



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:58 PM EDT

PDB ID : 4YSZ / pdb_00004ysz
Title : Crystal structure of Mitochondrial rhodoquinol-fumarate reductase from *Ascaris suum* with 2-iodo-N-[3-(1-methylethoxy)phenyl]benzamide
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 : 2015-03-17
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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

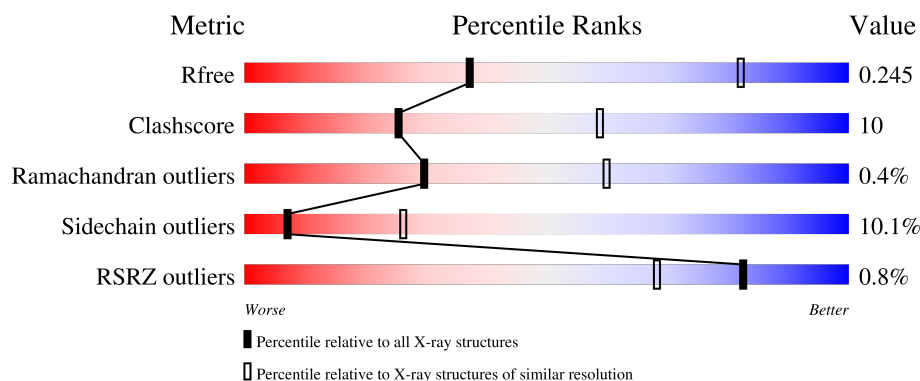
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	
1	E	645	
2	B	282	
2	F	282	

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Mol	Chain	Length	Quality of chain
3	C	188	
3	G	188	
4	D	156	
4	H	156	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MLI	E	701	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18361 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 flavoprotein.

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			

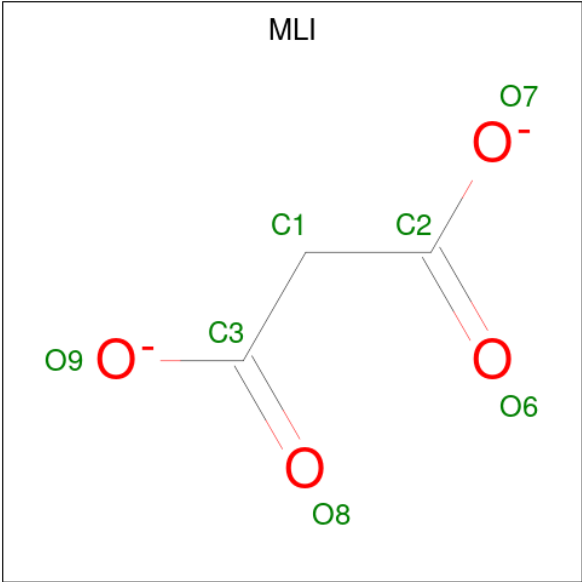
- Molecule 3 is a protein called Cytochrome b-large subunit.

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.

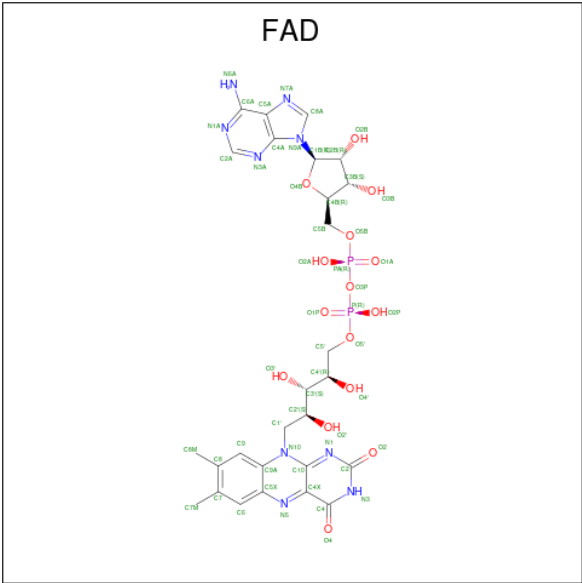
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			
4	H	129	Total	C	N	O	S	0	0	0
			998	659	165	169	5			

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



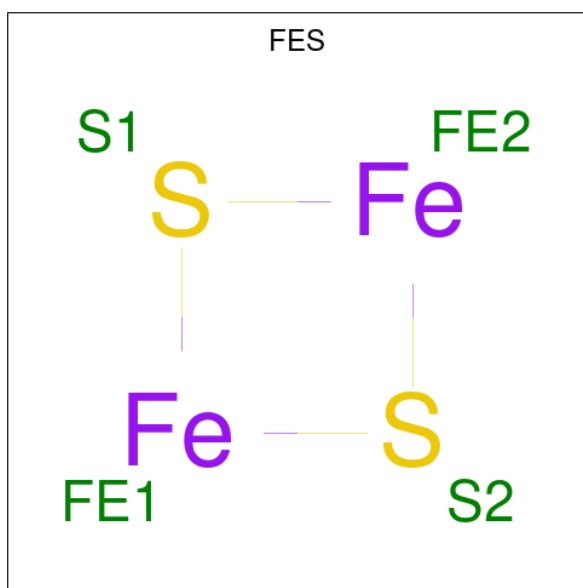
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	E	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



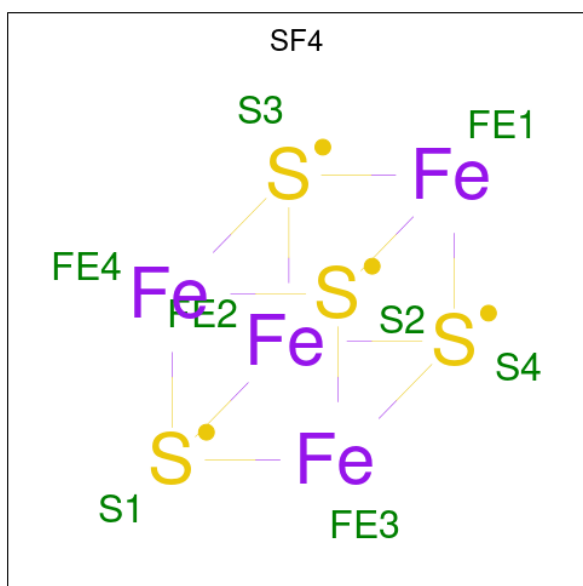
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0
			53	27	9	15	2	
6	E	1	Total	C	N	O	P	0
			53	27	9	15	2	

- 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).



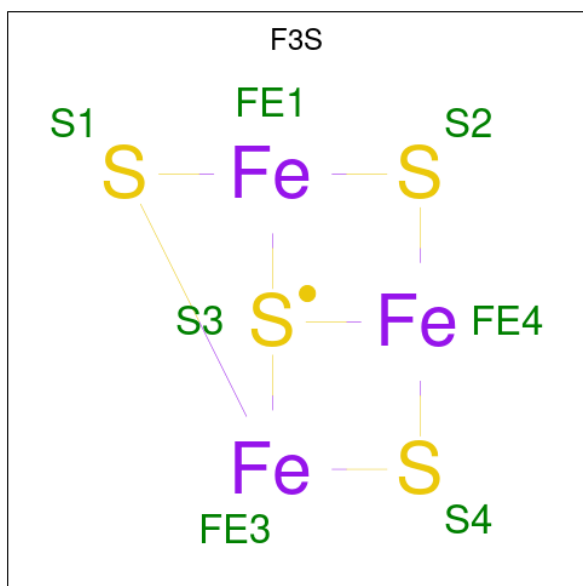
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		

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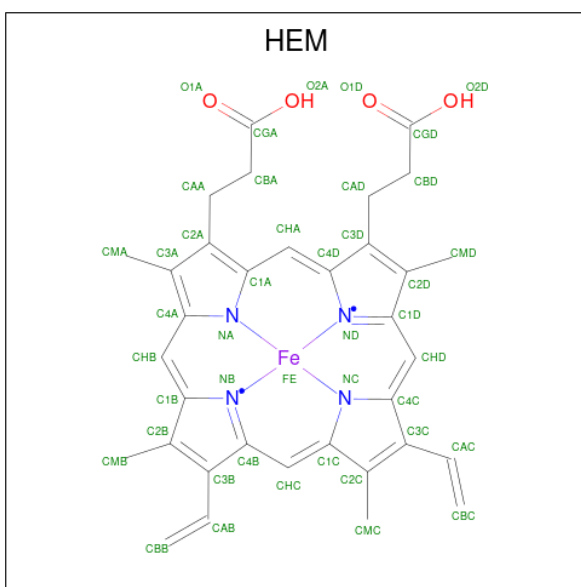
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	Fe	S	0	0
			8	4	4		

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



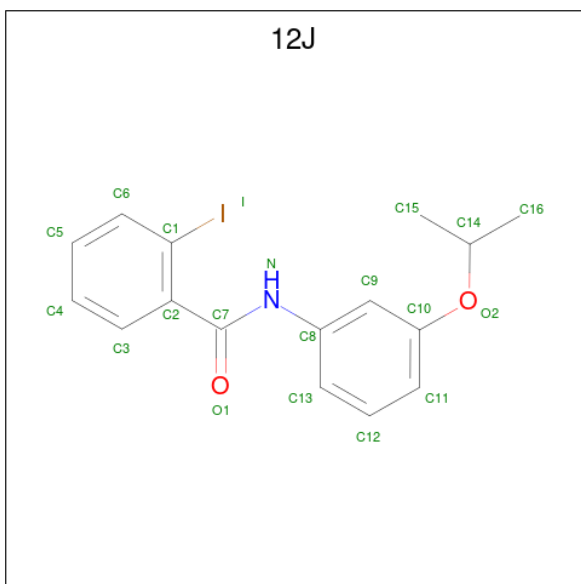
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			7	3	4		
9	F	1	Total	Fe	S	0	0
			7	3	4		

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		
10	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is 2-iodo-N-[3-(1-methylethoxy)phenyl]benzamide (CCD ID: 12J) (formula: $C_{16}H_{16}INO_2$).



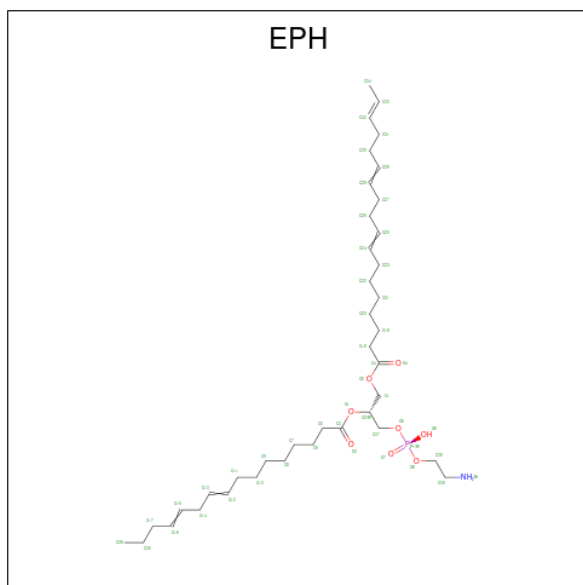
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	I	N	O	0	0
			20	16	1	1	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	G	1	Total	C	I	N	O	0	0
			20	16	1	1	2		

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (CCD ID: EPH) (formula: $C_{39}H_{68}NO_8P$).



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		

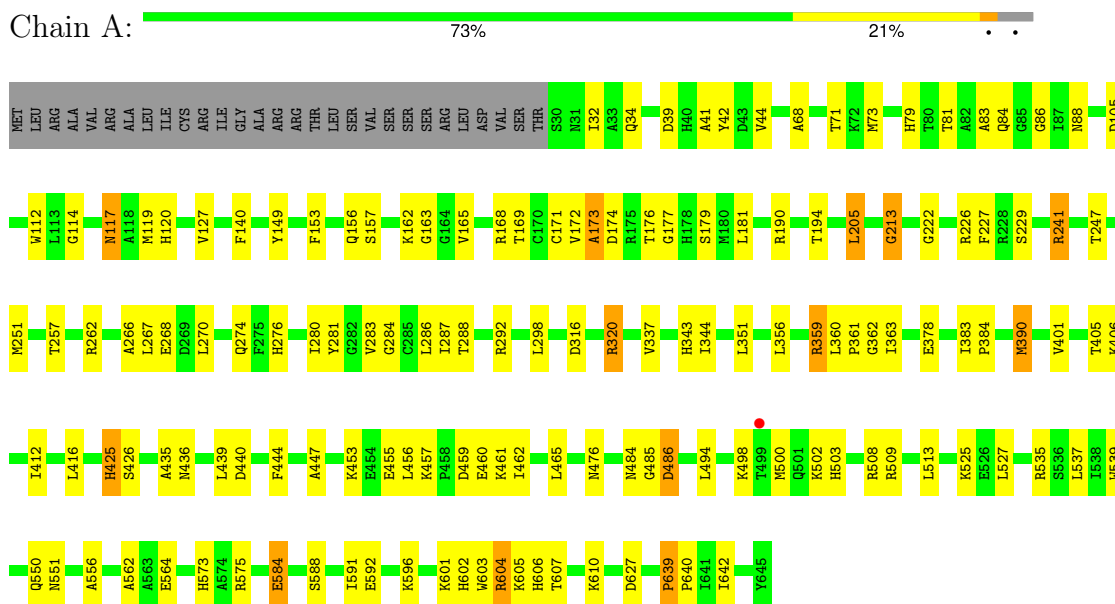
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	4	Total	O	0	0
			4	4		
13	B	2	Total	O	0	0
			2	2		
13	C	1	Total	O	0	0
			1	1		
13	D	1	Total	O	0	0
			1	1		
13	E	6	Total	O	0	0
			6	6		
13	H	1	Total	O	0	0
			1	1		

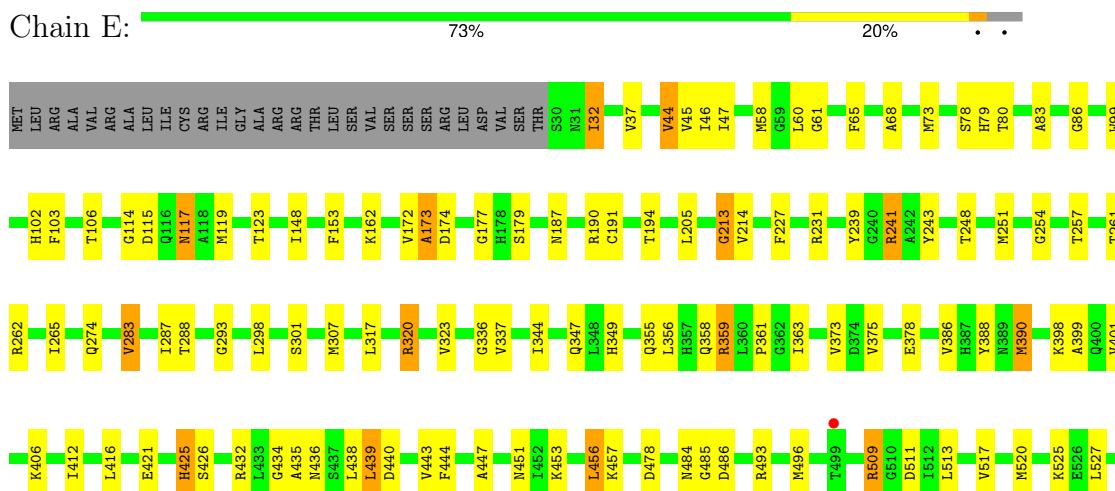
3 Residue-property plots

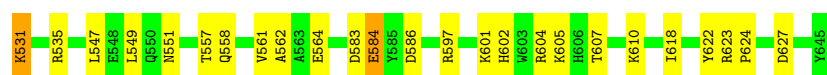
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

