



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 10:23 PM EST

PDB ID : 3VRB  
Title : Mitochondrial rhodoquinol-fumarate reductase from the parasitic nematode *Ascaris suum* with the specific inhibitor flutolanil and substrate fumarate  
Authors : Shimizu, H.; Shiba, T.; Inaoka, D.K.; Osanai, A.; Kita, K.; Sakamoto, K.; Harada, S.  
Deposited on : 2012-04-07  
Resolution : 2.91 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

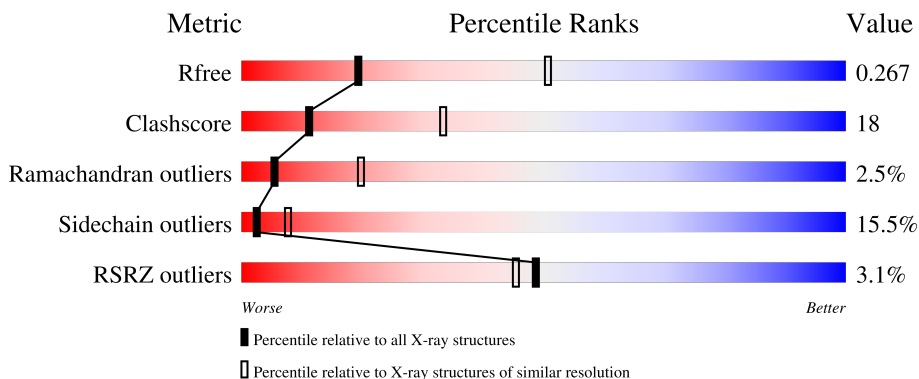
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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))
$R_{free}$	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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  $\geq 3$ , 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	 2% 53% 37% 5% 5%
1	E	645	 3% 54% 36% 5% 5%
2	B	282	 53% 31% 8% 12%
2	F	282	 4% 51% 27% 8% 12%

*Continued on next page...*

Continued from previous page...

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	FUM	E	701	-	-	X	-
7	FES	F	301	-	-	X	-
8	SF4	B	302	-	-	X	-
8	SF4	F	302	-	-	X	-
9	F3S	B	303	-	-	X	-

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 18242 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 Flavoprotein subunit of complex II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	613	Total 4758	C 2983	N 851	O 896	S 28	0	0	0
1	E	613	Total 4758	C 2983	N 851	O 896	S 28	0	0	0

- Molecule 2 is a protein called Iron-sulfur subunit of succinate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	249	Total 1973	C 1254	N 337	O 359	S 23	0	0	0
2	F	249	Total 1973	C 1254	N 337	O 359	S 23	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	153	Total 1217	C 813	N 204	O 194	S 6	0	0	0
3	G	150	Total 1195	C 798	N 201	O 190	S 6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	129	Total 994	C 658	N 165	O 166	S 5	0	0	0
4	H	129	Total 994	C 658	N 165	O 166	S 5	0	0	0

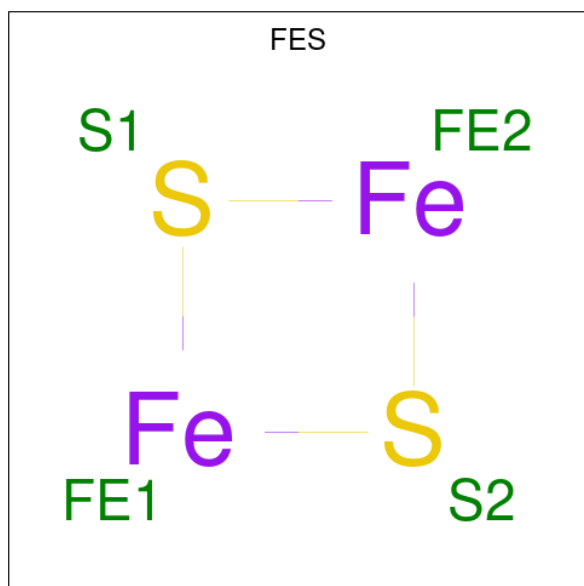
- Molecule 5 is FUMARIC ACID (three-letter code: FUM) (formula: C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>).



Continued from previous page...

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

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



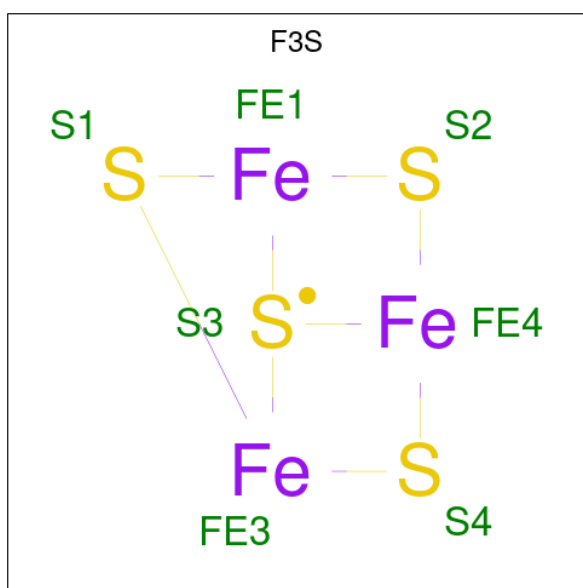
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	B	1	4	2	2	0	0
7	F	1	4	2	2	0	0

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



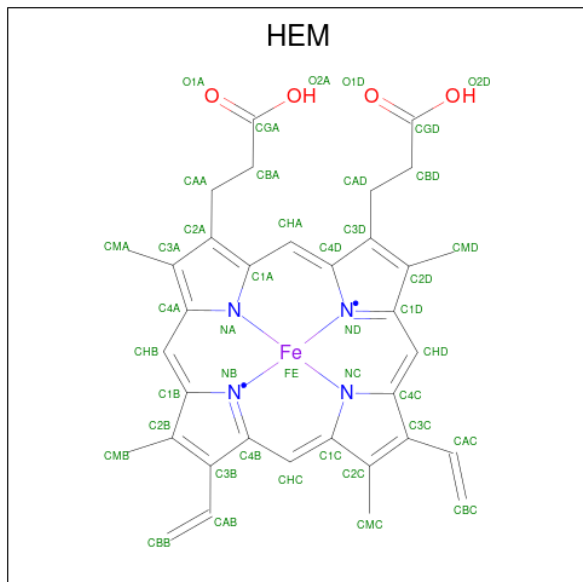
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Fe S	0	0
			8	4 4		
8	F	1	Total	Fe S	0	0
			8	4 4		

- Molecule 9 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



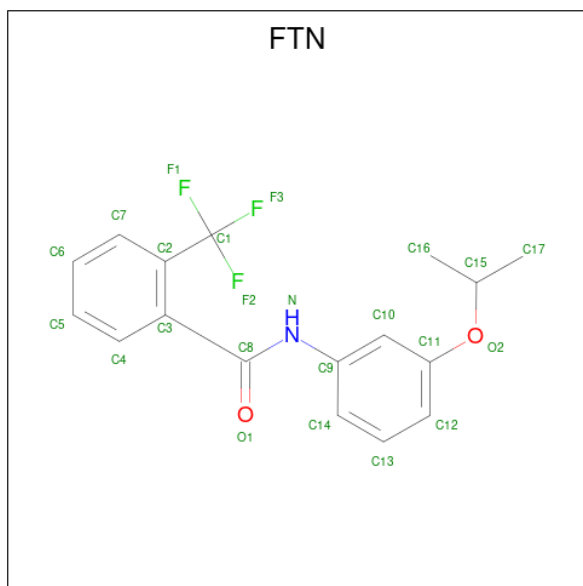
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Fe S	0	0
			7	3 4		
9	F	1	Total	Fe S	0	0
			7	3 4		

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



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

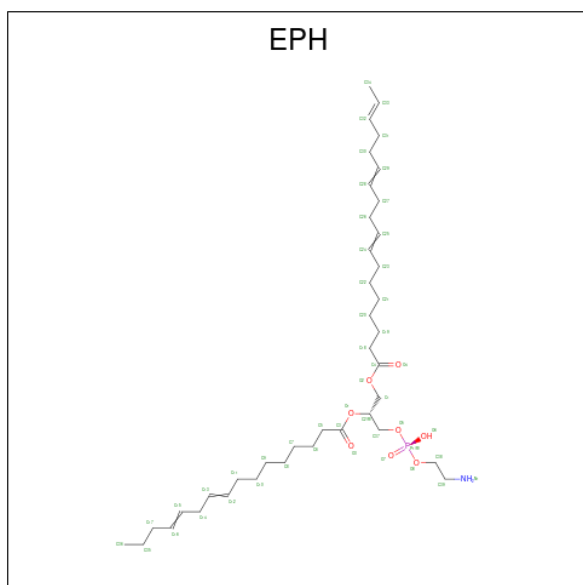
- Molecule 11 is N-[3-(1-methylethoxy)phenyl]-2-(trifluoromethyl)benzamide (three-letter code: FTN) (formula:  $C_{17}H_{16}F_3NO_2$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	F	N	O	0	0
			23	17	3	1	2		
11	F	1	Total	C	F	N	O	0	0
			23	17	3	1	2		

- Molecule 12 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: C<sub>39</sub>H<sub>68</sub>NO<sub>8</sub>P).

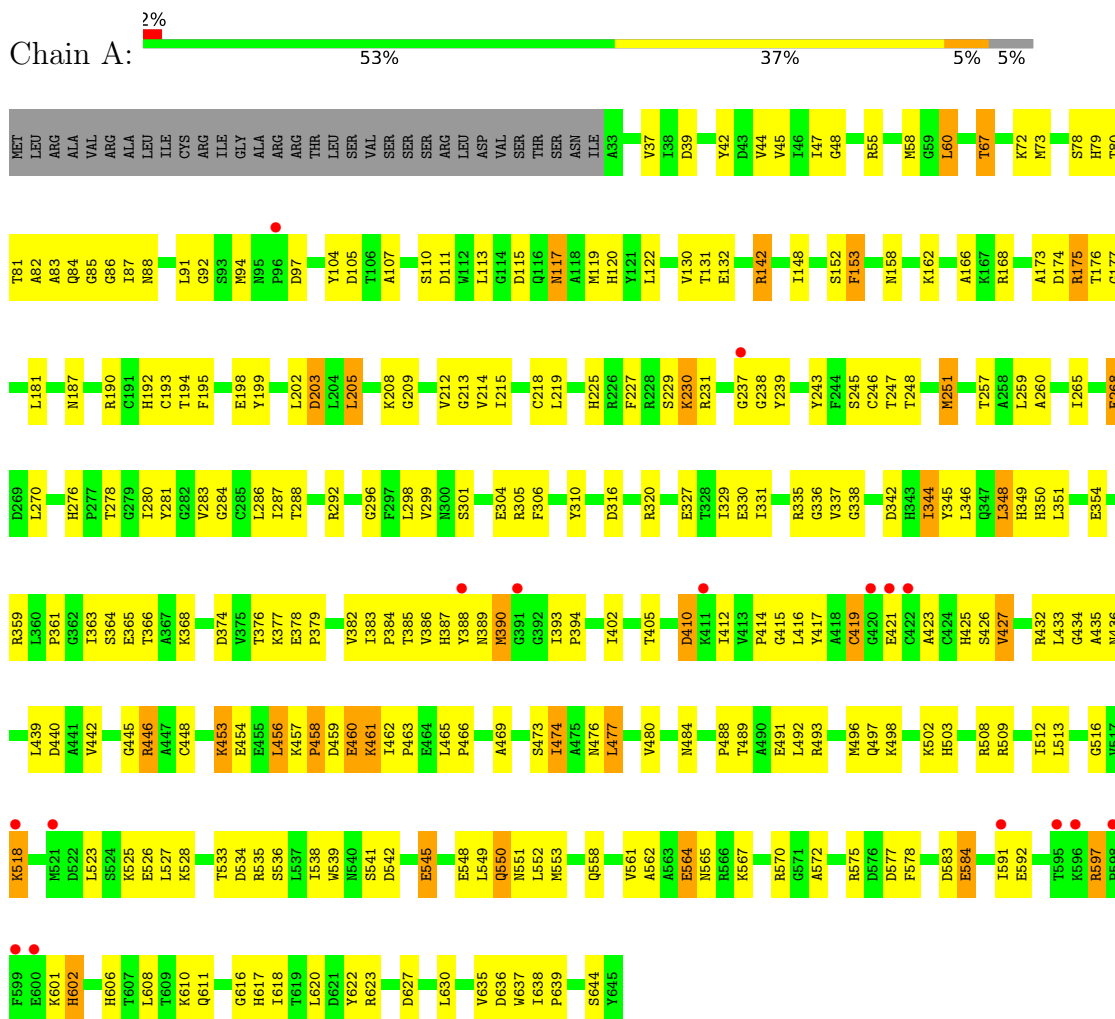


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
12	H	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

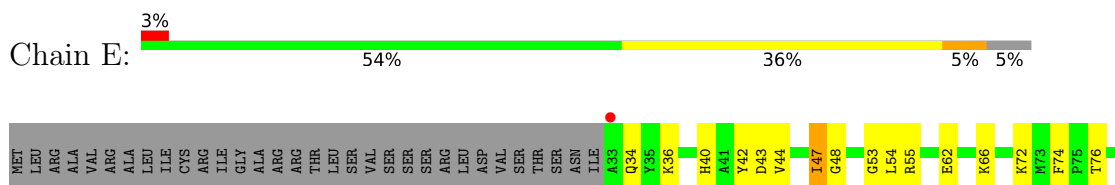
### 3 Residue-property plots [i](#)

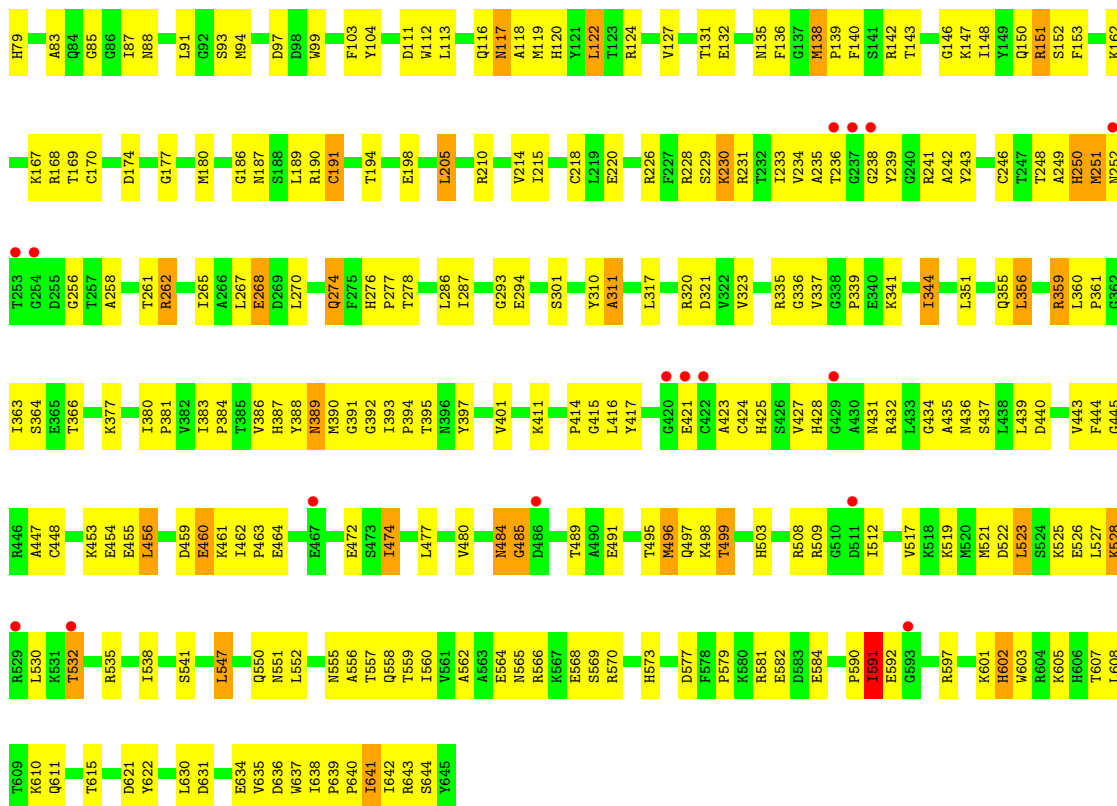
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Flavoprotein subunit of complex II

