



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:15 am BST

PDB ID : 1ZOY  
Title : Crystal Structure of Mitochondrial Respiratory Complex II from porcine heart at 2.4 Angstroms  
Authors : Sun, F.; Huo, X.; Zhai, Y.; Wang, A.; Xu, J.; Su, D.; Bartlam, M.; Rao, Z.  
Deposited on : 2005-05-15  
Resolution : 2.40 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.

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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	:	2.11
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)	:	2.11

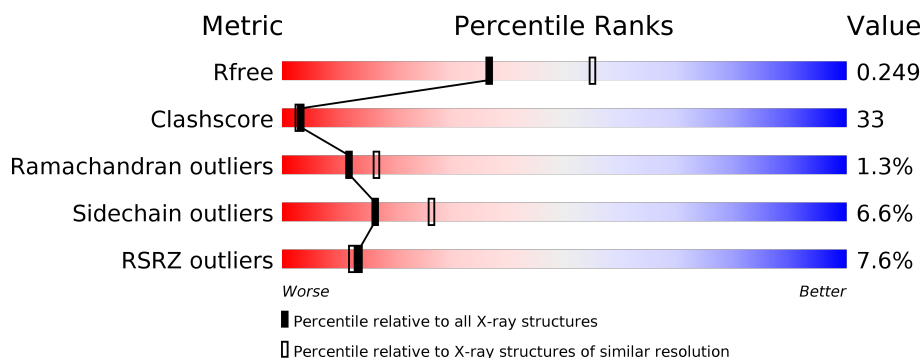
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	622	<div> <div>10%</div> <div> <div>48%</div> <div>45%</div> <div>5%</div> </div> </div>
2	B	252	<div> <div>6%</div> <div> <div>57%</div> <div>32%</div> <div>6%</div> <div>5%</div> </div> </div>
3	C	140	<div> <div>4%</div> <div> <div>56%</div> <div>40%</div> </div> </div>
4	D	103	<div> <div>4%</div> <div> <div>56%</div> <div>39%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	F3S	B	304	-	-	X	-
9	UQ1	B	1201	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 9024 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 FAD-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4729	2954	848	895	32			

- Molecule 2 is a protein called Iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1922	1214	326	360	22			

- Molecule 3 is a protein called Large cytochrome binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	138	Total	C	N	O	S	0	0	0
			1064	695	179	183	7			

- Molecule 4 is a protein called Small cytochrome binding protein.

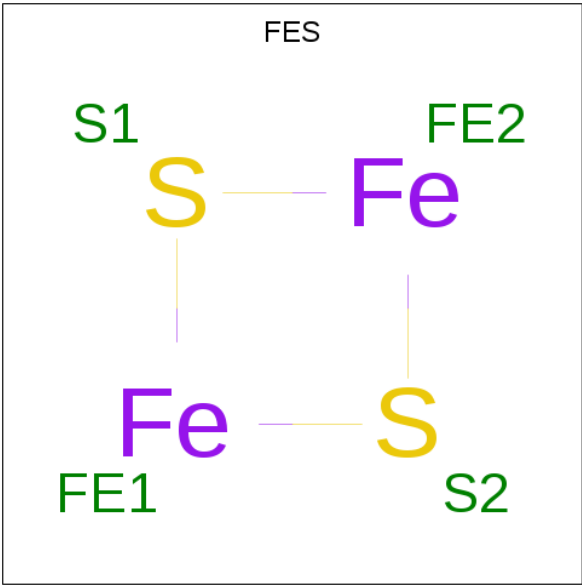
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			765	499	128	133	5			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



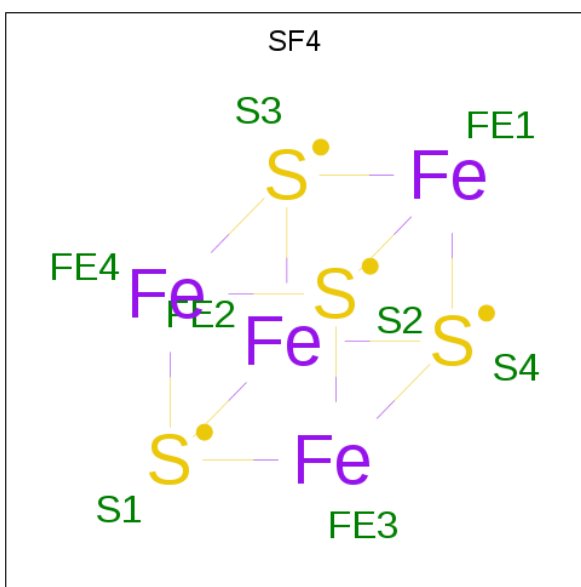
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



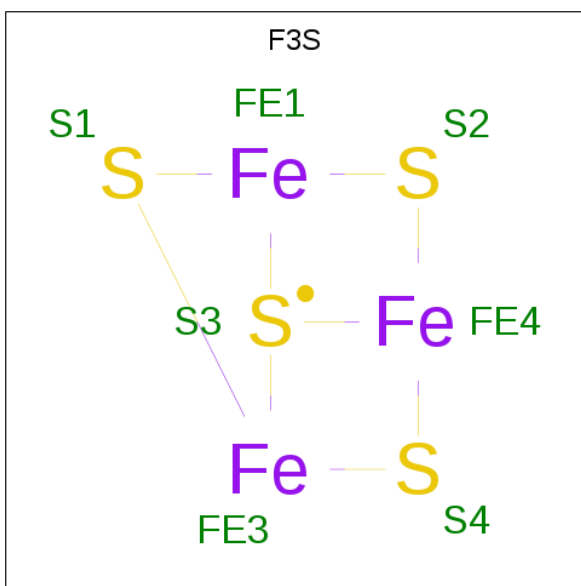
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



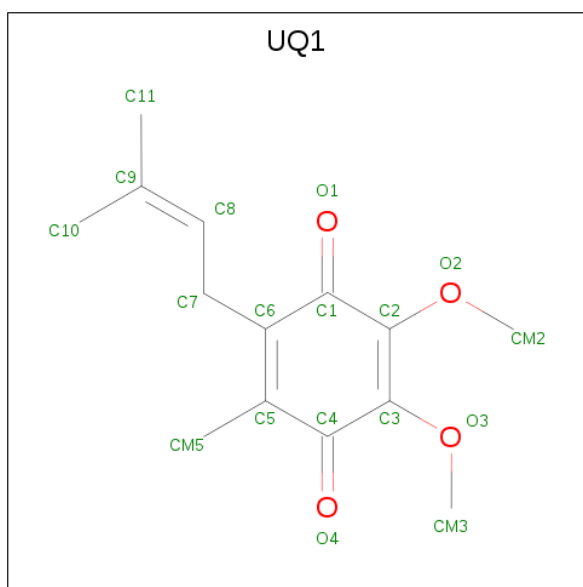
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



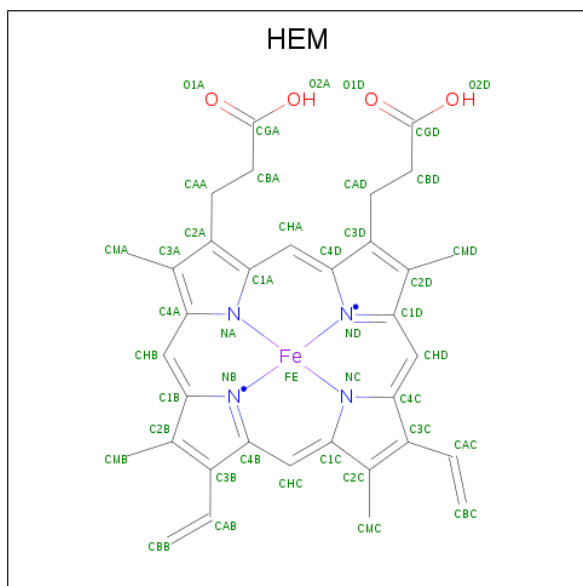
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

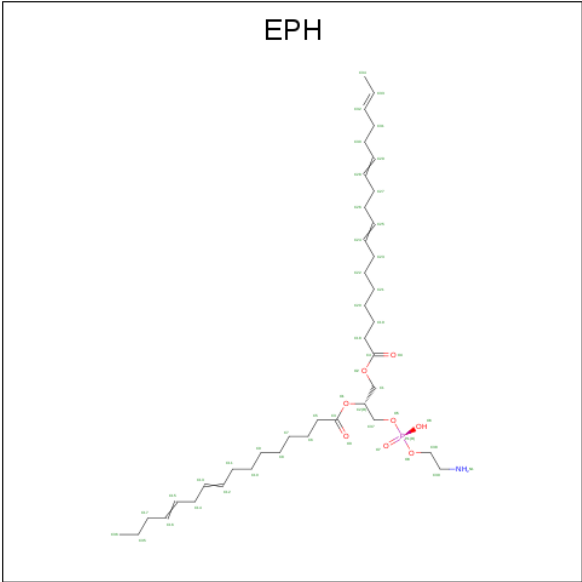
- Molecule 9 is UBIQUINONE-1 (three-letter code: UQ1) (formula:  $\text{C}_{14}\text{H}_{18}\text{O}_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	O		4	0
			18	14	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
11	D	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
11	D	1	Total	C	N	O	P	0	0
			36	26	1	8	1		

- Molecule 12 is water.