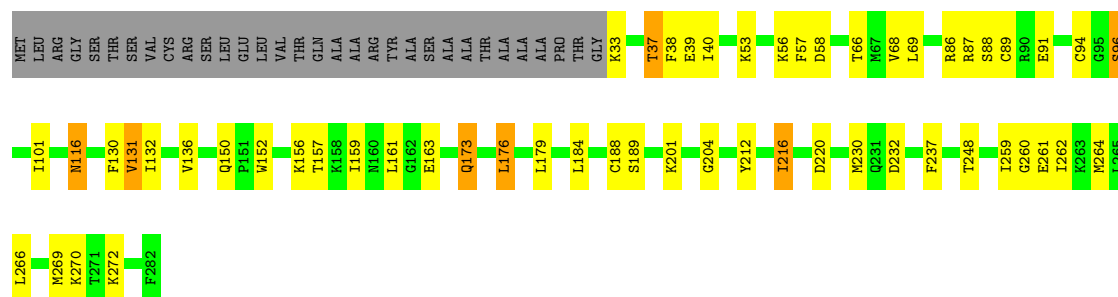


• Molecule 1: Succinate dehydrogenase flavoprotein

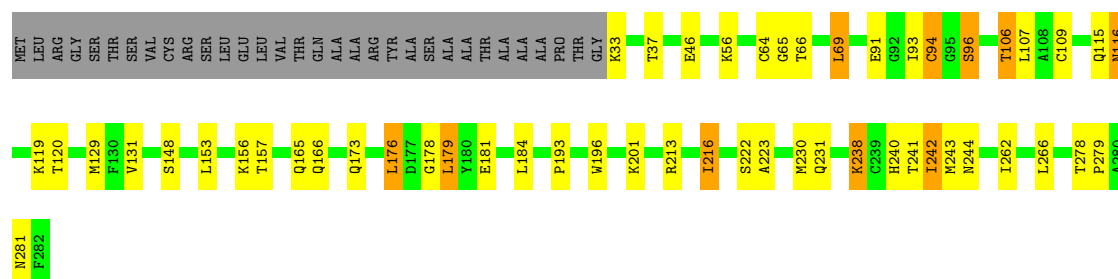




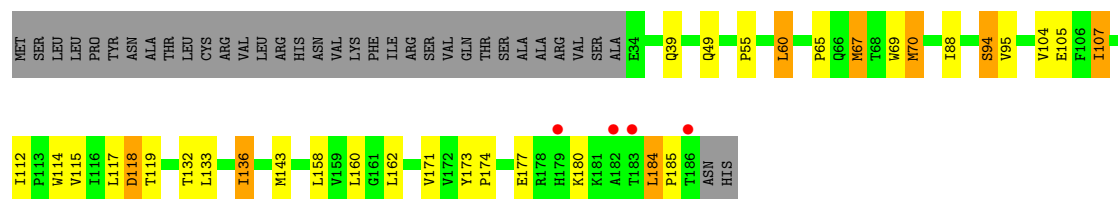
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



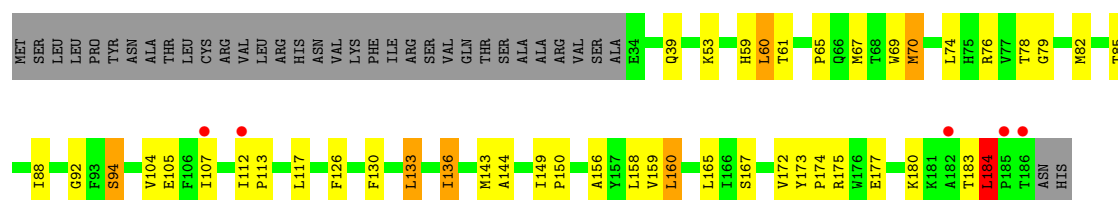
- Molecule 2: Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial



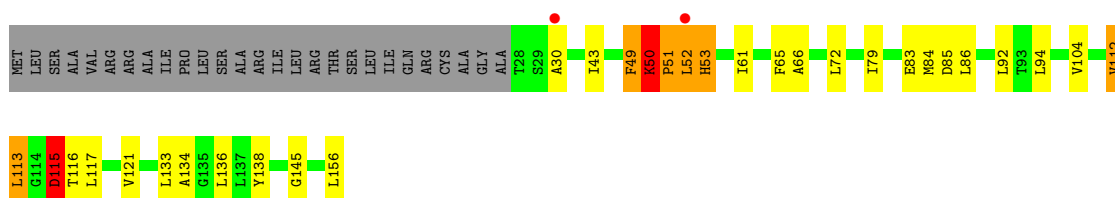
- Molecule 3: Cytochrome b-large subunit



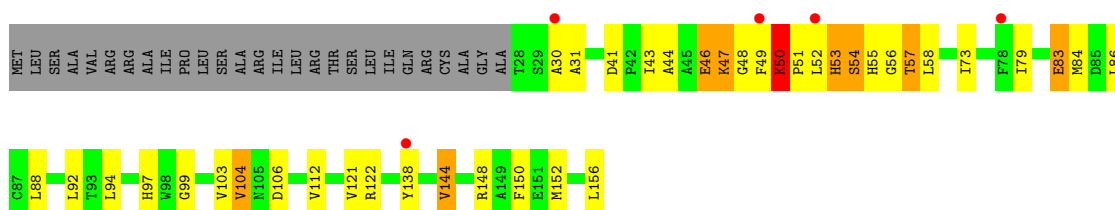
- Molecule 3: Cytochrome b-large subunit



- 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	123.93Å 126.97Å 219.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 3.30 29.82 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.82-3.30) 97.3 (29.82-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.179 , 0.250 0.180 , 0.245	Depositor DCC
R_{free} test set	2624 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18361	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: FES, EPH, HEM, F3S, 12J, FAD, SF4, MLI

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	0.64	1/4889 (0.0%)	0.90	5/6605 (0.1%)
1	E	0.63	2/4889 (0.0%)	0.92	8/6605 (0.1%)
2	B	0.61	0/2029	0.92	5/2739 (0.2%)
2	F	0.67	1/2029 (0.0%)	0.88	0/2739
3	C	0.62	0/1255	0.85	0/1709
3	G	0.64	0/1255	0.91	1/1709 (0.1%)
4	D	0.78	0/1030	0.96	1/1406 (0.1%)
4	H	0.79	3/1030 (0.3%)	0.97	4/1406 (0.3%)
All	All	0.65	7/18406 (0.0%)	0.91	24/24918 (0.1%)

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
4	D	0	1
4	H	0	2
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	94	CYS	C-N	6.77	1.43	1.33
1	A	173	ALA	CA-C	-6.53	1.47	1.53
1	E	173	ALA	CA-C	-6.53	1.47	1.53
4	H	73	ILE	CA-CB	5.37	1.57	1.54
1	E	173	ALA	C-O	-5.33	1.19	1.24
4	H	55	HIS	CG-ND1	-5.31	1.32	1.38
4	H	55	HIS	CA-C	-5.08	1.46	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ALA	CB-CA-C	-8.33	106.97	116.63
4	H	47	LYS	N-CA-C	-7.14	99.88	110.23
1	E	173	ALA	CB-CA-C	-6.52	109.04	116.54
1	E	283	VAL	N-CA-C	6.49	117.58	112.12
1	E	425	HIS	N-CA-C	6.47	119.64	111.69
1	E	283	VAL	CB-CA-C	-6.41	104.63	110.91
2	B	163	GLU	N-CA-C	6.39	118.05	111.14
1	E	86	GLY	N-CA-C	6.34	119.38	110.38
2	B	204	GLY	CA-C-N	6.21	126.12	119.28
2	B	204	GLY	C-N-CA	6.21	126.12	119.28
1	A	213	GLY	N-CA-C	6.04	118.11	110.38
4	D	115	ASP	N-CA-C	5.93	117.41	111.07
1	E	213	GLY	N-CA-C	5.93	117.97	110.38
1	A	425	HIS	N-CA-C	5.89	118.66	111.82
4	H	50	LYS	CA-C-N	5.81	125.75	119.76
4	H	50	LYS	C-N-CA	5.81	125.75	119.76
1	E	373	VAL	N-CA-C	5.58	115.90	107.75
4	H	57	THR	N-CA-C	-5.50	105.28	111.28
1	E	288	THR	N-CA-C	5.42	117.29	110.24
1	A	127	VAL	CB-CA-C	-5.39	104.98	112.04
1	A	639	PRO	O-C-N	5.34	123.66	121.15
3	G	184	LEU	N-CA-C	5.34	114.28	108.14
2	B	132	ILE	N-CA-C	-5.13	106.80	111.67
2	B	161	LEU	N-CA-C	5.10	117.50	111.33

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	30	ALA	Peptide
4	H	30	ALA	Peptide
4	H	50	LYS	Peptide

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	4720	76	0
1	E	4787	0	4720	84	0
2	B	1985	0	2001	25	0
2	F	1985	0	2001	26	0
3	C	1217	0	1265	30	0
3	G	1217	0	1265	26	0
4	D	998	0	985	45	0
4	H	998	0	985	49	0
5	A	7	0	2	1	0
5	E	7	0	2	2	0
6	A	53	0	31	4	0
6	E	53	0	31	5	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	6	0
10	G	43	0	30	7	0
11	C	20	0	16	4	0
11	G	20	0	16	4	0
12	D	44	0	53	0	0
12	H	44	0	53	2	0
13	A	4	0	0	0	0
13	B	2	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	6	0	0	0	0
13	H	1	0	0	0	0
All	All	18361	0	18206	350	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 10.