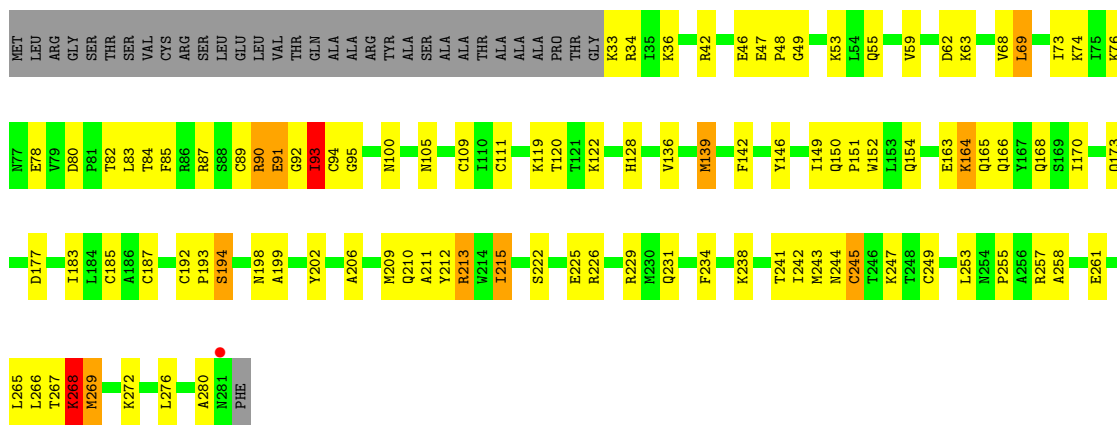


#### • Molecule 1: Flavoprotein subunit of complex II

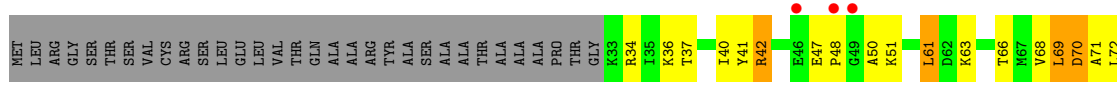


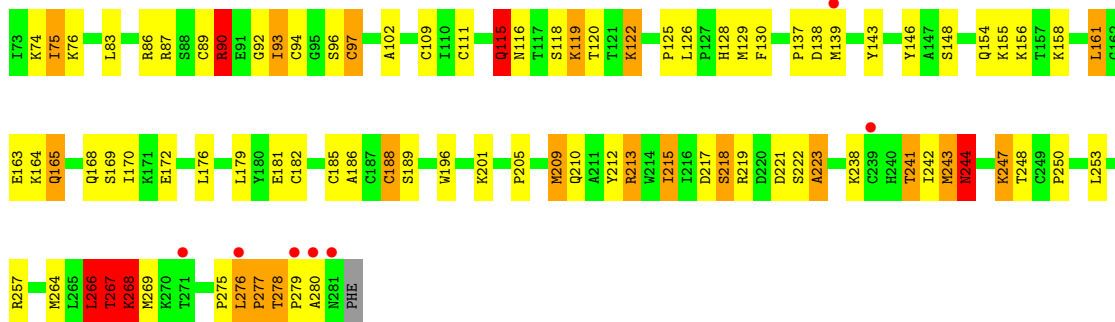


● Molecule 2: Iron-sulfur subunit of succinate dehydrogenase

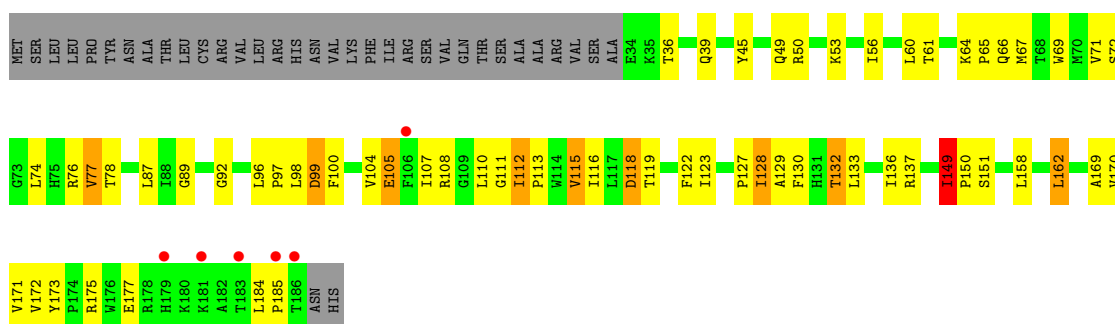


● Molecule 2: Iron-sulfur subunit of succinate dehydrogenase

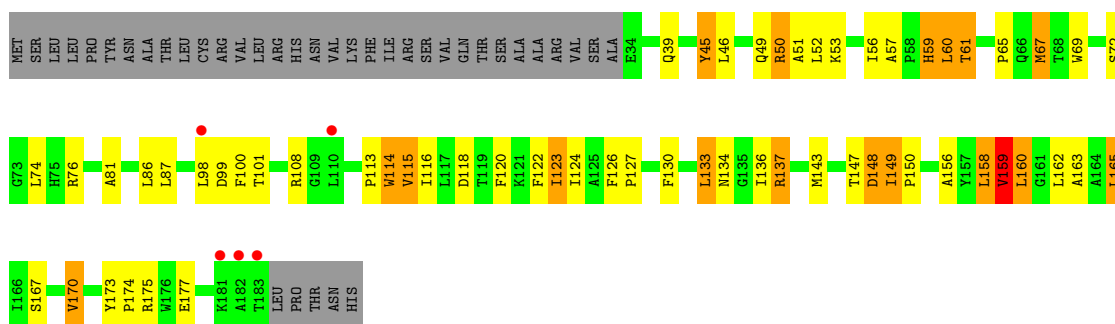




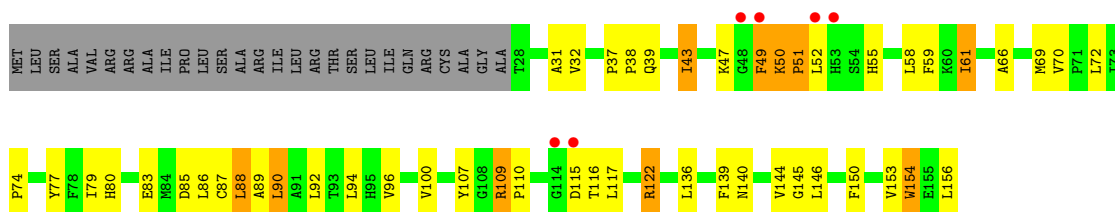
• Molecule 3: Cytochrome b-large subunit



• Molecule 3: Cytochrome b-large subunit

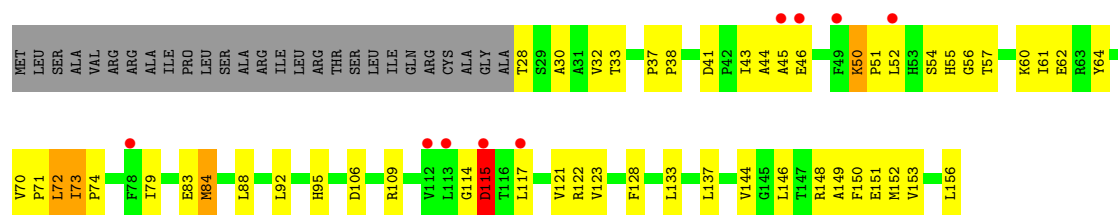


• Molecule 4: Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial



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

Chain H: 6% 49% 31% 17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.31Å 131.65Å 222.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.39 – 2.91 35.39 – 2.91	Depositor EDS
% Data completeness (in resolution range)	74.0 (35.39-2.91) 74.0 (35.39-2.91)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 2.90Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.204 , 0.272 0.199 , 0.267	Depositor DCC
$R_{free}$ test set	2986 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.5	Xtrriage
Anisotropy	0.130	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18242	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FAD, SF4, EPH, F3S, FUM, FTN, HEM

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	0.61	0/4859	0.73	0/6564
1	E	0.66	1/4859 (0.0%)	0.73	0/6564
2	B	0.70	1/2016 (0.0%)	0.75	0/2723
2	F	0.74	1/2016 (0.0%)	0.77	0/2723
3	C	0.63	0/1255	0.72	0/1709
3	G	0.57	0/1232	0.69	0/1676
4	D	0.64	0/1026	0.72	0/1402
4	H	0.62	0/1026	0.72	0/1402
All	All	0.65	3/18289 (0.0%)	0.73	0/24763

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	91	GLU	CG-CD	6.03	1.60	1.51
2	F	97	CYS	CB-SG	-5.54	1.72	1.81
1	E	268	GLU	CG-CD	5.20	1.59	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4758	0	4692	198	0
1	E	4758	0	4692	164	0
2	B	1973	0	1996	64	0
2	F	1973	0	1996	79	0
3	C	1217	0	1265	50	0
3	G	1195	0	1240	48	0
4	D	994	0	977	37	0
4	H	994	0	977	32	0
5	A	8	0	1	3	0
5	E	8	0	1	5	0
6	A	53	0	31	8	0
6	E	53	0	31	5	0
7	B	4	0	0	0	0
7	F	4	0	0	2	0
8	B	8	0	0	2	0
8	F	8	0	0	4	0
9	B	7	0	0	2	0
9	F	7	0	0	0	0
10	C	43	0	30	6	0
10	G	43	0	30	5	0
11	C	23	0	16	4	0
11	F	23	0	16	1	0
12	D	44	0	53	5	0
12	H	44	0	53	1	0
All	All	18242	0	18097	644	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 18.

All (644) 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	1.34	1.37
1:A:79:HIS:CE1	6:A:702:FAD:HM82	1.60	1.35
1:E:79:HIS:NE2	6:E:702:FAD:HM82	0.89	1.21
1:A:79:HIS:NE2	6:A:702:FAD:HM81	1.62	1.09
2:B:268:LYS:HG3	2:B:269:MET:H	1.13	1.06
3:C:149:ILE:HG12	3:C:150:PRO:HD3	1.36	1.05
1:E:79:HIS:CE1	6:E:702:FAD:HM82	1.92	1.03
3:G:115:VAL:HG23	3:G:116:ILE:HD12	1.38	1.03
4:D:50:LYS:H	4:D:51:PRO:HD2	1.20	0.98
2:B:245:CYS:HG	9:B:303:F3S:FE3	0.73	0.98

