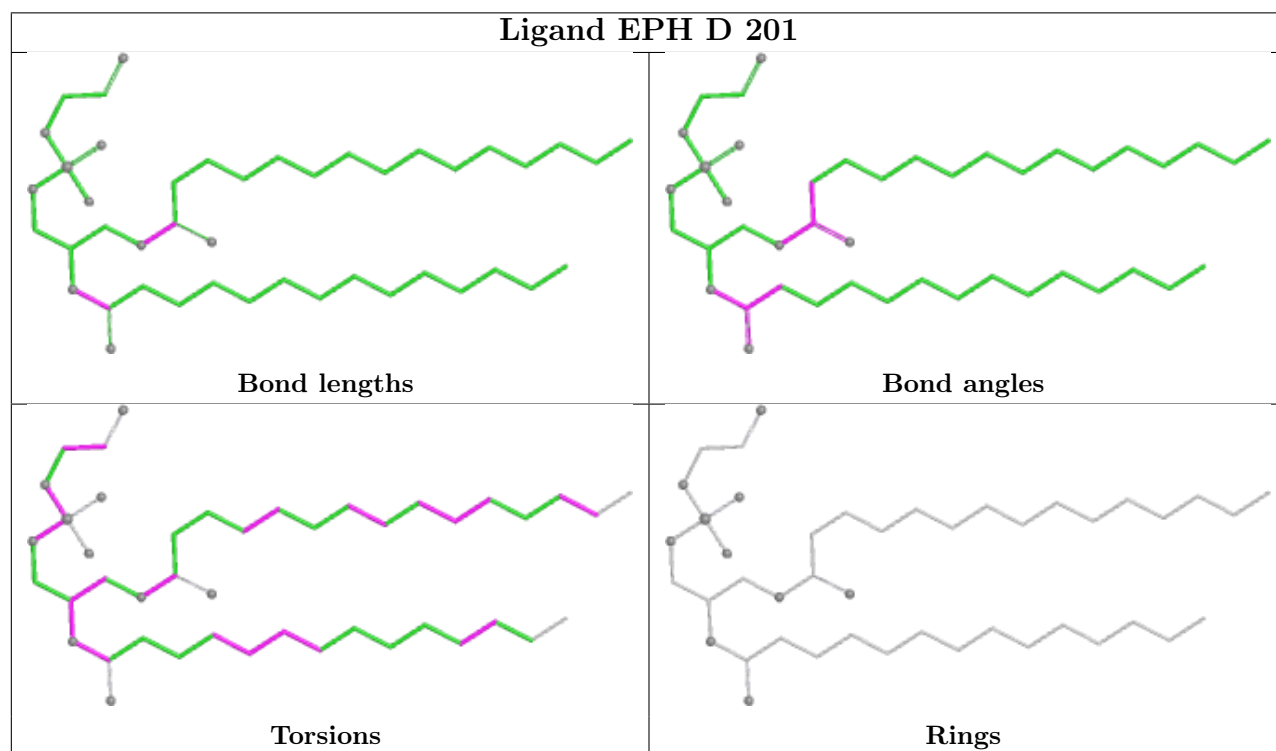
There are no ring outliers.

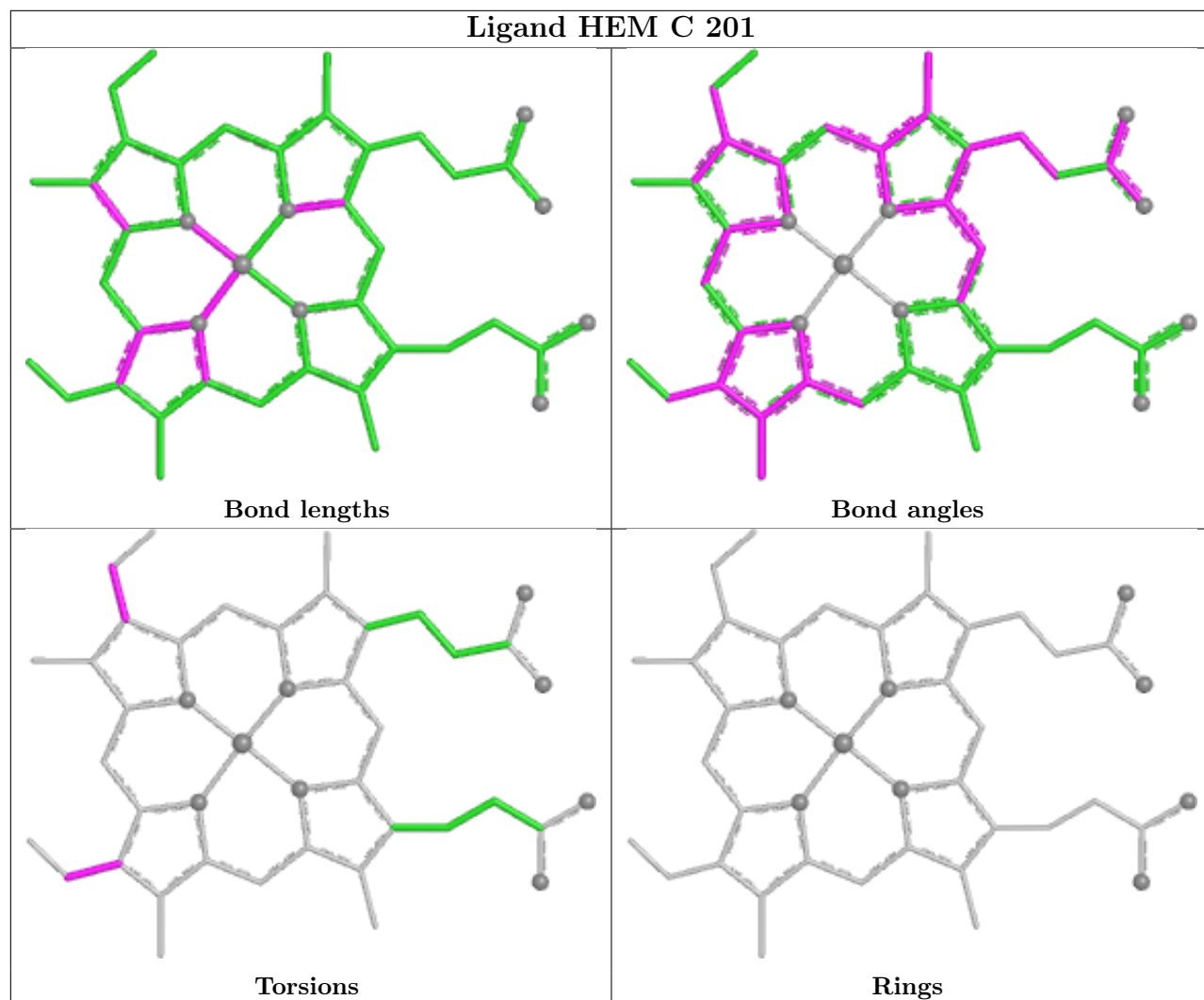
9 monomers are involved in 28 short contacts:

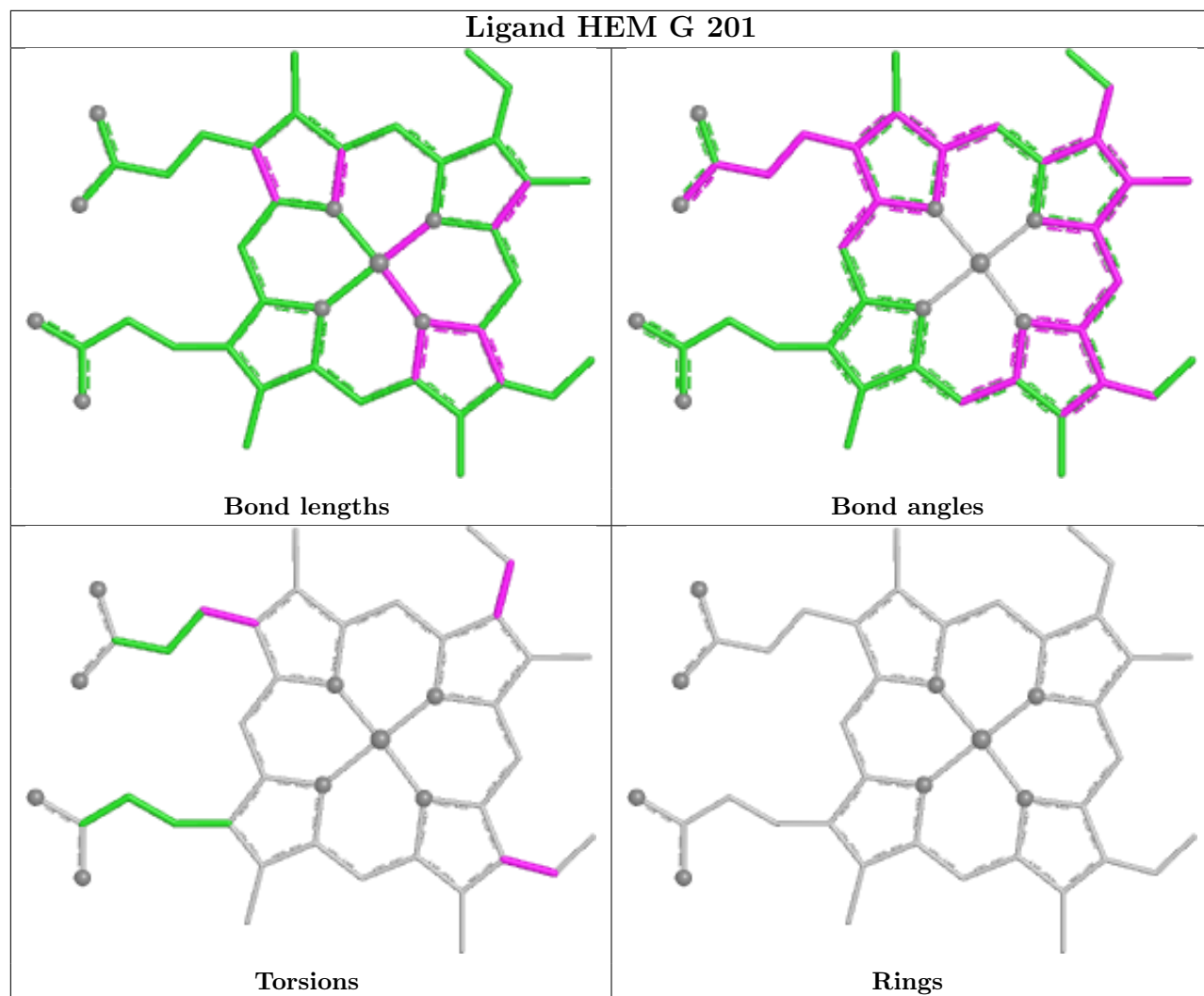
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	201	HEM	4	0
5	A	701	MLI	1	0
10	G	201	HEM	4	0
11	C	202	4YP	1	0
11	G	202	4YP	1	0
12	H	201	EPH	2	0
5	E	701	MLI	1	0
6	A	702	FAD	8	0
6	E	702	FAD	6	0

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.