All (350) 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)
4:D:112:VAL:C	4:D:113:LEU:HD23	1.39	1.44
1:A:79:HIS:NE2	6:A:702:FAD:HM82	1.36	1.40
4:D:112:VAL:HG12	4:D:113:LEU:CD2	1.77	1.13
4:H:50:LYS:N	4:H:50:LYS:HD2	1.59	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:112:VAL:HG12	4:D:113:LEU:HD21	1.14	1.11
4:D:113:LEU:HD23	4:D:113:LEU:N	1.50	1.11
4:H:52:LEU:C	4:H:53:HIS:CD2	2.30	1.09
4:D:50:LYS:N	4:D:51:PRO:CD	2.15	1.09
4:H:46:GLU:HA	4:H:46:GLU:OE2	1.47	1.06
4:D:52:LEU:C	4:D:53:HIS:HD2	1.64	1.05
1:A:172:VAL:HG12	1:A:172:VAL:O	1.55	1.04
4:D:112:VAL:C	4:D:113:LEU:CD2	2.31	1.04
4:D:50:LYS:H	4:D:51:PRO:CD	1.68	1.03
1:E:79:HIS:NE2	6:E:702:FAD:HM81	1.74	1.02
4:H:50:LYS:N	4:H:51:PRO:HD3	1.73	1.01
4:D:112:VAL:CG1	4:D:113:LEU:HD21	1.92	0.98
4:D:50:LYS:N	4:D:51:PRO:HD2	1.77	0.98
4:D:52:LEU:C	4:D:53:HIS:CD2	2.41	0.98
4:D:50:LYS:H	4:D:51:PRO:HD3	1.27	0.98
4:H:51:PRO:HB2	4:H:53:HIS:NE2	1.78	0.97
4:H:51:PRO:CB	4:H:53:HIS:NE2	2.30	0.95
4:D:113:LEU:CD2	4:D:113:LEU:N	2.30	0.94
4:H:50:LYS:N	4:H:51:PRO:CD	2.30	0.94
4:D:53:HIS:CD2	4:D:53:HIS:N	2.30	0.94
4:D:52:LEU:CA	4:D:53:HIS:HD2	1.80	0.94
1:A:79:HIS:NE2	6:A:702:FAD:C8M	2.29	0.93
4:H:50:LYS:N	4:H:50:LYS:CD	2.30	0.93
4:H:52:LEU:C	4:H:53:HIS:HD2	1.80	0.88
4:H:51:PRO:C	4:H:53:HIS:NE2	2.32	0.87
2:F:94:CYS:SG	2:F:96:SER:OG	2.32	0.87
4:H:49:PHE:O	4:H:49:PHE:CD1	2.30	0.84
4:D:49:PHE:CD1	4:D:49:PHE:O	2.30	0.84
4:D:112:VAL:CG1	4:D:113:LEU:CD2	2.56	0.80
4:D:52:LEU:CA	4:D:53:HIS:CD2	2.65	0.80
1:E:79:HIS:NE2	6:E:702:FAD:C8M	2.44	0.79
2:F:242:ILE:O	2:F:243:MET:HB2	1.82	0.78
1:A:79:HIS:CD2	6:A:702:FAD:HM82	2.18	0.77
4:H:49:PHE:C	4:H:51:PRO:HD2	2.10	0.76
4:H:49:PHE:C	4:H:51:PRO:CD	2.59	0.76
1:E:307:MET:HE2	1:E:323:VAL:HG22	1.68	0.76
4:D:112:VAL:O	4:D:113:LEU:HD23	1.86	0.74
4:H:46:GLU:OE2	4:H:46:GLU:CA	2.30	0.74
1:A:172:VAL:O	1:A:173:ALA:HB3	1.87	0.73
1:A:172:VAL:O	1:A:172:VAL:CG1	2.30	0.72
4:H:49:PHE:O	4:H:49:PHE:CG	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:513:LEU:HD13	1:E:564:GLU:HA	1.71	0.72
4:H:53:HIS:CD2	4:H:53:HIS:N	2.57	0.72
1:E:320:ARG:HH12	5:E:701:MLI:C2	2.04	0.71
2:F:116:ASN:C	2:F:116:ASN:HD22	1.97	0.71
1:A:604:ARG:NH1	1:A:627:ASP:OD2	2.23	0.71
10:C:201:HEM:HBD1	10:C:201:HEM:HHA	1.72	0.71
1:E:174:ASP:HB2	1:E:361:PRO:HD2	1.73	0.70
1:E:562:ALA:HB1	1:E:607:THR:HG21	1.72	0.70
4:H:52:LEU:N	4:H:53:HIS:CD2	2.59	0.69
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.75	0.69
2:F:240:HIS:C	2:F:241:THR:OG1	2.35	0.69
4:H:50:LYS:CD	4:H:50:LYS:H	2.03	0.68
2:F:240:HIS:O	2:F:241:THR:OG1	2.12	0.68
1:E:274:GLN:HB2	1:E:390:MET:HE1	1.75	0.68
3:G:74:LEU:HD23	3:G:130:PHE:CE1	2.29	0.68
1:A:205:LEU:HD23	1:A:465:LEU:HD21	1.75	0.67
1:E:47:ILE:HD11	1:E:214:VAL:CG2	2.25	0.67
4:D:112:VAL:O	4:D:113:LEU:CD2	2.42	0.66
2:B:94:CYS:SG	2:B:96:SER:OG	2.53	0.66
1:A:476:ASN:HD21	1:A:550:GLN:HE22	1.42	0.65
2:F:240:HIS:C	2:F:241:THR:HG1	2.05	0.65
4:D:115:ASP:OD2	4:D:115:ASP:N	2.29	0.65
4:D:51:PRO:O	4:D:53:HIS:NE2	2.30	0.65
4:H:52:LEU:O	4:H:53:HIS:HD2	1.79	0.64
4:D:52:LEU:N	4:D:53:HIS:HD2	1.95	0.64
4:H:50:LYS:H	4:H:51:PRO:HD3	1.63	0.64
1:E:262:ARG:HH22	1:E:551:ASN:HD21	1.45	0.63
1:A:222:GLY:HA3	1:A:537:LEU:HB3	1.81	0.63
11:C:202:12J:O1	11:C:202:12J:I	2.87	0.63
3:C:69:TRP:CE3	11:C:202:12J:H14	2.34	0.62
1:A:267:LEU:HD12	1:A:270:LEU:HD11	1.81	0.62
4:H:51:PRO:HB2	4:H:53:HIS:CE1	2.34	0.62
2:B:68:VAL:HG11	2:B:101:ILE:HD13	1.80	0.62
1:E:190:ARG:HG3	4:H:43:ILE:HD11	1.81	0.62
1:A:425:HIS:N	1:A:426:SER:HA	2.13	0.62
10:G:201:HEM:HBD1	10:G:201:HEM:HHA	1.82	0.62
2:B:237:PHE:CE1	2:B:266:LEU:HD23	2.35	0.61
3:C:107:ILE:HD11	4:D:156:LEU:HD13	1.82	0.61
1:E:356:LEU:HD23	1:E:375:VAL:HG23	1.82	0.61
1:E:103:PHE:HA	1:E:123:THR:HG21	1.82	0.61
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:231:GLN:HB3	4:H:54:SER:HA	1.83	0.60
1:E:583:ASP:O	1:E:597:ARG:NH2	2.34	0.60
4:D:52:LEU:N	4:D:53:HIS:CD2	2.70	0.60
1:E:79:HIS:CD2	6:E:702:FAD:C8M	2.85	0.60
1:E:47:ILE:HD11	1:E:214:VAL:HG21	1.84	0.59
1:A:42:TYR:O	1:A:229:SER:HA	2.01	0.59
1:A:320:ARG:HH12	5:A:701:MLI:C2	2.15	0.59
1:A:602:HIS:O	1:A:605:LYS:HE2	2.02	0.59
4:H:104:VAL:HG13	4:H:121:VAL:HG12	1.84	0.59
1:A:584:GLU:OE2	1:A:604:ARG:NH2	2.36	0.59
4:D:49:PHE:CD1	4:D:49:PHE:C	2.80	0.59
1:E:425:HIS:N	1:E:426:SER:HA	2.18	0.59
1:A:88:ASN:ND2	1:A:156:GLN:HE22	2.02	0.58
4:H:52:LEU:CA	4:H:53:HIS:CD2	2.86	0.58
2:B:188:CYS:SG	2:B:189:SER:N	2.77	0.58
2:F:116:ASN:C	2:F:116:ASN:ND2	2.62	0.57
4:H:88:LEU:O	4:H:92:LEU:HB2	2.04	0.57
3:C:69:TRP:CH2	3:C:70:MET:HE3	2.39	0.57
4:H:83:GLU:CD	4:H:83:GLU:H	2.11	0.57
4:H:41:ASP:HB3	4:H:44:ALA:HB3	1.87	0.57
1:A:500:MET:HE1	1:A:556:ALA:O	2.06	0.56
4:H:51:PRO:C	4:H:53:HIS:CD2	2.83	0.56
4:D:51:PRO:C	4:D:53:HIS:CD2	2.84	0.56
1:E:172:VAL:O	1:E:173:ALA:C	2.47	0.56
1:E:485:GLY:O	1:E:531:LYS:HB2	2.05	0.56
1:A:603:TRP:HA	1:A:605:LYS:HE2	1.88	0.55
4:D:104:VAL:HG13	4:D:121:VAL:HG12	1.88	0.55
1:E:32:ILE:HG13	1:E:32:ILE:O	2.07	0.55
1:A:274:GLN:HB2	1:A:390:MET:HE1	1.89	0.55
4:D:51:PRO:C	4:D:53:HIS:HE2	2.13	0.55
3:C:112:ILE:HD11	3:C:117:LEU:CD2	2.37	0.54
1:A:588:SER:HB3	1:A:642:ILE:HD11	1.89	0.54
2:F:238:LYS:HE3	4:H:106:ASP:OD1	2.08	0.54
3:G:158:LEU:C	3:G:158:LEU:HD23	2.33	0.54
3:C:60:LEU:HA	11:C:202:12J:H15A	1.89	0.54
1:A:174:ASP:OD2	1:A:362:GLY:N	2.41	0.54
1:A:266:ALA:HB2	1:A:610:LYS:HG2	1.90	0.54
11:G:202:12J:O1	11:G:202:12J:I	2.96	0.54
2:F:242:ILE:O	2:F:243:MET:CB	2.50	0.53
1:E:117:ASN:N	1:E:117:ASN:HD22	2.06	0.53
2:F:242:ILE:HG22	2:F:244:ASN:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLY:HA3	1:A:227:PHE:O	2.08	0.53
2:B:212:TYR:OH	2:B:261:GLU:HG2	2.09	0.53
4:D:51:PRO:C	4:D:53:HIS:NE2	2.67	0.53
2:B:269:MET:CE	3:C:143:MET:HE3	2.39	0.53
1:A:117:ASN:H	1:A:117:ASN:HD22	1.57	0.53
2:F:179:LEU:HD23	2:F:216:ILE:HD11	1.91	0.53
1:E:47:ILE:HD11	1:E:214:VAL:HG22	1.90	0.52
1:E:557:THR:O	1:E:561:VAL:HG13	2.09	0.52
10:G:201:HEM:HHC	10:G:201:HEM:HBB2	1.91	0.52
3:G:112:ILE:HD11	3:G:117:LEU:HD21	1.91	0.52
1:A:41:ALA:HB1	1:A:462:ILE:HD13	1.92	0.52
1:E:401:VAL:HG21	1:E:416:LEU:HG	1.91	0.52
1:A:174:ASP:OD2	1:A:363:ILE:N	2.41	0.52
1:A:251:MET:HE2	2:B:87:ARG:O	2.10	0.51
1:A:513:LEU:HD13	1:A:564:GLU:HA	1.92	0.51
10:C:201:HEM:HHC	10:C:201:HEM:HBB2	1.92	0.51
1:E:79:HIS:CD2	6:E:702:FAD:HM83	2.46	0.51
1:E:172:VAL:O	1:E:172:VAL:HG12	2.09	0.51
3:G:74:LEU:HD23	3:G:130:PHE:CZ	2.45	0.51
1:A:117:ASN:HD22	1:A:117:ASN:N	2.08	0.51
4:H:52:LEU:O	4:H:53:HIS:CD2	2.57	0.51
1:E:486:ASP:OD2	1:E:486:ASP:N	2.30	0.51
1:A:84:GLN:OE1	1:A:288:THR:HB	2.10	0.51
1:A:172:VAL:O	1:A:173:ALA:CB	2.54	0.51
1:E:301:SER:HB3	1:E:336:GLY:O	2.10	0.51
3:G:94:SER:HA	4:H:138:TYR:CZ	2.46	0.51
3:G:104:VAL:HG13	4:H:156:LEU:HD21	1.93	0.51
3:G:126:PHE:HA	3:G:167:SER:OG	2.11	0.51
3:G:133:LEU:O	3:G:136:ILE:HG23	2.11	0.51
1:A:486:ASP:OD2	1:A:486:ASP:N	2.44	0.50
1:E:174:ASP:OD1	1:E:174:ASP:O	2.30	0.50
3:C:136:ILE:HD12	3:C:136:ILE:C	2.37	0.50
1:A:591:ILE:N	1:A:591:ILE:HD12	2.27	0.50
3:G:60:LEU:HD12	3:G:61:THR:HG23	1.94	0.50
1:E:73:MET:SD	1:E:251:MET:HG3	2.51	0.50
4:D:112:VAL:HG12	4:D:113:LEU:HD23	1.78	0.50
1:A:584:GLU:CD	1:A:604:ARG:NH2	2.69	0.50
2:B:116:ASN:C	2:B:116:ASN:ND2	2.69	0.50
1:E:388:TYR:CE1	1:E:421:GLU:HG3	2.47	0.50
1:A:114:GLY:C	1:A:119:MET:HE2	2.37	0.49
3:C:95:VAL:HG12	3:C:95:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:493:ARG:HB2	1:E:549:LEU:HD13	1.94	0.49
4:H:46:GLU:O	4:H:48:GLY:O	2.30	0.49
4:H:94:LEU:O	4:H:97:HIS:HB3	2.11	0.49
1:A:105:ASP:OD2	1:A:157:SER:N	2.39	0.49
1:A:247:THR:HG22	1:A:284:GLY:O	2.12	0.49
2:F:153:LEU:HD21	2:F:166:GLN:HE22	1.77	0.49
2:B:86:ARG:CZ	2:B:136:VAL:HG13	2.43	0.49
3:C:158:LEU:CD2	3:C:162:LEU:HD12	2.43	0.49
1:E:45:VAL:HG21	1:E:227:PHE:HB3	1.95	0.49
2:B:131:VAL:HG22	3:C:55:PRO:HG2	1.95	0.48
3:G:173:TYR:HB3	3:G:174:PRO:HD3	1.93	0.48
1:A:359:ARG:O	1:A:360:LEU:HD23	2.13	0.48
1:A:73:MET:SD	1:A:251:MET:HG3	2.53	0.48
1:A:174:ASP:HB2	1:A:361:PRO:HD2	1.95	0.48
3:C:180:LYS:O	3:C:184:LEU:HB3	2.13	0.48
1:E:293:GLY:HA2	1:E:317:LEU:HD21	1.96	0.48
1:E:602:HIS:O	1:E:605:LYS:NZ	2.44	0.48
3:C:184:LEU:HD22	3:C:185:PRO:O	2.14	0.47
1:E:114:GLY:C	1:E:119:MET:HE2	2.39	0.47
1:A:86:GLY:HA2	1:A:176:THR:HG21	1.95	0.47
1:A:584:GLU:CD	1:A:604:ARG:HH21	2.22	0.47
3:G:69:TRP:CE2	11:G:202:12J:H14	2.49	0.47
1:A:42:TYR:CD2	1:A:68:ALA:HB2	2.49	0.47
2:B:130:PHE:CD2	3:C:49:GLN:HB3	2.50	0.47
1:E:355:GLN:O	1:E:359:ARG:HB2	2.14	0.47
2:B:37:THR:HB	2:B:58:ASP:OD2	2.15	0.47
1:E:604:ARG:HH22	1:E:627:ASP:CG	2.22	0.47
4:H:49:PHE:C	4:H:50:LYS:HD2	2.32	0.47
2:B:201:LYS:HA	3:C:39:GLN:HG2	1.97	0.47
1:A:39:ASP:OD1	1:A:226:ARG:NH1	2.48	0.47
4:D:50:LYS:N	4:D:51:PRO:HD3	1.96	0.47
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.96	0.47
2:B:230:MET:HE3	2:B:262:ILE:HG21	1.97	0.47
1:E:44:VAL:HB	1:E:231:ARG:HB2	1.97	0.47
1:E:293:GLY:CA	1:E:317:LEU:HD21	2.45	0.47
1:E:509:ARG:NH1	1:E:511:ASP:OD2	2.39	0.47
2:F:69:LEU:HD12	2:F:109:CYS:HB3	1.97	0.46
1:A:562:ALA:HB1	1:A:607:THR:HG21	1.97	0.46
4:H:46:GLU:O	4:H:47:LYS:C	2.56	0.46
1:E:451:ASN:HD22	1:E:451:ASN:N	2.14	0.46
2:F:193:PRO:O	2:F:196:TRP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:TRP:CZ3	11:C:202:12J:H14	2.51	0.46
1:E:241:ARG:HA	1:E:241:ARG:HD2	1.77	0.46
10:G:201:HEM:HHD	10:G:201:HEM:HBC2	1.98	0.46
1:A:169:THR:HG23	1:A:435:ALA:CB	2.45	0.46
1:A:286:LEU:HD22	6:A:702:FAD:C6	2.46	0.46
1:E:584:GLU:HA	1:E:602:HIS:CD2	2.50	0.46
1:A:459:ASP:OD1	1:A:460:GLU:N	2.49	0.46
2:F:106:THR:HG23	2:F:107:LEU:N	2.31	0.46
1:A:476:ASN:HD21	1:A:550:GLN:NE2	2.10	0.46
2:B:40:ILE:HD12	2:B:57:PHE:CD1	2.51	0.46
3:C:112:ILE:HD11	3:C:117:LEU:HD23	1.98	0.46
1:E:243:TYR:CD2	1:E:386:VAL:HG21	2.51	0.46
2:F:64:CYS:SG	2:F:65:GLY:N	2.89	0.46
2:F:230:MET:HE3	2:F:262:ILE:HG23	1.97	0.46
10:G:201:HEM:HAD1	4:H:99:GLY:CA	2.46	0.46
1:E:265:ILE:HD13	1:E:401:VAL:HG11	1.98	0.45
2:F:173:GLN:O	2:F:176:LEU:HB2	2.17	0.45
3:C:94:SER:HA	4:D:138:TYR:CZ	2.51	0.45
3:C:158:LEU:HD21	3:C:162:LEU:HD12	1.99	0.45
1:E:451:ASN:N	1:E:451:ASN:ND2	2.64	0.45
3:C:67:MET:HA	3:C:67:MET:HE3	1.97	0.45
10:C:201:HEM:HHA	10:C:201:HEM:CBD	2.45	0.45
10:C:201:HEM:HBC2	10:C:201:HEM:HHD	1.97	0.45
1:E:99:TRP:O	1:E:102:HIS:HB3	2.16	0.45
1:E:347:GLN:HG3	1:E:349:HIS:CE1	2.50	0.45
1:A:262:ARG:HH22	1:A:551:ASN:ND2	2.14	0.45
2:B:38:PHE:O	2:B:56:LYS:HA	2.16	0.45
4:D:116:THR:OG1	4:D:117:LEU:N	2.48	0.45
3:G:180:LYS:O	3:G:184:LEU:HB3	2.16	0.45
4:H:51:PRO:HB3	4:H:53:HIS:NE2	2.26	0.45
1:A:276:HIS:CE1	1:A:286:LEU:HD11	2.52	0.45
2:B:220:ASP:O	2:B:272:LYS:NZ	2.49	0.45
3:C:115:VAL:O	3:C:119:THR:OG1	2.32	0.45
3:G:69:TRP:CD2	11:G:202:12J:H14	2.52	0.45
1:E:241:ARG:NH2	1:E:248:THR:O	2.50	0.45
1:A:140:PHE:HA	1:A:172:VAL:HG22	1.98	0.44
2:B:150:GLN:HA	2:B:152:TRP:CZ3	2.52	0.44
3:C:118:ASP:HB3	3:C:171:VAL:CG1	2.47	0.44
1:A:190:ARG:HG3	4:D:43:ILE:HD11	2.00	0.44
4:D:52:LEU:HA	4:D:53:HIS:CD2	2.52	0.44
1:E:439:LEU:HD22	1:E:443:VAL:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:VAL:HG13	4:D:156:LEU:HD21	1.99	0.44
1:E:558:GLN:HA	1:E:618:ILE:HD13	1.99	0.44
1:A:476:ASN:ND2	1:A:550:GLN:HE22	2.12	0.44
2:B:116:ASN:C	2:B:116:ASN:HD22	2.26	0.44
2:B:216:ILE:CD1	2:B:216:ILE:C	2.91	0.44
3:G:107:ILE:HD11	4:H:156:LEU:HD13	1.99	0.44
1:E:444:PHE:HA	1:E:447:ALA:HB3	1.98	0.44
1:E:605:LYS:HD2	1:E:622:TYR:HB3	2.00	0.44
3:G:76:ARG:CZ	4:H:103:VAL:HG22	2.48	0.44
4:H:51:PRO:CA	4:H:53:HIS:NE2	2.81	0.44
1:A:508:ARG:HB3	1:A:513:LEU:HD11	1.99	0.44
1:E:73:MET:HE3	1:E:78:SER:HA	1.99	0.44
10:G:201:HEM:HAD1	4:H:99:GLY:HA3	1.99	0.44
4:H:144:VAL:HG11	4:H:152:MET:SD	2.58	0.44
3:C:184:LEU:C	3:C:184:LEU:HD13	2.43	0.44
1:A:494:LEU:HG	1:A:498:LYS:HD2	2.00	0.43
3:C:107:ILE:HD11	4:D:156:LEU:CD1	2.48	0.43
1:A:174:ASP:OD2	1:A:362:GLY:CA	2.65	0.43
1:E:438:LEU:HG	6:E:702:FAD:C2	2.48	0.43
1:A:267:LEU:CD1	1:A:270:LEU:HD11	2.48	0.43
1:E:46:ILE:HD11	1:E:60:LEU:HD12	2.01	0.43
1:E:496:MET:HG3	1:E:520:MET:HE1	2.00	0.43
2:B:264:MET:HE3	2:B:270:LYS:HG3	2.00	0.43
3:C:173:TYR:HB3	3:C:174:PRO:HD3	1.99	0.43
1:E:517:VAL:HG13	1:E:561:VAL:HG12	2.00	0.43
4:H:52:LEU:N	4:H:53:HIS:HD2	2.15	0.43
4:D:133:LEU:O	4:D:134:ALA:C	2.62	0.43
1:E:239:TYR:HB3	1:E:254:GLY:HA3	2.01	0.43
2:B:39:GLU:HG2	2:B:56:LYS:HD2	1.99	0.43
1:E:58:MET:HE3	1:E:187:ASN:HB3	2.01	0.43
1:E:172:VAL:O	1:E:173:ALA:HB3	2.18	0.43
1:A:105:ASP:OD2	1:A:168:ARG:NH2	2.52	0.43
1:A:241:ARG:HA	1:A:241:ARG:HD2	1.93	0.43
1:E:45:VAL:HG22	1:E:68:ALA:HB3	2.00	0.43
1:E:439:LEU:HD22	1:E:443:VAL:CG2	2.49	0.43
4:D:50:LYS:H	4:D:51:PRO:HD2	1.48	0.43
1:E:65:PHE:CE2	1:E:456:LEU:HD13	2.53	0.43
2:F:230:MET:HE3	2:F:262:ILE:CG2	2.49	0.42
1:A:573:HIS:CE1	1:A:575:ARG:HG2	2.54	0.42
1:E:601:LYS:HZ3	1:E:601:LYS:HG3	1.73	0.42
1:E:623:ARG:HG3	1:E:624:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:ILE:O	2:B:266:LEU:HB2	2.19	0.42
1:E:320:ARG:NH1	5:E:701:MLI:C2	2.79	0.42
1:E:307:MET:CE	1:E:323:VAL:HG22	2.43	0.42
3:G:156:ALA:O	3:G:160:LEU:HD22	2.20	0.42
4:D:72:LEU:O	4:D:72:LEU:HD23	2.20	0.42
4:H:56:GLY:O	4:H:57:THR:C	2.59	0.42
3:C:132:THR:HG23	10:C:201:HEM:CBB	2.50	0.42
3:C:136:ILE:HD12	3:C:136:ILE:O	2.20	0.42
1:A:604:ARG:NH1	1:A:627:ASP:CG	2.78	0.41
2:B:173:GLN:O	2:B:176:LEU:HB2	2.20	0.41
4:D:65:PHE:CE2	4:D:94:LEU:HD23	2.55	0.41
1:E:561:VAL:HG21	1:E:618:ILE:HG21	2.02	0.41
3:G:78:THR:O	3:G:82:MET:HG3	2.20	0.41
1:A:149:TYR:CD2	1:A:171:CYS:SG	3.13	0.41
2:F:222:SER:O	2:F:223:ALA:C	2.62	0.41
1:A:112:TRP:CE2	1:A:640:PRO:HA	2.55	0.41
1:E:115:ASP:HB3	1:E:117:ASN:HD21	1.85	0.41
3:G:69:TRP:CZ3	3:G:70:MET:HE3	2.55	0.41
1:A:639:PRO:HA	1:A:640:PRO:HD3	1.97	0.41
1:A:292:ARG:HD2	1:A:316:ASP:O	2.21	0.41
3:C:114:TRP:CE2	3:C:115:VAL:HG23	2.56	0.41
1:E:243:TYR:CG	1:E:386:VAL:HG21	2.56	0.41
1:A:401:VAL:HG21	1:A:416:LEU:HG	2.02	0.41
1:A:444:PHE:HA	1:A:447:ALA:HB3	2.03	0.41
10:C:201:HEM:HMB2	4:D:66:ALA:HB1	2.02	0.41
1:E:61:GLY:HA3	1:E:191:CYS:HB2	2.03	0.41
2:F:178:GLY:N	2:F:181:GLU:OE1	2.52	0.41
1:A:268:GLU:HG3	1:A:606:HIS:HB3	2.03	0.41
1:A:383:ILE:O	1:A:384:PRO:C	2.62	0.41
3:C:158:LEU:C	3:C:158:LEU:HD23	2.46	0.41
1:E:213:GLY:HA3	1:E:227:PHE:O	2.21	0.41
1:E:398:LYS:O	1:E:399:ALA:HB3	2.21	0.41
1:E:586:ASP:OD1	1:E:586:ASP:C	2.64	0.41
1:E:623:ARG:CG	1:E:624:PRO:HD2	2.51	0.41
4:H:150:PHE:HB3	12:H:201:EPH:H2	2.03	0.41
1:A:81:THR:HB	1:A:181:LEU:HD23	2.03	0.41
1:A:502:LYS:HD3	1:A:503:HIS:CE1	2.55	0.41
4:D:112:VAL:CG1	4:D:113:LEU:HD23	2.40	0.41
1:E:37:VAL:HB	4:H:31:ALA:HB2	2.03	0.41
1:E:434:GLY:O	1:E:435:ALA:HB3	2.21	0.41
3:G:149:ILE:HB	3:G:150:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:ILE:H	2:F:165:GLN:HE22	1.68	0.41
1:E:432:ARG:HH21	1:E:435:ALA:H	1.70	0.41
1:E:32:ILE:HG23	1:E:478:ASP:OD1	2.21	0.40
2:F:213:ARG:HD3	2:F:213:ARG:C	2.47	0.40
3:G:82:MET:HE3	10:G:201:HEM:C3C	2.56	0.40
4:H:83:GLU:CD	4:H:83:GLU:N	2.80	0.40
1:A:280:ILE:HD11	1:A:287:ILE:HD11	2.02	0.40
3:C:65:PRO:HA	3:C:69:TRP:CZ2	2.56	0.40
1:E:287:ILE:HG23	1:E:363:ILE:HD13	2.03	0.40
3:G:88:ILE:O	3:G:92:GLY:HA3	2.21	0.40
3:G:143:MET:O	3:G:144:ALA:HB3	2.21	0.40
2:F:193:PRO:HG3	11:G:202:12J:H16A	2.03	0.40
1:A:281:TYR:CD1	1:A:343:HIS:HB3	2.57	0.40
2:B:259:ILE:O	2:B:260:GLY:C	2.63	0.40
4:D:85:ASP:OD1	4:D:145:GLY:HA3	2.21	0.40
3:G:65:PRO:HA	3:G:69:TRP:CZ2	2.56	0.40
3:G:79:GLY:C	10:G:201:HEM:HMD3	2.46	0.40
3:G:85:THR:HG21	12:H:201:EPH:C27	2.51	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%)	573 (93%)	39 (6%)	2 (0%)	36	65
1	E	614/645 (95%)	583 (95%)	30 (5%)	1 (0%)	43	71
2	B	248/282 (88%)	232 (94%)	14 (6%)	2 (1%)	16	45
2	F	248/282 (88%)	231 (93%)	16 (6%)	1 (0%)	30	60
3	C	151/188 (80%)	142 (94%)	9 (6%)	0	100	100
3	G	151/188 (80%)	140 (93%)	10 (7%)	1 (1%)	18	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	127/156 (81%)	120 (94%)	6 (5%)	1 (1%)	16	45
4	H	127/156 (81%)	123 (97%)	4 (3%)	0	100	100
All	All	2280/2542 (90%)	2144 (94%)	128 (6%)	8 (0%)	30	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	485	GLY
1	E	80	THR
2	B	88	SER
2	B	232	ASP
3	G	113	PRO
4	D	50	LYS
1	A	163	GLY
2	F	279	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%)	455 (91%)	47 (9%)	8	30
1	E	502/527 (95%)	464 (92%)	38 (8%)	12	37
2	B	220/242 (91%)	201 (91%)	19 (9%)	10	33
2	F	220/242 (91%)	192 (87%)	28 (13%)	4	18
3	C	127/158 (80%)	114 (90%)	13 (10%)	7	26
3	G	127/158 (80%)	110 (87%)	17 (13%)	4	16
4	D	98/119 (82%)	83 (85%)	15 (15%)	3	13
4	H	98/119 (82%)	84 (86%)	14 (14%)	3	14
All	All	1894/2092 (90%)	1703 (90%)	191 (10%)	7	26