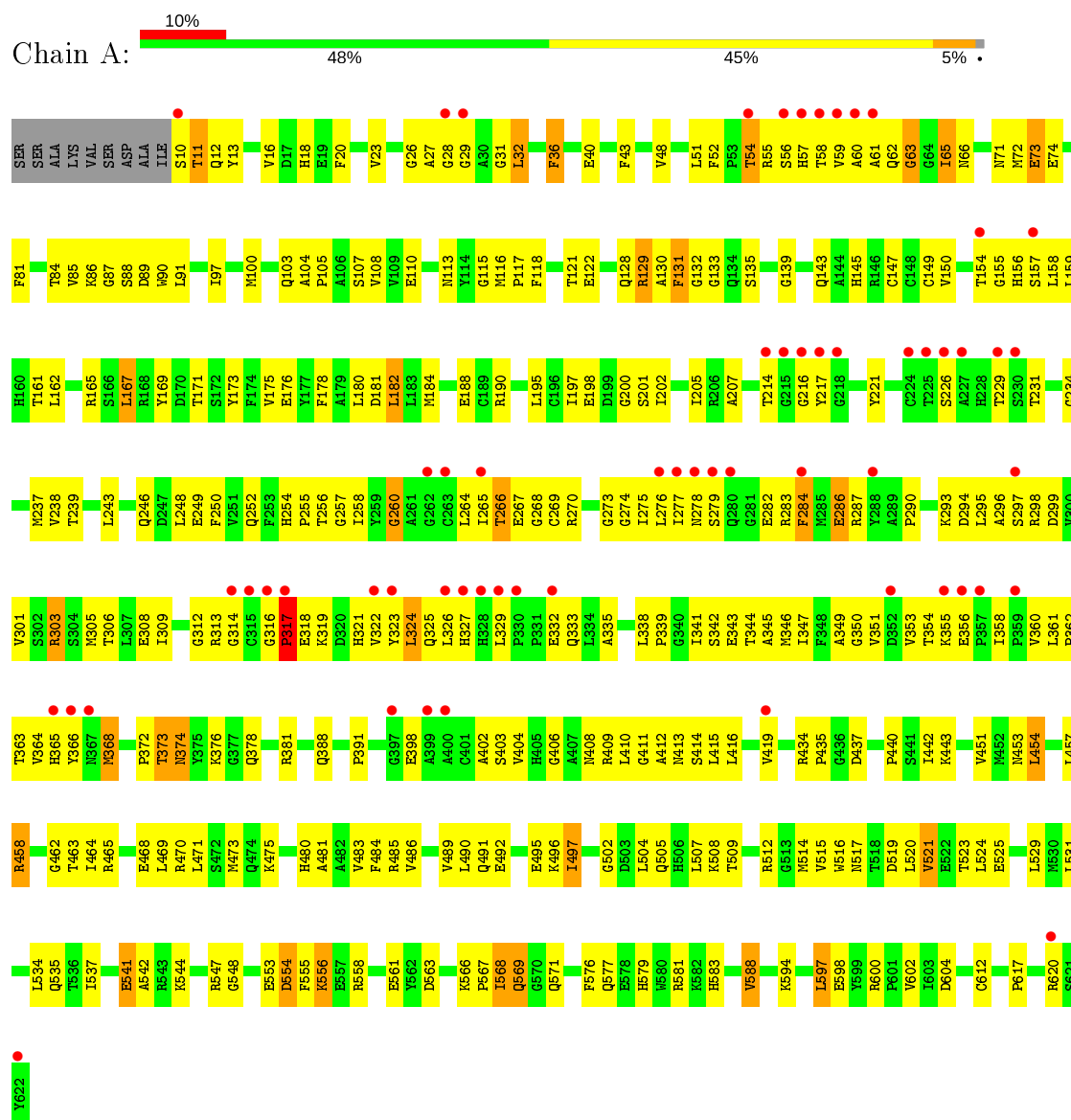
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	195	Total	O	0	0
			195	195		
12	B	91	Total	O	0	0
			91	91		
12	C	24	Total	O	0	0
			24	24		
12	D	21	Total	O	0	0
			21	21		



### 3 Residue-property plots

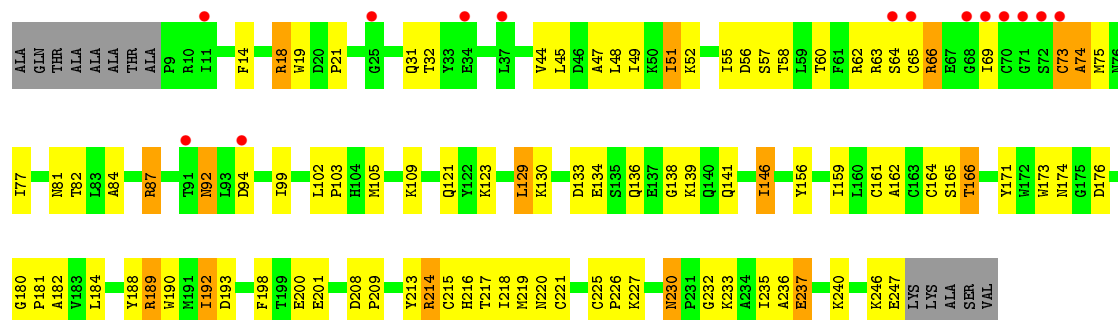
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

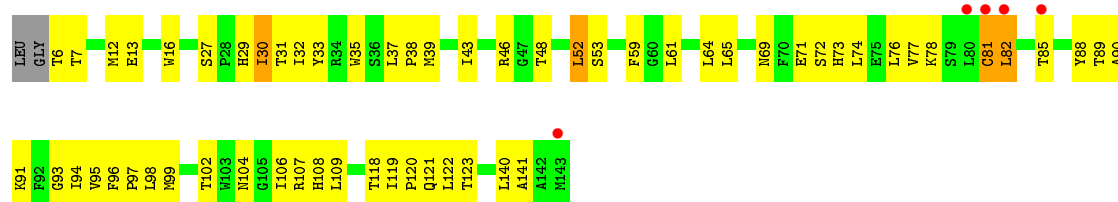


#### • Molecule 2: Iron-sulfur protein

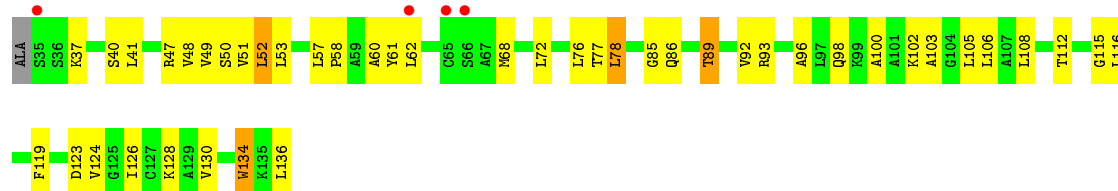




• Molecule 3: Large cytochrome binding protein



• Molecule 4: Small cytochrome binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.24Å 83.56Å 293.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 48.08 – 2.37	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 79.6 (48.08-2.37)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.213 , 0.259 0.204 , 0.249	Depositor DCC
$R_{free}$ test set	5757 reflections (9.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: SF4, F3S, FES, EPH, UQ1, HEM, FAD

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	0.38	0/4828	0.67	1/6531 (0.0%)
2	B	0.42	1/1964 (0.1%)	0.65	0/2648
3	C	0.37	0/1091	0.56	0/1483
4	D	0.38	0/784	0.56	0/1066
All	All	0.38	1/8667 (0.0%)	0.64	1/11728 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	73	CYS	CB-SG	-6.65	1.71	1.82

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	ALA	N-CA-C	-5.42	96.36	111.00

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	4729	0	4618	366	0
2	B	1922	0	1900	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1064	0	1104	63	0
4	D	765	0	773	49	0
5	A	53	0	29	14	0
6	B	4	0	0	0	0
7	B	8	0	0	0	0
8	B	7	0	0	3	0
9	B	18	0	18	3	0
10	C	43	0	30	7	0
11	D	80	0	94	4	0
12	A	195	0	0	49	0
12	B	91	0	0	18	0
12	C	24	0	0	13	0
12	D	21	0	0	7	0
All	All	9024	0	8566	567	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 33.