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:ILE:HD12	1:E:234:VAL:HA	1.44	0.96
3:C:123:ILE:O	3:C:127:PRO:HD2	1.66	0.95
1:A:117:ASN:H	1:A:117:ASN:HD22	1.11	0.94
1:A:44:VAL:HG11	1:A:60:LEU:HD22	1.51	0.92
1:A:115:ASP:HB3	1:A:117:ASN:HD21	1.35	0.92
4:D:50:LYS:N	4:D:51:PRO:HD2	1.85	0.91
2:F:97:CYS:HG	7:F:301:FES:FE1	0.74	0.91
1:E:79:HIS:CD2	6:E:702:FAD:HM82	2.05	0.90
1:A:42:TYR:O	1:A:229:SER:HA	1.70	0.90
2:B:268:LYS:CG	2:B:269:MET:H	1.85	0.88
3:C:133:LEU:O	3:C:136:ILE:HG13	1.74	0.88
4:H:70:VAL:O	4:H:74:PRO:HD2	1.74	0.87
3:G:149:ILE:HD13	3:G:149:ILE:H	1.40	0.87
1:A:202:LEU:HB2	1:A:215:ILE:HG23	1.57	0.86
2:B:268:LYS:HG3	2:B:269:MET:N	1.92	0.85
1:A:541:SER:HB2	2:B:84:THR:HG23	1.59	0.85
3:C:149:ILE:HD13	3:C:149:ILE:H	1.42	0.85
1:E:97:ASP:OD2	1:E:168:ARG:NH1	2.10	0.84
1:A:268:GLU:HB3	1:A:608:LEU:HD23	1.58	0.84
1:A:230:LYS:O	1:A:231:ARG:HD3	1.78	0.84
1:E:557:THR:O	1:E:560:ILE:HG22	1.76	0.84
3:C:158:LEU:O	3:C:162:LEU:HB2	1.77	0.83
4:D:80:HIS:HE1	12:D:201:EPH:H371	1.42	0.83
1:E:120:HIS:CD2	1:E:630:LEU:HD12	2.14	0.83
1:A:278:THR:HG21	1:A:346:LEU:HD22	1.61	0.82
1:A:327:GLU:OE2	1:A:384:PRO:HD3	1.79	0.82
2:F:89:CYS:O	2:F:90:ARG:HD2	1.80	0.81
1:E:495:THR:O	1:E:499:THR:HG23	1.80	0.81
4:D:50:LYS:H	4:D:51:PRO:CD	1.93	0.81
2:F:264:MET:SD	3:G:143:MET:HA	2.21	0.80
3:G:76:ARG:HG2	10:G:201:HEM:O2D	1.82	0.80
1:A:205:LEU:HB3	1:A:212:VAL:HG22	1.62	0.80
1:A:565:ASN:ND2	1:A:622:TYR:OH	2.13	0.80
1:E:79:HIS:CD2	6:E:702:FAD:C8M	2.64	0.79
2:F:115:GLN:HE21	2:F:115:GLN:HA	1.47	0.78
1:A:205:LEU:HB3	1:A:212:VAL:CG2	2.13	0.78
1:A:239:TYR:H	1:A:389:ASN:ND2	1.81	0.78
1:E:135:ASN:ND2	2:F:161:LEU:O	2.16	0.78
2:F:188:CYS:SG	8:F:302:SF4:S3	2.82	0.77
2:F:268:LYS:CG	2:F:269:MET:H	1.97	0.77
3:G:173:TYR:HB3	3:G:174:PRO:HD3	1.66	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:201:HEM:HBD1	10:C:201:HEM:HHA	1.68	0.76
4:D:80:HIS:CE1	12:D:201:EPH:H371	2.21	0.75
3:C:110:LEU:O	3:C:112:ILE:HG13	1.84	0.75
1:A:83:ALA:HB3	1:A:177:GLY:HA3	1.68	0.74
1:E:276:HIS:CE1	1:E:286:LEU:HD11	2.21	0.74
1:A:476:ASN:O	1:A:480:VAL:HG23	1.87	0.74
1:A:117:ASN:H	1:A:117:ASN:ND2	1.83	0.74
3:C:76:ARG:NH1	4:D:107:TYR:CE1	2.56	0.74
1:A:132:GLU:OE1	1:A:446:ARG:NH1	2.22	0.73
1:A:493:ARG:O	1:A:497:GLN:HG3	1.87	0.73
1:A:120:HIS:HD2	1:A:630:LEU:H	1.35	0.73
1:A:104:TYR:HD2	1:A:105:ASP:OD1	1.72	0.72
1:E:301:SER:HB3	1:E:336:GLY:O	1.89	0.72
2:F:268:LYS:HG2	2:F:269:MET:H	1.55	0.72
2:B:76:LYS:HA	2:B:80:ASP:O	1.89	0.72
1:E:582:GLU:HG3	1:E:603:TRP:HD1	1.54	0.72
3:C:100:PHE:O	3:C:104:VAL:HG23	1.91	0.71
2:F:115:GLN:HA	2:F:115:GLN:NE2	2.05	0.71
1:A:213:GLY:HA3	1:A:227:PHE:O	1.90	0.70
2:B:93:ILE:HD13	2:B:93:ILE:O	1.91	0.70
3:G:133:LEU:O	3:G:136:ILE:HG13	1.93	0.68
1:A:78:SER:O	1:A:81:THR:HG22	1.92	0.68
1:E:83:ALA:HB3	1:E:177:GLY:HA3	1.73	0.68
2:F:146:TYR:HE1	2:F:210:GLN:HG2	1.57	0.68
3:G:126:PHE:HB3	3:G:127:PRO:HD3	1.76	0.68
3:G:126:PHE:HA	3:G:167:SER:OG	1.94	0.68
3:C:149:ILE:HD13	3:C:149:ILE:N	2.10	0.67
1:A:174:ASP:OD1	1:A:174:ASP:O	2.12	0.67
2:F:86:ARG:NH1	2:F:137:PRO:HD2	2.10	0.67
1:A:48:GLY:HA2	6:A:702:FAD:H1B	1.76	0.67
2:B:154:GLN:HG3	2:B:222:SER:OG	1.94	0.67
1:A:545:GLU:OE2	1:A:545:GLU:HA	1.93	0.66
2:B:245:CYS:SG	9:B:303:F3S:S1	2.94	0.66
1:A:115:ASP:HB3	1:A:117:ASN:ND2	2.10	0.66
2:B:150:GLN:O	2:B:226:ARG:NH1	2.28	0.66
4:H:73:ILE:HG22	4:H:74:PRO:HD3	1.76	0.66
3:C:128:ILE:O	3:C:132:THR:OG1	2.14	0.66
1:E:241:ARG:HH11	1:E:250:HIS:CE1	2.14	0.66
2:F:94:CYS:SG	2:F:96:SER:HB2	2.36	0.65
1:E:262:ARG:NH1	1:E:551:ASN:HD21	1.94	0.65
10:G:201:HEM:HBA2	10:G:201:HEM:HHA	1.78	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ARG:NH2	5:A:701:FUM:O7	2.29	0.65
1:E:294:GLU:HG3	1:E:360:LEU:HD11	1.79	0.65
2:B:89:CYS:HB3	2:B:94:CYS:HB3	1.76	0.65
1:E:74:PHE:CD2	1:E:76:THR:HB	2.32	0.65
1:E:383:ILE:HG23	1:E:384:PRO:O	1.96	0.65
2:B:193:PRO:HD2	2:B:242:ILE:HD13	1.78	0.64
1:E:230:LYS:HD2	1:E:462:ILE:HA	1.76	0.64
1:E:351:LEU:HB2	1:E:356:LEU:HD11	1.79	0.64
1:E:391:GLY:HA2	1:E:424:CYS:HB2	1.78	0.64
1:E:454:GLU:OE2	1:E:454:GLU:N	2.30	0.64
4:D:69:MET:HG2	4:D:69:MET:O	1.98	0.64
1:A:246:CYS:O	2:B:90:ARG:NH2	2.30	0.64
2:F:179:LEU:HD23	2:F:213:ARG:HA	1.80	0.64
4:H:32:VAL:HG22	4:H:33:THR:H	1.62	0.64
1:A:268:GLU:HB3	1:A:608:LEU:CD2	2.28	0.64
3:C:105:GLU:C	3:C:107:ILE:H	2.01	0.64
3:G:148:ASP:OD2	3:G:150:PRO:HD2	1.97	0.64
1:A:148:ILE:H	2:B:165:GLN:HE22	1.43	0.64
1:A:276:HIS:CE1	1:A:286:LEU:HD11	2.33	0.64
3:C:69:TRP:CE3	11:C:202:FTN:H15	2.33	0.64
2:F:169:SER:OG	2:F:172:GLU:HG3	1.97	0.63
2:F:36:LYS:HB2	2:F:61:LEU:CD1	2.28	0.63
1:A:148:ILE:N	2:B:165:GLN:HE22	1.97	0.63
1:A:374:ASP:OD1	1:A:376:THR:OG1	2.16	0.63
1:A:378:GLU:HB3	1:A:379:PRO:HD2	1.80	0.63
1:E:239:TYR:H	1:E:389:ASN:HD21	1.47	0.63
1:E:484:ASN:O	1:E:485:GLY:O	2.16	0.63
1:E:388:TYR:CE1	1:E:421:GLU:HG3	2.33	0.62
3:G:163:ALA:O	3:G:167:SER:HB2	1.98	0.62
1:E:231:ARG:HD3	1:E:415:GLY:HA2	1.82	0.62
2:B:95:GLY:HA2	2:B:183:ILE:HD12	1.82	0.62
1:A:281:TYR:HA	1:A:383:ILE:HG22	1.81	0.62
2:B:212:TYR:OH	2:B:261:GLU:HG2	2.00	0.62
1:E:508:ARG:HH11	1:E:573:HIS:CD2	2.18	0.62
2:F:276:LEU:HG	2:F:277:PRO:HD2	1.81	0.62
4:H:73:ILE:HG22	4:H:74:PRO:CD	2.29	0.62
3:G:115:VAL:HG23	3:G:116:ILE:CD1	2.24	0.61
2:B:146:TYR:HE1	2:B:210:GLN:HG2	1.66	0.61
3:C:112:ILE:H	3:C:112:ILE:HD12	1.66	0.61
1:E:74:PHE:HD2	1:E:76:THR:HB	1.65	0.61
2:B:149:ILE:HD13	2:B:211:ALA:HA	1.81	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ILE:HG12	1:A:345:TYR:N	2.15	0.61
1:E:148:ILE:H	2:F:165:GLN:HE22	1.49	0.61
4:H:44:ALA:O	4:H:46:GLU:N	2.34	0.61
2:F:115:GLN:HE21	2:F:115:GLN:CA	2.13	0.61
2:F:242:ILE:O	2:F:243:MET:HB2	2.01	0.60
3:C:76:ARG:NH1	4:D:107:TYR:HE1	1.99	0.60
1:E:320:ARG:HH12	5:E:701:FUM:C6	2.14	0.60
1:E:503:HIS:HD2	1:E:512:ILE:HG22	1.66	0.60
2:B:36:LYS:HE3	2:B:119:LYS:O	2.01	0.60
1:A:488:PRO:HG2	1:A:491:GLU:HB2	1.83	0.60
1:A:584:GLU:O	1:A:597:ARG:HG3	2.02	0.60
1:E:508:ARG:HH11	1:E:573:HIS:HD2	1.50	0.60
2:F:212:TYR:HA	2:F:215:ILE:HG13	1.84	0.60
2:F:36:LYS:HB2	2:F:61:LEU:HD11	1.82	0.60
2:F:102:ALA:HA	2:F:122:LYS:HE2	1.84	0.60
3:C:149:ILE:H	3:C:149:ILE:CD1	2.15	0.60
1:E:508:ARG:NH1	1:E:573:HIS:HD2	2.00	0.59
2:F:116:ASN:ND2	2:F:118:SER:OG	2.33	0.59
1:A:456:LEU:O	1:A:458:PRO:HD3	2.02	0.59
1:E:93:SER:H	1:E:150:GLN:HE22	1.50	0.59
1:E:336:GLY:HA3	1:E:341:LYS:O	2.02	0.59
2:B:69:LEU:HD12	2:B:109:CYS:HB3	1.84	0.59
1:A:402:ILE:HG22	1:A:412:ILE:HA	1.84	0.59
1:E:112:TRP:CE2	1:E:640:PRO:HA	2.38	0.59
2:B:215:ILE:HD11	2:B:265:LEU:HD12	1.84	0.58
3:G:126:PHE:HB3	3:G:127:PRO:CD	2.33	0.58
1:A:82:ALA:O	1:A:84:GLN:HG3	2.03	0.58
4:H:54:SER:C	4:H:56:GLY:H	2.05	0.58
1:E:186:GLY:HA2	1:E:189:LEU:HD12	1.85	0.58
3:G:86:LEU:HD11	4:H:92:LEU:HD23	1.86	0.58
3:C:170:VAL:HG11	12:D:201:EPH:H61	1.85	0.58
1:A:611:GLN:HE21	1:A:616:GLY:HA2	1.68	0.58
2:B:242:ILE:O	2:B:243:MET:HB2	2.04	0.57
2:F:74:LYS:O	2:F:76:LYS:N	2.37	0.57
2:B:95:GLY:CA	2:B:183:ILE:HD12	2.35	0.57
3:C:113:PRO:HB2	3:C:116:ILE:HD13	1.86	0.57
1:A:388:TYR:CE1	1:A:421:GLU:HG3	2.38	0.57
1:E:361:PRO:O	1:E:364:SER:HB2	2.05	0.57
1:E:87:ILE:O	1:E:169:THR:HA	2.05	0.57
2:F:97:CYS:SG	2:F:109:CYS:SG	3.03	0.57
3:G:81:ALA:HB1	12:H:201:EPH:H301	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:TYR:O	1:E:229:SER:HA	2.04	0.57
1:A:79:HIS:CE1	6:A:702:FAD:C8M	2.49	0.56
1:A:536:SER:HB2	2:B:46:GLU:OE1	2.05	0.56
1:A:47:ILE:HD11	1:A:214:VAL:HG21	1.86	0.56
1:A:549:LEU:O	1:A:552:LEU:N	2.31	0.56
4:D:55:HIS:O	4:D:55:HIS:ND1	2.38	0.56
1:E:519:LYS:O	1:E:523:LEU:HD12	2.05	0.56
10:G:201:HEM:HHA	10:G:201:HEM:HBD1	1.88	0.56
4:H:32:VAL:HG22	4:H:33:THR:N	2.19	0.56
1:A:378:GLU:HB3	1:A:379:PRO:CD	2.35	0.56
1:A:37:VAL:HB	4:D:31:ALA:HB3	1.85	0.56
1:A:457:LYS:C	1:A:459:ASP:H	2.09	0.56
1:A:81:THR:HB	1:A:181:LEU:HD23	1.88	0.56
1:A:280:ILE:HD11	1:A:287:ILE:HD11	1.88	0.56
1:E:174:ASP:HB2	1:E:361:PRO:HD2	1.86	0.56
3:C:76:ARG:HE	10:C:201:HEM:CGD	2.18	0.56
1:A:202:LEU:HB2	1:A:215:ILE:CG2	2.34	0.56
1:A:209:GLY:O	1:A:414:PRO:HD2	2.06	0.56
1:E:94:MET:HG3	1:E:167:LYS:HD3	1.88	0.56
1:E:320:ARG:NH1	5:E:701:FUM:C6	2.69	0.56
2:F:182:CYS:HG	8:F:302:SF4:FE3	1.20	0.56
2:F:201:LYS:HA	3:G:39:GLN:HG2	1.88	0.56
1:A:503:HIS:HD2	1:A:516:GLY:CA	2.20	0.55
4:D:70:VAL:O	4:D:74:PRO:HD2	2.06	0.55
3:C:69:TRP:CD2	11:C:202:FTN:H15	2.42	0.55
2:F:217:ASP:C	2:F:219:ARG:H	2.09	0.55
2:B:226:ARG:HG2	2:B:229:ARG:NH2	2.22	0.55
1:E:117:ASN:ND2	1:E:118:ALA:H	2.05	0.55
1:A:337:VAL:HG12	1:A:344:ILE:HA	1.89	0.55
3:G:74:LEU:HG	3:G:130:PHE:CE1	2.42	0.55
1:A:231:ARG:HD2	1:A:415:GLY:HA2	1.88	0.55
1:A:298:LEU:HD12	1:A:344:ILE:HD11	1.87	0.55
1:E:43:ASP:OD1	1:E:66:LYS:N	2.33	0.55
3:G:50:ARG:HG3	3:G:51:ALA:N	2.22	0.55
2:F:47:GLU:OE2	2:F:50:ALA:HB2	2.08	0.54
2:F:89:CYS:HB3	2:F:94:CYS:HB3	1.89	0.54
3:G:101:THR:HG23	4:H:152:MET:HE3	1.88	0.54
1:A:453:LYS:O	1:A:453:LYS:HG3	2.07	0.54
1:A:523:LEU:C	1:A:525:LYS:H	2.09	0.54
1:A:611:GLN:HE21	1:A:616:GLY:CA	2.19	0.54
3:C:45:TYR:CZ	3:C:49:GLN:HG3	2.42	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:GLN:OE1	1:E:34:GLN:HA	2.07	0.54
1:E:87:ILE:HG22	1:E:170:CYS:HB2	1.88	0.54
3:C:76:ARG:HG2	10:C:201:HEM:O2D	2.07	0.54
4:D:122:ARG:NH1	4:D:122:ARG:HG3	2.21	0.54
3:C:105:GLU:C	3:C:107:ILE:N	2.60	0.54
1:A:203:ASP:H	1:A:215:ILE:HG22	1.72	0.54
1:E:495:THR:O	1:E:499:THR:CG2	2.55	0.54
2:F:154:GLN:HG3	2:F:222:SER:OG	2.08	0.54
2:B:187:CYS:HB2	8:B:302:SF4:S3	2.48	0.54
2:F:222:SER:O	2:F:223:ALA:C	2.44	0.54
2:F:128:HIS:HA	3:G:56:ILE:HG22	1.89	0.54
2:B:76:LYS:HD2	2:B:83:LEU:O	2.08	0.54
3:G:159:VAL:HG12	3:G:160:LEU:N	2.23	0.54
4:D:122:ARG:HG3	4:D:122:ARG:HH11	1.72	0.53
1:A:117:ASN:HD22	1:A:117:ASN:N	1.93	0.53
1:A:117:ASN:ND2	1:A:117:ASN:N	2.53	0.53
1:A:542:ASP:O	1:A:545:GLU:HB2	2.08	0.53
1:A:58:MET:CE	1:A:187:ASN:HB3	2.38	0.53
3:C:123:ILE:O	3:C:127:PRO:CD	2.48	0.53
2:F:267:THR:HG21	4:H:60:LYS:HB2	1.91	0.53
10:G:201:HEM:NC	4:H:95:HIS:CD2	2.76	0.53
4:H:133:LEU:HG	4:H:137:LEU:HD12	1.90	0.53
1:A:584:GLU:HG3	1:A:602:HIS:CE1	2.44	0.53
4:D:109:ARG:CB	4:D:110:PRO:HD2	2.38	0.53
4:D:140:ASN:HD22	4:D:145:GLY:HA2	1.74	0.53
1:A:107:ALA:O	1:A:110:SER:OG	2.25	0.53
1:A:79:HIS:CE1	1:A:248:THR:HA	2.44	0.53
3:C:116:ILE:HD12	3:C:116:ILE:H	1.74	0.53
1:A:459:ASP:OD1	1:A:460:GLU:N	2.34	0.52
4:D:109:ARG:HB2	4:D:110:PRO:HD2	1.90	0.52
1:E:321:ASP:OD2	1:E:643:ARG:NH1	2.38	0.52
2:F:40:ILE:HG22	2:F:41:TYR:O	2.09	0.52
1:A:115:ASP:O	1:A:119:MET:HG3	2.09	0.52
4:D:88:LEU:O	4:D:92:LEU:HB2	2.09	0.52
2:F:268:LYS:CG	2:F:269:MET:N	2.70	0.52
3:G:134:ASN:O	3:G:137:ARG:N	2.41	0.52
3:G:100:PHE:CD1	4:H:144:VAL:HG21	2.44	0.52
3:G:123:ILE:HG22	3:G:123:ILE:O	2.09	0.52
1:E:72:LYS:O	1:E:198:GLU:HA	2.09	0.52
1:E:270:LEU:O	1:E:559:THR:HG23	2.09	0.52
1:A:86:GLY:HA2	1:A:176:THR:HG21	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:LEU:HD22	1:E:214:VAL:N	2.25	0.52
1:E:360:LEU:HB3	1:E:363:ILE:HD11	1.92	0.52
1:E:388:TYR:CE2	1:E:432:ARG:HD2	2.45	0.52
1:A:301:SER:HB3	1:A:336:GLY:O	2.10	0.52
1:A:466:PRO:HG2	1:A:469:ALA:HB2	1.91	0.52
2:B:268:LYS:CG	2:B:269:MET:N	2.55	0.52
2:F:119:LYS:HE2	2:F:119:LYS:HA	1.92	0.52
2:F:247:LYS:O	2:F:247:LYS:HG3	2.09	0.52
1:A:117:ASN:O	1:A:120:HIS:HB3	2.09	0.51
1:A:508:ARG:O	1:A:575:ARG:HA	2.10	0.51
1:A:513:LEU:HD13	1:A:564:GLU:HA	1.90	0.51
1:E:320:ARG:HH11	1:E:432:ARG:HH12	1.58	0.51
1:A:567:LYS:HB3	1:A:578:PHE:CE1	2.45	0.51
4:D:139:PHE:HE2	4:D:145:GLY:O	1.94	0.51
1:E:48:GLY:O	1:E:53:GLY:HA3	2.10	0.51
1:E:138:MET:SD	1:E:180:MET:HA	2.50	0.51
1:A:327:GLU:O	1:A:331:ILE:HG12	2.10	0.51
1:E:277:PRO:HB3	1:E:323:VAL:HG12	1.91	0.51
1:A:608:LEU:HD11	1:A:623:ARG:HB2	1.92	0.51
1:E:395:THR:HG22	1:E:401:VAL:HA	1.92	0.51
1:E:459:ASP:OD1	1:E:460:GLU:N	2.40	0.51
3:C:105:GLU:HA	3:C:108:ARG:H	1.75	0.51
2:F:115:GLN:NE2	2:F:115:GLN:CA	2.70	0.51
1:A:320:ARG:HH12	5:A:701:FUM:C5	2.25	0.50
1:E:274:GLN:HB3	1:E:388:TYR:HB3	1.93	0.50
1:A:503:HIS:CD2	1:A:516:GLY:CA	2.94	0.50
1:A:549:LEU:O	1:A:551:ASN:N	2.44	0.50
1:E:445:GLY:O	1:E:448:CYS:HB2	2.12	0.50
1:A:230:LYS:C	1:A:231:ARG:HD3	2.32	0.50
1:A:502:LYS:HB3	1:A:503:HIS:ND1	2.26	0.50
1:E:231:ARG:HE	1:E:456:LEU:HD23	1.77	0.50
3:G:149:ILE:HG12	3:G:150:PRO:HD3	1.92	0.50
1:E:562:ALA:HB1	1:E:607:THR:HG21	1.94	0.50
1:A:47:ILE:HD11	1:A:214:VAL:CG2	2.41	0.50
1:E:215:ILE:HG13	1:E:226:ARG:HG3	1.93	0.50
1:E:241:ARG:NH2	1:E:246:CYS:SG	2.85	0.50
2:B:210:GLN:O	2:B:213:ARG:HB3	2.12	0.50
2:F:268:LYS:HG2	2:F:269:MET:N	2.24	0.50
1:E:140:PHE:HB3	1:E:148:ILE:HG23	1.94	0.50
3:C:128:ILE:HD13	12:D:201:EPH:H221	1.94	0.50
3:G:87:LEU:HD22	4:H:128:PHE:CE1	2.46	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:217:ASP:OD1	2:F:219:ARG:HB2	2.12	0.49
1:A:192:HIS:HE1	4:D:43:ILE:HG22	1.77	0.49
1:A:363:ILE:HG13	1:A:364:SER:N	2.27	0.49
2:F:122:LYS:H	2:F:122:LYS:CE	2.25	0.49
1:A:434:GLY:O	1:A:435:ALA:HB3	2.12	0.49
2:B:206:ALA:O	2:B:209:MET:HB3	2.13	0.49
2:F:172:GLU:OE2	2:F:275:PRO:HD2	2.12	0.49
2:B:74:LYS:O	2:B:78:GLU:HG3	2.12	0.49
1:E:93:SER:H	1:E:150:GLN:NE2	2.10	0.49
1:E:642:ILE:O	1:E:642:ILE:HD12	2.13	0.49
2:B:241:THR:HB	2:B:243:MET:HE3	1.95	0.49
2:B:185:CYS:SG	8:B:302:SF4:S3	3.10	0.49
1:E:635:VAL:HG22	1:E:636:ASP:N	2.28	0.49
3:G:116:ILE:HD12	3:G:116:ILE:H	1.76	0.49
3:G:122:PHE:C	3:G:124:ILE:H	2.16	0.49
4:H:84:MET:HA	4:H:84:MET:HE2	1.94	0.49
2:B:267:THR:OG1	2:B:268:LYS:N	2.46	0.49
1:E:54:LEU:O	1:E:55:ARG:C	2.50	0.49
1:E:278:THR:OG1	1:E:287:ILE:O	2.30	0.49
1:E:522:ASP:O	1:E:526:GLU:HG2	2.12	0.49
2:F:205:PRO:O	2:F:209:MET:HB3	2.13	0.49
3:G:100:PHE:HD1	4:H:144:VAL:HG21	1.78	0.49
3:G:134:ASN:OD1	3:G:137:ARG:NH1	2.46	0.49
1:A:205:LEU:HD22	1:A:214:VAL:N	2.27	0.49
1:E:236:THR:OG1	1:E:256:GLY:HA3	2.13	0.49
1:A:72:LYS:HE3	1:A:251:MET:HG3	1.95	0.48
1:A:292:ARG:HA	1:A:296:GLY:O	2.12	0.48
2:F:139:MET:HG2	2:F:143:TYR:CZ	2.47	0.48
2:F:217:ASP:O	2:F:219:ARG:N	2.46	0.48
1:A:199:TYR:CE2	1:A:218:CYS:HB2	2.48	0.48
2:B:68:VAL:HG23	2:B:111:CYS:O	2.13	0.48
1:A:44:VAL:HG13	1:A:67:THR:HG23	1.93	0.48