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ILE
1	A	34	GLN
1	A	44	VAL
1	A	71	THR
1	A	117	ASN
1	A	120	HIS
1	A	153	PHE
1	A	162	LYS
1	A	165	VAL
1	A	179	SER
1	A	194	THR
1	A	205	LEU
1	A	241	ARG
1	A	257	THR
1	A	283	VAL
1	A	298	LEU
1	A	320	ARG
1	A	337	VAL
1	A	344	ILE
1	A	351	LEU
1	A	356	LEU
1	A	359	ARG
1	A	378	GLU
1	A	390	MET
1	A	405	THR
1	A	406	LYS
1	A	412	ILE
1	A	436	ASN
1	A	439	LEU
1	A	440	ASP
1	A	453	LYS
1	A	455	GLU
1	A	456	LEU
1	A	457	LYS
1	A	461	LYS
1	A	484	ASN
1	A	486	ASP
1	A	509	ARG
1	A	525	LYS
1	A	527	LEU
1	A	535	ARG
1	A	539	TRP
1	A	584	GLU

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Mol	Chain	Res	Type
1	A	592	GLU
1	A	596	LYS
1	A	601	LYS
1	A	604	ARG
2	B	33	LYS
2	B	37	THR
2	B	53	LYS
2	B	66	THR
2	B	69	LEU
2	B	89	CYS
2	B	91	GLU
2	B	96	SER
2	B	116	ASN
2	B	131	VAL
2	B	156	LYS
2	B	157	THR
2	B	159	ILE
2	B	173	GLN
2	B	176	LEU
2	B	179	LEU
2	B	184	LEU
2	B	216	ILE
2	B	248	THR
3	C	60	LEU
3	C	67	MET
3	C	70	MET
3	C	88	ILE
3	C	94	SER
3	C	105	GLU
3	C	107	ILE
3	C	118	ASP
3	C	133	LEU
3	C	136	ILE
3	C	160	LEU
3	C	177	GLU
3	C	184	LEU
4	D	49	PHE
4	D	50	LYS
4	D	51	PRO
4	D	52	LEU
4	D	53	HIS
4	D	61	ILE

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Mol	Chain	Res	Type
4	D	79	ILE
4	D	83	GLU
4	D	84	MET
4	D	86	LEU
4	D	92	LEU
4	D	112	VAL
4	D	113	LEU
4	D	115	ASP
4	D	136	LEU
1	E	32	ILE
1	E	44	VAL
1	E	106	THR
1	E	117	ASN
1	E	153	PHE
1	E	162	LYS
1	E	179	SER
1	E	194	THR
1	E	205	LEU
1	E	241	ARG
1	E	257	THR
1	E	261	THR
1	E	283	VAL
1	E	298	LEU
1	E	320	ARG
1	E	337	VAL
1	E	344	ILE
1	E	358	GLN
1	E	359	ARG
1	E	378	GLU
1	E	390	MET
1	E	406	LYS
1	E	412	ILE
1	E	436	ASN
1	E	439	LEU
1	E	440	ASP
1	E	453	LYS
1	E	456	LEU
1	E	457	LYS
1	E	484	ASN
1	E	509	ARG
1	E	525	LYS
1	E	527	LEU

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Mol	Chain	Res	Type
1	E	531	LYS
1	E	535	ARG
1	E	547	LEU
1	E	584	GLU
1	E	610	LYS
2	F	33	LYS
2	F	37	THR
2	F	46	GLU
2	F	56	LYS
2	F	66	THR
2	F	69	LEU
2	F	91	GLU
2	F	93	ILE
2	F	96	SER
2	F	106	THR
2	F	115	GLN
2	F	116	ASN
2	F	119	LYS
2	F	120	THR
2	F	129	MET
2	F	131	VAL
2	F	148	SER
2	F	156	LYS
2	F	157	THR
2	F	176	LEU
2	F	179	LEU
2	F	184	LEU
2	F	216	ILE
2	F	238	LYS
2	F	242	ILE
2	F	266	LEU
2	F	278	THR
2	F	281	ASN
3	G	53	LYS
3	G	59	HIS
3	G	60	LEU
3	G	67	MET
3	G	70	MET
3	G	94	SER
3	G	105	GLU
3	G	133	LEU
3	G	136	ILE

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Mol	Chain	Res	Type
3	G	159	VAL
3	G	160	LEU
3	G	165	LEU
3	G	172	VAL
3	G	175	ARG
3	G	177	GLU
3	G	183	THR
3	G	184	LEU
4	H	46	GLU
4	H	50	LYS
4	H	53	HIS
4	H	54	SER
4	H	58	LEU
4	H	79	ILE
4	H	83	GLU
4	H	84	MET
4	H	86	LEU
4	H	104	VAL
4	H	112	VAL
4	H	122	ARG
4	H	144	VAL
4	H	148	ARG

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

Mol	Chain	Res	Type
1	A	88	ASN
1	A	117	ASN
1	A	150	GLN
1	A	158	ASN
1	A	250	HIS
1	A	358	GLN
1	A	436	ASN
1	A	497	GLN
1	A	503	HIS
1	A	550	GLN
1	A	551	ASN
2	B	55	GLN
2	B	100	ASN
2	B	105	ASN
2	B	116	ASN
2	B	198	ASN