All (567) 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:57:HIS:NE2	5:A:700:FAD:HM81	1.69	1.07
1:A:150:VAL:H	1:A:154:THR:HG22	0.92	1.07
1:A:57:HIS:CE1	5:A:700:FAD:C8M	2.39	1.05
1:A:150:VAL:N	1:A:154:THR:HG22	1.76	1.01
3:C:52:LEU:HB3	10:C:1305:HEM:HAC	1.39	1.00
1:A:71:ASN:HB2	1:A:128:GLN:HE21	1.25	0.98
1:A:374:ASN:HB3	12:A:794:HOH:O	1.63	0.97
1:A:322:VAL:HG12	1:A:323:TYR:H	1.30	0.96
1:A:353:VAL:HG12	1:A:358:ILE:HD11	1.45	0.96
1:A:190:ARG:HD2	1:A:440:PRO:HB2	1.48	0.94
1:A:113:ASN:HD22	2:B:138:GLY:H	1.12	0.89
1:A:202:ILE:HD13	1:A:451:VAL:HG22	1.54	0.89
1:A:264:LEU:HD12	1:A:265:ILE:H	1.40	0.86
4:D:106:LEU:HB3	12:D:1318:HOH:O	1.76	0.85
1:A:157:SER:O	1:A:161:THR:HG23	1.77	0.85
1:A:248:LEU:HD12	1:A:535:GLN:HB2	1.58	0.84
1:A:457:LEU:HD23	1:A:523:THR:HG22	1.59	0.84
1:A:150:VAL:H	1:A:154:THR:CG2	1.85	0.84
1:A:216:GLY:HA3	1:A:398:GLU:OE2	1.80	0.82
1:A:237:MET:HB3	12:A:857:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:GLU:OE2	1:A:581:ARG:HD3	1.78	0.81
1:A:368:MET:CE	1:A:408:ASN:HA	2.11	0.81
3:C:69:ASN:HD21	3:C:71:GLU:HB2	1.45	0.81
1:A:465:ARG:HB3	1:A:468:GLU:HG3	1.63	0.81
1:A:61:ALA:HB3	1:A:155:GLY:HA3	1.63	0.80
4:D:72:LEU:O	4:D:76:LEU:HB2	1.81	0.79
1:A:258:ILE:HD12	1:A:258:ILE:H	1.47	0.79
1:A:345:ALA:O	1:A:349:ALA:HB3	1.82	0.79
1:A:256:THR:HA	1:A:360:VAL:HB	1.65	0.79
4:D:92:VAL:HB	12:D:1323:HOH:O	1.83	0.78
2:B:230:ASN:ND2	2:B:233:LYS:H	1.82	0.78
1:A:115:GLY:HA3	12:A:890:HOH:O	1.82	0.78
1:A:71:ASN:HB2	1:A:128:GLN:NE2	1.99	0.78
1:A:279:SER:HB3	1:A:314:GLY:O	1.84	0.77
1:A:129:ARG:HG3	1:A:129:ARG:HH11	1.49	0.77
4:D:124:VAL:HG12	4:D:128:LYS:HB3	1.67	0.76
1:A:465:ARG:HD3	12:A:846:HOH:O	1.86	0.76
1:A:57:HIS:HB3	12:A:790:HOH:O	1.85	0.76
2:B:103:PRO:HD2	2:B:166:THR:HG23	1.68	0.75
1:A:254:HIS:O	1:A:362:PRO:HA	1.85	0.75
1:A:409:ARG:HE	1:A:414:SER:HB2	1.52	0.75
1:A:258:ILE:HG22	1:A:260:GLY:H	1.51	0.75
1:A:563:ASP:HB3	1:A:571:GLN:HE22	1.52	0.75
3:C:91:LYS:O	3:C:95:VAL:HG23	1.86	0.75
1:A:113:ASN:ND2	2:B:138:GLY:H	1.83	0.74
1:A:171:THR:HB	1:A:173:TYR:CE1	2.22	0.74
1:A:368:MET:HE1	1:A:408:ASN:HA	1.69	0.74
1:A:269:CYS:SG	1:A:341:ILE:HD13	2.28	0.74
1:A:571:GLN:HB3	12:A:844:HOH:O	1.89	0.73
1:A:256:THR:HG22	1:A:360:VAL:HG21	1.70	0.73
1:A:303:ARG:HG2	1:A:303:ARG:HH11	1.54	0.72
1:A:345:ALA:HB1	1:A:358:ILE:HD12	1.71	0.72
1:A:579:HIS:HD2	1:A:581:ARG:H	1.36	0.72
1:A:458:ARG:HG3	1:A:458:ARG:HH11	1.55	0.72
3:C:30:ILE:HD13	3:C:31:THR:H	1.54	0.71
1:A:512:ARG:HH11	1:A:512:ARG:HG3	1.56	0.71
12:A:890:HOH:O	2:B:129:LEU:HB2	1.91	0.71
2:B:215:CYS:HA	12:B:1260:HOH:O	1.89	0.71
1:A:278:ASN:HD21	1:A:282:GLU:HB3	1.55	0.70
2:B:92:ASN:HD22	2:B:92:ASN:C	1.93	0.70
1:A:275:ILE:HG22	1:A:276:LEU:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HG22	5:A:700:FAD:O4'	1.91	0.70
1:A:58:THR:HG23	5:A:700:FAD:O1A	1.90	0.70
4:D:124:VAL:CG1	4:D:128:LYS:HB3	2.21	0.70
1:A:361:LEU:HD12	1:A:362:PRO:HD2	1.74	0.70
3:C:106:ILE:HA	12:C:1329:HOH:O	1.90	0.70
1:A:544:LYS:HG2	1:A:555:PHE:CE2	2.26	0.70
1:A:57:HIS:NE2	5:A:700:FAD:C8	2.52	0.70
1:A:161:THR:HG22	12:B:1215:HOH:O	1.92	0.70
1:A:284:PHE:HD2	1:A:284:PHE:N	1.89	0.70
1:A:403:SER:HA	12:A:739:HOH:O	1.91	0.69
1:A:269:CYS:HB3	1:A:326:LEU:HD21	1.74	0.69
1:A:16:VAL:HG23	12:A:831:HOH:O	1.91	0.69
1:A:116:MET:HA	1:A:161:THR:HG21	1.75	0.69
1:A:246:GLN:HE22	1:A:600:ARG:HE	1.39	0.69
1:A:568:ILE:HD12	12:A:844:HOH:O	1.93	0.69
2:B:92:ASN:ND2	2:B:94:ASP:H	1.90	0.69
1:A:182:LEU:HB2	12:A:857:HOH:O	1.92	0.69
1:A:353:VAL:CG1	1:A:358:ILE:HD11	2.23	0.69
2:B:92:ASN:HD21	2:B:94:ASP:HB2	1.56	0.69
1:A:29:GLY:H	1:A:58:THR:HG21	1.58	0.69
1:A:299:ASP:HB3	1:A:408:ASN:ND2	2.09	0.68
1:A:486:VAL:CG1	1:A:553:GLU:HB2	2.23	0.68
1:A:87:GLY:HA2	1:A:620:ARG:HH12	1.58	0.68
1:A:190:ARG:HD2	1:A:440:PRO:CB	2.22	0.68
1:A:178:PHE:HB2	1:A:197:ILE:HD11	1.74	0.68
1:A:492:GLU:O	1:A:496:LYS:HB2	1.92	0.68
1:A:71:ASN:H	1:A:128:GLN:HE22	1.39	0.68
1:A:57:HIS:HE1	1:A:226:SER:HA	1.58	0.68
1:A:284:PHE:CD2	1:A:284:PHE:N	2.61	0.68
1:A:255:PRO:HG2	1:A:270:ARG:HH12	1.59	0.67
2:B:109:LYS:HG2	12:B:1245:HOH:O	1.94	0.67
1:A:298:ARG:HE	1:A:409:ARG:HH12	1.43	0.67
4:D:60:ALA:HA	4:D:68:MET:HG2	1.76	0.66
8:B:304:F3S:S1	8:B:304:F3S:FE3	1.88	0.66
1:A:376:LYS:HB2	12:A:794:HOH:O	1.95	0.66
1:A:71:ASN:H	1:A:128:GLN:NE2	1.94	0.66
1:A:554:ASP:HB2	1:A:555:PHE:CD2	2.31	0.66
3:C:52:LEU:HD21	3:C:98:LEU:HA	1.77	0.66
1:A:246:GLN:NE2	1:A:600:ARG:HE	1.93	0.65
1:A:264:LEU:HD12	1:A:265:ILE:N	2.12	0.65
12:C:1322:HOH:O	4:D:116:LEU:HD21	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:304:F3S:FE4	8:B:304:F3S:S2	1.89	0.64
1:A:516:TRP:HB3	2:B:60:THR:HG21	1.80	0.64
1:A:252:GLN:CD	1:A:298:ARG:HD2	2.18	0.64
1:A:508:LYS:HE2	1:A:509:THR:O	1.97	0.64
1:A:181:ASP:HA	1:A:237:MET:HG2	1.80	0.63
1:A:368:MET:HE3	1:A:408:ASN:HA	1.79	0.63
2:B:102:LEU:HD22	2:B:166:THR:HG21	1.78	0.63
3:C:46:ARG:NE	10:C:1305:HEM:O2D	2.32	0.63
1:A:26:GLY:O	1:A:31:GLY:HA3	1.98	0.63
3:C:37:LEU:HB3	3:C:38:PRO:HD3	1.80	0.63
1:A:182:LEU:HD22	12:A:857:HOH:O	1.98	0.63
1:A:282:GLU:OE1	1:A:287:ARG:HD2	1.98	0.62
1:A:54:THR:O	1:A:59:VAL:HG21	1.99	0.62
2:B:92:ASN:HD22	2:B:94:ASP:H	1.45	0.62
1:A:458:ARG:NH1	1:A:458:ARG:HG3	2.11	0.62
1:A:57:HIS:CE1	1:A:226:SER:HA	2.35	0.62
3:C:74:LEU:HD22	4:D:136:LEU:HD13	1.81	0.62
1:A:453:ASN:O	1:A:457:LEU:HD13	1.99	0.62
3:C:53:SER:HA	10:C:1305:HEM:HBC1	1.80	0.62
1:A:563:ASP:CB	1:A:571:GLN:HE22	2.11	0.62
1:A:464:ILE:O	1:A:508:LYS:N	2.26	0.62
3:C:91:LYS:HB3	12:C:1323:HOH:O	1.99	0.62
1:A:214:THR:OG1	1:A:234:GLY:HA3	1.99	0.62
1:A:346:MET:HA	1:A:351:VAL:H	1.64	0.62
1:A:52:PHE:HB3	1:A:55:ARG:HG2	1.82	0.61
2:B:188:TYR:O	2:B:192:ILE:HD12	1.99	0.61
2:B:77:ILE:HD12	2:B:99:ILE:HG13	1.82	0.61
1:A:180:LEU:HA	12:A:853:HOH:O	1.99	0.61
1:A:171:THR:HB	1:A:173:TYR:CZ	2.35	0.61
9:B:1201:UQ1:HM52	3:C:43:ILE:HD11	1.83	0.61
2:B:219:MET:HE1	2:B:232:GLY:HA3	1.82	0.61
3:C:30:ILE:HD13	3:C:31:THR:N	2.16	0.61
1:A:161:THR:HB	12:A:881:HOH:O	1.99	0.61
1:A:597:LEU:HD23	1:A:597:LEU:N	2.15	0.61
2:B:219:MET:CE	2:B:232:GLY:HA3	2.31	0.61
1:A:59:VAL:CG2	1:A:159:LEU:HD23	2.30	0.60
1:A:60:ALA:HB1	5:A:700:FAD:HM72	1.82	0.60
2:B:47:ALA:O	2:B:51:ILE:HG23	2.01	0.60
3:C:73:HIS:O	3:C:76:LEU:HB3	2.01	0.60
4:D:85:GLY:O	4:D:89:THR:HG23	2.01	0.60