3:C:136:ILE:HD12	3:C:137:ARG:N	2.28	0.48
2:F:92:GLY:HA2	7:F:301:FES:S2	2.53	0.48
1:A:246:CYS:HA	1:A:385:THR:HG22	1.95	0.48
1:A:363:ILE:HG13	1:A:364:SER:H	1.78	0.48
1:A:445:GLY:O	1:A:448:CYS:HB2	2.13	0.48
1:A:549:LEU:HD12	1:A:549:LEU:HA	1.65	0.48
2:B:128:HIS:HA	3:C:56:ILE:HG22	1.95	0.48
2:B:241:THR:O	2:B:243:MET:HG2	2.13	0.48
2:F:276:LEU:O	2:F:278:THR:N	2.46	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:41:ASP:HB3	4:H:44:ALA:HB3	1.94	0.48
1:A:365:GLU:OE2	1:A:365:GLU:HA	2.12	0.48
2:B:249:CYS:SG	2:B:253:LEU:HB2	2.54	0.48
3:G:156:ALA:O	3:G:160:LEU:HB2	2.14	0.48
4:D:89:ALA:HB1	4:D:136:LEU:HD23	1.96	0.48
1:A:257:THR:HA	1:A:393:ILE:HD11	1.96	0.48
3:C:74:LEU:HD23	3:C:130:PHE:CZ	2.47	0.48
1:E:582:GLU:HG3	1:E:603:TRP:CD1	2.42	0.48
1:A:239:TYR:H	1:A:389:ASN:HD21	1.58	0.48
1:A:243:TYR:CG	1:A:386:VAL:HG21	2.48	0.48
3:C:92:GLY:O	3:C:96:LEU:HB2	2.14	0.48
1:E:117:ASN:ND2	1:E:118:ALA:N	2.62	0.48
1:E:243:TYR:CD2	1:E:386:VAL:HG21	2.49	0.48
1:E:496:MET:HG3	1:E:497:GLN:N	2.29	0.48
1:A:120:HIS:CD2	1:A:630:LEU:H	2.23	0.48
1:A:425:HIS:HB2	1:A:427:VAL:HG22	1.95	0.47
4:D:58:LEU:O	4:D:61:ILE:HG12	2.13	0.47
1:E:434:GLY:O	1:E:435:ALA:HB3	2.14	0.47
1:A:435:ALA:HA	6:A:702:FAD:O2	2.13	0.47
1:A:299:VAL:HG13	1:A:304:GLU:H	1.79	0.47
2:B:128:HIS:HA	3:C:56:ILE:CG2	2.45	0.47
3:C:76:ARG:O	3:C:77:VAL:C	2.51	0.47
2:F:185:CYS:O	2:F:186:ALA:HB3	2.13	0.47
1:A:55:ARG:O	1:A:55:ARG:NH2	2.45	0.47
1:E:432:ARG:HE	1:E:437:SER:HB2	1.79	0.47
4:H:28:THR:C	4:H:30:ALA:H	2.17	0.47
1:A:148:ILE:HG13	2:B:165:GLN:NE2	2.29	0.47
1:A:306:PHE:O	1:A:310:TYR:HD2	1.96	0.47
1:A:577:ASP:N	1:A:577:ASP:OD2	2.47	0.47
2:F:68:VAL:HG23	2:F:111:CYS:O	2.13	0.47
1:E:294:GLU:HG3	1:E:360:LEU:CD1	2.45	0.47
3:G:114:TRP:O	3:G:118:ASP:OD1	2.33	0.47
1:A:187:ASN:OD1	1:A:190:ARG:NH1	2.47	0.47
1:A:523:LEU:HA	1:A:526:GLU:HG3	1.96	0.47
1:A:549:LEU:O	1:A:550:GLN:C	2.52	0.47
3:C:64:LYS:O	3:C:66:GLN:HG3	2.14	0.47
1:E:79:HIS:CD2	6:E:702:FAD:HM81	2.45	0.47
1:E:143:THR:O	1:E:146:GLY:N	2.36	0.47
1:E:566:ARG:NH1	1:E:568:GLU:OE2	2.43	0.47
2:F:179:LEU:HD21	2:F:212:TYR:CD2	2.50	0.47
2:B:136:VAL:HG12	2:B:136:VAL:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:ASN:HA	1:E:168:ARG:O	2.14	0.47
2:F:42:ARG:HE	2:F:83:LEU:HD12	1.80	0.47
1:A:296:GLY:HA3	1:A:348:LEU:HD23	1.97	0.47
1:E:190:ARG:HG3	4:H:43:ILE:HD12	1.96	0.47
1:E:444:PHE:HA	1:E:447:ALA:HB3	1.97	0.47
2:F:70:ASP:OD1	2:F:70:ASP:N	2.48	0.47
2:F:279:PRO:O	2:F:280:ALA:HB3	2.15	0.47
3:G:149:ILE:HD13	3:G:149:ILE:N	2.20	0.47
4:D:150:PHE:O	4:D:153:VAL:HG22	2.15	0.47
1:E:40:HIS:HB3	1:E:42:TYR:HE1	1.80	0.47
1:E:239:TYR:HA	1:E:252:ASN:O	2.15	0.47
1:E:519:LYS:O	1:E:522:ASP:HB2	2.15	0.47
1:E:556:ALA:O	1:E:557:THR:C	2.53	0.47
1:E:602:HIS:O	1:E:605:LYS:HE2	2.14	0.47
1:A:198:GLU:HB3	1:A:219:LEU:HD12	1.98	0.46
1:A:331:ILE:HG23	1:A:342:ASP:HA	1.97	0.46
1:A:410:ASP:OD2	1:A:410:ASP:N	2.48	0.46
1:A:446:ARG:HD2	1:A:446:ARG:O	2.14	0.46
2:B:198:ASN:O	2:B:199:ALA:C	2.52	0.46
4:H:54:SER:C	4:H:56:GLY:N	2.68	0.46
1:A:320:ARG:NH1	5:A:701:FUM:C6	2.78	0.46
1:A:534:ASP:HB2	2:B:82:THR:HG22	1.97	0.46
2:B:225:GLU:N	2:B:225:GLU:OE2	2.48	0.46
2:F:250:PRO:HD2	8:F:302:SF4:S3	2.55	0.46
4:H:50:LYS:HG3	4:H:50:LYS:O	2.15	0.46
1:E:48:GLY:HA3	1:E:235:ALA:O	2.15	0.46
1:E:635:VAL:HG22	1:E:636:ASP:H	1.79	0.46
4:H:150:PHE:O	4:H:151:GLU:C	2.54	0.46
1:A:245:SER:OG	1:A:385:THR:HG23	2.15	0.46
2:B:89:CYS:O	2:B:90:ARG:HD2	2.16	0.46
10:C:201:HEM:HMB3	4:D:66:ALA:HB1	1.97	0.46
1:E:131:THR:O	1:E:132:GLU:C	2.53	0.46
2:F:86:ARG:HH12	2:F:137:PRO:HD2	1.81	0.46
3:C:71:VAL:HG12	3:C:72:SER:N	2.29	0.46
1:A:237:GLY:HA2	1:A:421:GLU:HB3	1.98	0.46
1:E:555:ASN:O	1:E:559:THR:OG1	2.29	0.46
2:F:102:ALA:HA	2:F:122:LYS:CE	2.46	0.46
2:F:188:CYS:SG	8:F:302:SF4:S4	3.14	0.46
2:B:85:PHE:CD1	2:B:85:PHE:N	2.83	0.46
3:C:169:ALA:O	3:C:173:TYR:HB3	2.16	0.46
4:D:92:LEU:HA	4:D:92:LEU:HD12	1.64	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:150:PHE:HA	4:D:153:VAL:HG22	1.98	0.46
1:E:355:GLN:O	1:E:359:ARG:HB2	2.17	0.46
1:A:280:ILE:HG13	1:A:287:ILE:HG12	1.97	0.45
1:A:442:VAL:O	1:A:446:ARG:HB2	2.16	0.45
11:F:304:FTN:C5	3:G:76:ARG:HG3	2.46	0.45
1:A:203:ASP:HA	1:A:259:LEU:HG	1.99	0.45
1:A:419:CYS:HA	1:A:423:ALA:HB2	1.98	0.45
1:E:47:ILE:CD1	1:E:234:VAL:HG22	2.47	0.45
1:E:321:ASP:HB3	1:E:431:ASN:ND2	2.31	0.45
3:G:116:ILE:HD12	3:G:116:ILE:N	2.31	0.45
2:B:268:LYS:NZ	2:B:268:LYS:HB3	2.31	0.45
1:E:120:HIS:CD2	1:E:630:LEU:HB2	2.51	0.45
1:E:293:GLY:HA2	1:E:317:LEU:HD21	1.98	0.45
2:F:128:HIS:HA	3:G:56:ILE:CG2	2.47	0.45
1:A:58:MET:HE3	1:A:187:ASN:HB3	1.98	0.45
1:A:130:VAL:HG12	1:A:131:THR:N	2.31	0.45
2:B:231:GLN:HE22	4:D:52:LEU:CD2	2.29	0.45
1:E:143:THR:OG1	1:E:147:LYS:N	2.50	0.45
1:E:267:LEU:HD12	1:E:270:LEU:HD11	1.99	0.45
1:E:388:TYR:CZ	1:E:421:GLU:HG3	2.52	0.45
1:A:85:GLY:HA3	1:A:153:PHE:CZ	2.51	0.45
1:E:249:ALA:C	1:E:251:MET:H	2.20	0.45
2:F:74:LYS:C	2:F:76:LYS:H	2.20	0.45
1:E:276:HIS:O	1:E:384:PRO:HA	2.15	0.45
1:E:310:TYR:O	1:E:311:ALA:HB2	2.17	0.45
3:G:65:PRO:HA	3:G:69:TRP:CZ2	2.52	0.45
4:H:146:LEU:O	4:H:149:ALA:HB3	2.17	0.45
1:A:432:ARG:NH2	6:A:702:FAD:N1	2.65	0.45
3:C:149:ILE:N	3:C:149:ILE:CD1	2.77	0.45
1:E:432:ARG:NH2	5:E:701:FUM:O8	2.44	0.45
1:E:464:GLU:OE1	1:E:464:GLU:HA	2.16	0.45
2:F:268:LYS:HE2	2:F:268:LYS:HB3	1.61	0.45
3:G:158:LEU:O	3:G:159:VAL:C	2.54	0.45
1:A:85:GLY:HA3	1:A:153:PHE:HZ	1.81	0.45
1:A:122:LEU:HG	1:A:439:LEU:HD12	1.98	0.45
1:A:276:HIS:O	1:A:384:PRO:HA	2.16	0.45
3:C:129:ALA:O	3:C:133:LEU:HD13	2.17	0.45
4:D:77:TYR:HA	12:D:201:EPH:H11	1.98	0.45
1:A:111:ASP:O	1:A:570:ARG:HD3	2.17	0.45
1:E:344:ILE:HD13	1:E:344:ILE:H	1.81	0.45
1:A:80:THR:HB	1:A:181:LEU:HD22	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HD13	1:A:427:VAL:HG11	1.99	0.44
1:A:270:LEU:HD12	1:A:558:GLN:HB3	1.98	0.44
1:A:523:LEU:HB3	1:A:553:MET:HE1	1.99	0.44
2:B:47:GLU:HG2	2:B:48:PRO:HD2	2.00	0.44
1:A:113:LEU:O	1:A:606:HIS:CE1	2.71	0.44
1:E:122:LEU:HD12	1:E:443:VAL:HG21	1.99	0.44
2:F:122:LYS:HE2	2:F:122:LYS:H	1.82	0.44
1:E:233:ILE:HG12	1:E:417:TYR:HB2	1.99	0.44
2:F:130:PHE:O	2:F:138:ASP:N	2.40	0.44
4:H:71:PRO:O	4:H:73:ILE:N	2.50	0.44
1:A:509:ARG:HB3	1:A:512:ILE:HD12	2.00	0.44
3:C:132:THR:HG23	10:C:201:HEM:HAB	1.99	0.44
1:E:590:PRO:O	1:E:592:GLU:N	2.51	0.44
2:F:181:GLU:HB2	2:F:253:LEU:HD21	1.99	0.44
1:A:87:ILE:HD11	1:A:439:LEU:HA	1.99	0.44
1:A:523:LEU:C	1:A:525:LYS:N	2.71	0.44
1:E:99:TRP:CZ2	1:E:124:ARG:HG3	2.53	0.44
1:E:428:HIS:HB3	1:E:432:ARG:HB2	1.99	0.44
1:E:517:VAL:O	1:E:521:MET:HG2	2.18	0.44
2:F:242:ILE:O	2:F:243:MET:CB	2.65	0.44
2:B:100:ASN:HB2	2:B:105:ASN:ND2	2.33	0.44
1:E:268:GLU:HG2	1:E:394:PRO:HG3	1.98	0.44
1:A:58:MET:HE1	1:A:187:ASN:HB3	2.00	0.44
1:A:92:GLY:C	1:A:94:MET:H	2.21	0.44
1:A:329:ILE:HG22	1:A:330:GLU:N	2.32	0.44
1:E:85:GLY:O	1:E:151:ARG:NH2	2.51	0.44
1:E:393:ILE:HA	1:E:394:PRO:HD3	1.86	0.44
1:E:525:LYS:C	1:E:527:LEU:H	2.21	0.44
1:E:621:ASP:C	1:E:622:TYR:CD1	2.91	0.44
4:H:153:VAL:O	4:H:156:LEU:HG	2.17	0.44
1:A:513:LEU:HB3	1:A:564:GLU:HB2	2.00	0.44
1:E:62:GLU:HB2	1:E:191:CYS:HB3	2.00	0.44
1:E:242:ALA:HB2	1:E:552:LEU:HD22	1.99	0.44
1:E:474:ILE:HD12	1:E:474:ILE:O	2.18	0.44
3:G:76:ARG:HH22	4:H:106:ASP:CG	2.20	0.44
1:A:567:LYS:HG2	1:A:578:PHE:CZ	2.53	0.43
4:D:96:VAL:O	4:D:100:VAL:HG13	2.18	0.43
1:E:47:ILE:H	1:E:47:ILE:HG13	1.59	0.43
2:F:215:ILE:H	2:F:215:ILE:HG12	1.44	0.43
1:A:337:VAL:HG22	1:A:338:GLY:H	1.82	0.43
1:A:461:LYS:HE2	1:A:461:LYS:HB3	1.90	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:201:HEM:HHA	10:C:201:HEM:CBD	2.42	0.43
1:E:258:ALA:O	1:E:262:ARG:HB2	2.18	0.43
1:E:320:ARG:HH11	1:E:432:ARG:NH1	2.16	0.43
3:G:113:PRO:HB2	3:G:116:ILE:HD13	1.99	0.43
1:E:87:ILE:CG2	1:E:170:CYS:HB2	2.48	0.43
1:E:103:PHE:O	1:E:104:TYR:C	2.56	0.43
2:F:189:SER:OG	2:F:205:PRO:HD2	2.18	0.43
1:A:73:MET:CE	1:A:78:SER:HA	2.48	0.43
1:E:528:LYS:HD3	1:E:528:LYS:N	2.33	0.43
1:A:276:HIS:HB2	1:A:387:HIS:CB	2.48	0.43
1:A:329:ILE:O	1:A:330:GLU:C	2.56	0.43
1:A:390:MET:CE	1:A:572:ALA:HB2	2.49	0.43
3:C:115:VAL:HG23	3:C:116:ILE:HD12	2.01	0.43
4:D:55:HIS:CE1	4:D:59:PHE:HB2	2.54	0.43
1:E:151:ARG:HA	1:E:167:LYS:HE2	1.99	0.43
1:E:638:ILE:HA	1:E:639:PRO:HD3	1.80	0.43
1:A:97:ASP:OD1	1:A:168:ARG:NH1	2.52	0.43
1:A:45:VAL:HG23	1:A:229:SER:HB3	2.01	0.43
4:D:37:PRO:HA	4:D:38:PRO:HD2	1.84	0.43
1:A:230:LYS:CD	1:A:462:ILE:HG12	2.49	0.43
1:A:457:LYS:C	1:A:459:ASP:N	2.72	0.43
3:C:36:THR:OG1	3:C:39:GLN:HG3	2.18	0.43
1:E:432:ARG:HH22	5:E:701:FUM:C6	2.30	0.43
2:F:126:LEU:HB2	2:F:129:MET:HG3	2.00	0.43
2:F:155:LYS:HA	2:F:221:ASP:HB2	2.01	0.43
1:A:460:GLU:HG2	1:A:461:LYS:N	2.32	0.43
1:E:286:LEU:HD22	1:E:387:HIS:HE1	1.84	0.43
1:E:477:LEU:HD12	1:E:547:LEU:HD21	2.01	0.43
4:H:73:ILE:HD12	4:H:73:ILE:HA	1.72	0.43
1:E:220:GLU:O	1:E:538:ILE:HG23	2.19	0.43
1:E:321:ASP:H	1:E:431:ASN:HD21	1.67	0.43
2:B:212:TYR:O	2:B:213:ARG:C	2.57	0.42
11:C:202:FTN:O1	11:C:202:FTN:F1	2.27	0.42
1:E:138:MET:HG3	1:E:139:PRO:HD2	2.02	0.42
1:E:558:GLN:NE2	1:E:611:GLN:OE1	2.51	0.42
2:F:196:TRP:CZ3	3:G:59:HIS:HB2	2.54	0.42
2:F:212:TYR:HA	2:F:215:ILE:CG1	2.49	0.42
3:G:165:LEU:HD22	3:G:165:LEU:HA	1.89	0.42
1:A:120:HIS:CD2	1:A:630:LEU:HB2	2.55	0.42
2:B:202:TYR:HA	2:B:234:PHE:O	2.19	0.42
1:A:541:SER:HB3	2:B:76:LYS:HZ3	1.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:ILE:HG12	1:E:384:PRO:HD2	2.02	0.42
3:G:76:ARG:HE	10:G:201:HEM:CGD	2.31	0.42
4:H:144:VAL:HG11	4:H:152:MET:SD	2.59	0.42
2:B:139:MET:O	2:B:142:PHE:HB3	2.18	0.42
3:C:77:VAL:O	3:C:78:THR:C	2.58	0.42
4:D:87:CYS:HA	4:D:90:LEU:HB2	2.01	0.42
1:E:320:ARG:HH12	5:E:701:FUM:C5	2.32	0.42
1:E:392:GLY:H	1:E:424:CYS:HB2	1.84	0.42
2:F:125:PRO:HG2	3:G:57:ALA:HB1	2.01	0.42
3:C:118:ASP:O	3:C:171:VAL:HG11	2.20	0.42
1:E:112:TRP:CH2	1:E:641:ILE:HG13	2.55	0.42
1:E:116:GLN:HA	1:E:119:MET:HE2	2.01	0.42
1:E:210:ARG:HG3	1:E:414:PRO:HB2	2.01	0.42
2:F:69:LEU:O	2:F:72:LEU:HB2	2.19	0.42
4:H:54:SER:O	4:H:56:GLY:N	2.52	0.42
1:E:631:ASP:HB3	1:E:634:GLU:HB2	2.00	0.42
1:A:503:HIS:CD2	1:A:516:GLY:HA2	2.54	0.42
2:B:151:PRO:HD2	2:B:152:TRP:CE3	2.54	0.42
4:D:117:LEU:HD23	4:D:117:LEU:O	2.20	0.42
1:E:591:ILE:HD12	1:E:591:ILE:H	1.85	0.42
3:G:67:MET:HE2	3:G:67:MET:HA	2.01	0.42
1:A:416:LEU:C	1:A:417:TYR:HD1	2.23	0.42
3:C:162:LEU:HA	3:C:162:LEU:HD22	1.74	0.42
2:F:241:THR:O	2:F:241:THR:OG1	2.32	0.42
3:G:122:PHE:C	3:G:124:ILE:N	2.73	0.42
1:A:203:ASP:HB2	1:A:473:SER:OG	2.19	0.42
4:D:110:PRO:HB3	4:D:115:ASP:OD2	2.20	0.42
1:E:480:VAL:HG21	1:E:550:GLN:HE22	1.85	0.42
1:A:260:ALA:HB1	1:A:265:ILE:HB	2.02	0.41
1:A:561:VAL:HG23	1:A:562:ALA:N	2.35	0.41
1:A:73:MET:HE1	1:A:78:SER:HA	2.01	0.41
1:A:158:ASN:HD21	1:A:166:ALA:HA	1.85	0.41
1:A:238:GLY:HA3	1:A:389:ASN:HD22	1.85	0.41
1:A:349:HIS:HB2	1:A:376:THR:O	2.21	0.41
1:E:238:GLY:HA3	1:E:389:ASN:ND2	2.35	0.41
1:E:380:ILE:HA	1:E:381:PRO:HD2	1.91	0.41
2:F:71:ALA:O	2:F:75:ILE:HG23	2.21	0.41
2:F:266:LEU:O	2:F:267:THR:HG23	2.20	0.41
1:A:88:ASN:HD21	1:A:435:ALA:HB3	1.84	0.41
1:A:212:VAL:O	1:A:229:SER:N	2.48	0.41
3:C:97:PRO:HD2	3:C:98:LEU:HD12	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:GLU:C	1:E:423:ALA:H	2.23	0.41
1:E:528:LYS:N	1:E:528:LYS:CD	2.84	0.41
4:H:37:PRO:O	4:H:38:PRO:C	2.57	0.41
1:A:72:LYS:NZ	1:A:548:GLU:OE1	2.36	0.41
1:A:175:ARG:HH21	1:A:361:PRO:HB2	1.85	0.41
1:A:195:PHE:HD1	4:D:39:GLN:HE22	1.67	0.41
2:B:192:CYS:SG	2:B:194:SER:HB2	2.61	0.41
1:E:91:LEU:HD23	1:E:127:VAL:HG13	2.01	0.41
1:A:122:LEU:HG	1:A:439:LEU:CD1	2.51	0.41
1:A:432:ARG:HG2	1:A:433:LEU:O	2.19	0.41
1:A:516:GLY:O	1:A:518:LYS:N	2.53	0.41
1:E:277:PRO:HB2	1:E:278:THR:HG23	2.01	0.41
2:B:42:ARG:HG3	2:B:55:GLN:HE21	1.85	0.41
3:C:107:ILE:HD11	4:D:156:LEU:HD22	2.03	0.41
3:G:45:TYR:O	3:G:49:GLN:HG2	2.19	0.41
4:H:71:PRO:C	4:H:73:ILE:H	2.23	0.41
1:A:305:ARG:NH2	1:A:316:ASP:OD1	2.54	0.41
2:B:92:GLY:HA2	2:B:109:CYS:SG	2.60	0.41
3:G:149:ILE:H	3:G:149:ILE:CD1	2.12	0.41
1:A:247:THR:HA	1:A:284:GLY:O	2.21	0.41
1:A:296:GLY:HA2	1:A:350:HIS:HE1	1.86	0.41
1:A:638:ILE:HA	1:A:639:PRO:HD3	1.82	0.41
2:B:255:PRO:O	2:B:258:ALA:HB3	2.21	0.41
3:C:64:LYS:HA	3:C:65:PRO:HD2	1.72	0.41
1:E:104:TYR:HA	1:E:638:ILE:HD12	2.02	0.41
1:E:570:ARG:NH1	1:E:581:ARG:HG2	2.35	0.41
1:A:278:THR:HG22	1:A:382:VAL:HG21	2.02	0.41
1:A:466:PRO:HG2	1:A:469:ALA:CB	2.51	0.41
2:B:163:GLU:O	2:B:164:LYS:O	2.39	0.41
2:B:226:ARG:HG2	2:B:229:ARG:HH21	1.84	0.41
3:C:99:ASP:OD1	3:C:99:ASP:C	2.59	0.41
4:H:114:GLY:O	4:H:115:ASP:C	2.60	0.41
1:A:393:ILE:HA	1:A:394:PRO:HD3	1.74	0.41
1:A:474:ILE:O	1:A:477:LEU:HB3	2.21	0.41
1:A:538:ILE:O	1:A:539:TRP:C	2.59	0.41
2:B:215:ILE:HD11	2:B:265:LEU:CD1	2.50	0.41
3:G:60:LEU:HD12	3:G:61:THR:H	1.86	0.41
3:C:122:PHE:HA	3:C:171:VAL:HG21	2.02	0.40
4:D:50:LYS:O	4:D:51:PRO:C	2.60	0.40
4:D:153:VAL:HG23	4:D:154:TRP:HE3	1.85	0.40
1:E:43:ASP:O	1:E:230:LYS:HB2	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:532:THR:OG1	1:E:535:ARG:NH2	2.54	0.40
2:F:244:ASN:HD22	2:F:244:ASN:HA	1.58	0.40
1:A:225:HIS:HB3	1:A:227:PHE:CE1	2.56	0.40
1:A:270:LEU:HD12	1:A:558:GLN:CB	2.51	0.40
1:E:639:PRO:HA	1:E:640:PRO:HD3	1.97	0.40
1:A:142:ARG:HG2	2:B:168:GLN:O	2.21	0.40
1:A:203:ASP:N	1:A:215:ILE:HG22	2.37	0.40
1:A:435:ALA:HA	6:A:702:FAD:C2	2.52	0.40
1:A:608:LEU:CD1	1:A:623:ARG:HB2	2.52	0.40
1:E:136:PHE:CD1	1:E:187:ASN:OD1	2.75	0.40
2:F:42:ARG:NE	2:F:83:LEU:HD12	2.36	0.40
2:F:168:GLN:NE2	2:F:218:SER:OG	2.54	0.40
3:C:87:LEU:C	3:C:89:GLY:N	2.75	0.40
3:C:116:ILE:HD12	3:C:116:ILE:N	2.36	0.40
1:E:401:VAL:HG21	1:E:416:LEU:HG	2.02	0.40
1:A:492:LEU:HD21	1:A:527:LEU:HD12	2.03	0.40
1:A:610:LYS:O	1:A:618:ILE:HA	2.22	0.40
11:C:202:FTN:O1	11:C:202:FTN:C14	2.67	0.40
1:E:569:SER:HB2	1:E:579:PRO:C	2.42	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	611/645 (95%)	523 (86%)	81 (13%)	7 (1%)	14	41
1	E	611/645 (95%)	535 (88%)	68 (11%)	8 (1%)	12	36
2	B	247/282 (88%)	209 (85%)	33 (13%)	5 (2%)	7	26
2	F	247/282 (88%)	202 (82%)	29 (12%)	16 (6%)	1	3
3	C	151/188 (80%)	122 (81%)	25 (17%)	4 (3%)	5	19