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Mol	Chain	Res	Type
2	B	210	GLN
4	D	53	HIS
4	D	140	ASN
1	E	88	ASN
1	E	117	ASN
1	E	125	ASN
1	E	158	ASN
1	E	187	ASN
1	E	349	HIS
1	E	358	GLN
1	E	428	HIS
1	E	436	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	115	GLN
2	F	116	ASN
2	F	145	GLN
2	F	154	GLN
2	F	165	GLN
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	H	201	-	43,43,48	1.18	2 (4%)	46,48,53	1.23	5 (10%)
10	HEM	G	201	3,4	50,50,50	1.64	8 (16%)	67,82,82	1.94	21 (31%)
6	FAD	A	702	-	58,58,58	1.52	11 (18%)	85,89,89	1.75	23 (27%)
5	MLI	A	701	-	6,6,6	1.19	0	7,7,7	1.11	0
7	FES	F	301	2	0,4,4	-	-	-	-	-
10	HEM	C	201	3,4	50,50,50	1.60	7 (14%)	67,82,82	1.95	21 (31%)
12	EPH	D	201	-	43,43,48	1.11	2 (4%)	46,48,53	1.12	4 (8%)
5	MLI	E	701	-	6,6,6	1.11	0	7,7,7	1.13	0
11	12J	G	202	-	21,21,21	1.39	2 (9%)	28,28,28	2.00	2 (7%)
8	SF4	F	302	2	0,12,12	-	-	-	-	-
9	F3S	B	303	2	0,9,9	-	-	-	-	-
8	SF4	B	302	2	0,12,12	-	-	-	-	-
9	F3S	F	303	2	0,9,9	-	-	-	-	-
11	12J	C	202	-	21,21,21	1.53	2 (9%)	28,28,28	1.18	2 (7%)
7	FES	B	301	2	0,4,4	-	-	-	-	-
6	FAD	E	702	-	58,58,58	1.50	9 (15%)	85,89,89	1.95	28 (32%)

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	H	201	-	-	25/47/47/52	-
10	HEM	G	201	3,4	-	6/14/54/54	-
7	FES	B	301	2	-	-	0/1/1/1
5	MLI	A	701	-	-	0/4/4/4	-
7	FES	F	301	2	-	-	0/1/1/1
10	HEM	C	201	3,4	-	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	EPH	D	201	-	-	21/47/47/52	-
5	MLI	E	701	-	-	0/4/4/4	-
11	12J	G	202	-	-	3/12/12/12	0/2/2/2
8	SF4	F	302	2	-	-	0/6/5/5
9	F3S	B	303	2	-	-	0/3/3/3
8	SF4	B	302	2	-	-	0/6/5/5
9	F3S	F	303	2	-	-	0/3/3/3
11	12J	C	202	-	-	4/12/12/12	0/2/2/2
6	FAD	A	702	-	-	6/34/50/50	0/6/6/6
6	FAD	E	702	-	-	4/34/50/50	0/6/6/6

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	702	FAD	C9A-C5X	5.49	1.50	1.41
10	G	201	HEM	FE-NB	5.18	2.10	1.94
6	A	702	FAD	C9A-C5X	5.01	1.49	1.41
10	C	201	HEM	FE-NB	4.97	2.10	1.94
11	C	202	12J	C2-C7	-4.94	1.40	1.50
12	H	201	EPH	O2-C4	4.92	1.47	1.33
11	G	202	12J	C2-C7	-4.63	1.40	1.50
12	H	201	EPH	O1-C3	4.60	1.47	1.34
12	D	201	EPH	O2-C4	4.51	1.46	1.33
6	E	702	FAD	C5A-C4A	4.42	1.47	1.39
12	D	201	EPH	O1-C3	4.37	1.46	1.34
11	C	202	12J	C8-N	-4.20	1.33	1.41
10	C	201	HEM	FE-NC	4.19	2.09	1.95
6	A	702	FAD	C5A-C4A	3.92	1.46	1.39
10	G	201	HEM	FE-NC	3.89	2.08	1.95
10	G	201	HEM	C1B-NB	-3.75	1.33	1.40
10	C	201	HEM	C1B-NB	-3.63	1.34	1.40
6	E	702	FAD	C8-C7	3.62	1.49	1.40
6	A	702	FAD	C8-C7	3.34	1.49	1.40
6	A	702	FAD	P-O3P	3.08	1.62	1.59
10	C	201	HEM	C3B-C4B	3.06	1.50	1.44
11	G	202	12J	C8-N	-2.97	1.35	1.41
6	A	702	FAD	C4A-N9A	-2.90	1.31	1.37
10	G	201	HEM	C4B-NB	-2.80	1.33	1.38
10	G	201	HEM	C3B-C4B	2.78	1.50	1.44
6	A	702	FAD	C5A-N7A	-2.72	1.34	1.39
6	E	702	FAD	C5A-C6A	2.64	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	702	FAD	C8A-N7A	2.54	1.36	1.31
6	A	702	FAD	PA-O3P	2.49	1.62	1.59
10	G	201	HEM	C4D-ND	-2.40	1.36	1.40
6	E	702	FAD	C4A-N9A	-2.39	1.32	1.37
10	G	201	HEM	C1C-C2C	-2.39	1.40	1.45
6	E	702	FAD	C4X-N5	2.38	1.35	1.30
6	A	702	FAD	C4-N3	-2.36	1.34	1.38
6	E	702	FAD	C9-C8	-2.36	1.36	1.39
6	A	702	FAD	C5X-N5	-2.34	1.35	1.39
10	C	201	HEM	C1C-C2C	-2.29	1.40	1.45
6	A	702	FAD	C8A-N7A	2.28	1.36	1.31
10	C	201	HEM	C4D-ND	-2.22	1.36	1.40
10	G	201	HEM	C1D-ND	-2.18	1.34	1.38
10	C	201	HEM	C4B-NB	-2.16	1.34	1.38
6	E	702	FAD	C5A-N7A	-2.12	1.35	1.39
6	A	702	FAD	C5A-C6A	2.05	1.46	1.41

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	202	12J	C10-O2-C14	8.91	131.15	119.43
10	G	201	HEM	CAD-C3D-C4D	5.87	134.92	124.70
6	E	702	FAD	C5A-C4A-N3A	-5.43	119.24	126.72
10	C	201	HEM	CAD-C3D-C4D	5.17	133.71	124.70
6	E	702	FAD	C8M-C8-C9	-4.72	111.26	119.57
10	C	201	HEM	C1B-NB-C4B	4.58	110.63	105.21
6	A	702	FAD	C4A-N9A-C8A	4.34	110.29	105.74
12	H	201	EPH	O1-C3-C5	4.26	120.70	111.48
6	A	702	FAD	N3A-C2A-N1A	-4.23	122.18	128.58
6	E	702	FAD	N3A-C4A-N9A	4.15	134.22	127.17
12	D	201	EPH	O1-C3-C5	4.15	120.45	111.48
12	H	201	EPH	O2-C4-C18	4.13	124.43	111.83
11	C	202	12J	C10-O2-C14	4.01	124.70	119.43
6	A	702	FAD	C5A-C4A-N3A	-3.97	121.24	126.72
10	G	201	HEM	CBD-CAD-C3D	3.94	123.43	112.53
10	C	201	HEM	O2D-CGD-CBD	3.93	126.42	114.00
10	G	201	HEM	CHD-C1D-ND	3.85	128.56	124.42
10	C	201	HEM	C3B-C4B-NB	-3.84	106.71	109.47
6	E	702	FAD	O2-C2-N1	-3.84	115.43	121.80
10	C	201	HEM	CHD-C1D-ND	3.82	128.54	124.42
6	E	702	FAD	C2A-N3A-C4A	3.82	121.16	111.83
6	E	702	FAD	N3A-C2A-N1A	-3.76	122.89	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	201	HEM	C1B-NB-C4B	3.75	109.64	105.21
6	E	702	FAD	C8M-C8-C7	3.72	128.36	120.76
10	G	201	HEM	CAC-C3C-C4C	3.70	133.66	124.82
6	E	702	FAD	C5X-C9A-N10	3.64	121.26	117.97
6	A	702	FAD	N3A-C4A-N9A	3.62	133.32	127.17
6	E	702	FAD	O3P-P-O1P	-3.61	99.83	110.70
6	E	702	FAD	C4-C4X-N5	3.60	123.18	118.21
10	C	201	HEM	CAC-C3C-C4C	3.60	133.41	124.82
6	E	702	FAD	C4A-C5A-N7A	-3.58	106.49	110.58
10	G	201	HEM	CAD-C3D-C2D	-3.56	121.20	127.87
6	A	702	FAD	O4B-C1B-N9A	3.48	114.77	108.09
10	C	201	HEM	CBD-CAD-C3D	3.43	122.01	112.53
6	A	702	FAD	C2A-N3A-C4A	3.37	120.06	111.83
12	D	201	EPH	O2-C4-C18	3.32	121.97	111.83
10	G	201	HEM	CHB-C1B-NB	3.28	128.42	124.37
12	H	201	EPH	O2-C4-O4	-3.27	115.45	123.63
6	E	702	FAD	C4A-N9A-C8A	3.15	109.05	105.74
6	A	702	FAD	C4-C4X-N5	3.14	122.55	118.21
10	C	201	HEM	CAD-C3D-C2D	-3.11	122.04	127.87
6	A	702	FAD	N9A-C8A-N7A	-3.10	109.53	113.94
6	E	702	FAD	C9-C9A-N10	-3.06	117.73	121.85
10	C	201	HEM	O2D-CGD-O1D	-3.02	115.56	123.33
6	E	702	FAD	O4B-C1B-N9A	2.98	113.81	108.09
6	A	702	FAD	O2-C2-N1	-2.91	116.96	121.80
10	G	201	HEM	CHA-C4D-C3D	-2.88	119.92	125.23
10	G	201	HEM	CAC-C3C-C2C	-2.86	119.12	128.43
6	A	702	FAD	C4A-C5A-N7A	-2.83	107.35	110.58
12	D	201	EPH	O1-C3-O3	-2.83	117.09	123.70
6	E	702	FAD	C4X-C10-N10	2.80	120.49	116.48
10	C	201	HEM	CHD-C1D-C2D	-2.78	120.63	125.03
10	C	201	HEM	CHB-C1B-NB	2.78	127.81	124.37
10	C	201	HEM	CHA-C4D-C3D	-2.77	120.12	125.23
12	D	201	EPH	O2-C4-O4	-2.75	116.75	123.63
10	G	201	HEM	C3B-C4B-NB	-2.74	107.50	109.47
10	G	201	HEM	CHC-C1C-NC	2.73	127.42	124.45
10	G	201	HEM	CHA-C4D-ND	2.66	127.65	124.37
10	C	201	HEM	CAC-C3C-C2C	-2.64	119.84	128.43
6	A	702	FAD	O4-C4-C4X	-2.64	119.56	126.53
6	A	702	FAD	C2A-N1A-C6A	2.61	123.02	118.73
6	E	702	FAD	O4-C4-C4X	-2.60	119.66	126.53
10	G	201	HEM	CMD-C2D-C1D	2.60	129.09	125.03
6	A	702	FAD	O2A-PA-O1A	2.53	124.22	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	201	EPH	C1-O2-C4	2.53	126.37	117.12
6	A	702	FAD	C5A-N7A-C8A	2.50	107.39	103.45
6	E	702	FAD	C5A-N7A-C8A	2.50	107.38	103.45
6	E	702	FAD	O2A-PA-O1A	2.49	124.02	112.44
10	C	201	HEM	CHC-C1C-NC	2.46	127.13	124.45
6	A	702	FAD	C4A-N9A-C1B	-2.46	120.88	126.63
10	C	201	HEM	CHA-C4D-ND	2.45	127.40	124.37
6	E	702	FAD	C6A-C5A-N7A	2.44	136.80	132.09
6	E	702	FAD	C9A-C5X-N5	-2.43	119.88	122.45
6	E	702	FAD	C1'-C2'-C3'	2.42	116.22	109.66
6	E	702	FAD	C9A-N10-C10	-2.41	117.08	120.75
10	C	201	HEM	CMD-C2D-C1D	2.40	128.79	125.03
10	G	201	HEM	C4B-C3B-C2B	-2.40	105.07	107.28
6	A	702	FAD	C6A-C5A-N7A	2.40	136.71	132.09
6	E	702	FAD	N9A-C8A-N7A	-2.39	110.54	113.94
10	G	201	HEM	C4C-NC-C1C	2.38	109.70	105.82
6	A	702	FAD	C4X-C10-N10	2.38	119.89	116.48
10	G	201	HEM	CHD-C1D-C2D	-2.37	121.29	125.03
6	A	702	FAD	C10-N1-C2	2.36	121.95	116.85
10	G	201	HEM	O2D-CGD-O1D	-2.32	117.36	123.33
10	G	201	HEM	CHD-C4C-C3C	2.29	129.07	125.21
10	C	201	HEM	CHC-C4B-NB	2.29	126.89	124.42
11	G	202	12J	C8-C9-C10	2.24	122.49	119.18
6	A	702	FAD	C8M-C8-C9	-2.23	115.64	119.57
6	A	702	FAD	C4X-C4-N3	2.20	118.87	113.25
6	E	702	FAD	O2-C2-N3	2.19	122.78	118.58
6	A	702	FAD	C2B-C1B-N9A	-2.18	107.88	113.30
6	E	702	FAD	C4'-C3'-C2'	-2.17	109.96	113.57
11	C	202	12J	C8-N-C7	-2.16	120.91	126.61
6	A	702	FAD	C4X-C10-N1	-2.16	119.29	124.59
12	H	201	EPH	O1-C3-O3	-2.16	118.66	123.70
10	G	201	HEM	CAB-C3B-C2B	-2.11	121.56	128.43
10	C	201	HEM	C3D-C4D-ND	2.08	112.45	110.17
10	G	201	HEM	C4D-C3D-C2D	-2.07	103.88	106.89
6	A	702	FAD	C4'-C3'-C2'	-2.06	110.15	113.57
10	C	201	HEM	C4C-NC-C1C	2.04	109.15	105.82
6	E	702	FAD	C10-N1-C2	2.04	121.27	116.85
10	C	201	HEM	CAB-C3B-C2B	-2.03	121.83	128.43
10	G	201	HEM	CAB-C3B-C4B	2.03	133.36	124.39
6	E	702	FAD	C4X-C4-N3	2.03	118.41	113.25
6	E	702	FAD	C2A-N1A-C6A	2.02	122.05	118.73
10	C	201	HEM	CAD-CBD-CGD	2.01	118.99	113.67