12:B:1282:HOH:O	3:C:12:MET:HE1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG12	1:A:323:TYR:N	2.09	0.60
4:D:72:LEU:HD21	11:D:1306:EPH:H101	1.83	0.60
3:C:123:THR:HA	12:C:1325:HOH:O	2.00	0.60
1:A:373:THR:CG2	1:A:374:ASN:O	2.48	0.60
2:B:45:LEU:HA	2:B:48:LEU:HD12	1.83	0.60
1:A:252:GLN:NE2	1:A:298:ARG:HD2	2.17	0.60
1:A:287:ARG:HD3	12:A:848:HOH:O	2.00	0.60
4:D:57:LEU:HB2	4:D:58:PRO:HD3	1.84	0.60
1:A:248:LEU:HD12	1:A:535:GLN:CB	2.32	0.60
1:A:265:ILE:HD12	1:A:360:VAL:HG12	1.84	0.59
1:A:97:ILE:HG12	1:A:404:VAL:HG23	1.84	0.59
1:A:130:ALA:HB2	1:A:145:HIS:CD2	2.38	0.59
2:B:230:ASN:C	2:B:230:ASN:HD22	2.06	0.59
1:A:443:LYS:HB3	12:A:799:HOH:O	2.02	0.59
1:A:473:MET:HG3	1:A:497:ILE:HD11	1.84	0.59
1:A:117:PRO:HD2	1:A:157:SER:OG	2.02	0.59
1:A:11:THR:O	1:A:11:THR:HG22	2.03	0.59
12:B:1251:HOH:O	3:C:27:SER:HB2	2.02	0.59
1:A:238:VAL:HG13	1:A:243:LEU:HB2	1.84	0.59
1:A:497:ILE:HG23	1:A:534:LEU:HD12	1.85	0.59
1:A:556:LYS:H	1:A:556:LYS:HD2	1.68	0.59
2:B:214:ARG:NH2	4:D:86:GLN:OE1	2.31	0.59
1:A:188:GLU:HG2	1:A:391:PRO:HB2	1.85	0.58
3:C:95:VAL:HG11	3:C:140:LEU:HB2	1.84	0.58
11:D:1306:EPH:H24	11:D:1306:EPH:H13	1.84	0.58
1:A:313:ARG:HB3	12:A:858:HOH:O	2.03	0.58
1:A:458:ARG:HG2	1:A:520:LEU:HD22	1.84	0.58
1:A:502:GLY:O	1:A:505:GLN:HG2	2.03	0.58
1:A:198:GLU:O	1:A:515:VAL:HG13	2.03	0.58
1:A:62:GLN:HB2	1:A:266:THR:HB	1.84	0.58
1:A:491:GLN:O	1:A:495:GLU:HG2	2.03	0.58
3:C:119:ILE:N	3:C:120:PRO:HD2	2.18	0.58
1:A:104:ALA:HB3	1:A:105:PRO:HD3	1.84	0.58
1:A:110:GLU:N	12:A:822:HOH:O	2.37	0.58
2:B:216:HIS:HD2	12:B:1272:HOH:O	1.87	0.58
1:A:373:THR:HG23	1:A:374:ASN:O	2.03	0.58
1:A:490:LEU:HD13	1:A:541:GLU:HA	1.84	0.58
2:B:159:ILE:HG22	2:B:159:ILE:O	2.04	0.58
4:D:37:LYS:HE3	4:D:41:LEU:HD21	1.86	0.58
2:B:176:ASP:CG	4:D:93:ARG:HH22	2.07	0.58
2:B:66:ARG:HD2	2:B:66:ARG:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:NH1	1:A:129:ARG:HG3	2.16	0.57
1:A:267:GLU:OE1	1:A:298:ARG:NH1	2.37	0.57
1:A:182:LEU:HD23	1:A:184:MET:HE3	1.86	0.57
1:A:290:PRO:O	1:A:293:LYS:HG3	2.05	0.57
2:B:174:ASN:HD22	4:D:93:ARG:NH1	2.02	0.57
3:C:69:ASN:ND2	3:C:71:GLU:HB2	2.18	0.57
1:A:26:GLY:HA2	5:A:700:FAD:H1B	1.87	0.57
1:A:246:GLN:HB2	1:A:372:PRO:HG3	1.87	0.56
1:A:409:ARG:NE	1:A:414:SER:HB2	2.19	0.56
3:C:141:ALA:HB1	12:C:1323:HOH:O	2.05	0.56
12:A:890:HOH:O	2:B:129:LEU:N	2.37	0.56
1:A:531:LEU:O	1:A:535:GLN:HG3	2.05	0.56
2:B:164:CYS:SG	2:B:165:SER:N	2.79	0.56
1:A:129:ARG:HH11	1:A:130:ALA:H	1.51	0.56
3:C:91:LYS:HD2	4:D:134:TRP:CE2	2.40	0.56
1:A:18:HIS:HB3	1:A:20:PHE:HE1	1.70	0.56
1:A:343:GLU:O	1:A:347:ILE:HG13	2.06	0.56
1:A:61:ALA:HA	5:A:700:FAD:N5	2.20	0.56
1:A:274:GLY:HA3	1:A:326:LEU:HD23	1.87	0.56
1:A:65:ILE:HD12	1:A:108:VAL:CG2	2.35	0.56
3:C:88:TYR:HB3	12:C:1317:HOH:O	2.06	0.56
1:A:182:LEU:HD23	1:A:184:MET:CE	2.35	0.55
1:A:410:LEU:O	1:A:413:ASN:HB2	2.06	0.55
4:D:48:VAL:O	4:D:51:VAL:HG22	2.05	0.55
1:A:541:GLU:HG3	1:A:542:ALA:N	2.21	0.55
1:A:81:PHE:O	1:A:85:VAL:HG12	2.07	0.55
2:B:165:SER:HA	2:B:181:PRO:HD2	1.89	0.55
4:D:123:ASP:OD1	4:D:124:VAL:HG23	2.07	0.55
3:C:59:PHE:HB3	12:C:1322:HOH:O	2.05	0.55
1:A:28:GLY:O	1:A:32:LEU:HB2	2.06	0.55
1:A:89:ASP:HB3	1:A:547:ARG:HG2	1.88	0.55
1:A:361:LEU:HD12	1:A:362:PRO:CD	2.38	0.54
1:A:554:ASP:HB2	1:A:555:PHE:CE2	2.43	0.54
1:A:594:LYS:HD3	12:A:842:HOH:O	2.07	0.54
3:C:64:LEU:HG	4:D:115:GLY:HA2	1.90	0.54
4:D:47:ARG:O	4:D:50:SER:HB2	2.08	0.54
1:A:103:GLN:HB2	12:A:753:HOH:O	2.07	0.54
2:B:198:PHE:HD2	2:B:201:GLU:HG3	1.73	0.54
1:A:264:LEU:HD22	1:A:365:HIS:CE1	2.42	0.54
1:A:314:GLY:HA3	1:A:319:LYS:CA	2.38	0.54
1:A:358:ILE:HG13	12:A:862:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:HIS:HE1	2:B:156:TYR:O	1.92	0.53
1:A:294:ASP:HA	12:A:859:HOH:O	2.08	0.53
1:A:355:LYS:O	1:A:356:GLU:HG2	2.08	0.53
1:A:471:LEU:HD11	1:A:475:LYS:NZ	2.24	0.53
1:A:59:VAL:HG22	1:A:159:LEU:HD23	1.89	0.53
1:A:10:SER:O	1:A:12:GLN:N	2.41	0.53
4:D:53:LEU:HD11	4:D:76:LEU:HD13	1.89	0.53
1:A:249:GLU:HG2	1:A:250:PHE:CD1	2.44	0.53
1:A:278:ASN:HB2	12:A:858:HOH:O	2.07	0.53
1:A:361:LEU:O	1:A:363:THR:HG23	2.07	0.53
1:A:143:GLN:NE2	1:A:295:LEU:HD23	2.24	0.53
2:B:92:ASN:C	2:B:92:ASN:ND2	2.60	0.53
1:A:457:LEU:HD23	1:A:523:THR:CG2	2.35	0.53
3:C:74:LEU:HD22	4:D:136:LEU:CD1	2.39	0.53
1:A:507:LEU:O	1:A:507:LEU:HD12	2.10	0.52
1:A:514:MET:HA	1:A:514:MET:HE3	1.91	0.52
1:A:470:ARG:NH2	12:A:817:HOH:O	2.43	0.52
2:B:200:GLU:OE2	2:B:247:GLU:HB3	2.09	0.52
1:A:130:ALA:HB2	1:A:145:HIS:HD2	1.75	0.52
1:A:118:PHE:HA	1:A:150:VAL:HG22	1.91	0.52
1:A:87:GLY:CA	1:A:620:ARG:HH12	2.21	0.52
1:A:158:LEU:HD23	1:A:415:LEU:HD22	1.92	0.52
2:B:105:MET:HE1	12:B:1271:HOH:O	2.08	0.52
1:A:322:VAL:O	1:A:323:TYR:HD1	1.92	0.52
1:A:514:MET:HA	1:A:514:MET:CE	2.40	0.52
1:A:277:ILE:HD13	1:A:325:GLN:HB2	1.92	0.52
1:A:509:THR:HG23	1:A:512:ARG:NH1	2.24	0.52
1:A:581:ARG:HH22	1:A:604:ASP:CG	2.12	0.52
3:C:52:LEU:HB3	10:C:1305:HEM:CAC	2.28	0.52
1:A:278:ASN:OD1	1:A:282:GLU:N	2.43	0.51
1:A:97:ILE:HA	1:A:404:VAL:HG23	1.92	0.51
1:A:373:THR:HG23	1:A:374:ASN:N	2.26	0.51
1:A:175:VAL:HG12	1:A:176:GLU:HG3	1.91	0.51
1:A:197:ILE:N	1:A:197:ILE:HD12	2.25	0.51
1:A:303:ARG:O	1:A:306:THR:HG22	2.10	0.51
2:B:173:TRP:CD1	9:B:1201:UQ1:HM22	2.46	0.51
2:B:136:GLN:OE1	2:B:139:LYS:HD2	2.11	0.51
2:B:56:ASP:OD1	2:B:58:THR:HB	2.09	0.51
3:C:96:PHE:HB3	3:C:97:PRO:CD	2.40	0.51
3:C:91:LYS:HG3	4:D:134:TRP:CH2	2.45	0.51
1:A:256:THR:HB	1:A:360:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:PHE:HD2	1:A:284:PHE:H	1.58	0.51
1:A:221:TYR:CG	1:A:364:VAL:HG21	2.46	0.51
2:B:92:ASN:HD21	2:B:94:ASP:CB	2.22	0.51
1:A:569:GLN:N	12:A:844:HOH:O	2.35	0.51
1:A:258:ILE:HD12	12:A:792:HOH:O	2.11	0.51
1:A:373:THR:CG2	1:A:374:ASN:N	2.73	0.51
1:A:61:ALA:HA	5:A:700:FAD:C5X	2.41	0.51
4:D:37:LYS:HE3	4:D:41:LEU:HD11	1.92	0.51
1:A:277:ILE:HD12	1:A:277:ILE:N	2.25	0.50
1:A:471:LEU:HD11	1:A:475:LYS:HZ3	1.74	0.50
1:A:113:ASN:HD22	2:B:138:GLY:N	1.95	0.50
2:B:161:CYS:O	2:B:162:ALA:HB3	2.10	0.50
1:A:275:ILE:HG22	1:A:276:LEU:N	2.22	0.50
1:A:597:LEU:H	1:A:597:LEU:HD23	1.77	0.50
1:A:265:ILE:HD12	1:A:360:VAL:CG1	2.41	0.50
1:A:346:MET:O	1:A:350:GLY:N	2.44	0.50
2:B:198:PHE:CD2	2:B:201:GLU:HG3	2.47	0.50
1:A:326:LEU:O	1:A:329:LEU:HD23	2.11	0.50
2:B:165:SER:OG	2:B:181:PRO:HD2	2.12	0.50
1:A:353:VAL:HG21	12:A:867:HOH:O	2.11	0.50