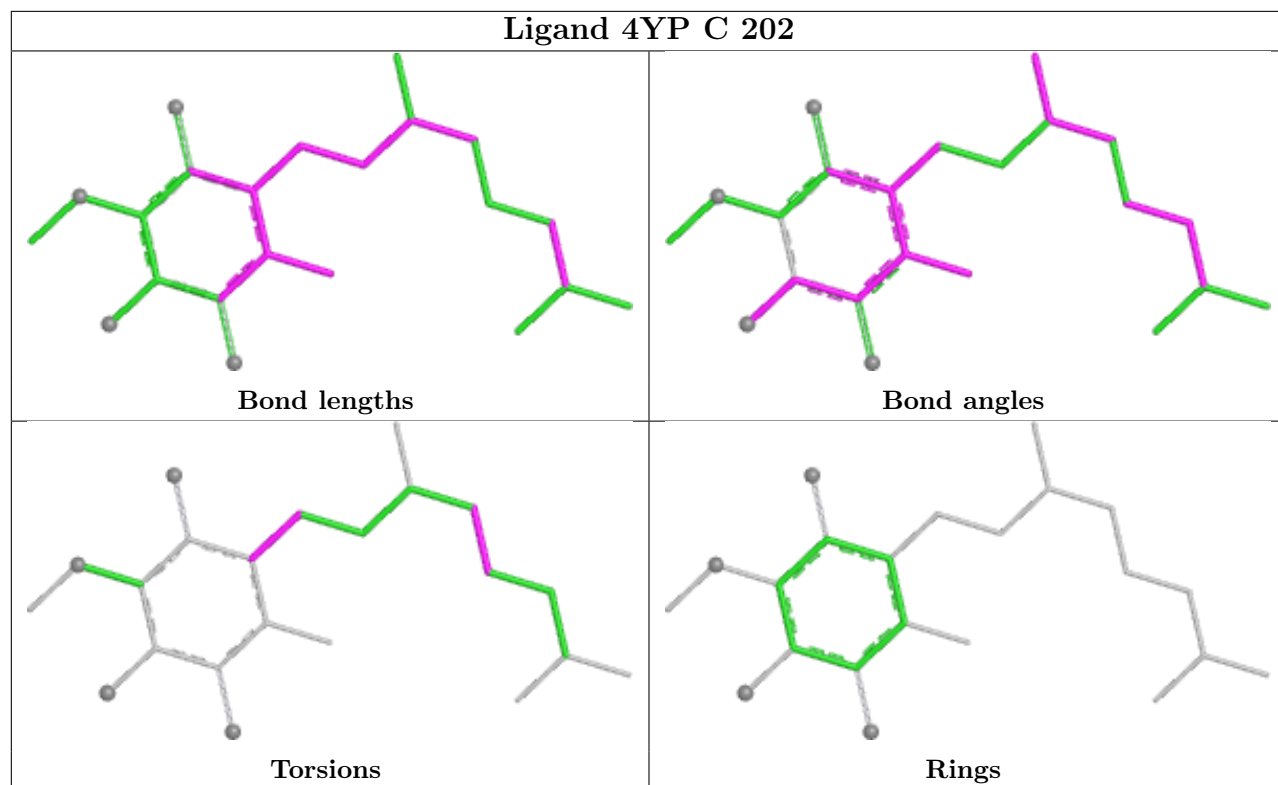
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