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	N10-C1'-C2'-C3'
6	A	702	FAD	PA-O3P-P-O5'
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	C	201	HEM	C2D-C3D-CAD-CBD
10	C	201	HEM	C4D-C3D-CAD-CBD
10	G	201	HEM	C2D-C3D-CAD-CBD
10	G	201	HEM	C4D-C3D-CAD-CBD
12	D	201	EPH	C37-O5-P1-O7
12	D	201	EPH	C37-O5-P1-O8
12	D	201	EPH	C5-C3-O1-C2
12	H	201	EPH	C18-C4-O2-C1
12	H	201	EPH	C37-O5-P1-O7
12	H	201	EPH	C37-O5-P1-O8
12	H	201	EPH	O3-C3-O1-C2
12	H	201	EPH	C13-C14-C15-C16
12	H	201	EPH	O4-C4-O2-C1
12	D	201	EPH	O4-C4-O2-C1
12	D	201	EPH	O3-C3-O1-C2
12	D	201	EPH	C18-C4-O2-C1
12	H	201	EPH	C5-C3-O1-C2
12	H	201	EPH	C19-C20-C21-C22
12	D	201	EPH	C4-C18-C19-C20
12	H	201	EPH	C11-C10-C9-C8
12	D	201	EPH	C11-C10-C9-C8
12	D	201	EPH	C7-C8-C9-C10
12	H	201	EPH	C6-C7-C8-C9
12	H	201	EPH	C7-C8-C9-C10
11	G	202	12J	C16-C14-O2-C10
12	H	201	EPH	C21-C22-C23-C24
12	D	201	EPH	O2-C1-C2-C37
12	D	201	EPH	C21-C22-C23-C24
12	H	201	EPH	O1-C2-C37-O5
6	A	702	FAD	P-O3P-PA-O1A
11	C	202	12J	C11-C10-O2-C14
12	H	201	EPH	O2-C1-C2-C37
12	D	201	EPH	C12-C13-C14-C15
12	H	201	EPH	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
11	C	202	12J	C9-C10-O2-C14
12	D	201	EPH	C28-C29-C30-C31
10	C	201	HEM	C3D-CAD-CBD-CGD
11	G	202	12J	C9-C10-O2-C14
11	G	202	12J	C11-C10-O2-C14
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
12	H	201	EPH	O2-C1-C2-O1
12	D	201	EPH	O2-C1-C2-O1
12	H	201	EPH	C10-C11-C12-C13
12	D	201	EPH	C37-O5-P1-O6
12	H	201	EPH	C37-O5-P1-O6
12	H	201	EPH	C38-O8-P1-O7
12	D	201	EPH	C9-C10-C11-C12
12	H	201	EPH	C28-C29-C30-C31
6	A	702	FAD	P-O3P-PA-O2A
12	D	201	EPH	C24-C25-C26-C27
12	D	201	EPH	C1-C2-O1-C3
12	H	201	EPH	C1-C2-C37-O5
12	D	201	EPH	C13-C14-C15-C16
12	H	201	EPH	C9-C10-C11-C12
10	G	201	HEM	C3D-CAD-CBD-CGD
12	D	201	EPH	C10-C11-C12-C13
12	H	201	EPH	C1-C2-O1-C3
11	C	202	12J	C13-C8-N-C7
12	D	201	EPH	C26-C27-C28-C29
12	H	201	EPH	C24-C25-C26-C27
11	C	202	12J	C9-C8-N-C7
6	A	702	FAD	O4B-C4B-C5B-O5B
12	H	201	EPH	C37-C2-O1-C3
6	E	702	FAD	PA-O3P-P-O2P
10	G	201	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

9 monomers are involved in 35 short contacts:

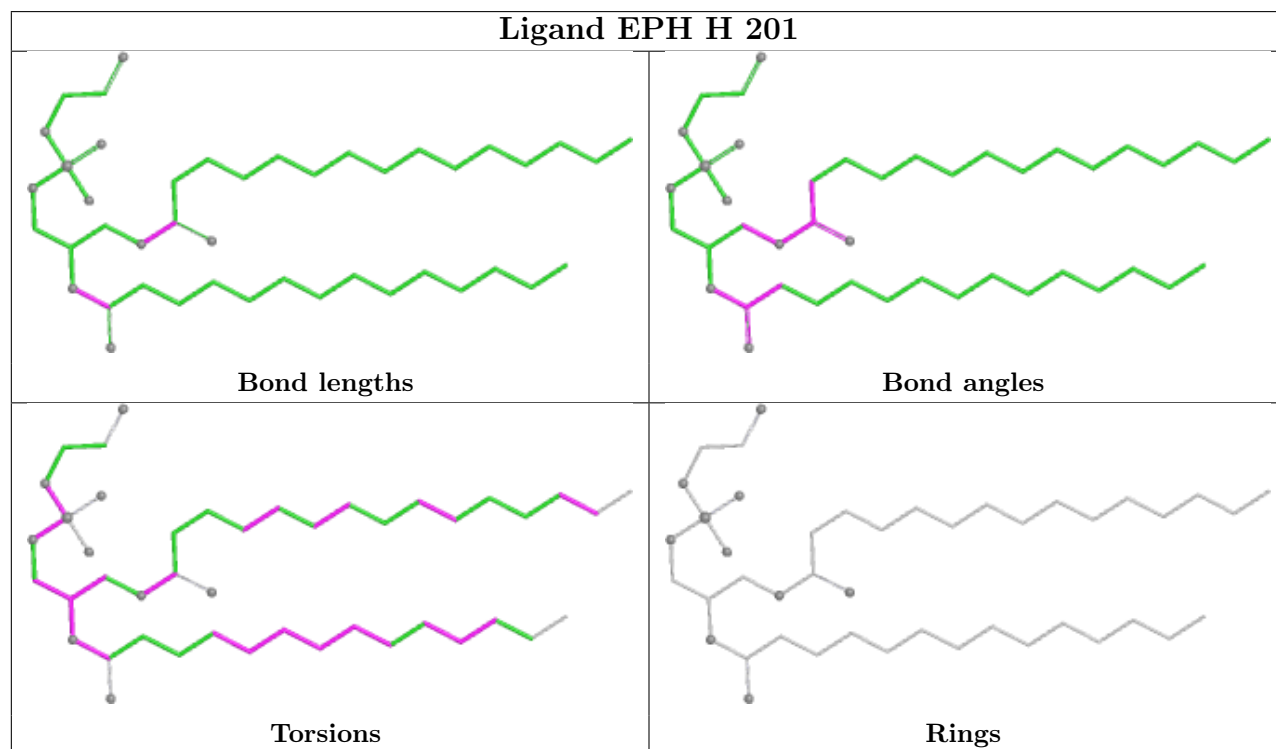
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	201	EPH	2	0
10	G	201	HEM	7	0
6	A	702	FAD	4	0

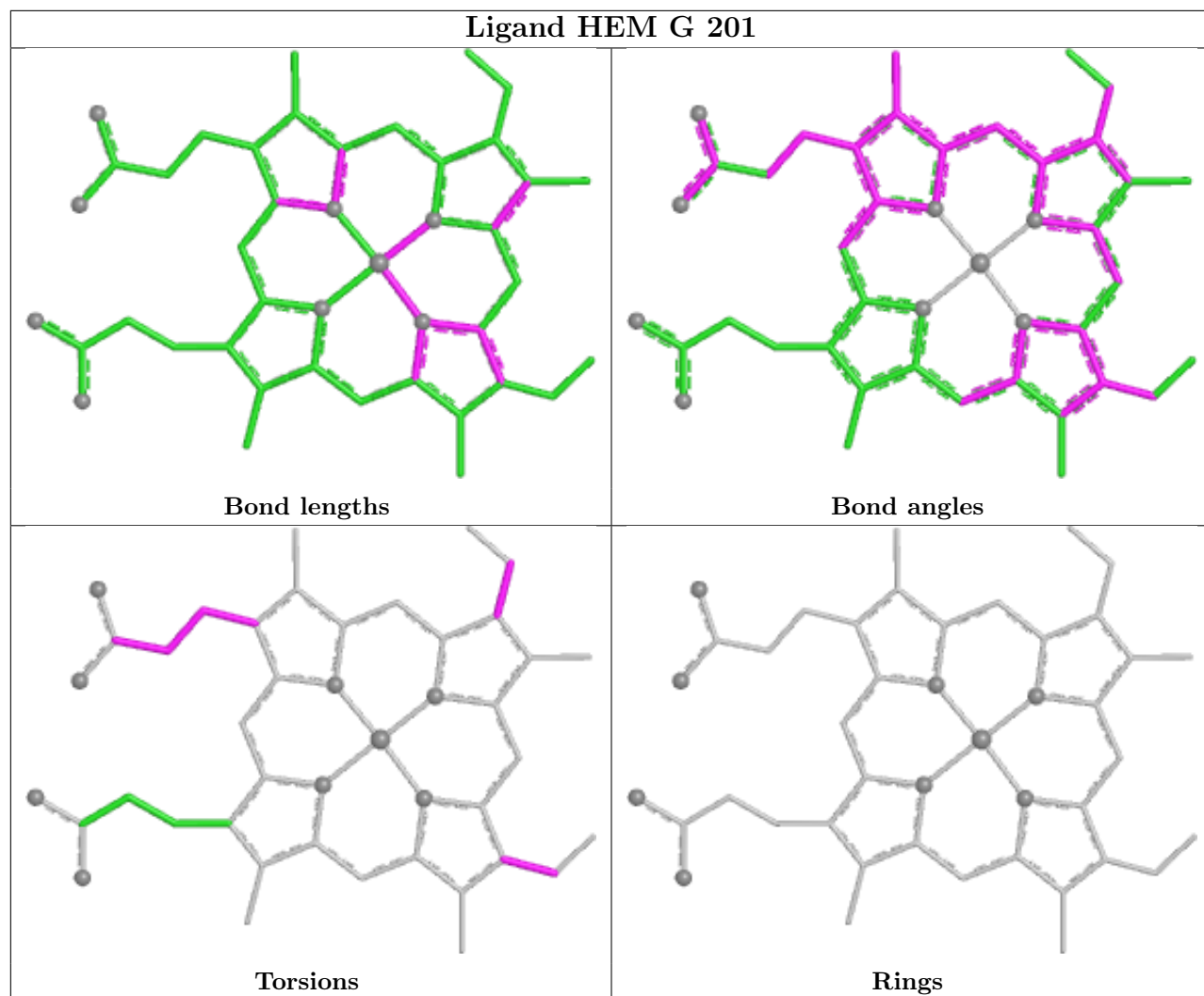
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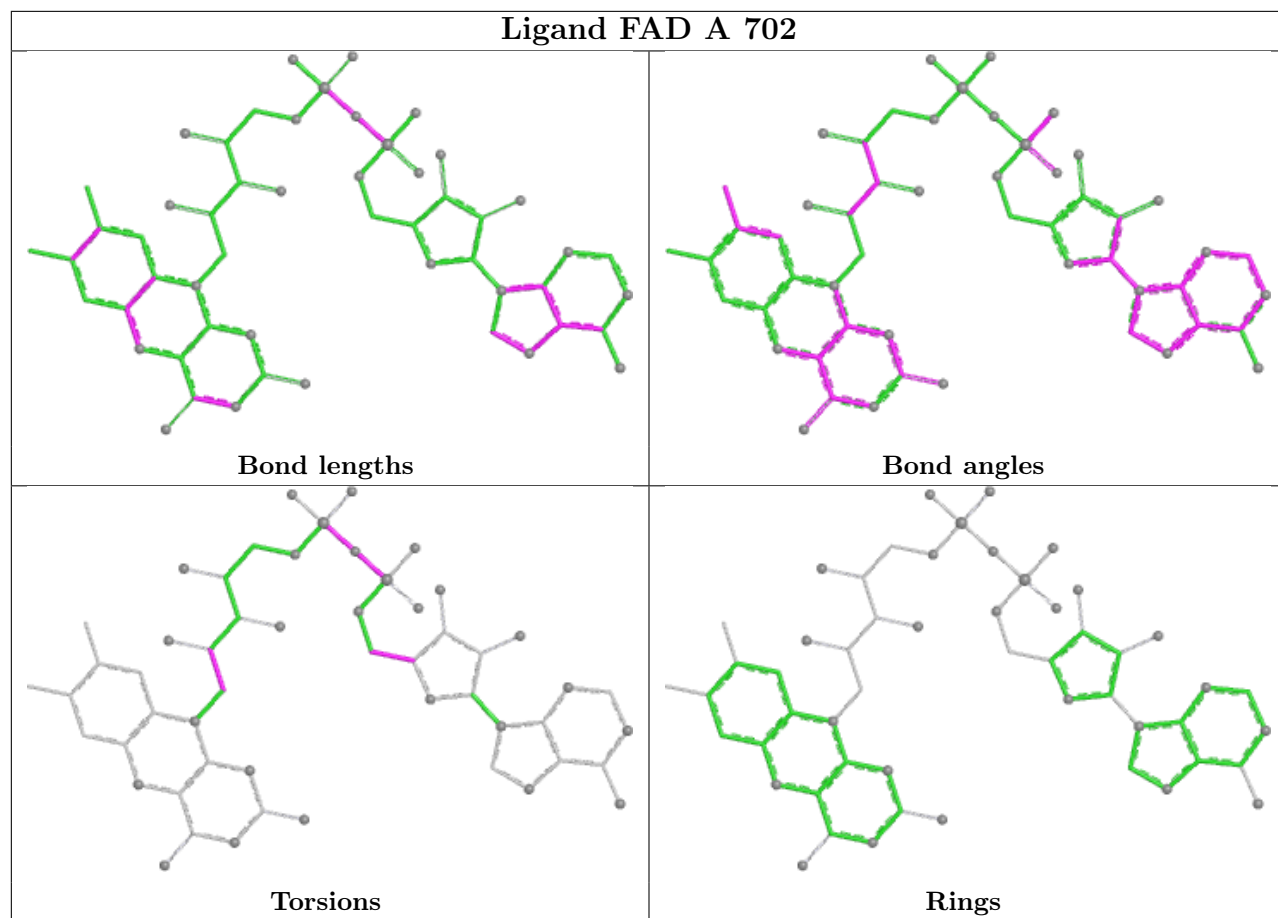
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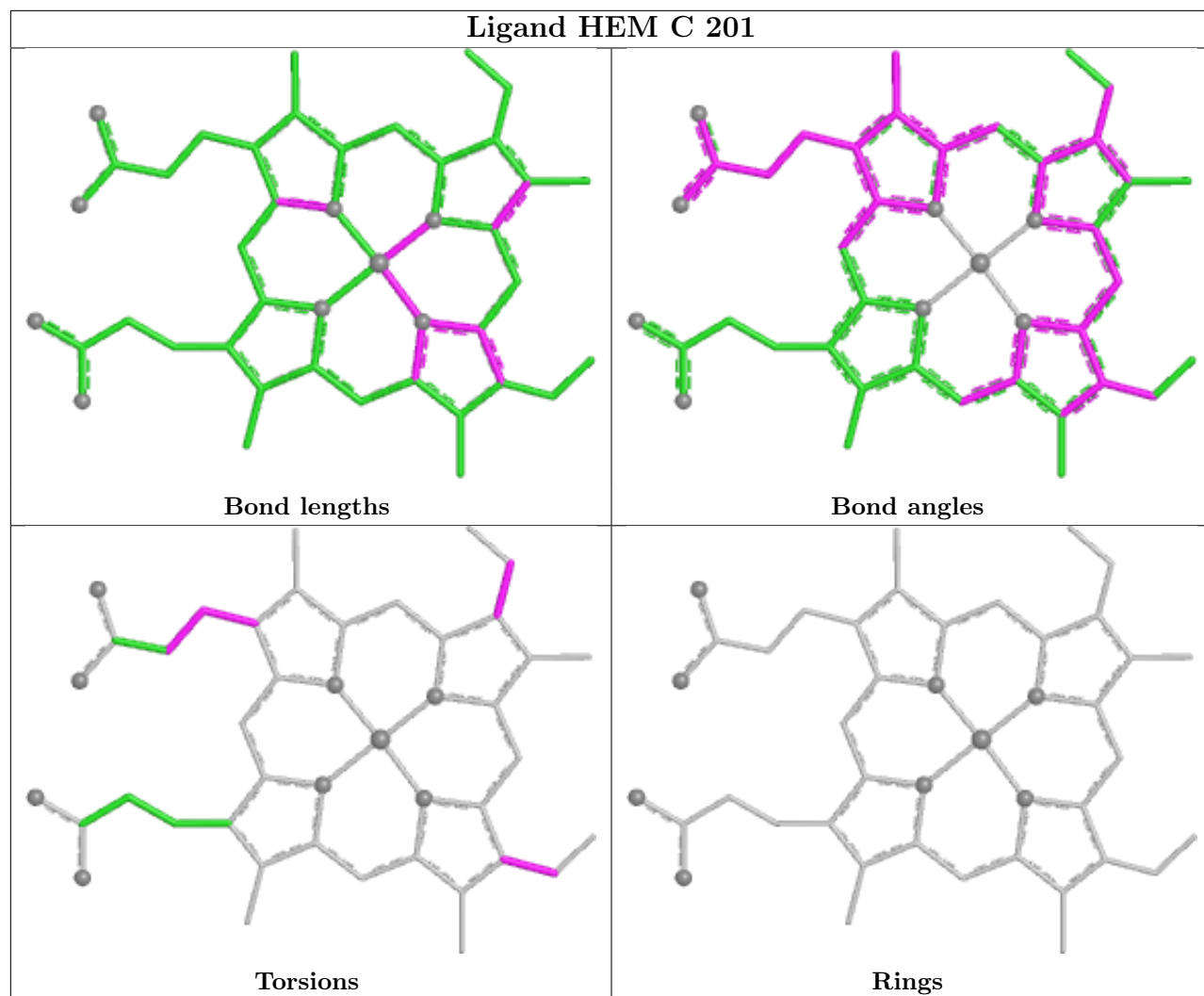
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	MLI	1	0
10	C	201	HEM	6	0
5	E	701	MLI	2	0
11	G	202	12J	4	0
11	C	202	12J	4	0
6	E	702	FAD	5	0