1:A:454:LEU:HD22	1:A:524:LEU:HD11	1.94	0.50
2:B:174:ASN:ND2	4:D:93:ARG:NH1	2.59	0.50
1:A:239:THR:CG2	1:A:588:VAL:HG13	2.40	0.50
1:A:254:HIS:HB2	1:A:365:HIS:HB2	1.93	0.50
2:B:109:LYS:HE2	12:B:1245:HOH:O	2.11	0.50
2:B:69:ILE:O	2:B:159:ILE:HD12	2.12	0.50
3:C:35:TRP:HZ3	3:C:43:ILE:HD11	1.77	0.50
1:A:312:GLY:C	1:A:313:ARG:HG3	2.32	0.49
1:A:517:ASN:HB2	12:A:807:HOH:O	2.12	0.49
2:B:45:LEU:O	2:B:49:ILE:HG12	2.12	0.49
3:C:77:VAL:HG12	3:C:82:LEU:HD21	1.94	0.49
1:A:43:PHE:CG	1:A:435:PRO:HG3	2.47	0.49
2:B:129:LEU:HD23	2:B:130:LYS:H	1.77	0.49
1:A:283:ARG:HH21	1:A:294:ASP:CG	2.16	0.49
1:A:517:ASN:OD1	1:A:519:ASP:HB3	2.13	0.49
1:A:266:THR:HG22	1:A:341:ILE:HG21	1.95	0.49
3:C:109:LEU:HD12	12:C:1329:HOH:O	2.12	0.49
2:B:215:CYS:SG	2:B:235:ILE:HG21	2.53	0.49
3:C:99:MET:HA	3:C:99:MET:HE2	1.95	0.49
4:D:68:MET:O	4:D:72:LEU:HB2	2.13	0.49
1:A:318:GLU:HB2	12:A:719:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:HB1	1:A:32:LEU:HD13	1.95	0.49
2:B:44:VAL:HG23	2:B:87:ARG:O	2.13	0.49
1:A:195:LEU:O	1:A:197:ILE:HD12	2.13	0.48
1:A:517:ASN:O	1:A:521:VAL:HG13	2.12	0.48
3:C:104:ASN:ND2	3:C:107:ARG:HE	2.11	0.48
3:C:48:THR:O	3:C:52:LEU:HB2	2.12	0.48
4:D:126:ILE:O	4:D:130:VAL:HG23	2.13	0.48
1:A:566:LYS:HB2	1:A:567:PRO:CD	2.43	0.48
2:B:214:ARG:HA	2:B:214:ARG:NE	2.27	0.48
1:A:254:HIS:HB2	1:A:365:HIS:CB	2.43	0.48
1:A:84:THR:HA	1:A:410:LEU:HD22	1.95	0.48
1:A:411:GLY:O	1:A:412:ALA:HB3	2.12	0.48
1:A:65:ILE:HD11	1:A:416:LEU:HD13	1.94	0.48
2:B:51:ILE:O	2:B:51:ILE:HD12	2.13	0.48
1:A:465:ARG:HG2	12:A:745:HOH:O	2.13	0.48
1:A:486:VAL:HG12	1:A:553:GLU:HB2	1.96	0.48
1:A:135:SER:OG	1:A:139:GLY:HA2	2.13	0.48
2:B:141:GLN:HG2	12:B:1231:HOH:O	2.12	0.48
2:B:180:GLY:O	2:B:184:LEU:HG	2.14	0.48
2:B:73:CYS:O	2:B:74:ALA:C	2.52	0.48
1:A:258:ILE:HD12	1:A:258:ILE:N	2.22	0.48
1:A:497:ILE:CG2	1:A:534:LEU:HD12	2.44	0.48
1:A:454:LEU:CD1	1:A:520:LEU:HD21	2.44	0.48
2:B:14:PHE:O	2:B:32:THR:HA	2.14	0.48
1:A:273:GLY:HA3	1:A:329:LEU:HD11	1.96	0.48
1:A:458:ARG:HH11	1:A:458:ARG:CG	2.24	0.48
2:B:174:ASN:ND2	4:D:93:ARG:HH11	2.12	0.48
1:A:303:ARG:HG3	1:A:484:PHE:CZ	2.49	0.48
1:A:354:THR:HG23	1:A:355:LYS:HG3	1.94	0.48
1:A:378:GLN:HG3	12:A:794:HOH:O	2.14	0.48
4:D:134:TRP:CD1	11:D:1306:EPH:H182	2.49	0.48
1:A:296:ALA:HB3	12:A:784:HOH:O	2.14	0.48
1:A:314:GLY:HA3	1:A:319:LYS:HA	1.96	0.48
4:D:89:THR:HG22	4:D:102:LYS:CE	2.44	0.48
1:A:10:SER:C	1:A:12:GLN:H	2.18	0.47
1:A:306:THR:HG21	1:A:483:VAL:HG11	1.96	0.47
1:A:458:ARG:NH2	1:A:514:MET:HE3	2.29	0.47
2:B:75:MET:HG3	2:B:77:ILE:HD11	1.95	0.47
2:B:18:ARG:HH11	2:B:18:ARG:HB3	1.78	0.47
12:A:890:HOH:O	2:B:190:TRP:CZ3	2.66	0.47
2:B:49:ILE:O	2:B:52:LYS:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ARG:NH1	1:A:512:ARG:HG3	2.26	0.47
1:A:231:THR:HA	1:A:529:LEU:HD21	1.96	0.47
2:B:66:ARG:CD	2:B:66:ARG:O	2.62	0.47
4:D:49:VAL:HG11	4:D:78:LEU:HD13	1.97	0.47
1:A:412:ALA:N	12:A:847:HOH:O	2.47	0.47
1:A:202:ILE:CD1	1:A:451:VAL:HG22	2.36	0.47
2:B:133:ASP:HB3	12:B:1273:HOH:O	2.15	0.47
1:A:63:GLY:N	5:A:700:FAD:O4	2.48	0.47
2:B:58:THR:HB	12:B:1257:HOH:O	2.13	0.47
1:A:36:PHE:CD1	1:A:36:PHE:C	2.88	0.47
1:A:366:TYR:CD2	1:A:409:ARG:HD3	2.50	0.47
1:A:454:LEU:CD2	1:A:524:LEU:HD11	2.45	0.47
2:B:58:THR:HG22	2:B:58:THR:O	2.13	0.47
1:A:13:TYR:OH	1:A:458:ARG:NH1	2.47	0.47
1:A:133:GLY:HA2	12:A:777:HOH:O	2.15	0.47
1:A:338:LEU:HB3	1:A:341:ILE:HG12	1.96	0.47
3:C:78:LYS:HA	3:C:82:LEU:HD12	1.96	0.47
1:A:10:SER:C	1:A:12:GLN:N	2.67	0.47
1:A:258:ILE:CD1	1:A:258:ILE:H	2.21	0.47
1:A:131:PHE:HE2	1:A:268:GLY:N	2.11	0.47
1:A:577:GLN:HG2	1:A:577:GLN:H	1.55	0.47
1:A:90:TRP:CD2	1:A:617:PRO:HA	2.50	0.47
1:A:90:TRP:CE2	1:A:617:PRO:HA	2.50	0.47
2:B:129:LEU:HD23	2:B:130:LYS:N	2.29	0.47
2:B:246:LYS:O	2:B:247:GLU:HB3	2.14	0.47
1:A:373:THR:HG21	12:A:732:HOH:O	2.14	0.46
2:B:99:ILE:N	2:B:99:ILE:HD12	2.30	0.46
4:D:61:TYR:CD2	4:D:62:LEU:HD23	2.50	0.46
1:A:470:ARG:HD2	12:A:762:HOH:O	2.15	0.46
2:B:65:CYS:O	2:B:66:ARG:HG3	2.15	0.46
12:A:830:HOH:O	3:C:6:THR:HG22	2.14	0.46
1:A:403:SER:N	12:A:746:HOH:O	2.46	0.46
2:B:189:ARG:NH2	2:B:193:ASP:OD1	2.49	0.46
2:B:236:ALA:O	2:B:240:LYS:HG3	2.15	0.46
1:A:36:PHE:HE2	1:A:162:LEU:HD22	1.80	0.46
1:A:305:MET:O	1:A:309:ILE:HG13	2.16	0.46
1:A:54:THR:HG23	12:A:843:HOH:O	2.15	0.46
1:A:265:ILE:CD1	1:A:358:ILE:HG21	2.45	0.46
3:C:118:THR:O	3:C:122:LEU:HB2	2.15	0.46
1:A:597:LEU:CD2	1:A:597:LEU:N	2.79	0.46
1:A:509:THR:HG23	1:A:512:ARG:HH12	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:ARG:NH1	12:D:1309:HOH:O	2.49	0.46
4:D:61:TYR:HD2	4:D:62:LEU:HD23	1.81	0.46
2:B:146:ILE:HG13	2:B:146:ILE:O	2.11	0.46
2:B:102:LEU:HB3	2:B:166:THR:HG21	1.97	0.46
2:B:188:TYR:OH	2:B:237:GLU:HG2	2.16	0.46
1:A:197:ILE:H	1:A:197:ILE:HD12	1.80	0.46
1:A:249:GLU:HG2	1:A:250:PHE:N	2.31	0.46
1:A:267:GLU:HB2	1:A:298:ARG:HH12	1.80	0.46
2:B:82:THR:HG21	2:B:87:ARG:NH2	2.31	0.46
1:A:265:ILE:HD13	1:A:358:ILE:HG21	1.98	0.45
1:A:454:LEU:HD11	1:A:520:LEU:HD21	1.97	0.45
3:C:104:ASN:HD21	3:C:107:ARG:HH21	1.63	0.45
4:D:52:LEU:HD12	4:D:52:LEU:HA	1.84	0.45
1:A:86:LYS:O	1:A:620:ARG:NH1	2.49	0.45
4:D:128:LYS:HE3	12:D:1319:HOH:O	2.17	0.45
1:A:195:LEU:HD11	1:A:200:GLY:HA2	1.98	0.45
1:A:250:PHE:O	1:A:368:MET:HG2	2.16	0.45
2:B:213:TYR:N	12:B:1242:HOH:O	2.46	0.45
2:B:227:LYS:HD2	12:B:1269:HOH:O	2.17	0.45
1:A:176:GLU:O	1:A:197:ILE:HD13	2.16	0.45
1:A:23:VAL:HG23	1:A:207:ALA:HB3	1.98	0.45
1:A:284:PHE:CD1	1:A:308:GLU:HG3	2.52	0.45
1:A:351:VAL:HG11	1:A:358:ILE:HD13	1.97	0.45
1:A:409:ARG:HE	1:A:414:SER:CB	2.24	0.45
3:C:29:HIS:CD2	3:C:30:ILE:HD12	2.51	0.45
1:A:521:VAL:O	1:A:525:GLU:HG3	2.16	0.45
1:A:73:GLU:HG2	1:A:74:GLU:O	2.17	0.45
2:B:181:PRO:HG3	8:B:304:F3S:S3	2.57	0.45
3:C:61:LEU:O	3:C:65:LEU:HG	2.16	0.45
1:A:72:MET:CE	1:A:121:THR:HG21	2.47	0.45
4:D:119:PHE:O	4:D:123:ASP:HB3	2.17	0.45
1:A:149:CYS:HB2	1:A:154:THR:HG21	1.98	0.45
2:B:213:TYR:HB2	12:B:1242:HOH:O	2.17	0.45
1:A:339:PRO:HG2	12:A:803:HOH:O	2.16	0.45
1:A:556:LYS:N	1:A:556:LYS:HD2	2.32	0.45
1:A:184:MET:HB2	1:A:184:MET:HE2	1.78	0.44
1:A:254:HIS:NE2	1:A:264:LEU:HD11	2.32	0.44
1:A:266:THR:HG22	1:A:341:ILE:CG2	2.47	0.44
1:A:297:SER:HB3	1:A:299:ASP:OD1	2.18	0.44
1:A:195:LEU:HD22	1:A:454:LEU:HD21	1.99	0.44