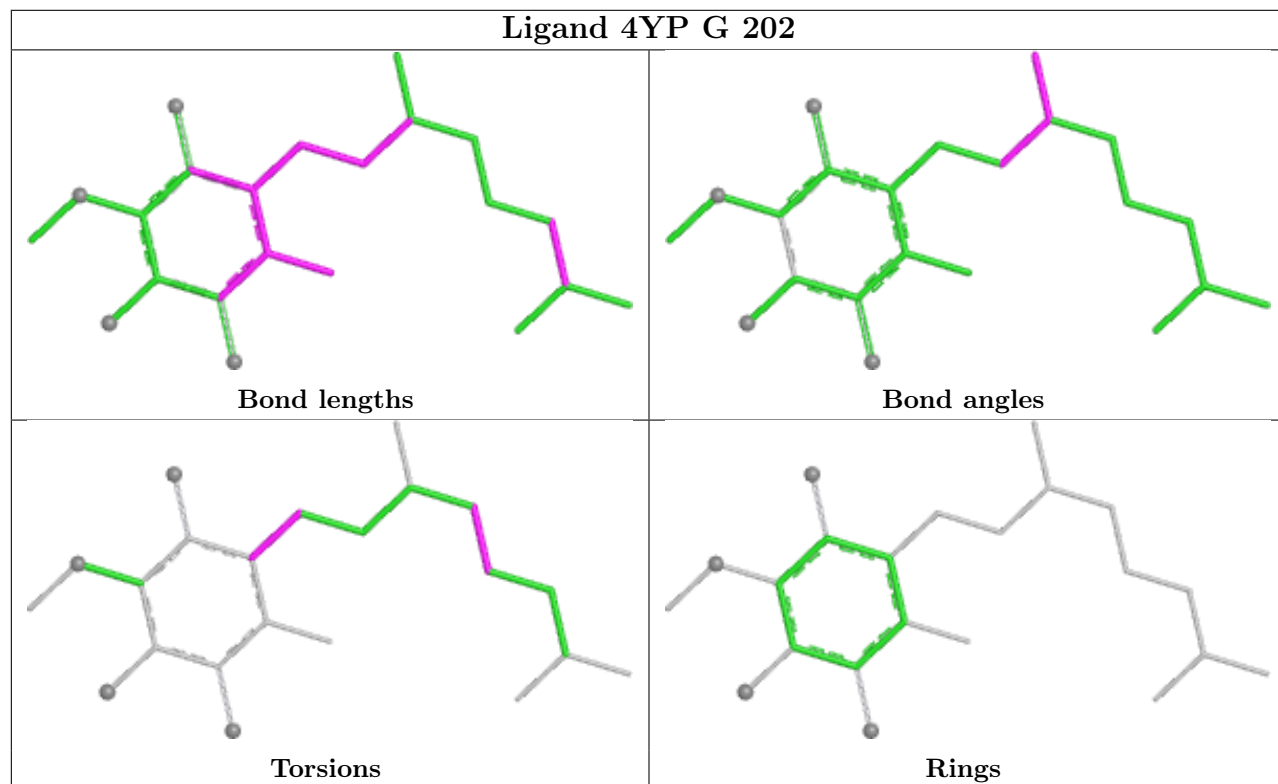


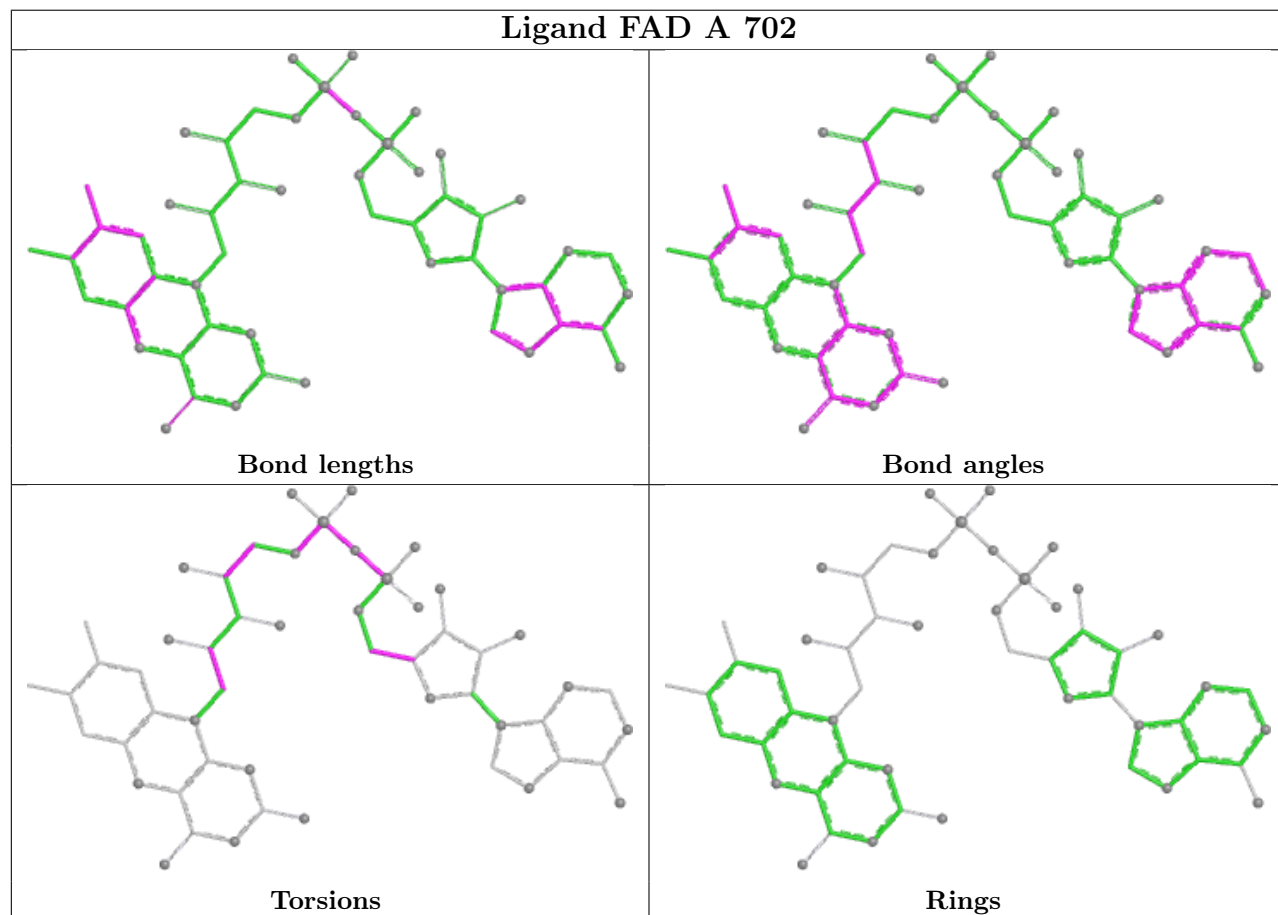
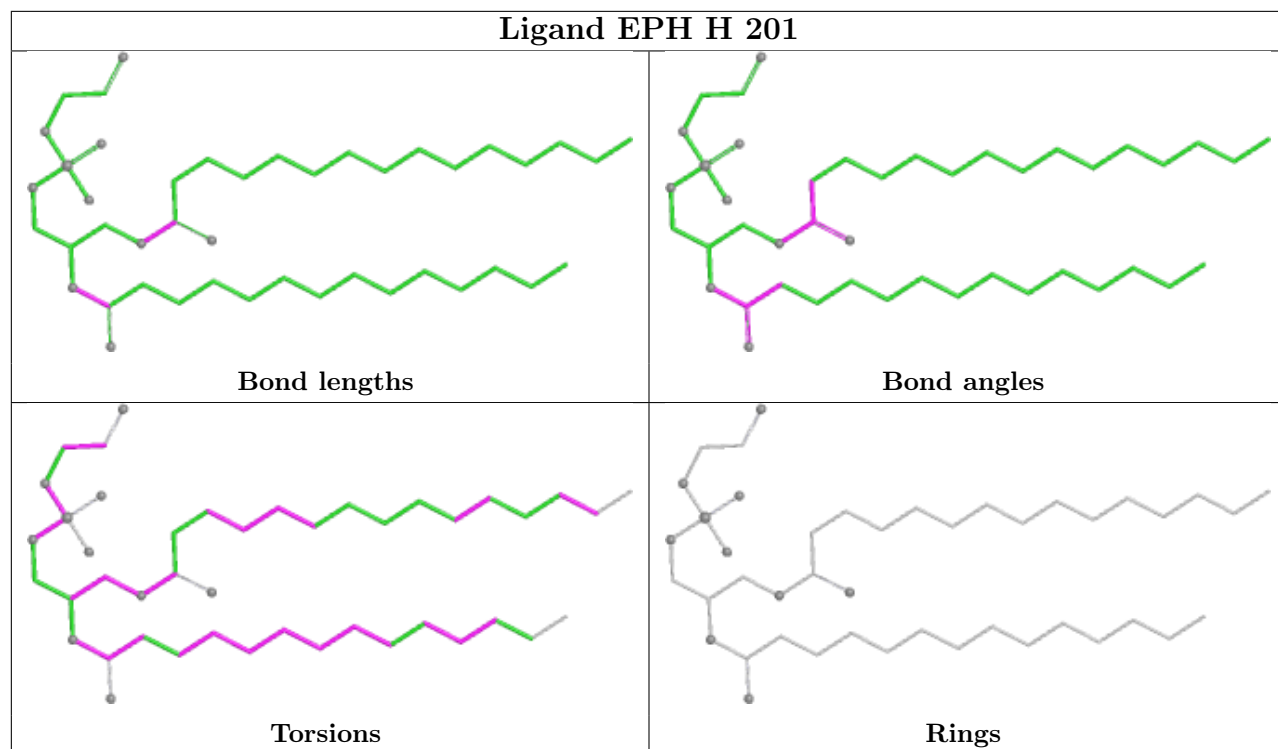