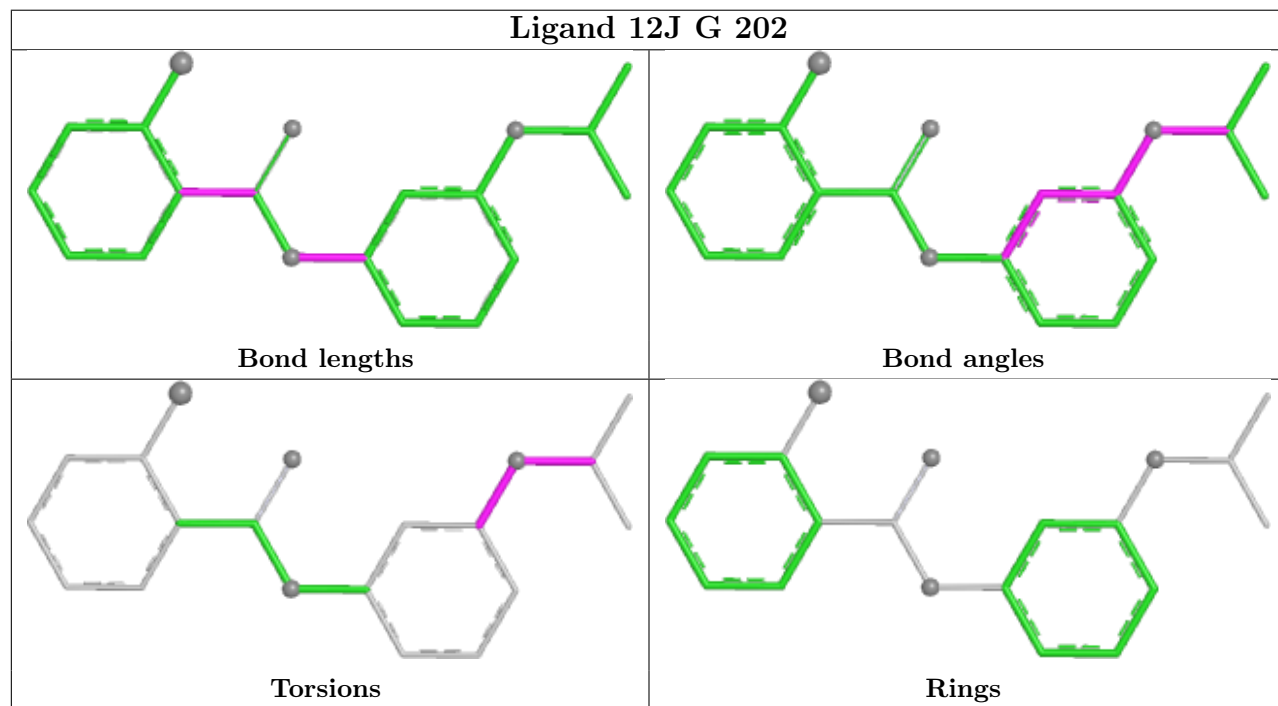
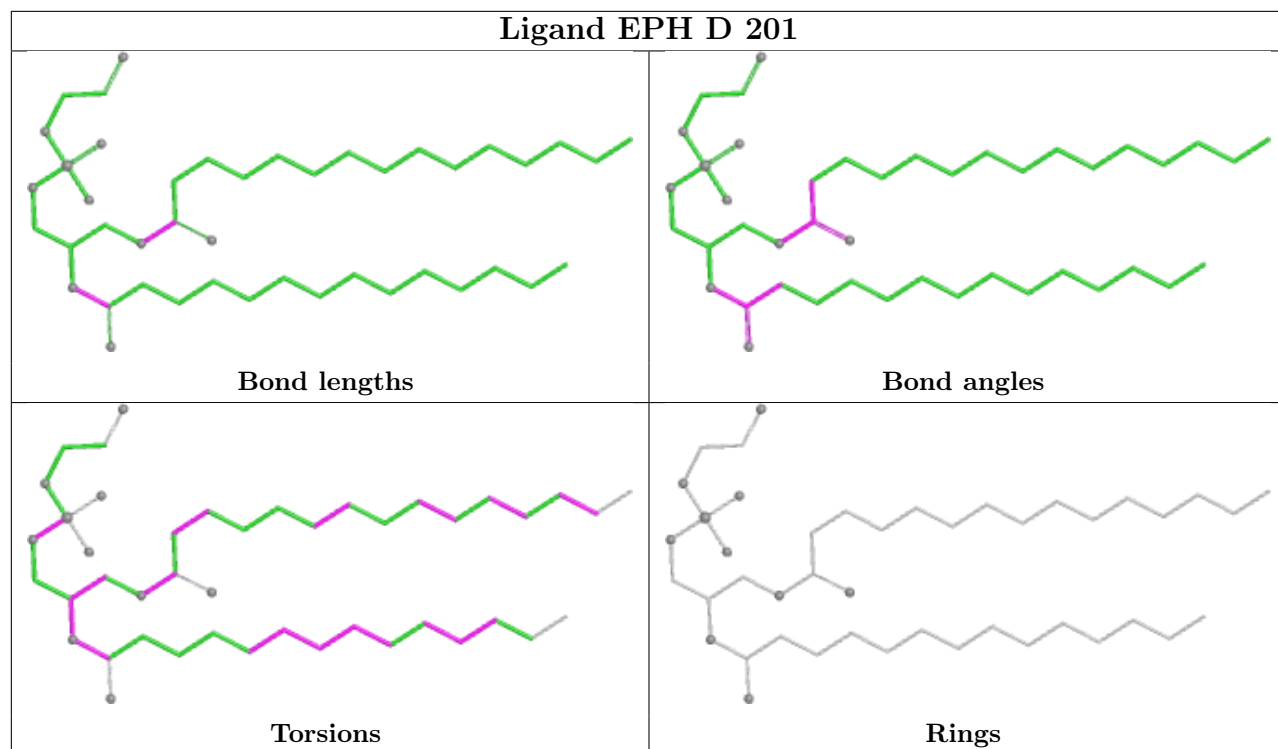
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



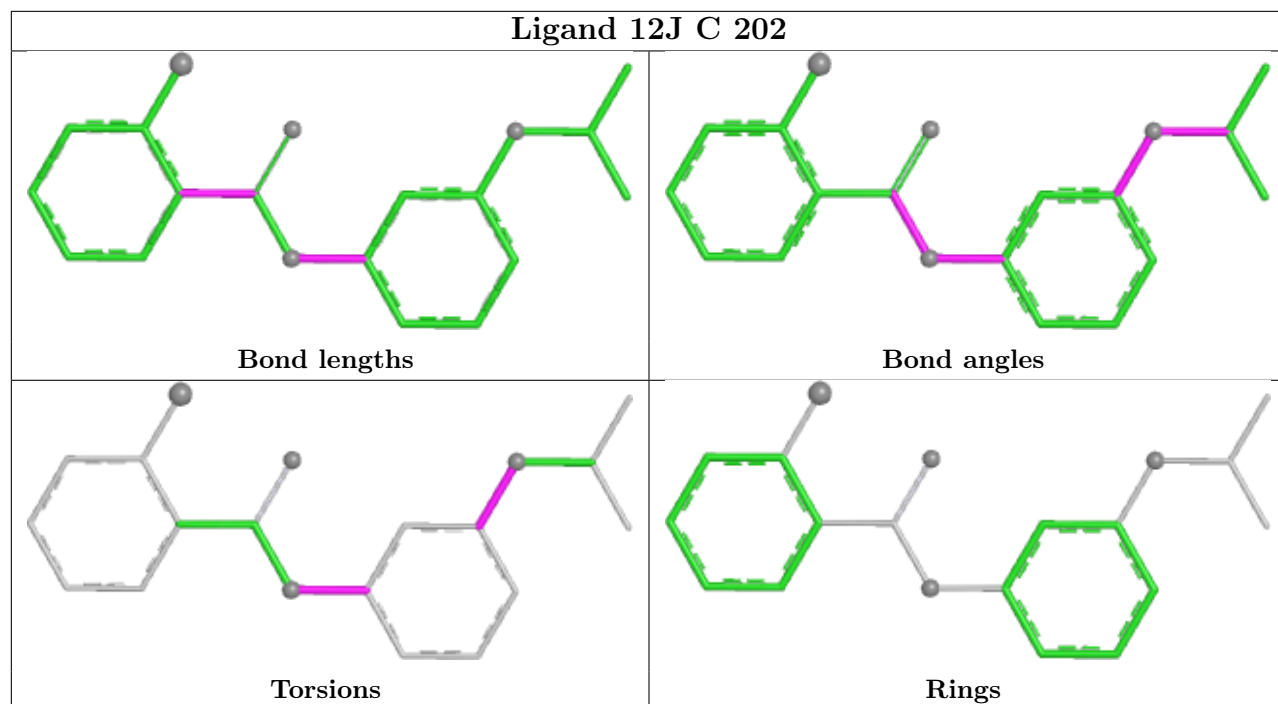




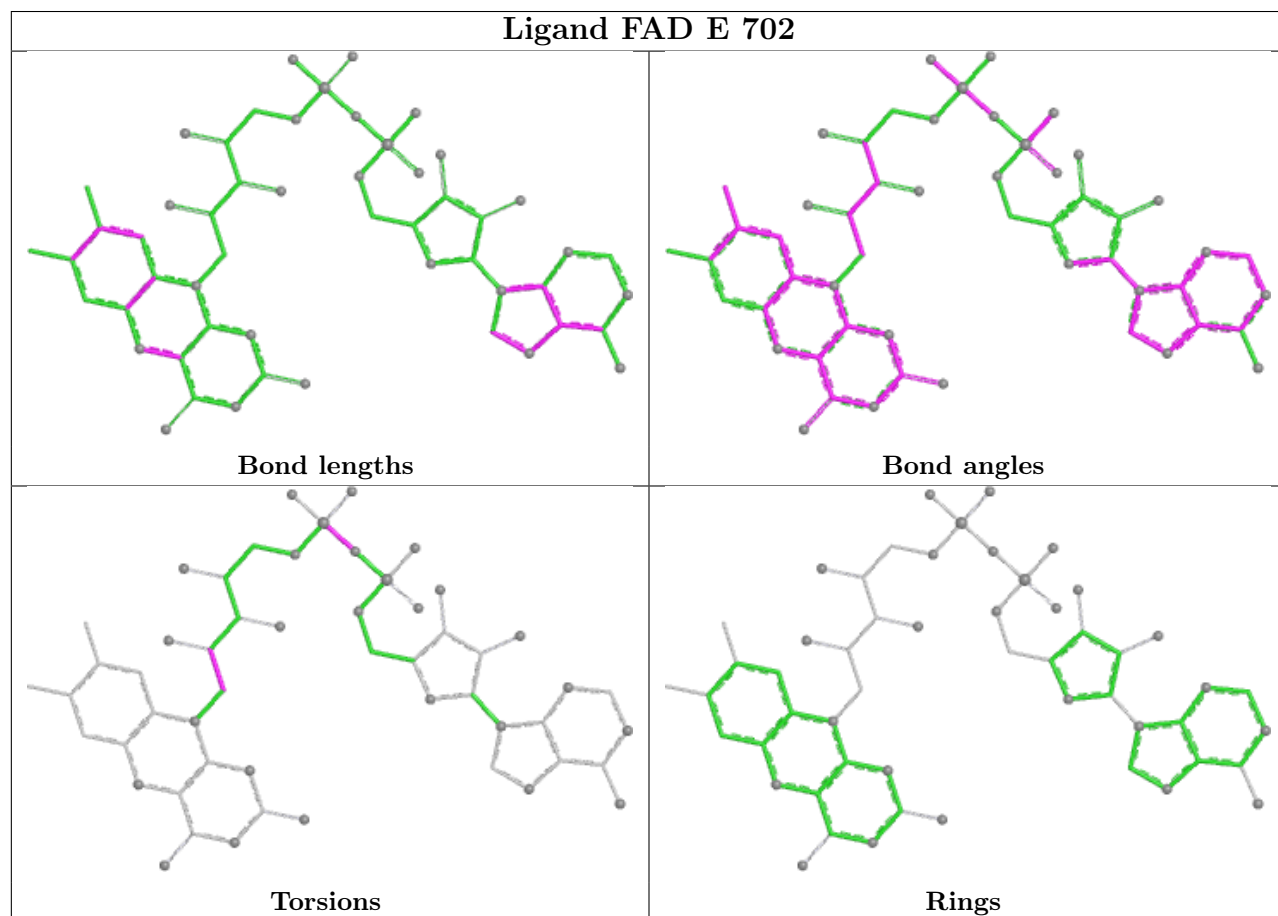




Ligand 12J C 202



Ligand FAD E 702



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%)	-0.50	1 (0%) 91 86	18, 55, 80, 108	1 (0%)
1	E	616/645 (95%)	-0.46	1 (0%) 91 86	19, 57, 83, 112	1 (0%)
2	B	250/282 (88%)	-0.47	0 100 100	35, 52, 78, 94	0
2	F	250/282 (88%)	-0.43	0 100 100	39, 55, 79, 109	0
3	C	153/188 (81%)	-0.26	4 (2%) 57 38	46, 62, 104, 151	0
3	G	153/188 (81%)	-0.00	5 (3%) 49 33	48, 68, 136, 211	0
4	D	129/156 (82%)	-0.25	2 (1%) 70 52	54, 66, 104, 141	0
4	H	129/156 (82%)	-0.09	5 (3%) 43 29	52, 72, 120, 154	0
All	All	2296/2542 (90%)	-0.39	18 (0%) 82 68	18, 58, 93, 211	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	499	THR	4.8
1	E	499	THR	4.2
4	H	52	LEU	3.8
3	G	185	PRO	3.8
3	G	107	ILE	3.3
3	C	186	THR	3.2
3	G	182	ALA	2.5
4	H	49	PHE	2.5
4	H	30	ALA	2.4
4	H	78	PHE	2.3
3	G	112	ILE	2.3
4	D	30	ALA	2.2
4	H	138	TYR	2.2
3	C	183	THR	2.2
4	D	52	LEU	2.1
3	C	182	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	179	HIS	2.0
3	G	186	THR	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](#)