1:A:129:ARG:O	1:A:147:CYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:CYS:CB	1:A:154:THR:HG21	2.47	0.44
1:A:72:MET:HE3	1:A:121:THR:CG2	2.48	0.44
2:B:121:GLN:NE2	2:B:171:TYR:OH	2.40	0.44
2:B:165:SER:HA	2:B:181:PRO:CD	2.47	0.44
3:C:32:ILE:HD12	3:C:33:TYR:N	2.32	0.44
3:C:90:ALA:O	3:C:94:ILE:HG12	2.17	0.44
11:D:1306:EPH:H11	12:D:1316:HOH:O	2.17	0.44
1:A:131:PHE:HE2	1:A:268:GLY:HA2	1.83	0.44
1:A:568:ILE:O	1:A:569:GLN:HB2	2.17	0.44
1:A:434:ARG:O	1:A:437:ASP:OD2	2.35	0.44
2:B:31:GLN:HG2	12:B:1259:HOH:O	2.17	0.44
3:C:102:THR:HG23	10:C:1305:HEM:HBB2	1.98	0.44
1:A:303:ARG:HH11	1:A:303:ARG:CG	2.25	0.44
1:A:554:ASP:N	1:A:554:ASP:OD1	2.39	0.44
2:B:133:ASP:HB3	12:B:1241:HOH:O	2.16	0.44
2:B:92:ASN:ND2	2:B:94:ASP:HB2	2.30	0.44
3:C:89:THR:N	12:C:1317:HOH:O	2.49	0.44
4:D:89:THR:HG22	4:D:102:LYS:HE2	1.99	0.44
3:C:122:LEU:HA	3:C:122:LEU:HD12	1.85	0.44
1:A:129:ARG:NH1	1:A:130:ALA:HB3	2.32	0.44
3:C:102:THR:OG1	10:C:1305:HEM:HBB2	2.18	0.44
3:C:7:THR:HB	12:C:1307:HOH:O	2.17	0.44
3:C:81:CYS:HA	12:C:1321:HOH:O	2.18	0.44
1:A:122:GLU:OE1	1:A:122:GLU:HA	2.18	0.43
1:A:303:ARG:HG2	1:A:303:ARG:NH1	2.29	0.43
1:A:324:LEU:HD12	1:A:360:VAL:HG11	1.99	0.43
1:A:88:SER:HB2	1:A:406:GLY:HA3	2.00	0.43
1:A:91:LEU:O	1:A:583:HIS:HE1	2.00	0.43
4:D:72:LEU:HB3	4:D:126:ILE:HD11	2.00	0.43
1:A:512:ARG:CG	1:A:512:ARG:HH11	2.27	0.43
1:A:239:THR:HG23	1:A:588:VAL:HG13	2.00	0.43
2:B:225:CYS:HA	2:B:226:PRO:HD3	1.91	0.43
3:C:74:LEU:O	3:C:77:VAL:N	2.45	0.43
3:C:88:TYR:HA	12:C:1323:HOH:O	2.18	0.43
1:A:338:LEU:N	1:A:339:PRO:CD	2.82	0.43
2:B:81:ASN:ND2	2:B:166:THR:HG23	2.34	0.43
2:B:176:ASP:HB3	3:C:16:TRP:CZ2	2.54	0.43
4:D:100:ALA:O	4:D:103:ALA:HB3	2.19	0.43
1:A:286:GLU:HG3	1:A:293:LYS:HE2	2.00	0.43
1:A:301:VAL:O	1:A:305:MET:HG3	2.19	0.43
1:A:360:VAL:HG23	12:A:788:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:VAL:HG12	1:A:554:ASP:OD1	2.18	0.43
1:A:65:ILE:HD13	1:A:65:ILE:C	2.39	0.43
2:B:74:ALA:HB3	12:B:1276:HOH:O	2.19	0.43
3:C:102:THR:HG23	10:C:1305:HEM:CBB	2.48	0.43
1:A:18:HIS:HB3	1:A:20:PHE:CE1	2.51	0.43
1:A:255:PRO:HA	1:A:362:PRO:HG3	2.00	0.43
1:A:458:ARG:NH2	1:A:514:MET:CE	2.82	0.43
2:B:230:ASN:CG	2:B:233:LYS:HB3	2.38	0.43
4:D:105:LEU:HD23	12:D:1317:HOH:O	2.18	0.43
1:A:107:SER:HB3	1:A:419:VAL:CG1	2.49	0.43
1:A:329:LEU:HD12	1:A:333:GLN:OE1	2.18	0.43
1:A:374:ASN:HA	1:A:374:ASN:HD22	1.58	0.43
2:B:66:ARG:C	2:B:66:ARG:HD2	2.39	0.43
2:B:164:CYS:HB2	2:B:221:CYS:HB2	2.00	0.43
1:A:576:PHE:HA	1:A:579:HIS:CE1	2.54	0.43
2:B:217:THR:O	2:B:217:THR:HG22	2.19	0.43
1:A:464:ILE:O	1:A:507:LEU:HA	2.19	0.42
2:B:19:TRP:CZ3	2:B:21:PRO:HG3	2.54	0.42
1:A:201:SER:HB2	12:A:831:HOH:O	2.18	0.42
3:C:38:PRO:HA	12:C:1309:HOH:O	2.19	0.42
1:A:150:VAL:HB	1:A:154:THR:HA	2.01	0.42
1:A:588:VAL:HA	1:A:594:LYS:O	2.18	0.42
1:A:316:GLY:O	1:A:317:PRO:C	2.57	0.42
1:A:409:ARG:HH21	5:A:700:FAD:C2	2.33	0.42
3:C:91:LYS:HD2	4:D:134:TRP:CD2	2.55	0.42
4:D:37:LYS:HB2	4:D:40:SER:OG	2.20	0.42
1:A:72:MET:HE3	1:A:121:THR:HG21	2.00	0.42
1:A:256:THR:CA	1:A:360:VAL:HB	2.45	0.42
2:B:218:ILE:HD11	12:B:1272:HOH:O	2.18	0.42
3:C:93:GLY:O	3:C:97:PRO:HD2	2.20	0.42
1:A:131:PHE:HE2	1:A:268:GLY:CA	2.33	0.42
1:A:131:PHE:CE2	1:A:268:GLY:HA2	2.54	0.42
1:A:303:ARG:NH2	1:A:548:GLY:O	2.53	0.42
1:A:324:LEU:O	1:A:358:ILE:N	2.52	0.42
2:B:246:LYS:O	2:B:247:GLU:CB	2.67	0.42
1:A:351:VAL:HG13	1:A:356:GLU:HB2	2.02	0.42
1:A:57:HIS:HA	12:A:797:HOH:O	2.18	0.42
4:D:72:LEU:HD23	4:D:126:ILE:CD1	2.48	0.42
1:A:221:TYR:CD2	1:A:364:VAL:HG21	2.55	0.42
1:A:40:GLU:HA	1:A:169:TYR:CE2	2.55	0.42
4:D:123:ASP:OD1	4:D:124:VAL:N	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:PHE:O	1:A:286:GLU:N	2.51	0.41
1:A:332:GLU:O	1:A:335:ALA:HB3	2.20	0.41
1:A:469:LEU:HD21	1:A:504:LEU:HD23	2.02	0.41
9:B:1201:UQ1:HM52	3:C:43:ILE:CD1	2.49	0.41
1:A:129:ARG:HA	1:A:129:ARG:HD2	1.62	0.41
1:A:257:GLY:HA2	12:A:792:HOH:O	2.19	0.41
1:A:284:PHE:HD1	1:A:308:GLU:HG3	1.85	0.41
1:A:282:GLU:HG2	1:A:283:ARG:N	2.35	0.41
1:A:298:ARG:HE	1:A:409:ARG:NH1	2.13	0.41
2:B:164:CYS:SG	2:B:182:ALA:HB2	2.60	0.41
1:A:276:LEU:C	1:A:277:ILE:HD12	2.40	0.41
1:A:100:MET:SD	1:A:404:VAL:HG21	2.61	0.41
1:A:481:ALA:HB2	1:A:537:ILE:HD13	2.03	0.41
1:A:56:SER:O	1:A:59:VAL:HG23	2.21	0.41
5:A:700:FAD:H4'	12:A:886:HOH:O	2.20	0.41
3:C:78:LYS:HA	3:C:82:LEU:CD1	2.50	0.41
1:A:65:ILE:HD13	1:A:66:ASN:N	2.35	0.41
1:A:167:LEU:HG	2:B:123:LYS:HG3	2.03	0.41
2:B:51:ILE:HA	2:B:55:ILE:HG12	2.02	0.41
2:B:73:CYS:HB3	2:B:84:ALA:H	1.85	0.41
3:C:118:THR:OG1	3:C:121:GLN:HB2	2.21	0.41
2:B:52:LYS:HD2	2:B:57:SER:HA	2.02	0.41
4:D:77:THR:HG22	4:D:112:THR:HG22	2.02	0.41
4:D:98:GLN:HG3	12:D:1323:HOH:O	2.21	0.41
1:A:26:GLY:HA2	5:A:700:FAD:C1B	2.50	0.41
1:A:341:ILE:HG13	1:A:342:SER:N	2.34	0.41
1:A:373:THR:HG22	1:A:374:ASN:O	2.21	0.41
2:B:208:ASP:HB2	2:B:209:PRO:HD2	2.02	0.41
1:A:327:HIS:ND1	1:A:355:LYS:HA	2.36	0.41
1:A:442:ILE:O	1:A:442:ILE:HG23	2.21	0.41
1:A:61:ALA:HA	5:A:700:FAD:C6	2.51	0.41
1:A:103:GLN:HG3	1:A:107:SER:OG	2.20	0.41
1:A:129:ARG:HH11	1:A:129:ARG:CG	2.25	0.41
1:A:516:TRP:CH2	2:B:62:ARG:HG2	2.56	0.41
3:C:109:LEU:HD13	4:D:51:VAL:HG12	2.02	0.41
1:A:217:TYR:CD1	1:A:217:TYR:O	2.74	0.41
1:A:59:VAL:CG2	1:A:159:LEU:CD2	2.99	0.41
3:C:104:ASN:HA	3:C:104:ASN:HD22	1.73	0.41
1:A:48:VAL:HG21	1:A:205:ILE:HD12	2.03	0.40
1:A:322:VAL:CG1	1:A:323:TYR:H	2.13	0.40
1:A:480:HIS:HD2	1:A:489:VAL:O	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:ASN:ND2	2:B:94:ASP:N	2.66	0.40
1:A:51:LEU:HD21	1:A:229:THR:HG21	2.03	0.40
1:A:81:PHE:CD2	1:A:612:CYS:SG	3.14	0.40
1:A:381:ARG:HD2	1:A:388:GLN:OE1	2.22	0.40
1:A:563:ASP:HB2	12:A:804:HOH:O	2.22	0.40
1:A:197:ILE:H	1:A:197:ILE:CD1	2.33	0.40
1:A:283:ARG:O	1:A:286:GLU:HB3	2.21	0.40
1:A:91:LEU:O	1:A:583:HIS:CE1	2.73	0.40
2:B:69:ILE:HD12	2:B:69:ILE:C	2.41	0.40
3:C:39:MET:O	3:C:43:ILE:HG13	2.21	0.40
1:A:451:VAL:O	1:A:454:LEU:HB3	2.21	0.40
2:B:136:GLN:O	2:B:139:LYS:HG2	2.22	0.40
3:C:85:THR:O	3:C:85:THR:HG22	2.22	0.40
4:D:72:LEU:HD23	4:D:126:ILE:HD11	2.02	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	611/622 (98%)	541 (88%)	61 (10%)	9 (2%)	10	14
2	B	237/252 (94%)	219 (92%)	16 (7%)	2 (1%)	19	29
3	C	136/140 (97%)	125 (92%)	9 (7%)	2 (2%)	10	14
4	D	100/103 (97%)	92 (92%)	7 (7%)	1 (1%)	15	23
All	All	1084/1117 (97%)	977 (90%)	93 (9%)	14 (1%)	12	17