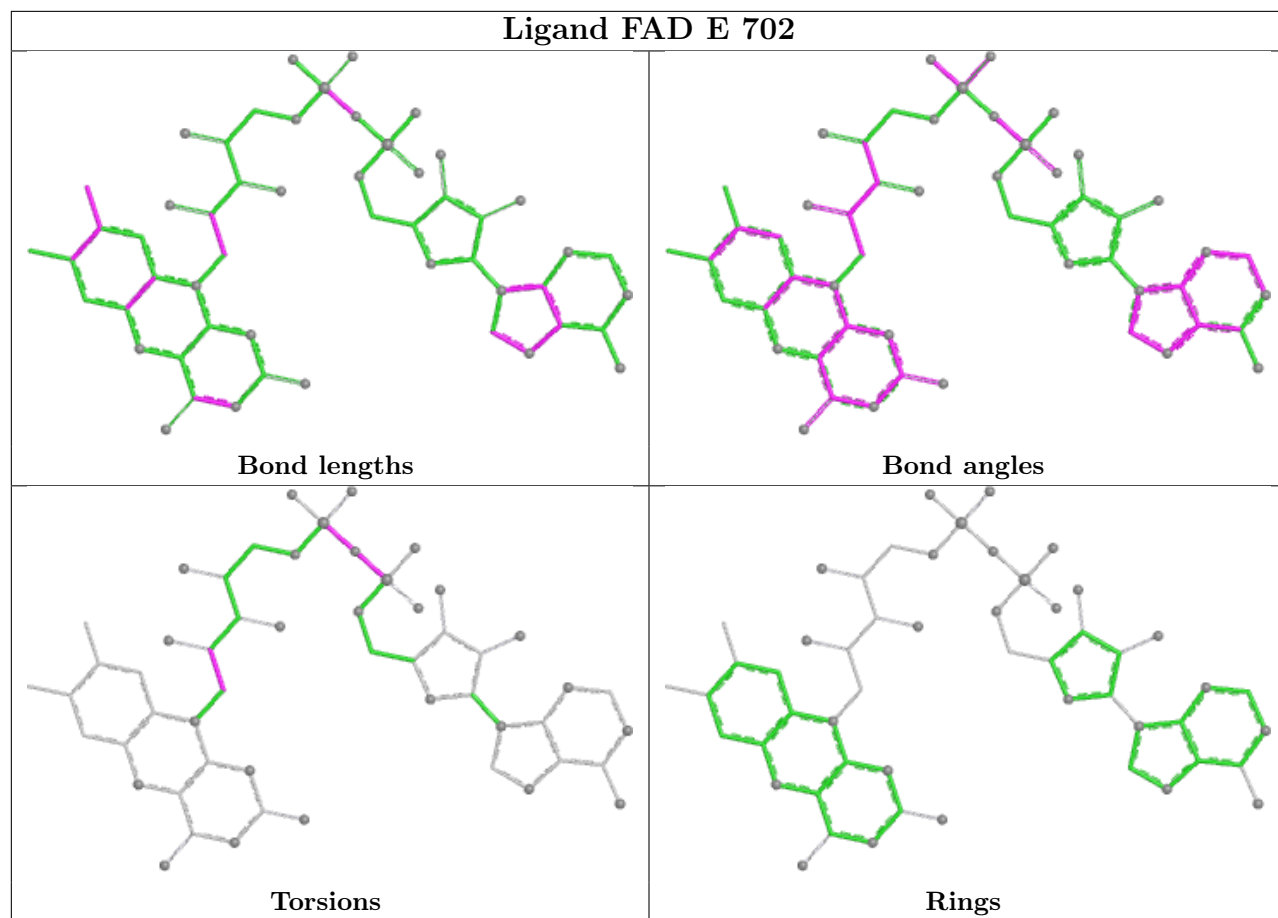
Ligand 4YP C 202



Ligand 4YP G 202







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	616/645 (95%)	-0.36	0 100 100	22, 37, 62, 87	0
1	E	616/645 (95%)	0.09	10 (1%) 70 69	27, 53, 85, 116	0
2	B	250/282 (88%)	-0.30	1 (0%) 88 89	24, 37, 70, 97	0
2	F	250/282 (88%)	-0.16	2 (0%) 82 82	24, 43, 73, 93	0
3	C	153/188 (81%)	0.12	2 (1%) 75 75	28, 55, 84, 112	0
3	G	153/188 (81%)	0.52	17 (11%) 10 9	33, 60, 134, 191	0
4	D	129/156 (82%)	0.12	3 (2%) 61 59	21, 50, 72, 97	1 (0%)
4	H	129/156 (82%)	0.27	6 (4%) 36 36	35, 59, 99, 130	0
All	All	2296/2542 (90%)	-0.06	41 (1%) 67 65	21, 47, 85, 191	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	185	PRO	5.3
3	G	186	THR	5.1
3	G	181	LYS	4.9
4	H	49	PHE	4.4
3	G	114	TRP	4.1
3	G	180	LYS	4.0
3	G	184	LEU	4.0
4	D	52	LEU	3.9
3	G	176	TRP	3.5
1	E	32	ILE	3.4
3	G	183	THR	3.4
4	H	52	LEU	3.3
4	H	28	THR	3.3
4	H	51	PRO	3.3
3	G	178	ARG	3.2
3	G	179	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	30	ALA	3.1
3	G	173	TYR	3.1
3	G	182	ALA	3.1
3	G	174	PRO	3.0
1	E	635	VAL	3.0
4	H	30	ALA	3.0
2	F	33	LYS	2.9
1	E	591	ILE	2.8
1	E	585	TYR	2.8
3	C	186	THR	2.8
1	E	590	PRO	2.8
1	E	30	SER	2.8
3	G	177	GLU	2.7
2	F	159	ILE	2.6
3	G	107	ILE	2.6
3	C	176	TRP	2.4
3	G	112	ILE	2.3