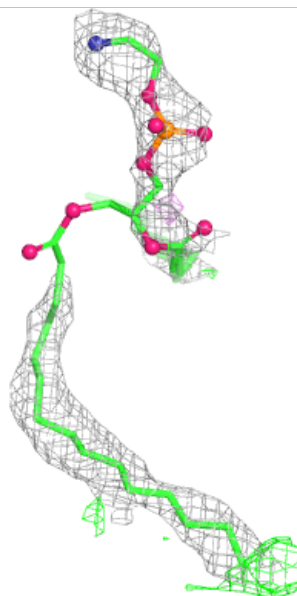
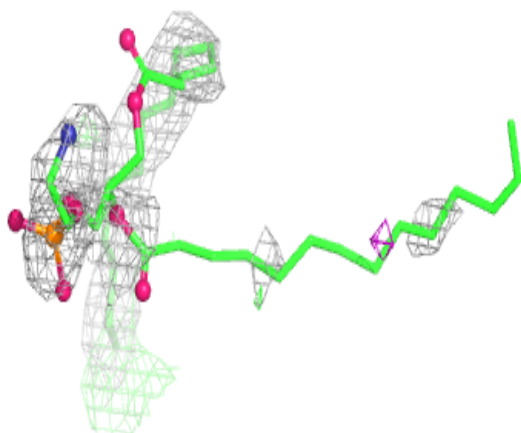
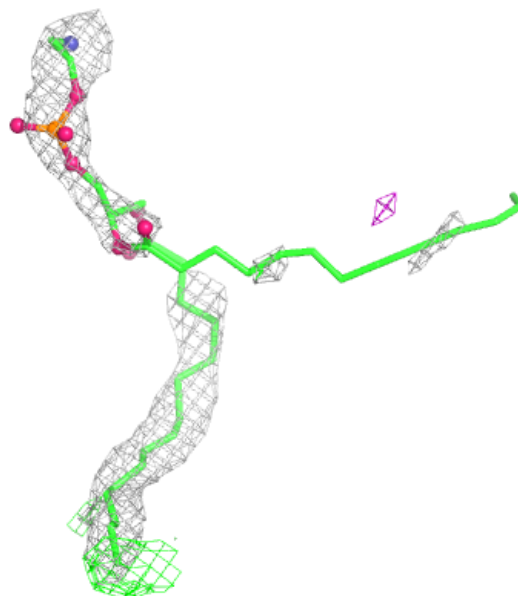
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	EPH	H	201	44/49	0.85	0.28	72,121,165,169	0
12	EPH	D	201	44/49	0.90	0.21	66,95,128,141	0
6	FAD	E	702	53/53	0.96	0.07	37,45,51,53	0
10	HEM	G	201	43/43	0.97	0.09	49,68,81,85	0
6	FAD	A	702	53/53	0.97	0.07	33,40,43,44	0
10	HEM	C	201	43/43	0.97	0.09	56,68,77,89	0
5	MLI	A	701	7/7	0.98	0.11	46,48,51,51	0
5	MLI	E	701	7/7	0.98	0.07	51,54,55,55	0
9	F3S	B	303	7/7	0.99	0.05	40,47,53,56	0
9	F3S	F	303	7/7	0.99	0.04	46,55,57,58	0
7	FES	B	301	4/4	0.99	0.03	44,46,48,49	0
7	FES	F	301	4/4	0.99	0.04	42,45,45,50	0
11	12J	C	202	20/20	0.99	0.08	61,70,76,77	0
11	12J	G	202	20/20	0.99	0.07	56,59,66,70	0
8	SF4	B	302	8/8	0.99	0.04	35,38,43,44	0
8	SF4	F	302	8/8	0.99	0.03	36,40,41,41	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.

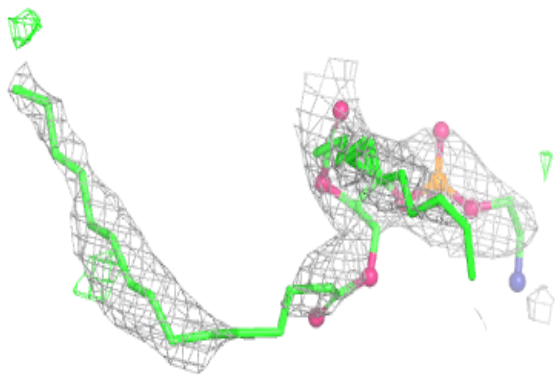
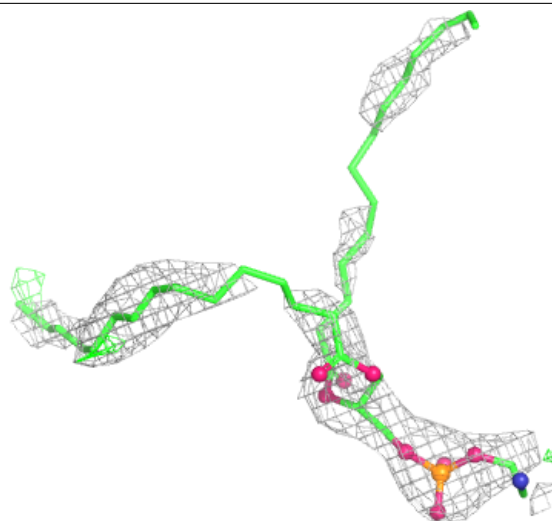
Electron density around EPH H 201:

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



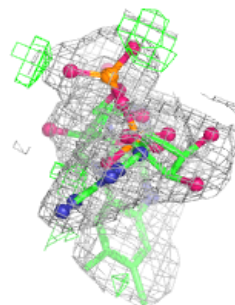
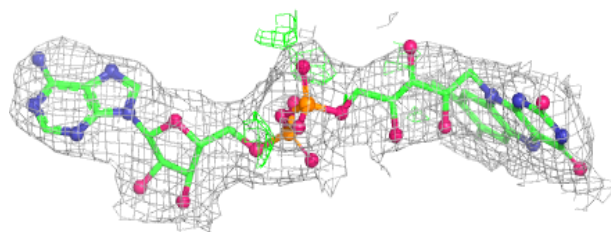
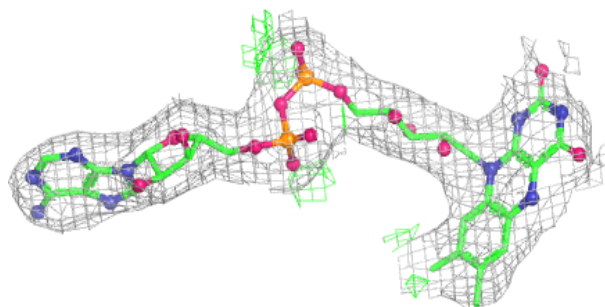
Electron density around EPH D 201:

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



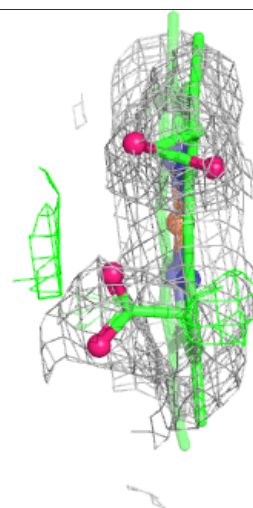
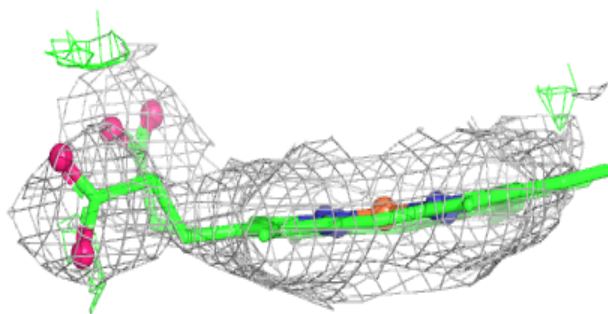
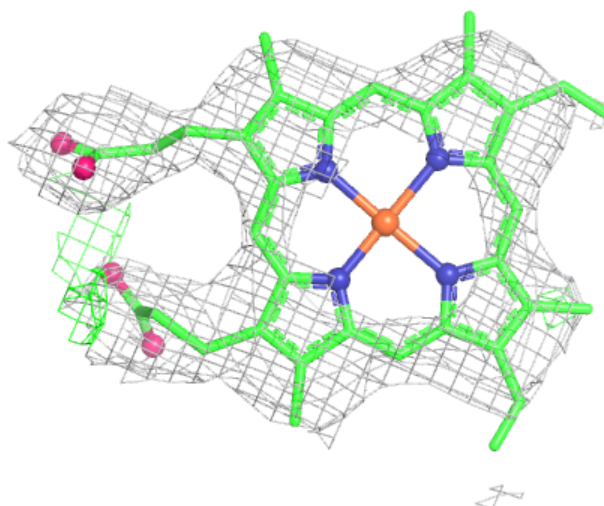
Electron density around FAD E 702:

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



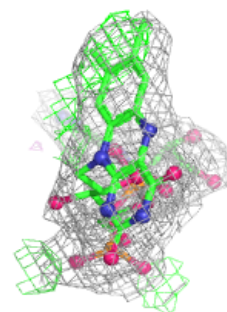
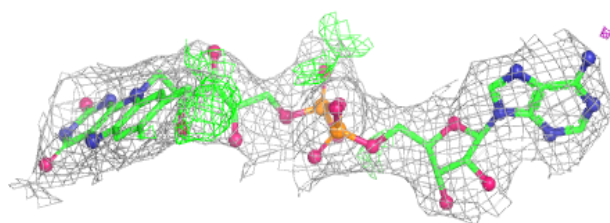
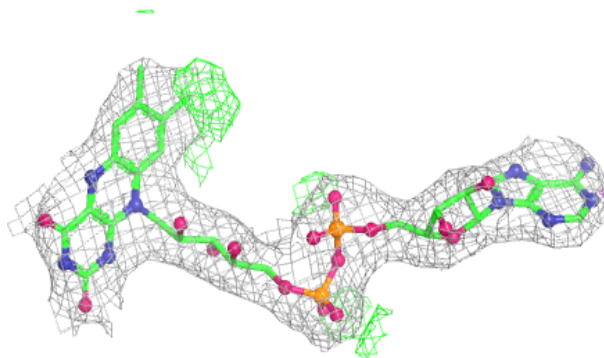
Electron density around HEM G 201:

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



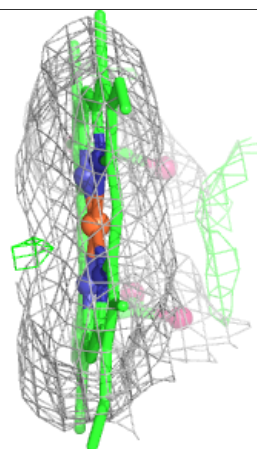
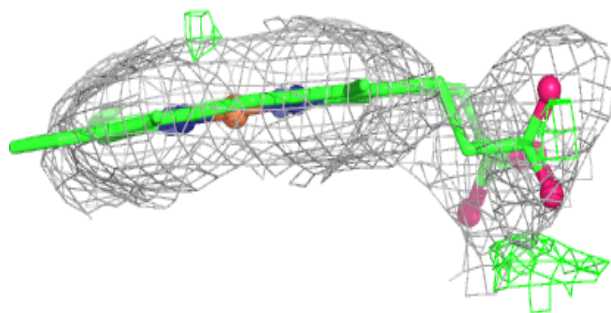
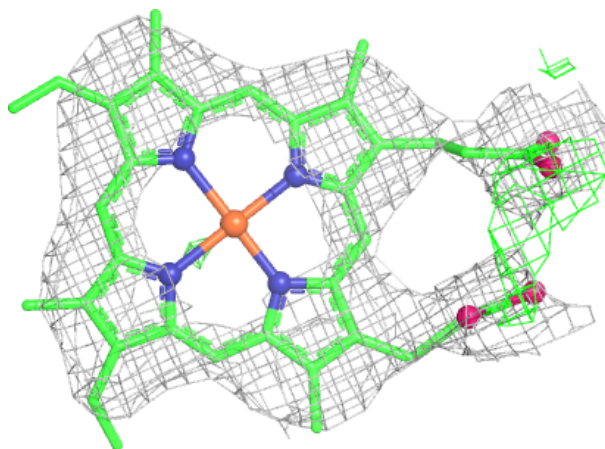
Electron density around FAD A 702:

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



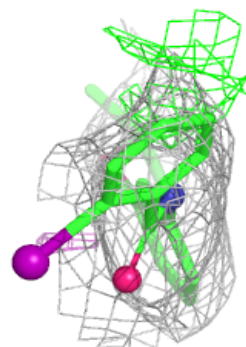
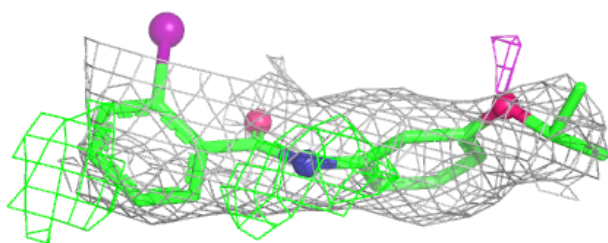
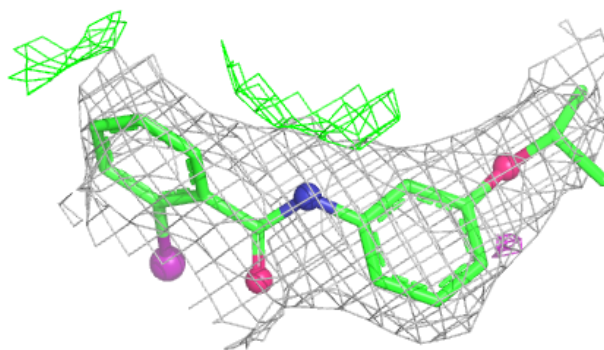
Electron density around HEM C 201:

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

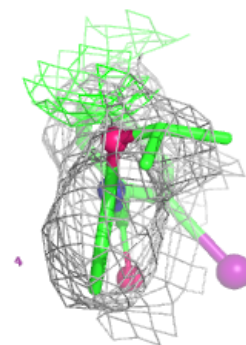
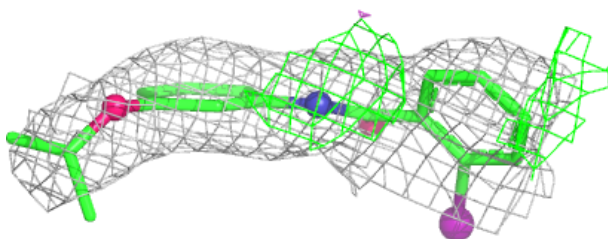
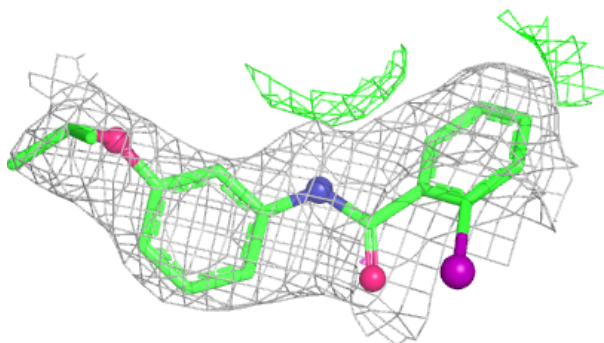


Electron density around 12J C 202:

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

**Electron density around 12J 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.