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	THR

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Mol	Chain	Res	Type
1	A	286	GLU
1	A	569	GLN
1	A	260	GLY
1	A	266	THR
1	A	317	PRO
2	B	74	ALA
3	C	82	LEU
1	A	63	GLY
2	B	64	SER
3	C	81	CYS
1	A	462	GLY
4	D	96	ALA
1	A	132	GLY

### 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	499/506 (99%)	465 (93%)	34 (7%)	16	25
2	B	214/221 (97%)	198 (92%)	16 (8%)	13	21
3	C	117/118 (99%)	112 (96%)	5 (4%)	29	46
4	D	76/76 (100%)	71 (93%)	5 (7%)	16	26
All	All	906/921 (98%)	846 (93%)	60 (7%)	16	26

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	36	PHE
1	A	54	THR
1	A	65	ILE
1	A	73	GLU
1	A	129	ARG
1	A	131	PHE
1	A	165	ARG

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Mol	Chain	Res	Type
1	A	167	LEU
1	A	182	LEU
1	A	284	PHE
1	A	303	ARG
1	A	317	PRO
1	A	321	HIS
1	A	324	LEU
1	A	344	THR
1	A	368	MET
1	A	373	THR
1	A	374	ASN
1	A	454	LEU
1	A	458	ARG
1	A	463	THR
1	A	485	ARG
1	A	497	ILE
1	A	521	VAL
1	A	541	GLU
1	A	554	ASP
1	A	556	LYS
1	A	558	ARG
1	A	568	ILE
1	A	588	VAL
1	A	597	LEU
1	A	598	GLU
1	A	602	VAL
2	B	18	ARG
2	B	51	ILE
2	B	63	ARG
2	B	66	ARG
2	B	87	ARG
2	B	92	ASN
2	B	129	LEU
2	B	134	GLU
2	B	146	ILE
2	B	166	THR
2	B	189	ARG
2	B	192	ILE
2	B	214	ARG
2	B	220	ASN
2	B	230	ASN
2	B	237	GLU

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Mol	Chain	Res	Type
3	C	13	GLU
3	C	30	ILE
3	C	52	LEU
3	C	72	SER
3	C	108	HIS
4	D	52	LEU
4	D	78	LEU
4	D	89	THR
4	D	108	LEU
4	D	134	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	113	ASN
1	A	128	GLN
1	A	145	HIS
1	A	156	HIS
1	A	246	GLN
1	A	254	HIS
1	A	374	ASN
1	A	378	GLN
1	A	384	ASN
1	A	408	ASN
1	A	453	ASN
1	A	461	ASN
1	A	474	GLN
1	A	527	GLN
1	A	550	HIS
1	A	571	GLN
1	A	579	HIS
2	B	31	GLN
2	B	39	ASN
2	B	92	ASN
2	B	121	GLN
2	B	174	ASN
2	B	186	GLN
2	B	220	ASN
2	B	230	ASN
3	C	17	ASN
3	C	29	HIS

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Mol	Chain	Res	Type
3	C	104	ASN
4	D	98	GLN
4	D	122	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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
11	EPH	D	1307	-	35,35,48	1.97	9 (25%)	37,40,53	2.37	4 (10%)
10	HEM	C	1305	3,4	27,50,50	0.99	1 (3%)	17,82,82	1.40	3 (17%)
6	FES	B	302	2	0,4,4	0.00	-	-		
8	F3S	B	304	2	0,9,9	0.00	-	-		
7	SF4	B	303	2	0,12,12	0.00	-	-		
11	EPH	D	1306	-	43,43,48	1.84	9 (20%)	45,48,53	2.23	5 (11%)
9	UQ1	B	1201	-	18,18,18	2.97	4 (22%)	22,25,25	2.95	8 (36%)
5	FAD	A	700	1	51,58,58	2.70	17 (33%)	60,89,89	2.05	6 (10%)

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
11	EPH	D	1307	-	-	7/39/39/52	-
10	HEM	C	1305	3,4	-	0/6/54/54	-
6	FES	B	302	2	-	-	0/1/1/1
8	F3S	B	304	2	-	-	0/3/3/3
7	SF4	B	303	2	-	-	0/6/5/5
11	EPH	D	1306	-	-	30/47/47/52	-
9	UQ1	B	1201	-	-	3/9/33/33	0/1/1/1
5	FAD	A	700	1	-	4/30/50/50	0/6/6/6

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	FAD	C9A-N10	8.71	1.50	1.38
9	B	1201	UQ1	C7-C6	8.69	1.65	1.51
9	B	1201	UQ1	C10-C9	7.78	1.71	1.50
5	A	700	FAD	C6-C7	6.95	1.55	1.37
11	D	1307	EPH	C29-C28	6.83	1.71	1.31
11	D	1306	EPH	C29-C28	6.68	1.70	1.31
5	A	700	FAD	C10-N1	5.67	1.40	1.33
5	A	700	FAD	C4-N3	5.45	1.42	1.33
5	A	700	FAD	C4X-N5	5.41	1.41	1.33
5	A	700	FAD	C4X-C10	5.24	1.44	1.38
5	A	700	FAD	C4A-N3A	4.57	1.42	1.35
11	D	1307	EPH	C25-C24	4.46	1.57	1.31
11	D	1306	EPH	C18-C4	-4.38	1.37	1.50
11	D	1306	EPH	C25-C24	3.78	1.53	1.31
11	D	1306	EPH	C13-C12	3.59	1.52	1.31
11	D	1307	EPH	P1-O7	3.56	1.63	1.50
5	A	700	FAD	C9-C8	3.39	1.46	1.37
11	D	1307	EPH	C26-C25	3.35	1.68	1.50
5	A	700	FAD	C5X-N5	3.20	1.40	1.35
11	D	1306	EPH	C27-C28	-3.20	1.32	1.50
11	D	1306	EPH	C15-C16	3.11	1.52	1.29
5	A	700	FAD	O2B-C2B	-3.10	1.35	1.43
11	D	1307	EPH	C18-C4	3.10	1.59	1.50
10	C	1305	HEM	C3B-C2B	-3.03	1.36	1.40
5	A	700	FAD	C9A-C5X	2.78	1.48	1.42
11	D	1306	EPH	P1-O7	2.77	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1201	UQ1	C7-C8	2.68	1.54	1.50
11	D	1306	EPH	C26-C25	2.62	1.64	1.50
5	A	700	FAD	C9-C9A	2.54	1.45	1.40
11	D	1307	EPH	C37-C2	2.47	1.58	1.50
11	D	1307	EPH	O2-C4	2.41	1.40	1.33
11	D	1306	EPH	C10-C11	-2.31	1.43	1.52
5	A	700	FAD	C4'-C3'	2.31	1.57	1.53
5	A	700	FAD	O4B-C1B	2.14	1.44	1.41
5	A	700	FAD	PA-O2A	-2.11	1.45	1.55
9	B	1201	UQ1	C6-C1	2.10	1.52	1.46
11	D	1307	EPH	C5-C3	2.08	1.56	1.50
5	A	700	FAD	C6A-C5A	-2.05	1.35	1.43
5	A	700	FAD	C2A-N1A	2.04	1.37	1.33
11	D	1307	EPH	P1-O5	2.03	1.67	1.59

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	1307	EPH	C27-C26-C25	12.73	146.29	112.92
11	D	1306	EPH	C27-C26-C25	11.98	144.32	112.92
5	A	700	FAD	C4-N3-C2	10.93	124.37	115.14
9	B	1201	UQ1	C8-C7-C6	9.58	137.88	112.05
9	B	1201	UQ1	C10-C9-C8	-6.59	103.59	122.65
11	D	1306	EPH	C15-C14-C13	5.56	139.41	112.02
5	A	700	FAD	C1'-N10-C10	4.99	122.88	118.41
5	A	700	FAD	C4X-C4-N3	-4.90	116.73	123.43
9	B	1201	UQ1	C11-C9-C10	-4.00	105.77	114.60
11	D	1307	EPH	C26-C27-C28	3.74	122.72	112.92
11	D	1306	EPH	C14-C15-C16	3.02	149.07	123.74
5	A	700	FAD	C10-C4X-N5	2.82	123.21	121.26
9	B	1201	UQ1	C7-C8-C9	-2.80	118.48	127.26
11	D	1306	EPH	C2-O1-C3	2.60	124.20	117.79
9	B	1201	UQ1	O1-C1-C6	-2.58	117.03	121.55
5	A	700	FAD	C4X-N5-C5X	2.43	119.20	116.77
10	C	1305	HEM	CMC-C2C-C3C	2.43	129.22	124.68
11	D	1307	EPH	C26-C25-C24	2.33	142.64	124.73
5	A	700	FAD	O5B-PA-O1A	-2.28	100.15	109.07
9	B	1201	UQ1	CM5-C5-C6	-2.27	120.69	124.40
10	C	1305	HEM	CMB-C2B-C3B	2.23	128.85	124.68
9	B	1201	UQ1	C11-C9-C8	2.23	129.08	122.65
10	C	1305	HEM	CMA-C3A-C4A	-2.19	125.09	128.46
11	D	1306	EPH	C6-C5-C3	-2.08	106.04	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1201	UQ1	CM3-O3-C3	-2.05	109.21	116.47
11	D	1307	EPH	C37-C2-C1	2.02	116.56	111.79