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	148/188 (79%)	117 (79%)	24 (16%)	7 (5%)	2	8
4	D	127/156 (81%)	106 (84%)	16 (13%)	5 (4%)	3	11
4	H	127/156 (81%)	99 (78%)	23 (18%)	5 (4%)	3	11
All	All	2269/2542 (89%)	1913 (84%)	299 (13%)	57 (2%)	5	20

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	550	GLN
2	B	164	LYS
4	D	47	LYS
4	D	51	PRO
1	E	485	GLY
2	F	90	ARG
2	F	218	SER
2	F	268	LYS
3	G	158	LEU
3	G	170	VAL
4	H	45	ALA
3	C	111	GLY
4	D	85	ASP
2	F	243	MET
2	F	266	LEU
2	F	277	PRO
3	G	159	VAL
4	H	55	HIS
1	A	489	THR
1	A	592	GLU
2	B	280	ALA
4	D	50	LYS
1	E	250	HIS
1	E	339	PRO
2	F	115	GLN
2	F	188	CYS
2	F	244	ASN
4	H	51	PRO
4	H	72	LEU
1	A	208	LYS
2	B	268	LYS
3	C	77	VAL
4	D	49	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	311	ALA
1	E	591	ILE
2	F	48	PRO
2	F	163	GLU
2	F	267	THR
3	G	52	LEU
4	H	115	ASP
1	A	173	ALA
1	A	458	PRO
2	B	93	ILE
3	C	185	PRO
1	E	111	ASP
2	F	93	ILE
2	F	161	LEU
3	G	61	THR
3	G	148	ASP
2	B	49	GLY
3	C	149	ILE
1	E	460	GLU
2	F	223	ALA
2	F	75	ILE
1	E	463	PRO
3	G	123	ILE
1	A	463	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	498/526 (95%)	431 (86%)	67 (14%)	4 10
1	E	498/526 (95%)	425 (85%)	73 (15%)	3 9
2	B	219/242 (90%)	187 (85%)	32 (15%)	3 9
2	F	219/242 (90%)	182 (83%)	37 (17%)	2 6
3	C	127/158 (80%)	107 (84%)	20 (16%)	2 7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	124/158 (78%)	99 (80%)	25 (20%)	1	3
4	D	96/119 (81%)	79 (82%)	17 (18%)	2	5
4	H	96/119 (81%)	77 (80%)	19 (20%)	1	3
All	All	1877/2090 (90%)	1587 (84%)	290 (16%)	2	8

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	60	LEU
1	A	67	THR
1	A	91	LEU
1	A	117	ASN
1	A	142	ARG
1	A	152	SER
1	A	153	PHE
1	A	162	LYS
1	A	175	ARG
1	A	193	CYS
1	A	194	THR
1	A	203	ASP
1	A	205	LEU
1	A	230	LYS
1	A	251	MET
1	A	268	GLU
1	A	283	VAL
1	A	288	THR
1	A	335	ARG
1	A	344	ILE
1	A	348	LEU
1	A	351	LEU
1	A	354	GLU
1	A	359	ARG
1	A	366	THR
1	A	368	LYS
1	A	377	LYS
1	A	390	MET
1	A	405	THR
1	A	410	ASP
1	A	419	CYS
1	A	426	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	427	VAL
1	A	436	ASN
1	A	440	ASP
1	A	446	ARG
1	A	453	LYS
1	A	454	GLU
1	A	456	LEU
1	A	460	GLU
1	A	461	LYS
1	A	465	LEU
1	A	474	ILE
1	A	477	LEU
1	A	484	ASN
1	A	496	MET
1	A	498	LYS
1	A	518	LYS
1	A	528	LYS
1	A	533	THR
1	A	535	ARG
1	A	545	GLU
1	A	564	GLU
1	A	583	ASP
1	A	584	GLU
1	A	591	ILE
1	A	597	ARG
1	A	601	LYS
1	A	602	HIS
1	A	617	HIS
1	A	620	LEU
1	A	627	ASP
1	A	635	VAL
1	A	636	ASP
1	A	637	TRP
1	A	644	SER
2	B	33	LYS
2	B	34	ARG
2	B	53	LYS
2	B	59	VAL
2	B	62	ASP
2	B	63	LYS
2	B	69	LEU
2	B	73	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	87	ARG
2	B	90	ARG
2	B	91	GLU
2	B	93	ILE
2	B	120	THR
2	B	122	LYS
2	B	139	MET
2	B	166	GLN
2	B	170	ILE
2	B	173	GLN
2	B	177	ASP
2	B	194	SER
2	B	213	ARG
2	B	215	ILE
2	B	238	LYS
2	B	244	ASN
2	B	245	CYS
2	B	247	LYS
2	B	257	ARG
2	B	266	LEU
2	B	268	LYS
2	B	269	MET
2	B	272	LYS
2	B	276	LEU
3	C	50	ARG
3	C	53	LYS
3	C	60	LEU
3	C	61	THR
3	C	67	MET
3	C	99	ASP
3	C	105	GLU
3	C	112	ILE
3	C	115	VAL
3	C	118	ASP
3	C	119	THR
3	C	128	ILE
3	C	132	THR
3	C	149	ILE
3	C	151	SER
3	C	162	LEU
3	C	172	VAL
3	C	175	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	177	GLU
3	C	184	LEU
4	D	32	VAL
4	D	43	ILE
4	D	49	PHE
4	D	61	ILE
4	D	72	LEU
4	D	79	ILE
4	D	83	GLU
4	D	86	LEU
4	D	88	LEU
4	D	90	LEU
4	D	94	LEU
4	D	109	ARG
4	D	116	THR
4	D	122	ARG
4	D	144	VAL
4	D	146	LEU
4	D	154	TRP
1	E	36	LYS
1	E	44	VAL
1	E	47	ILE
1	E	113	LEU
1	E	117	ASN
1	E	122	LEU
1	E	138	MET
1	E	142	ARG
1	E	151	ARG
1	E	152	SER
1	E	153	PHE
1	E	162	LYS
1	E	191	CYS
1	E	194	THR
1	E	205	LEU
1	E	218	CYS
1	E	228	ARG
1	E	230	LYS
1	E	248	THR
1	E	251	MET
1	E	261	THR
1	E	262	ARG
1	E	265	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	274	GLN
1	E	335	ARG
1	E	337	VAL
1	E	344	ILE
1	E	356	LEU
1	E	359	ARG
1	E	366	THR
1	E	377	LYS
1	E	389	ASN
1	E	390	MET
1	E	397	TYR
1	E	411	LYS
1	E	425	HIS
1	E	427	VAL
1	E	436	ASN
1	E	439	LEU
1	E	440	ASP
1	E	453	LYS
1	E	455	GLU
1	E	456	LEU
1	E	461	LYS
1	E	472	GLU
1	E	474	ILE
1	E	484	ASN
1	E	489	THR
1	E	491	GLU
1	E	496	MET
1	E	498	LYS
1	E	499	THR
1	E	509	ARG
1	E	523	LEU
1	E	528	LYS
1	E	530	LEU
1	E	532	THR
1	E	541	SER
1	E	547	LEU
1	E	564	GLU
1	E	565	ASN
1	E	577	ASP
1	E	584	GLU
1	E	591	ILE
1	E	597	ARG

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	601	LYS
1	E	602	HIS
1	E	608	LEU
1	E	610	LYS
1	E	615	THR
1	E	637	TRP
1	E	641	ILE
1	E	644	SER
2	F	34	ARG
2	F	37	THR
2	F	42	ARG
2	F	51	LYS
2	F	61	LEU
2	F	63	LYS
2	F	66	THR
2	F	69	LEU
2	F	70	ASP
2	F	87	ARG
2	F	90	ARG
2	F	93	ILE
2	F	115	GLN
2	F	119	LYS
2	F	120	THR
2	F	122	LYS
2	F	148	SER
2	F	156	LYS
2	F	158	LYS
2	F	164	LYS
2	F	165	GLN
2	F	170	ILE
2	F	176	LEU
2	F	209	MET
2	F	213	ARG
2	F	215	ILE
2	F	238	LYS
2	F	241	THR
2	F	244	ASN
2	F	247	LYS
2	F	248	THR
2	F	257	ARG
2	F	266	LEU
2	F	267	THR

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	268	LYS
2	F	276	LEU
2	F	278	THR
3	G	45	TYR
3	G	46	LEU
3	G	50	ARG
3	G	53	LYS
3	G	59	HIS
3	G	60	LEU
3	G	67	MET
3	G	72	SER
3	G	98	LEU
3	G	99	ASP
3	G	108	ARG
3	G	114	TRP
3	G	115	VAL
3	G	120	PHE
3	G	133	LEU
3	G	137	ARG
3	G	147	THR
3	G	149	ILE
3	G	159	VAL
3	G	160	LEU
3	G	162	LEU
3	G	165	LEU
3	G	170	VAL
3	G	175	ARG
3	G	177	GLU
4	H	50	LYS
4	H	52	LEU
4	H	57	THR
4	H	61	ILE
4	H	62	GLU
4	H	64	TYR
4	H	72	LEU
4	H	73	ILE
4	H	79	ILE
4	H	83	GLU
4	H	84	MET
4	H	88	LEU
4	H	109	ARG
4	H	115	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	H	117	LEU
4	H	121	VAL
4	H	122	ARG
4	H	123	VAL
4	H	148	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	88	ASN
1	A	117	ASN
1	A	120	HIS
1	A	125	ASN
1	A	158	ASN
1	A	192	HIS
1	A	349	HIS
1	A	355	GLN
1	A	389	ASN
1	A	436	ASN
1	A	451	ASN
1	A	484	ASN
1	A	497	GLN
1	A	550	GLN
1	A	551	ASN
1	A	565	ASN
1	A	606	HIS
2	B	55	GLN
2	B	100	ASN
2	B	105	ASN
2	B	140	ASN
2	B	145	GLN
2	B	165	GLN
3	C	59	HIS
4	D	80	HIS
4	D	140	ASN
1	E	88	ASN
1	E	117	ASN
1	E	120	HIS
1	E	125	ASN
1	E	150	GLN
1	E	156	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	159	ASN
1	E	178	HIS
1	E	182	HIS
1	E	250	HIS
1	E	349	HIS
1	E	389	ASN
1	E	431	ASN
1	E	436	ASN
1	E	476	ASN
1	E	484	ASN
1	E	503	HIS
1	E	550	GLN
1	E	551	ASN
1	E	573	HIS
1	E	606	HIS
2	F	44	ASN
2	F	100	ASN
2	F	105	ASN
2	F	115	GLN
2	F	116	ASN
2	F	145	GLN
2	F	165	GLN
2	F	168	GLN
2	F	244	ASN
4	H	140	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
9	F3S	F	303	2	0,9,9	-	-	-		
8	SF4	B	302	2	0,12,12	-	-	-		
6	FAD	A	702	1	53,58,58	1.24	4 (7%)	68,89,89	1.77	17 (25%)
12	EPH	D	201	-	43,43,48	1.83	9 (20%)	45,48,53	2.28	5 (11%)
12	EPH	H	201	-	43,43,48	1.90	10 (23%)	45,48,53	2.38	6 (13%)
5	FUM	E	701	-	7,7,7	1.29	1 (14%)	8,8,8	1.07	0
6	FAD	E	702	1	53,58,58	1.20	4 (7%)	68,89,89	1.56	13 (19%)
10	HEM	G	201	3,4	41,50,50	1.98	8 (19%)	45,82,82	1.74	12 (26%)
8	SF4	F	302	2	0,12,12	-	-	-		
7	FES	B	301	2	0,4,4	-	-	-		
11	FTN	C	202	-	24,24,24	3.33	9 (37%)	34,34,34	2.31	8 (23%)
10	HEM	C	201	3,4	41,50,50	1.96	9 (21%)	45,82,82	1.51	6 (13%)
9	F3S	B	303	2	0,9,9	-	-	-		
11	FTN	F	304	-	24,24,24	3.29	9 (37%)	34,34,34	2.40	7 (20%)
7	FES	F	301	2	0,4,4	-	-	-		
5	FUM	A	701	-	7,7,7	1.48	1 (14%)	8,8,8	1.83	3 (37%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	F3S	F	303	2	-	-	0/3/3/3
5	FUM	A	701	-	-	2/5/5/5	-
12	EPH	D	201	-	-	24/47/47/52	-
6	FAD	A	702	1	-	13/30/50/50	0/6/6/6
12	EPH	H	201	-	-	21/47/47/52	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SF4	B	302	2	-	-	0/6/5/5
5	FUM	E	701	-	-	4/5/5/5	-
6	FAD	E	702	1	-	12/30/50/50	0/6/6/6
8	SF4	F	302	2	-	-	0/6/5/5
11	FTN	C	202	-	-	5/18/18/18	0/2/2/2
7	FES	B	301	2	-	-	0/1/1/1
9	F3S	B	303	2	-	-	0/3/3/3
10	HEM	G	201	3,4	-	10/12/54/54	-
11	FTN	F	304	-	-	3/18/18/18	0/2/2/2
7	FES	F	301	2	-	-	0/1/1/1
10	HEM	C	201	3,4	-	6/12/54/54	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	202	FTN	C14-C9	8.49	1.53	1.39
11	F	304	FTN	C14-C9	8.08	1.52	1.39
10	G	201	HEM	C3D-C2D	7.71	1.53	1.36
10	C	201	HEM	C3D-C2D	7.53	1.52	1.36
12	H	201	EPH	C29-C28	6.93	1.71	1.31
12	D	201	EPH	C29-C28	6.93	1.71	1.31
11	C	202	FTN	C12-C11	6.88	1.52	1.38
11	C	202	FTN	C10-C11	6.55	1.50	1.38
11	F	304	FTN	C10-C11	6.52	1.50	1.38
11	F	304	FTN	C12-C11	6.50	1.51	1.38
11	F	304	FTN	C13-C14	6.03	1.51	1.38
11	C	202	FTN	C13-C14	5.72	1.51	1.38
10	C	201	HEM	C3C-C2C	-4.69	1.33	1.40
11	F	304	FTN	C9-N	-4.52	1.32	1.41
11	F	304	FTN	C3-C2	4.49	1.48	1.40
11	C	202	FTN	C9-N	-4.38	1.32	1.41
11	C	202	FTN	C3-C2	4.33	1.47	1.40
11	F	304	FTN	C10-C9	-4.22	1.32	1.39
6	E	702	FAD	C4X-N5	4.14	1.38	1.30
6	A	702	FAD	C2A-N3A	4.03	1.38	1.32
11	C	202	FTN	C10-C9	-3.97	1.33	1.39
6	E	702	FAD	C2A-N3A	3.89	1.38	1.32
12	H	201	EPH	C18-C4	-3.80	1.39	1.50
12	H	201	EPH	C25-C24	3.80	1.53	1.31
10	G	201	HEM	C3C-C2C	-3.78	1.35	1.40
12	D	201	EPH	C13-C12	3.75	1.53	1.31

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	201	EPH	C25-C24	3.74	1.53	1.31
12	D	201	EPH	C18-C4	-3.64	1.40	1.50
10	G	201	HEM	C3C-CAC	3.59	1.55	1.47
12	H	201	EPH	C13-C12	3.58	1.52	1.31
12	D	201	EPH	C15-C16	3.22	1.53	1.29
12	H	201	EPH	C15-C16	3.22	1.53	1.29
6	A	702	FAD	C4X-N5	3.19	1.36	1.30
10	G	201	HEM	CAB-C3B	3.02	1.55	1.47
12	D	201	EPH	C27-C28	-2.98	1.33	1.50
12	H	201	EPH	C27-C28	-2.91	1.33	1.50
6	A	702	FAD	C2A-N1A	2.83	1.39	1.33
12	D	201	EPH	P1-O7	2.82	1.60	1.50
12	H	201	EPH	P1-O7	2.81	1.60	1.50
12	H	201	EPH	C26-C25	2.78	1.65	1.50
10	C	201	HEM	C3C-CAC	2.77	1.53	1.47
11	C	202	FTN	C13-C12	-2.75	1.33	1.38
10	C	201	HEM	C3B-C2B	-2.67	1.31	1.37
11	C	202	FTN	O2-C11	2.60	1.43	1.38
12	D	201	EPH	C26-C25	2.58	1.64	1.50
6	A	702	FAD	C2B-C1B	-2.58	1.49	1.53
10	C	201	HEM	FE-ND	2.51	2.09	1.96
11	F	304	FTN	C13-C12	-2.47	1.33	1.38
10	C	201	HEM	CAB-C3B	2.46	1.54	1.47
6	E	702	FAD	C2A-N1A	2.38	1.38	1.33
6	E	702	FAD	C10-N1	2.33	1.38	1.33
10	C	201	HEM	CAA-C2A	2.32	1.55	1.52
12	H	201	EPH	O2-C4	2.25	1.39	1.33
10	G	201	HEM	CMD-C2D	2.23	1.55	1.50
12	H	201	EPH	C10-C11	-2.21	1.43	1.52
5	A	701	FUM	OXT-C	-2.19	1.24	1.30
11	F	304	FTN	O2-C11	2.13	1.42	1.38
10	G	201	HEM	CAD-C3D	2.12	1.56	1.51
12	D	201	EPH	C10-C11	-2.12	1.43	1.52
10	G	201	HEM	CMB-C2B	2.06	1.55	1.50
10	G	201	HEM	CHD-C1D	-2.06	1.35	1.41
5	E	701	FUM	O8-C6	-2.05	1.25	1.30
10	C	201	HEM	C4A-CHB	-2.01	1.35	1.41
10	C	201	HEM	CHD-C1D	-2.00	1.35	1.41

All (77) bond angle outliers are listed below:

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	201	EPH	C27-C26-C25	12.46	145.59	112.92
12	D	201	EPH	C27-C26-C25	11.58	143.28	112.92
11	F	304	FTN	C12-C11-C10	-8.59	108.73	120.53
11	C	202	FTN	C13-C14-C9	-6.91	111.46	119.72
11	C	202	FTN	C12-C11-C10	-6.74	111.27	120.53
11	F	304	FTN	C11-O2-C15	-6.35	111.24	119.37
11	F	304	FTN	C13-C14-C9	-6.13	112.39	119.72
12	D	201	EPH	C15-C14-C13	5.89	141.04	112.02
6	A	702	FAD	N3A-C2A-N1A	-5.83	119.57	128.68
12	H	201	EPH	C15-C14-C13	5.70	140.11	112.02
6	E	702	FAD	N3A-C2A-N1A	-5.59	119.94	128.68
10	G	201	HEM	CAD-C3D-C4D	4.68	132.84	124.66
10	G	201	HEM	C4D-ND-C1D	4.43	109.65	105.07
11	C	202	FTN	F3-C1-C2	-4.20	105.39	112.70
10	C	201	HEM	CAD-C3D-C4D	4.14	131.89	124.66
6	E	702	FAD	P-O3P-PA	-4.06	118.88	132.83
11	C	202	FTN	C14-C9-C10	4.06	124.46	119.65
6	A	702	FAD	O4B-C1B-C2B	-4.03	101.03	106.93
10	G	201	HEM	C4C-CHD-C1D	3.96	127.78	122.56
10	C	201	HEM	C4D-ND-C1D	3.86	109.06	105.07
6	A	702	FAD	P-O3P-PA	-3.86	119.59	132.83
6	A	702	FAD	C4-N3-C2	-3.67	118.86	125.64
12	H	201	EPH	C2-O1-C3	3.63	126.72	117.79
12	D	201	EPH	C2-O1-C3	3.42	126.21	117.79
6	A	702	FAD	C5'-C4'-C3'	3.19	118.37	112.20
5	A	701	FUM	C5-C4-C	-3.15	111.05	127.26
11	F	304	FTN	C9-N-C8	-3.07	118.60	126.58
10	G	201	HEM	CAA-CBA-CGA	-3.03	105.27	113.76
12	D	201	EPH	C14-C15-C16	3.02	149.09	123.74
12	H	201	EPH	C14-C15-C16	3.02	149.08	123.74
6	A	702	FAD	O2'-C2'-C3'	-2.99	101.83	109.10
6	A	702	FAD	O2B-C2B-C3B	2.98	121.46	111.82
11	C	202	FTN	C11-O2-C15	-2.93	115.63	119.37
11	F	304	FTN	C14-C9-C10	2.87	123.06	119.65
6	E	702	FAD	O4-C4-C4X	-2.87	118.98	126.60
10	G	201	HEM	CBA-CAA-C2A	2.83	117.45	112.62
6	E	702	FAD	C5B-C4B-C3B	-2.78	104.75	115.18
6	E	702	FAD	C4A-C5A-N7A	-2.76	106.53	109.40
11	C	202	FTN	O2-C11-C10	-2.74	105.35	119.42
6	A	702	FAD	C4-C4X-C10	2.74	121.39	116.79
6	A	702	FAD	C1'-C2'-C3'	2.72	117.40	109.79

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	702	FAD	C5B-C4B-C3B	-2.72	105.00	115.18
6	E	702	FAD	O4'-C4'-C5'	-2.65	103.96	109.92
10	C	201	HEM	C4D-C3D-C2D	-2.64	103.05	106.90
12	D	201	EPH	O5-P1-O7	-2.64	98.76	109.07
6	A	702	FAD	C4X-C10-N10	2.54	120.19	116.48
10	C	201	HEM	CAA-CBA-CGA	-2.51	106.72	113.76
6	E	702	FAD	C5X-C9A-N10	2.46	120.49	117.95
10	G	201	HEM	CAD-C3D-C2D	-2.43	123.34	127.88
6	A	702	FAD	C4'-C3'-C2'	-2.43	108.31	113.36
10	C	201	HEM	CBD-CAD-C3D	2.42	119.34	112.63
10	C	201	HEM	C2C-C3C-C4C	2.39	108.57	106.90
6	E	702	FAD	C4X-C4-N3	2.38	119.25	113.19
6	A	702	FAD	C4X-C4-N3	2.38	119.24	113.19
10	G	201	HEM	CBD-CAD-C3D	2.37	119.22	112.63
6	A	702	FAD	O4-C4-C4X	-2.32	120.45	126.60
6	E	702	FAD	C9A-C5X-N5	-2.30	119.93	122.43
10	G	201	HEM	CAA-C2A-C3A	-2.30	120.65	127.25
11	C	202	FTN	C10-C9-N	-2.29	112.71	120.18
6	A	702	FAD	C10-C4X-N5	-2.28	120.01	124.86
10	G	201	HEM	C2C-C3C-C4C	2.27	108.48	106.90
6	E	702	FAD	O2'-C2'-C3'	-2.23	103.67	109.10
11	F	304	FTN	O2-C11-C10	-2.23	107.99	119.42
6	E	702	FAD	C4-N3-C2	-2.21	121.55	125.64
6	A	702	FAD	C2B-C3B-C4B	-2.18	98.40	102.64
12	H	201	EPH	O2-C4-C18	2.18	118.74	111.91
12	H	201	EPH	C1-O2-C4	2.17	125.17	117.12
6	A	702	FAD	C4X-C10-N1	-2.16	119.71	124.73
5	A	701	FUM	O7-C6-C5	-2.16	114.25	120.99
10	G	201	HEM	CMC-C2C-C3C	2.15	128.71	124.68
10	G	201	HEM	C4A-C3A-C2A	2.13	108.47	107.00
10	G	201	HEM	C4D-C3D-C2D	-2.12	103.80	106.90
6	E	702	FAD	C1'-C2'-C3'	2.12	115.72	109.79
6	E	702	FAD	O3'-C3'-C2'	-2.09	103.76	108.81
5	A	701	FUM	C4-C5-C6	-2.08	116.57	127.26
11	C	202	FTN	C13-C12-C11	2.05	122.25	118.96
11	F	304	FTN	O2-C11-C12	-2.02	110.12	119.93

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	FAD	C5B-O5B-PA-O3P

Continued on next page...



*Continued from previous page...*

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	C2'-C3'-C4'-O4'
6	A	702	FAD	O3'-C3'-C4'-O4'
6	A	702	FAD	O3'-C3'-C4'-C5'
6	A	702	FAD	O4'-C4'-C5'-O5'
6	E	702	FAD	C5B-O5B-PA-O1A
6	E	702	FAD	C5B-O5B-PA-O2A
6	E	702	FAD	C3B-C4B-C5B-O5B
6	E	702	FAD	N10-C1'-C2'-O2'
6	E	702	FAD	N10-C1'-C2'-C3'
6	E	702	FAD	C2'-C3'-C4'-O4'
6	E	702	FAD	C2'-C3'-C4'-C5'
10	C	201	HEM	C2D-C3D-CAD-CBD
10	C	201	HEM	C4D-C3D-CAD-CBD
10	G	201	HEM	C1A-C2A-CAA-CBA
10	G	201	HEM	C3A-C2A-CAA-CBA
10	G	201	HEM	C2D-C3D-CAD-CBD
10	G	201	HEM	C4D-C3D-CAD-CBD
12	D	201	EPH	C25-C26-C27-C28
12	D	201	EPH	C38-O8-P1-O6
12	D	201	EPH	O8-C38-C39-N1
12	H	201	EPH	C5-C3-O1-C2
12	H	201	EPH	C14-C15-C16-C17
12	H	201	EPH	C38-O8-P1-O7
12	H	201	EPH	O3-C3-O1-C2
12	D	201	EPH	C27-C28-C29-C30
12	D	201	EPH	C11-C12-C13-C14
6	E	702	FAD	O3'-C3'-C4'-O4'
6	A	702	FAD	C2'-C3'-C4'-C5'
11	F	304	FTN	C10-C11-O2-C15
12	H	201	EPH	C3-C5-C6-C7
5	A	701	FUM	O-C-C4-C5
12	D	201	EPH	C3-C5-C6-C7
6	E	702	FAD	O4B-C4B-C5B-O5B
5	A	701	FUM	OXT-C-C4-C5
12	D	201	EPH	C38-O8-P1-O5
12	H	201	EPH	C37-O5-P1-O8
12	D	201	EPH	C18-C19-C20-C21
12	D	201	EPH	C7-C8-C9-C10
5	E	701	FUM	C4-C5-C6-O7
5	E	701	FUM	C4-C5-C6-O8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
12	D	201	EPH	C20-C21-C22-C23
12	H	201	EPH	C5-C6-C7-C8
6	E	702	FAD	O3'-C3'-C4'-C5'
12	H	201	EPH	C6-C7-C8-C9
12	H	201	EPH	C20-C21-C22-C23
6	A	702	FAD	C3B-C4B-C5B-O5B
12	D	201	EPH	C6-C7-C8-C9
12	D	201	EPH	C5-C6-C7-C8
12	D	201	EPH	C5-C3-O1-C2
6	A	702	FAD	O4B-C4B-C5B-O5B
12	D	201	EPH	O3-C3-O1-C2
6	A	702	FAD	C3'-C4'-C5'-O5'
12	H	201	EPH	C21-C22-C23-C24
12	H	201	EPH	C7-C8-C9-C10
12	D	201	EPH	C11-C10-C9-C8
11	C	202	FTN	C10-C11-O2-C15
10	G	201	HEM	C3D-CAD-CBD-CGD
12	D	201	EPH	C37-O5-P1-O8
12	H	201	EPH	C13-C14-C15-C16
11	F	304	FTN	C16-C15-O2-C11
11	C	202	FTN	C12-C11-O2-C15
11	F	304	FTN	C17-C15-O2-C11
12	D	201	EPH	C28-C29-C30-C31
12	H	201	EPH	C28-C29-C30-C31
10	G	201	HEM	C2B-C3B-CAB-CBB
5	E	701	FUM	OXT-C-C4-C5
12	H	201	EPH	C27-C28-C29-C30
12	H	201	EPH	C38-O8-P1-O5
12	D	201	EPH	C37-O5-P1-O6
12	H	201	EPH	C37-O5-P1-O6
5	E	701	FUM	O-C-C4-C5
12	D	201	EPH	C21-C22-C23-C24
10	G	201	HEM	C2A-CAA-CBA-CGA
11	C	202	FTN	C17-C15-O2-C11
12	H	201	EPH	C26-C27-C28-C29
12	D	201	EPH	C23-C24-C25-C26
12	D	201	EPH	C26-C27-C28-C29
12	H	201	EPH	C18-C19-C20-C21
10	C	201	HEM	CAA-CBA-CGA-O2A
11	C	202	FTN	C2-C3-C8-O1
12	H	201	EPH	O1-C2-C37-O5
10	C	201	HEM	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
10	G	201	HEM	CAA-CBA-CGA-O1A
10	G	201	HEM	CAA-CBA-CGA-O2A
12	H	201	EPH	C22-C23-C24-C25
10	C	201	HEM	C2B-C3B-CAB-CBB
6	E	702	FAD	O4'-C4'-C5'-O5'
10	C	201	HEM	C4B-C3B-CAB-CBB
10	G	201	HEM	C4B-C3B-CAB-CBB
12	D	201	EPH	C22-C23-C24-C25
6	E	702	FAD	C5B-O5B-PA-O3P
6	A	702	FAD	PA-O3P-P-O2P
11	C	202	FTN	C2-C3-C8-N
6	A	702	FAD	C5B-O5B-PA-O2A
12	D	201	EPH	C37-O5-P1-O7
12	D	201	EPH	C38-O8-P1-O7
12	H	201	EPH	C39-C38-O8-P1

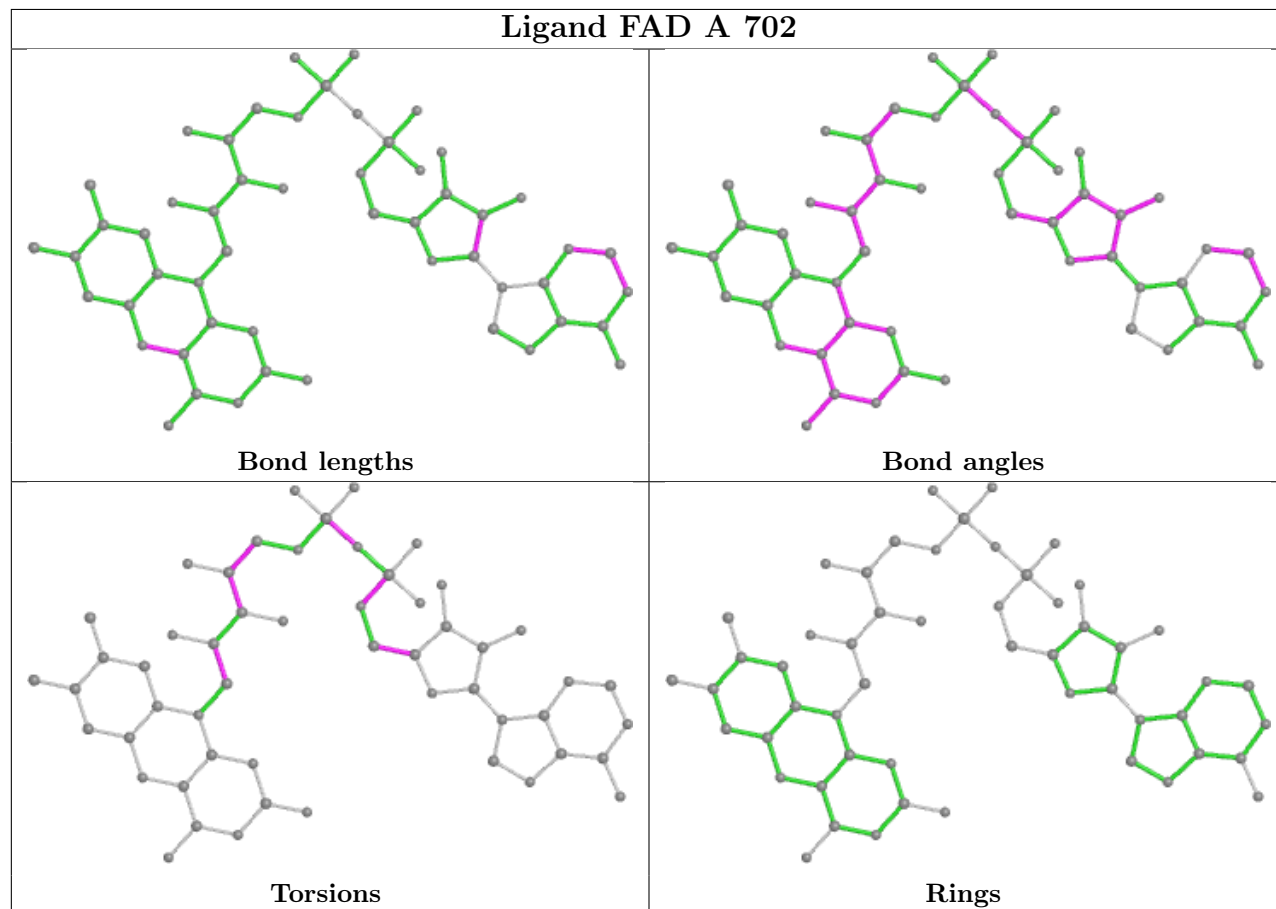
There are no ring outliers.

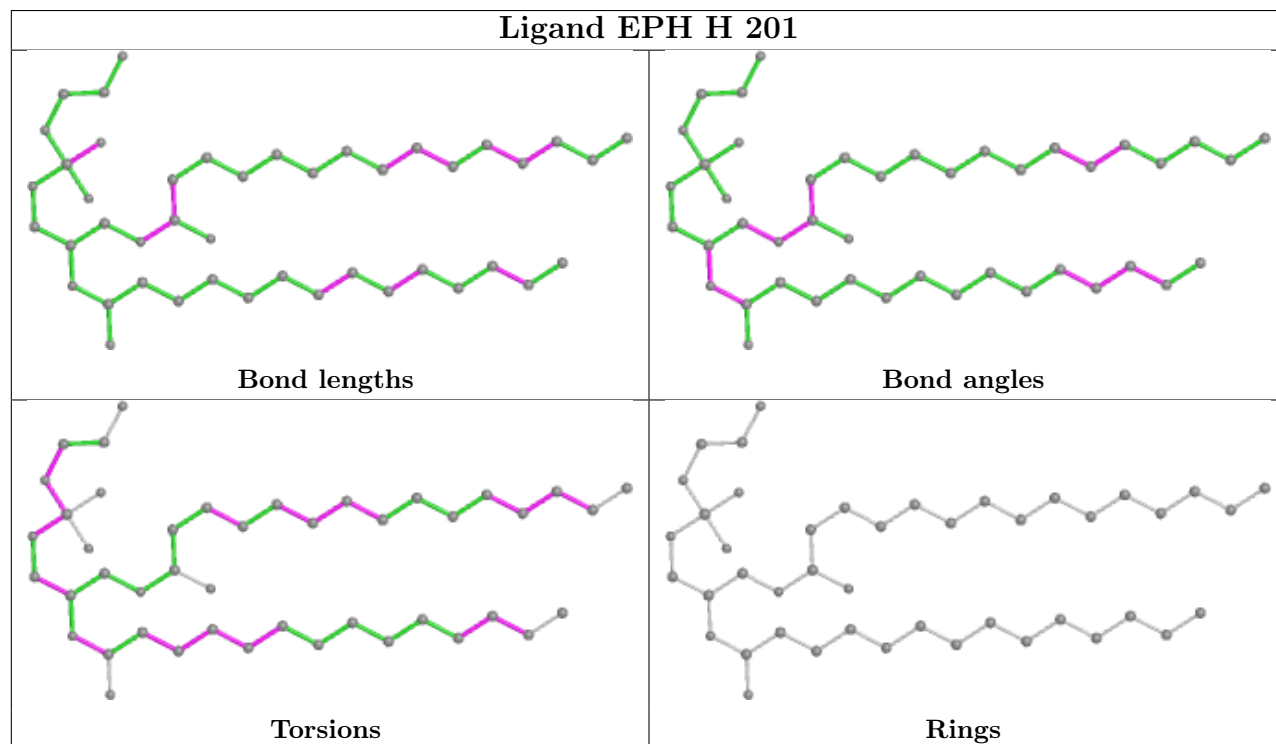
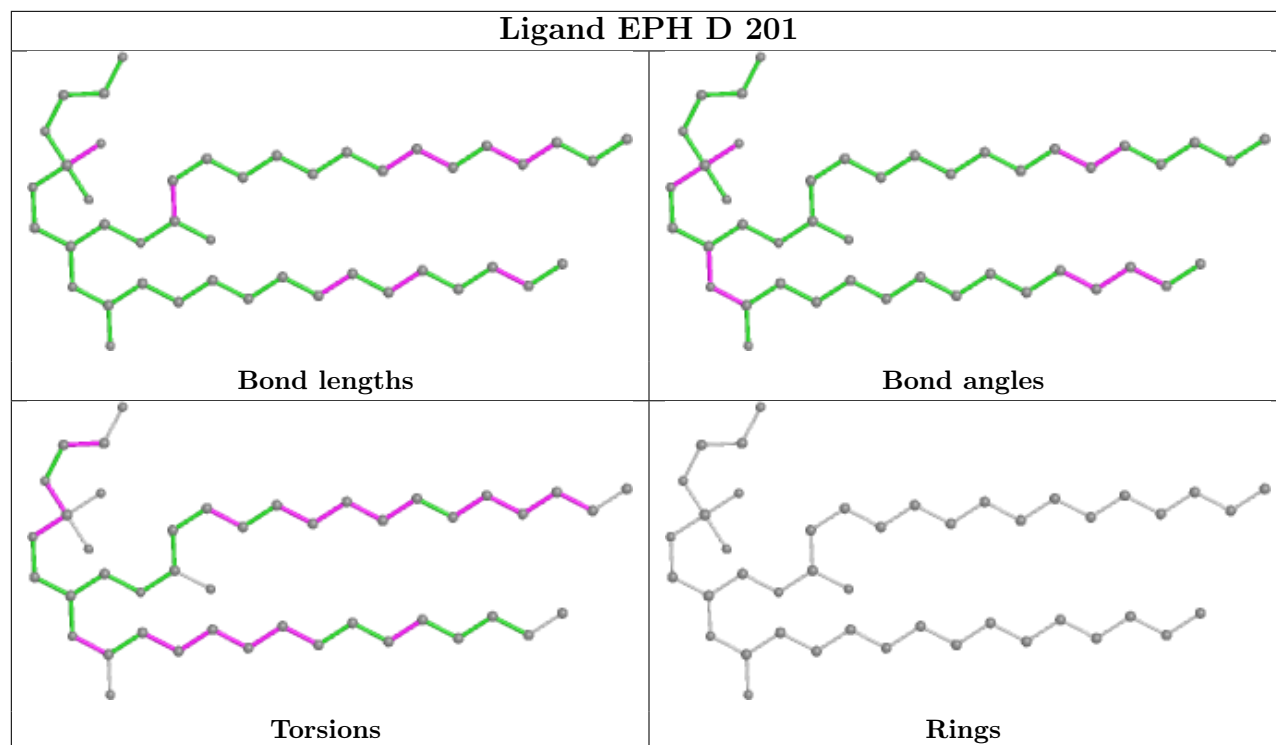
14 monomers are involved in 53 short contacts:

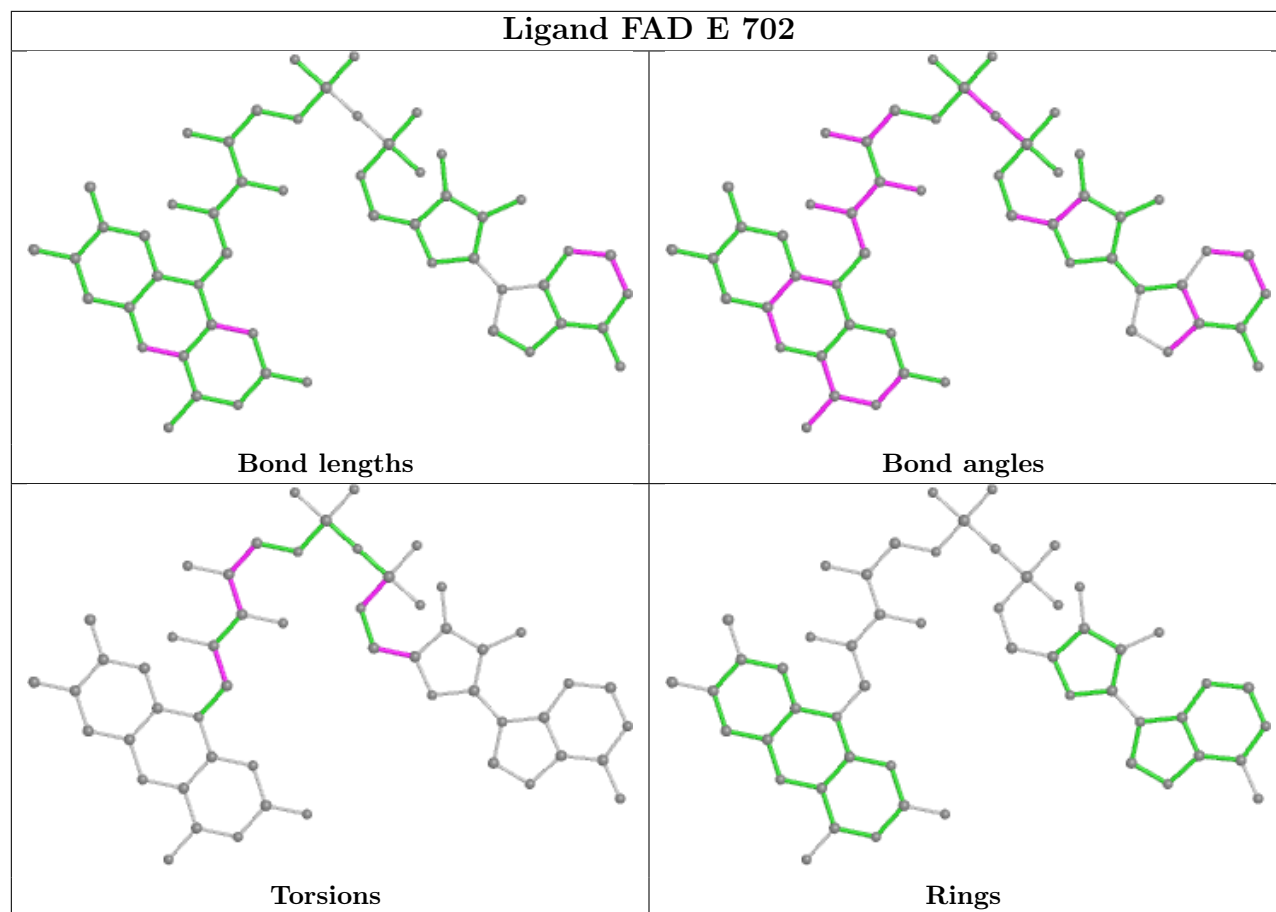
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	302	SF4	2	0
6	A	702	FAD	8	0
12	D	201	EPH	5	0
12	H	201	EPH	1	0
5	E	701	FUM	5	0
6	E	702	FAD	5	0
10	G	201	HEM	5	0
8	F	302	SF4	4	0
11	C	202	FTN	4	0
10	C	201	HEM	6	0
9	B	303	F3S	2	0
11	F	304	FTN	1	0
7	F	301	FES	2	0
5	A	701	FUM	3	0

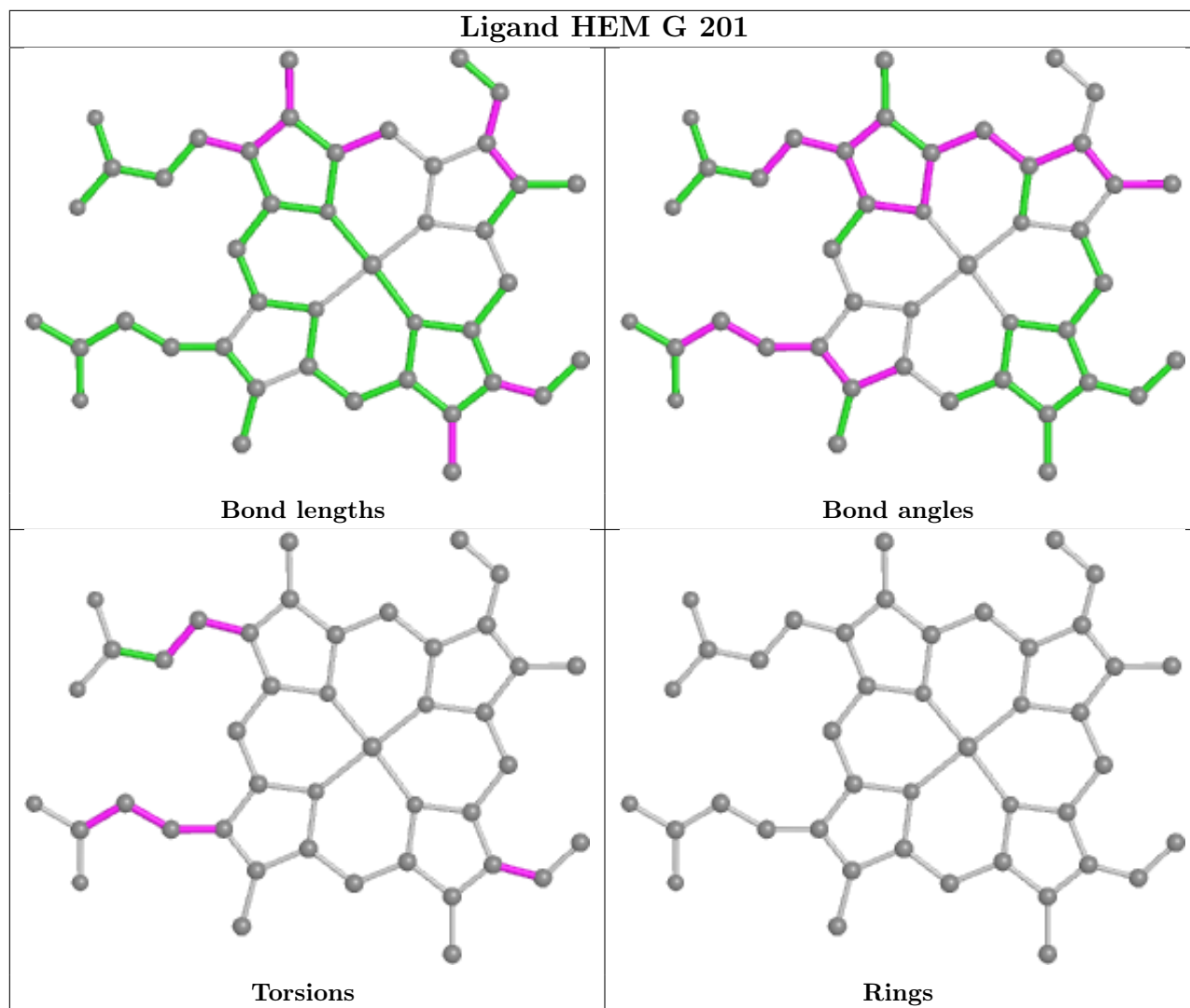
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

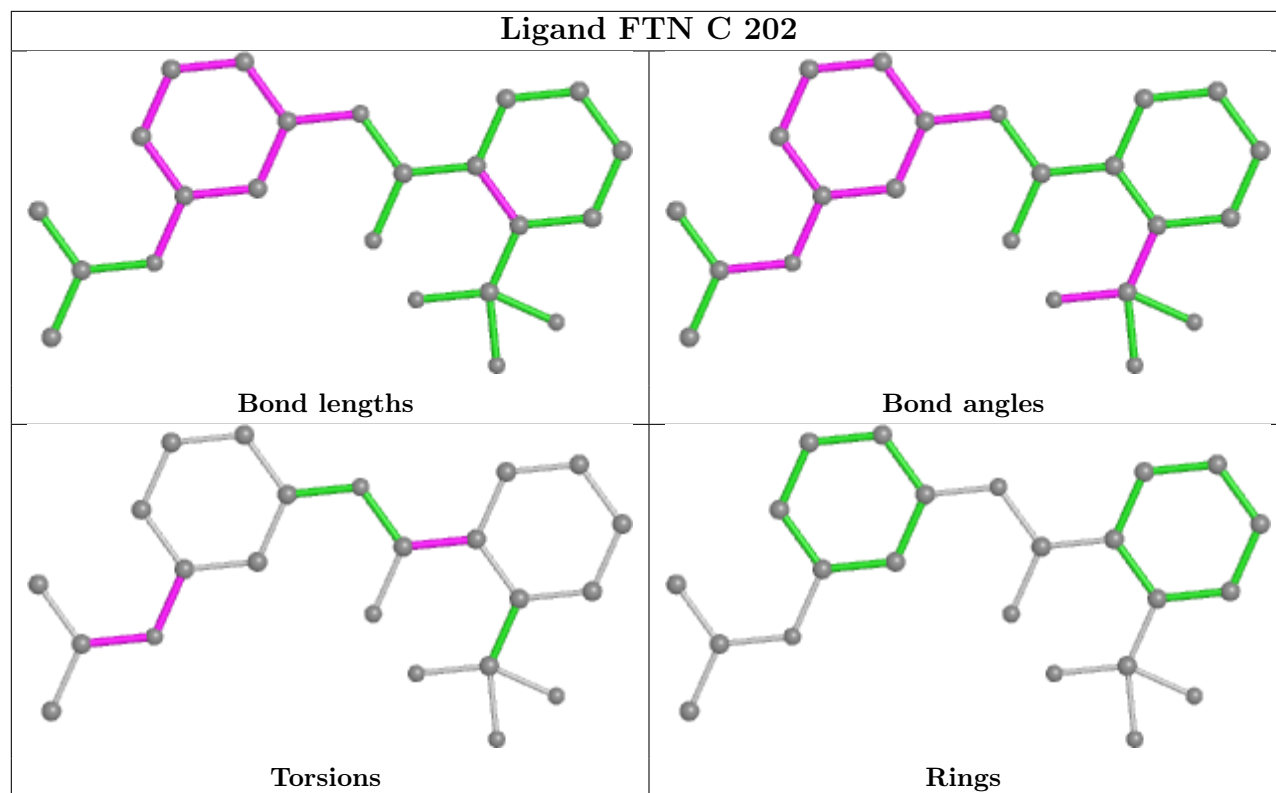
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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



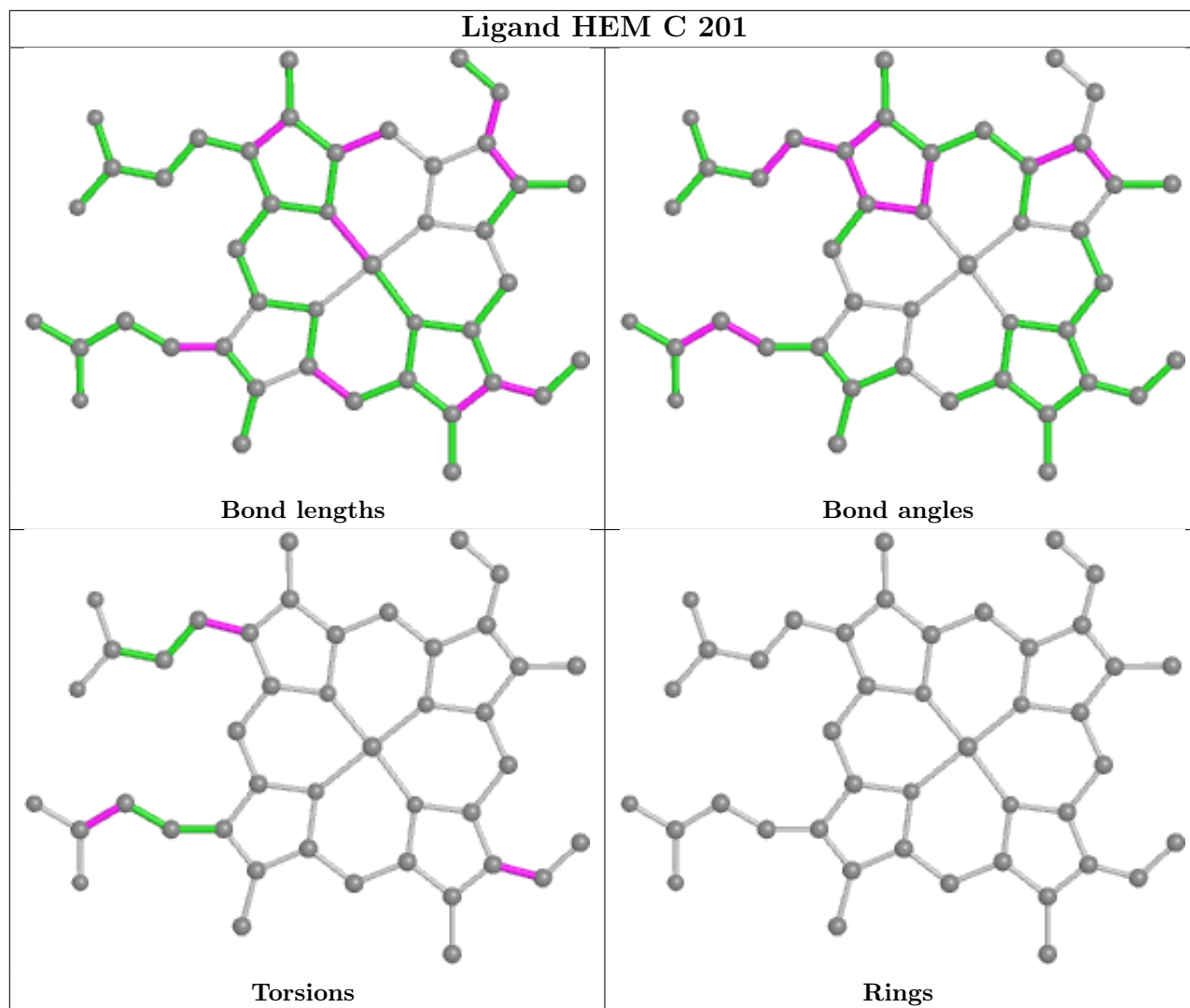


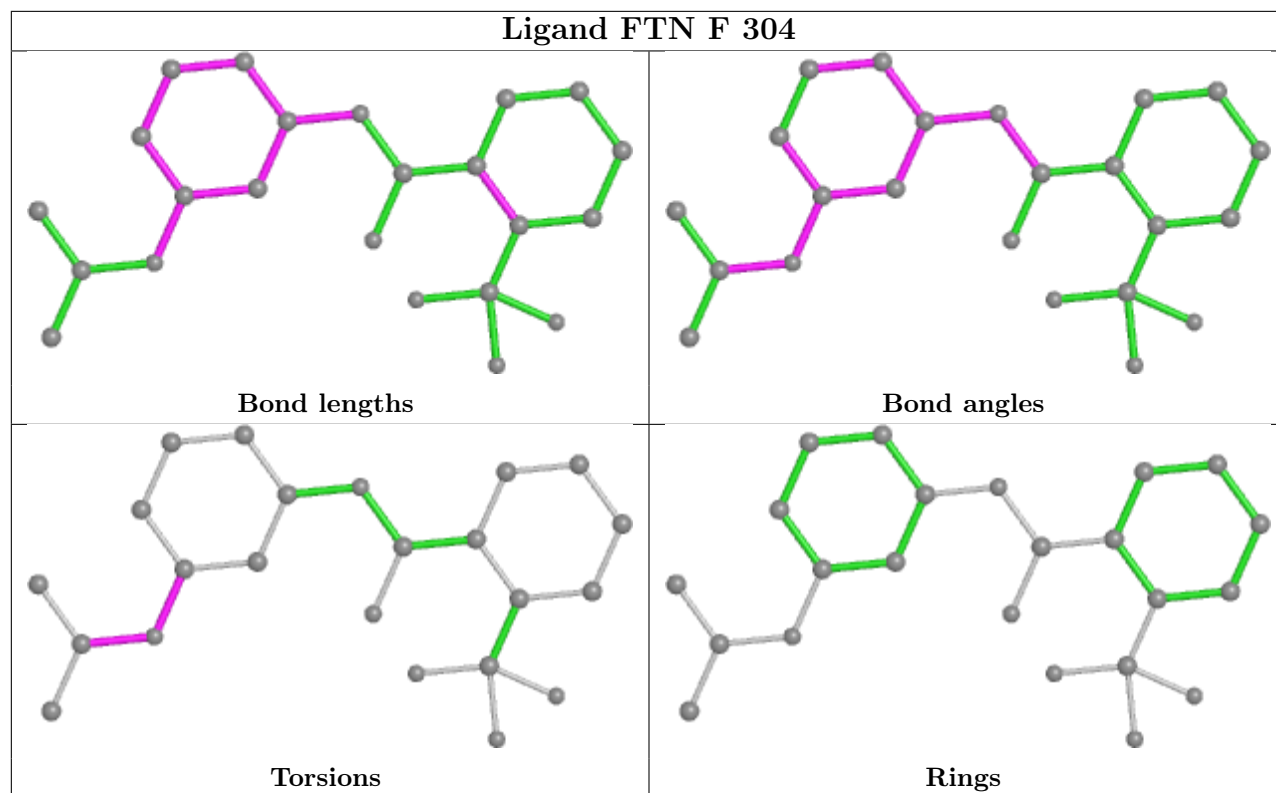












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	613/645 (95%)	0.04	16 (2%) 56 53	60, 90, 113, 124	0
1	E	613/645 (95%)	-0.02	17 (2%) 53 50	53, 83, 105, 113	0
2	B	249/282 (88%)	-0.14	1 (0%) 92 92	57, 78, 110, 123	0
2	F	249/282 (88%)	-0.09	10 (4%) 38 35	52, 71, 100, 114	0
3	C	153/188 (81%)	-0.06	6 (3%) 39 36	65, 89, 131, 148	0
3	G	150/188 (79%)	-0.25	5 (3%) 46 42	68, 87, 128, 135	0
4	D	129/156 (82%)	-0.17	6 (4%) 31 28	70, 92, 113, 123	0
4	H	129/156 (82%)	-0.10	9 (6%) 16 13	68, 91, 118, 128	0
All	All	2285/2542 (89%)	-0.05	70 (3%) 49 45	52, 86, 113, 148	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	185	PRO	6.5
4	D	49	PHE	5.9
3	C	186	THR	4.9
2	F	279	PRO	4.2
4	D	53	HIS	4.1
1	A	598	PRO	3.9
2	F	280	ALA	3.5
3	C	181	LYS	3.5
1	A	599	PHE	3.5
1	A	420	GLY	3.4
4	H	49	PHE	3.4
2	F	281	ASN	3.2
1	E	237	GLY	3.1
1	A	591	ILE	3.1
1	E	254	GLY	3.1
1	A	96	PRO	3.0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	G	181	LYS	3.0
3	C	183	THR	3.0
1	E	486	ASP	2.9
2	B	281	ASN	2.9
3	G	183	THR	2.8
4	D	52	LEU	2.8
1	E	253	THR	2.8
3	G	98	LEU	2.8
4	D	115	ASP	2.7
1	A	596	LYS	2.7
1	A	421	GLU	2.7
2	F	46	GLU	2.7
1	E	238	GLY	2.7
1	E	422	CYS	2.6
3	G	182	ALA	2.6
2	F	276	LEU	2.6
1	E	236	THR	2.6
1	E	252	ASN	2.6
2	F	271	THR	2.6
4	H	78	PHE	2.5
1	E	33	ALA	2.5
3	C	179	HIS	2.5
1	E	420	GLY	2.4
3	C	106	PHE	2.4
4	H	117	LEU	2.4
2	F	48	PRO	2.3
1	E	421	GLU	2.3
4	H	46	GLU	2.3
4	D	48	GLY	2.3
1	E	511	ASP	2.3
1	A	391	GLY	2.3
1	A	422	CYS	2.3
1	A	600	GLU	2.3
4	H	115	ASP	2.3
4	H	112	VAL	2.2
1	A	595	THR	2.2
4	H	52	LEU	2.2
4	D	114	GLY	2.2
4	H	45	ALA	2.2
4	H	113	LEU	2.1
3	G	110	LEU	2.1
1	A	237	GLY	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	532	THR	2.1
1	E	467	GLU	2.1
1	E	593	GLY	2.1
1	A	388	TYR	2.1
1	E	529	ARG	2.1
2	F	239	CYS	2.1
1	E	429	GLY	2.1
1	A	521	MET	2.1
2	F	49	GLY	2.0
2	F	139	MET	2.0
1	A	411	LYS	2.0
1	A	518	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