1	E	406	LYS	2.3
4	D	53	HIS	2.2
1	E	632	PRO	2.2
1	E	637	TRP	2.2
1	E	486	ASP	2.2
3	G	175	ARG	2.1
2	B	54	LEU	2.1
4	H	53	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

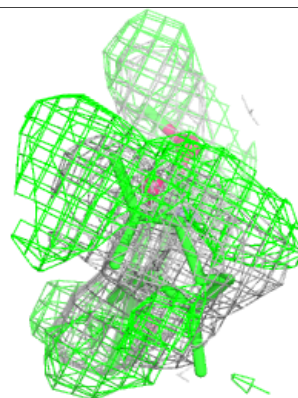
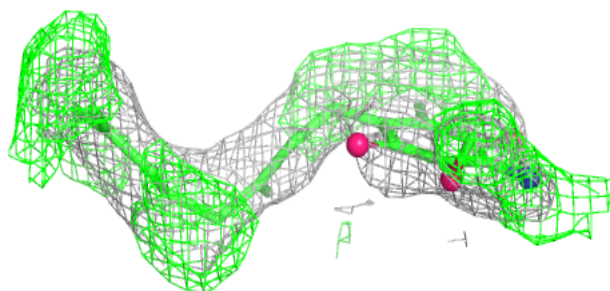
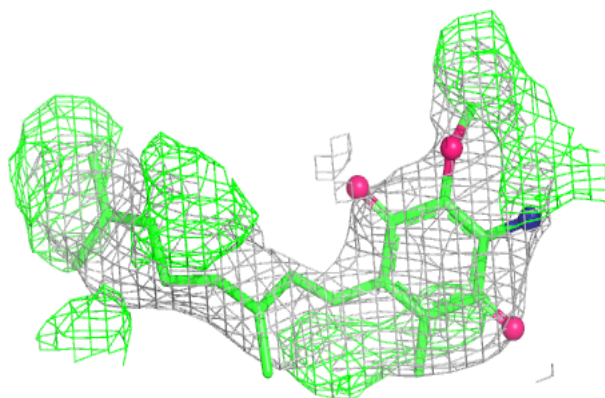
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	4YP	C	202	22/22	0.66	0.33	55,57,59,61	22
11	4YP	G	202	22/22	0.71	0.35	49,58,65,65	22
12	EPH	H	201	44/49	0.72	0.29	56,76,102,105	44
12	EPH	D	201	44/49	0.82	0.22	42,63,74,77	44
6	FAD	E	702	53/53	0.95	0.08	28,32,40,43	0
10	HEM	G	201	43/43	0.95	0.11	51,59,68,73	0
5	MLI	A	701	7/7	0.96	0.06	36,37,38,38	0
10	HEM	C	201	43/43	0.97	0.09	39,53,59,69	0
5	MLI	E	701	7/7	0.97	0.10	37,38,39,40	0
9	F3S	F	303	7/7	0.97	0.06	32,36,38,41	0
9	F3S	B	303	7/7	0.98	0.05	31,35,37,37	0
6	FAD	A	702	53/53	0.98	0.05	18,22,27,27	0
8	SF4	B	302	8/8	0.98	0.04	24,27,28,30	0
8	SF4	F	302	8/8	0.98	0.04	28,29,32,33	0
7	FES	B	301	4/4	0.99	0.03	22,24,26,31	0
7	FES	F	301	4/4	0.99	0.03	28,30,30,36	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.

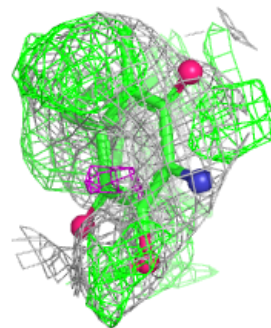
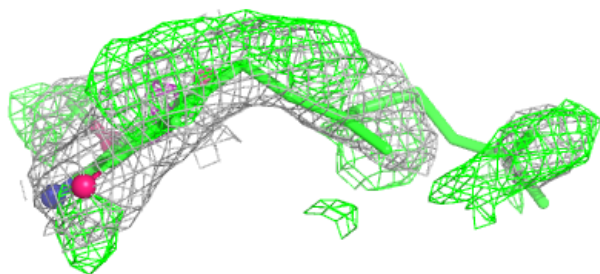
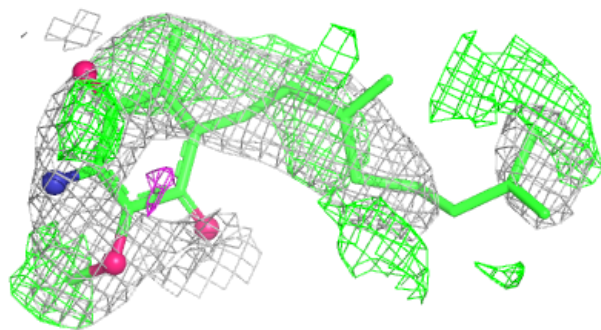
Electron density around 4YP C 202:

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



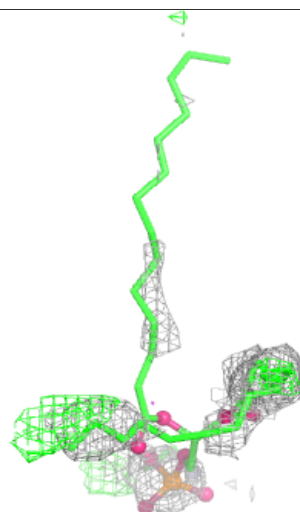
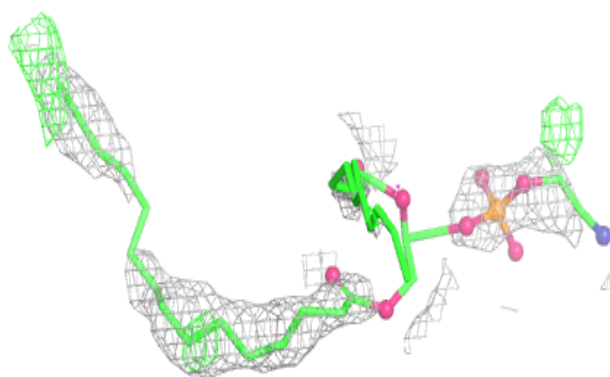
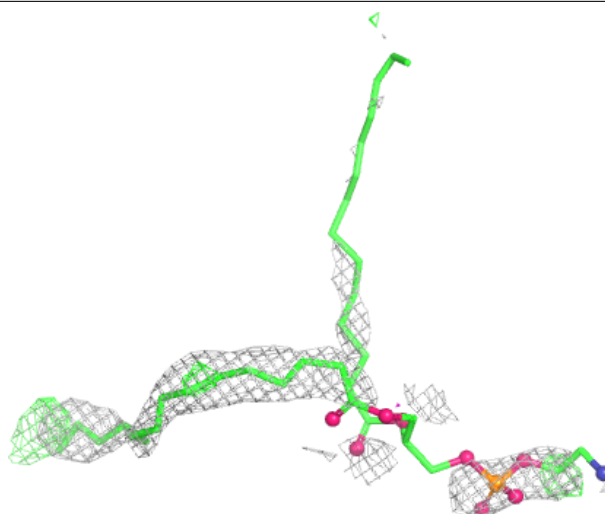
Electron density around 4YP G 202:

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



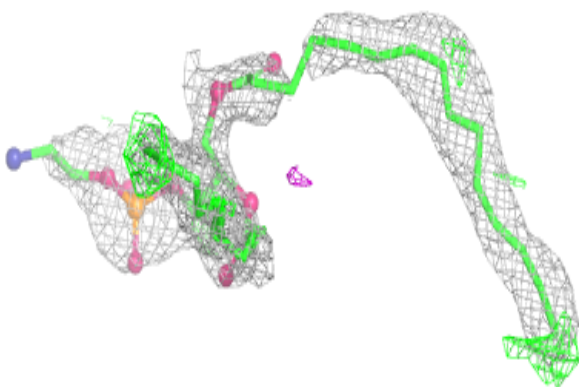
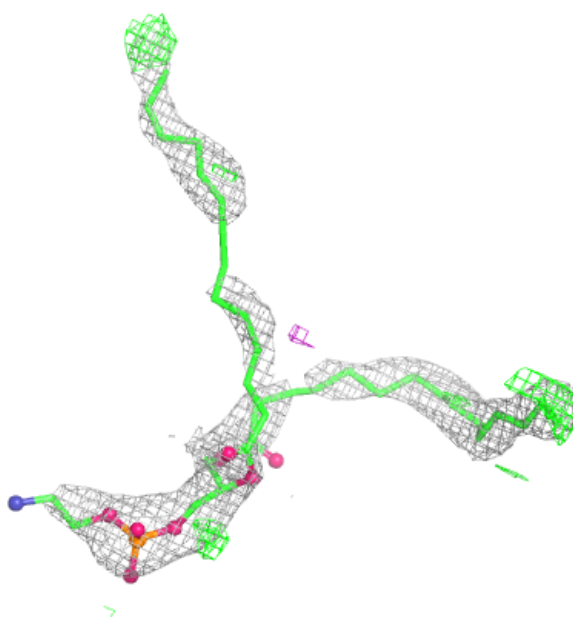
Electron density around EPH H 201:

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



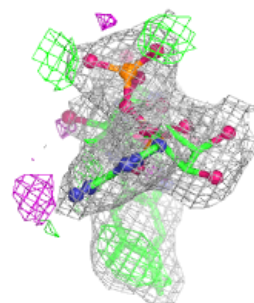
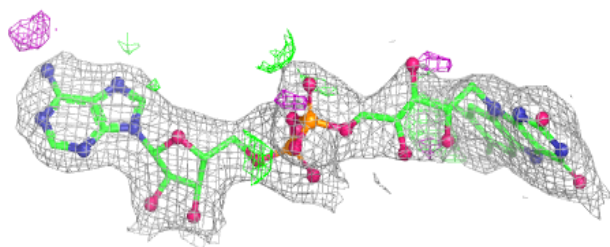
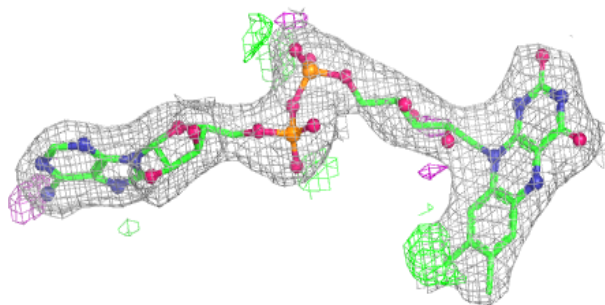
Electron density around EPH D 201:

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



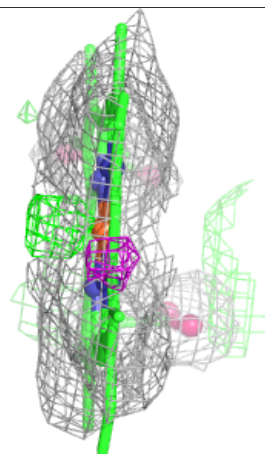
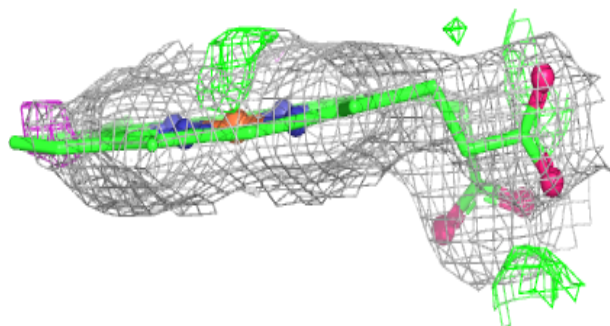
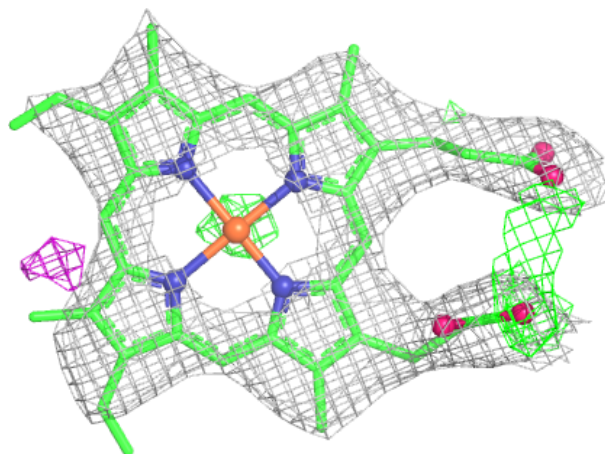
Electron density around FAD E 702:

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



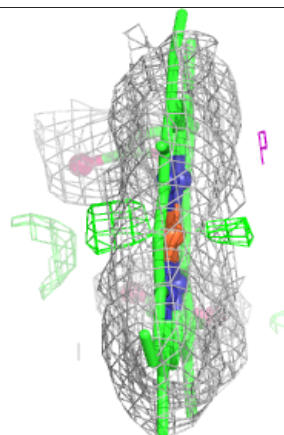
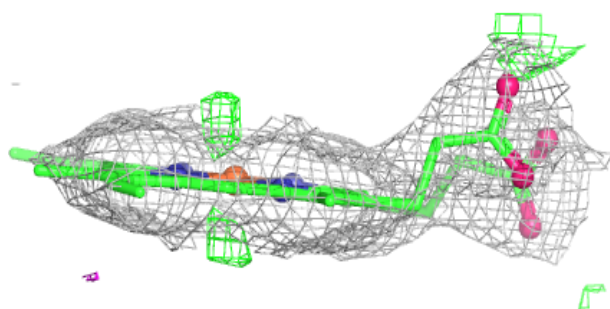
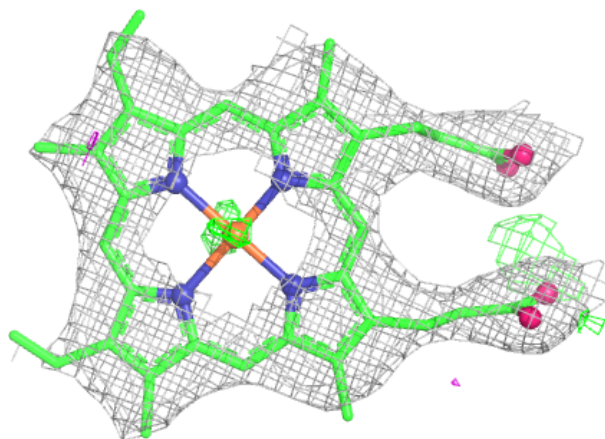
Electron density around HEM G 201:

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

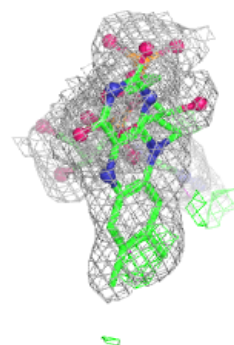
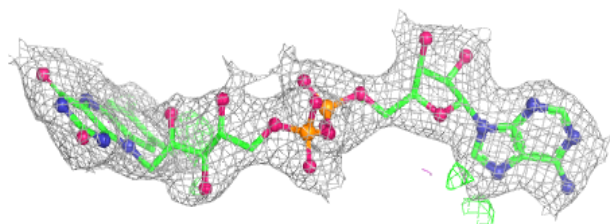
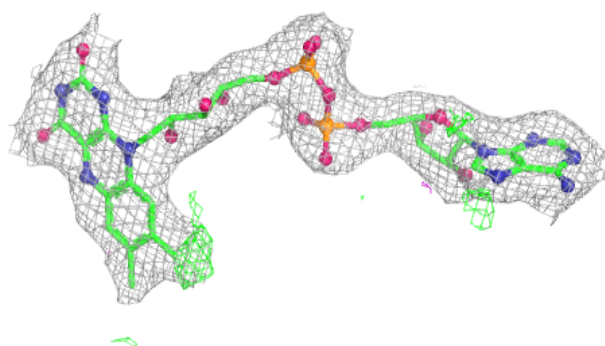


Electron density around HEM C 201:

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

**Electron density around FAD A 702:**

$2mF_o-DF_c$ (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.