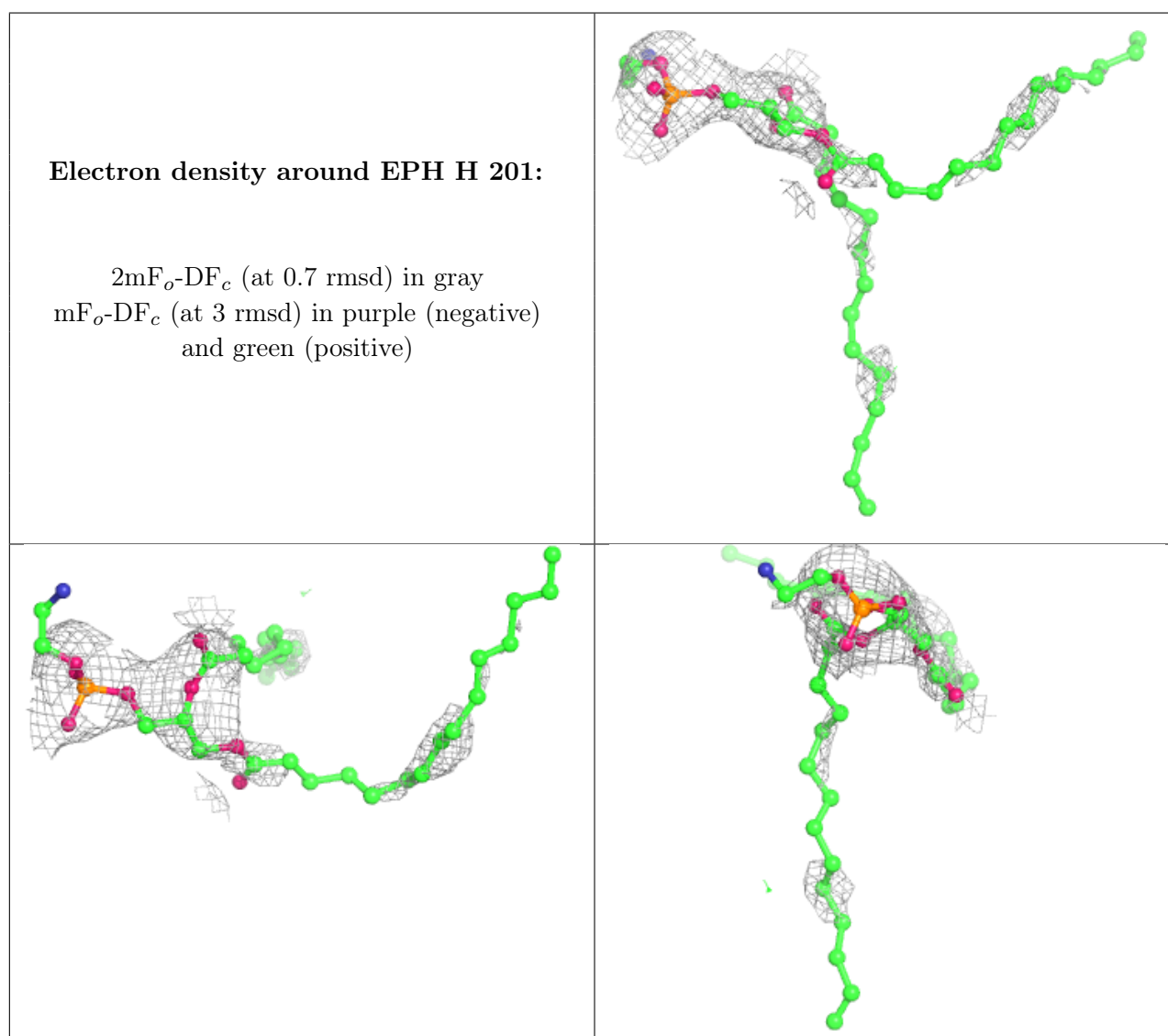
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	EPH	H	201	44/49	0.88	0.35	119,129,143,145	0
5	FUM	A	701	8/8	0.90	0.44	97,99,100,100	0
5	FUM	E	701	8/8	0.91	0.23	111,112,113,114	0
12	EPH	D	201	44/49	0.93	0.23	100,109,111,112	0
11	FTN	C	202	23/23	0.96	0.19	66,72,78,80	0
11	FTN	F	304	23/23	0.96	0.24	65,67,80,82	0
6	FAD	E	702	53/53	0.97	0.23	53,61,68,69	0
10	HEM	C	201	43/43	0.98	0.19	68,72,85,91	0
10	HEM	G	201	43/43	0.98	0.20	71,74,84,88	0
6	FAD	A	702	53/53	0.98	0.26	49,61,70,71	0
7	FES	F	301	4/4	0.99	0.17	62,66,68,68	0

*Continued on next page...*

Continued from previous page...

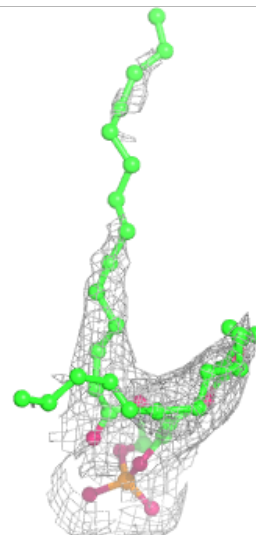
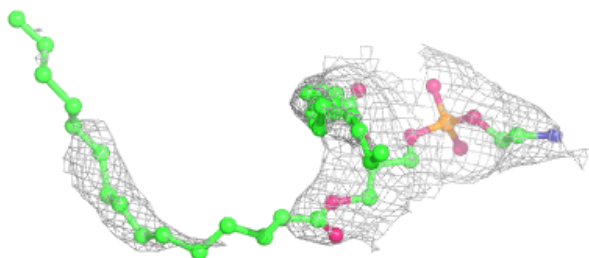
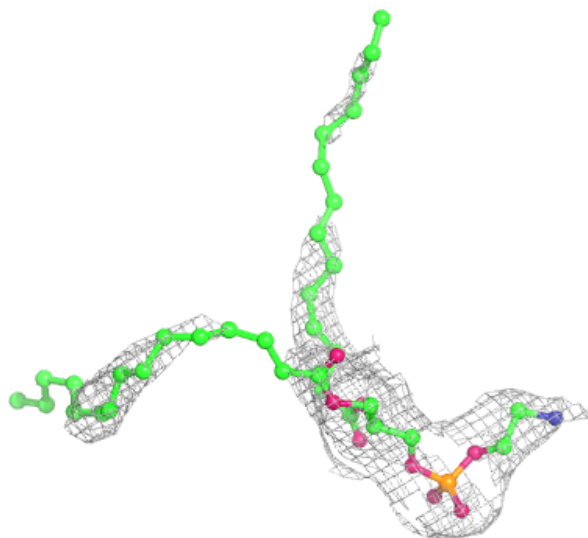
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	F3S	B	303	7/7	0.99	0.17	57,59,61,61	0
7	FES	B	301	4/4	1.00	0.16	62,63,65,68	0
9	F3S	F	303	7/7	1.00	0.20	57,58,60,60	0
8	SF4	B	302	8/8	1.00	0.19	55,58,60,60	0
8	SF4	F	302	8/8	1.00	0.18	52,53,55,58	0

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.



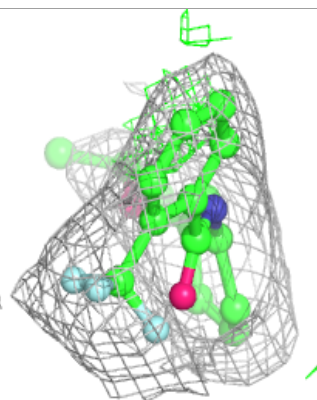
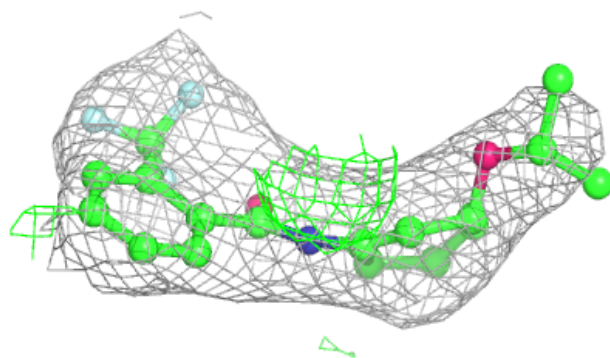
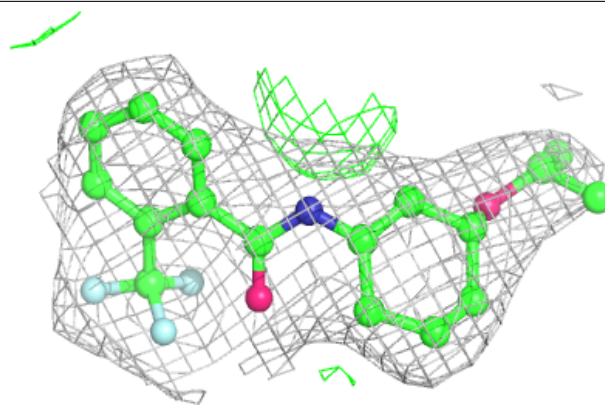
**Electron density around EPH D 201:**

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

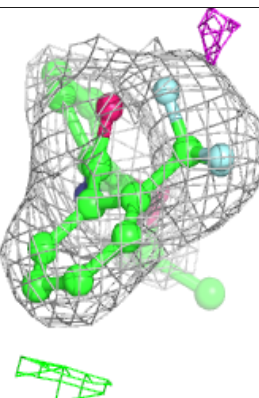
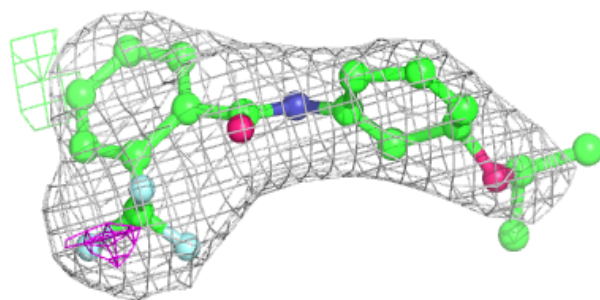
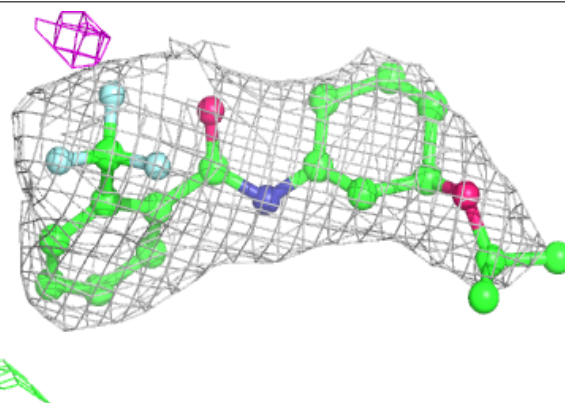


**Electron density around FTN C 202:**

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

**Electron density around FTN F 304:**

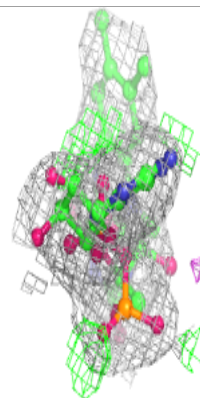
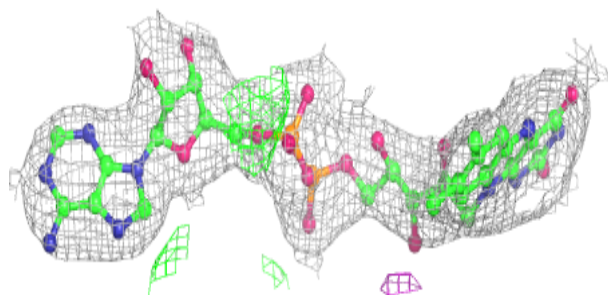
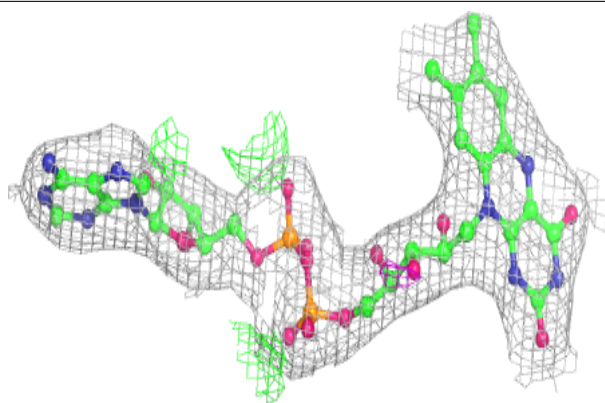
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



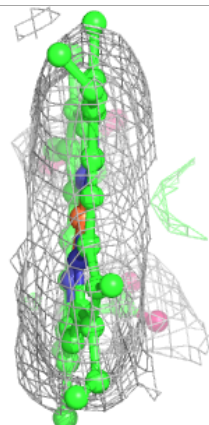
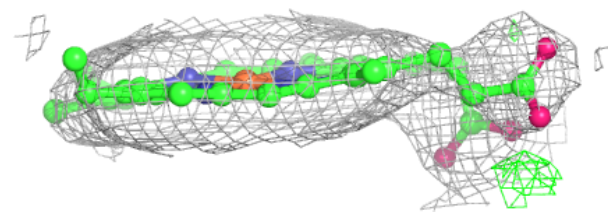
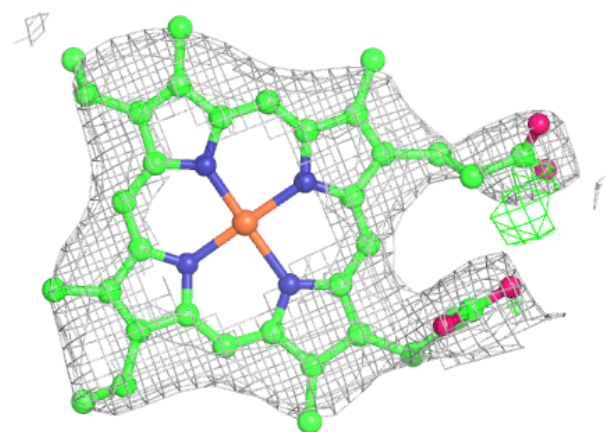


**Electron density around FAD E 702:**

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

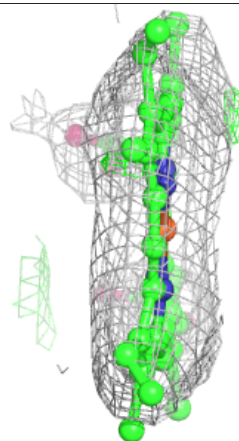
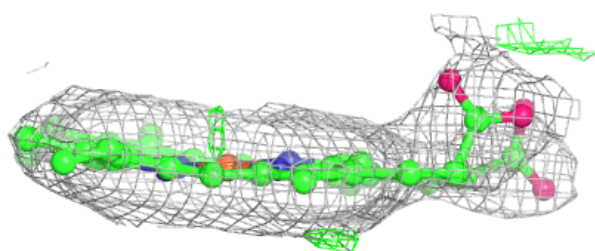
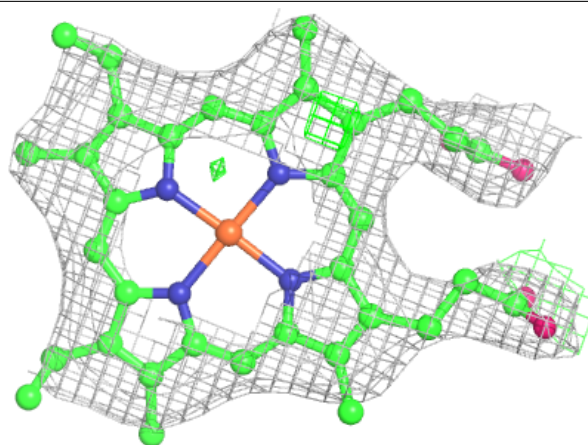
**Electron density around HEM C 201:**

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

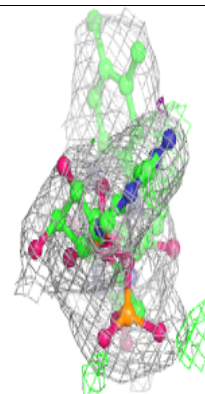
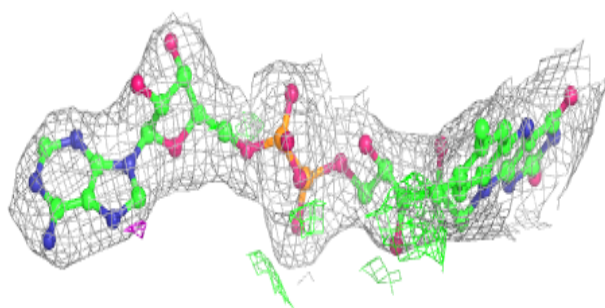
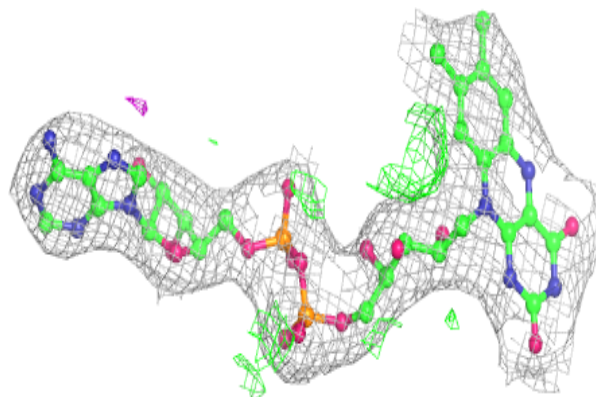


**Electron density around HEM G 201:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.