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	1307	EPH	C25-C26-C27-C28
11	D	1307	EPH	O8-C38-C39-N1
11	D	1306	EPH	C27-C28-C29-C30
11	D	1306	EPH	C28-C29-C30-C31
11	D	1306	EPH	C37-O5-P1-O6
11	D	1306	EPH	C37-O5-P1-O7
11	D	1306	EPH	C37-O5-P1-O8
11	D	1306	EPH	O3-C3-O1-C2
11	D	1306	EPH	C5-C3-O1-C2
11	D	1306	EPH	C14-C15-C16-C17
11	D	1306	EPH	C38-O8-P1-O7
11	D	1306	EPH	O8-C38-C39-N1
5	A	700	FAD	N10-C1'-C2'-O2'
5	A	700	FAD	N10-C1'-C2'-C3'
9	B	1201	UQ1	C7-C8-C9-C10
11	D	1307	EPH	C4-C18-C19-C20
11	D	1306	EPH	C23-C24-C25-C26
11	D	1306	EPH	C18-C4-O2-C1
11	D	1306	EPH	C11-C10-C9-C8
11	D	1306	EPH	C4-C18-C19-C20
11	D	1306	EPH	C11-C12-C13-C14
11	D	1306	EPH	C21-C22-C23-C24
11	D	1306	EPH	O4-C4-O2-C1
11	D	1306	EPH	C7-C8-C9-C10
11	D	1306	EPH	C18-C19-C20-C21
11	D	1306	EPH	O2-C1-C2-O1
11	D	1307	EPH	C27-C28-C29-C30
11	D	1306	EPH	O2-C1-C2-C37
11	D	1306	EPH	C12-C13-C14-C15
5	A	700	FAD	P-O3P-PA-O1A
11	D	1306	EPH	C38-O8-P1-O6
11	D	1306	EPH	C38-O8-P1-O5
11	D	1306	EPH	C2-C37-O5-P1
9	B	1201	UQ1	C7-C8-C9-C11
11	D	1306	EPH	C24-C25-C26-C27

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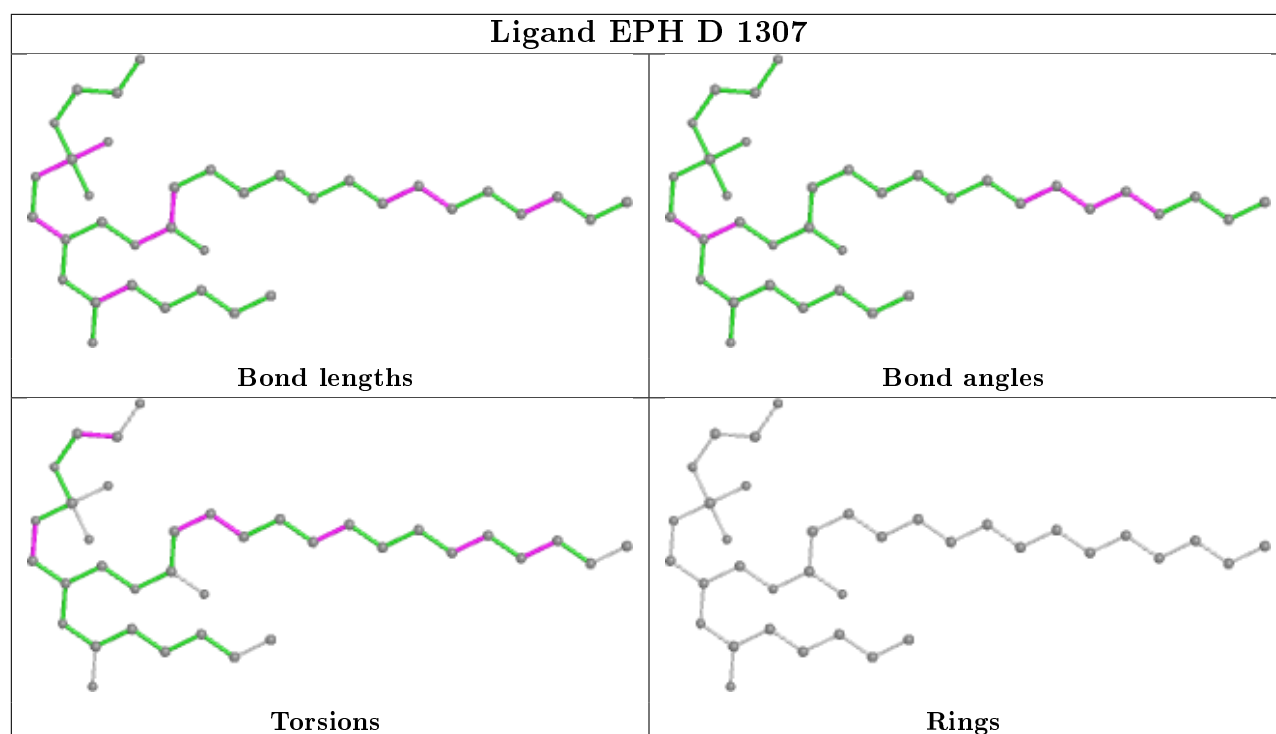
Mol	Chain	Res	Type	Atoms
11	D	1306	EPH	C1-C2-O1-C3
11	D	1306	EPH	C37-C2-O1-C3
11	D	1306	EPH	C5-C6-C7-C8
11	D	1306	EPH	C25-C26-C27-C28
11	D	1307	EPH	C21-C22-C23-C24
9	B	1201	UQ1	C1-C2-O2-CM2
11	D	1307	EPH	C18-C19-C20-C21
11	D	1307	EPH	C2-C37-O5-P1
5	A	700	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

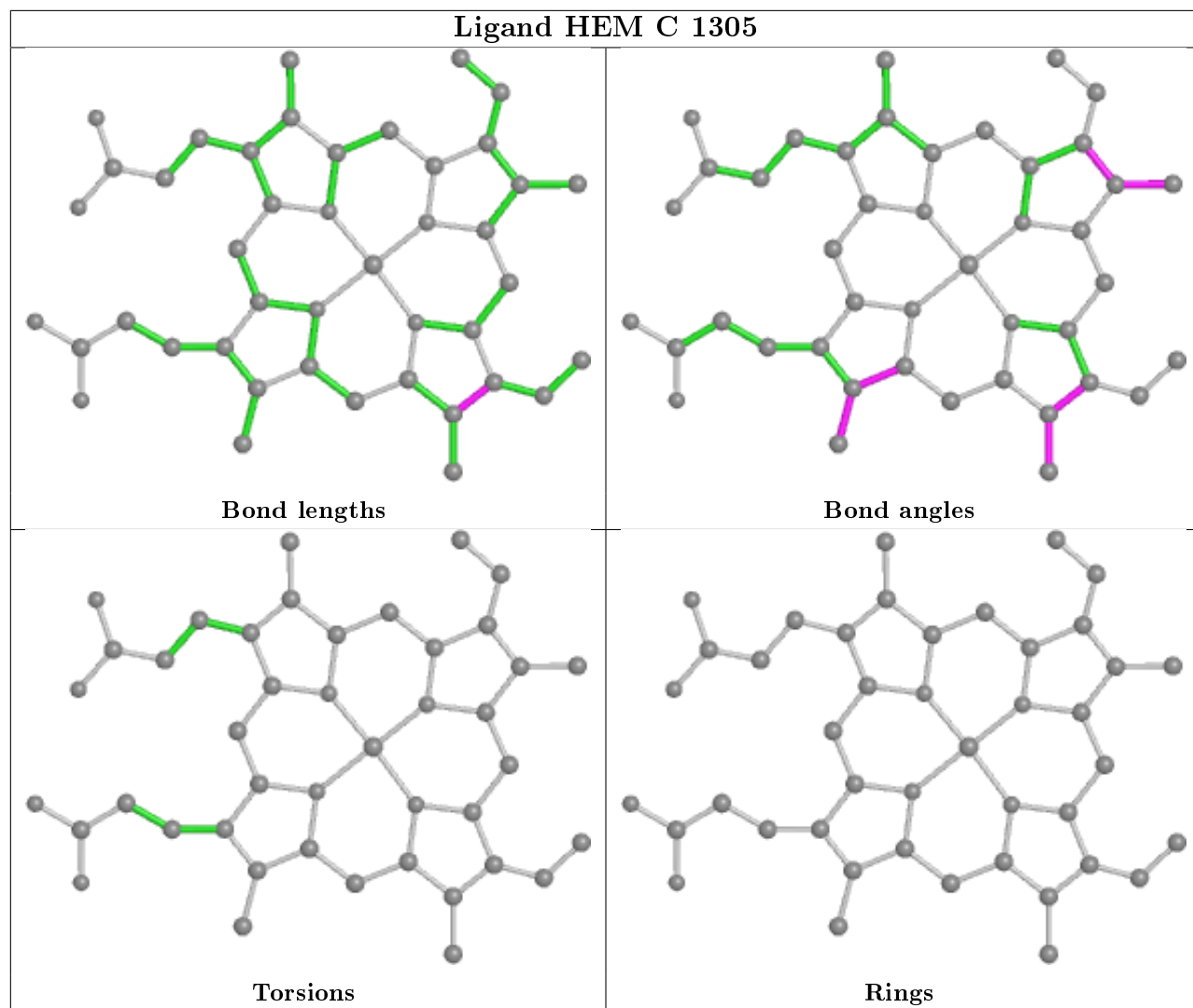
5 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1305	HEM	7	0
8	B	304	F3S	3	0
11	D	1306	EPH	4	0
9	B	1201	UQ1	3	0
5	A	700	FAD	14	0

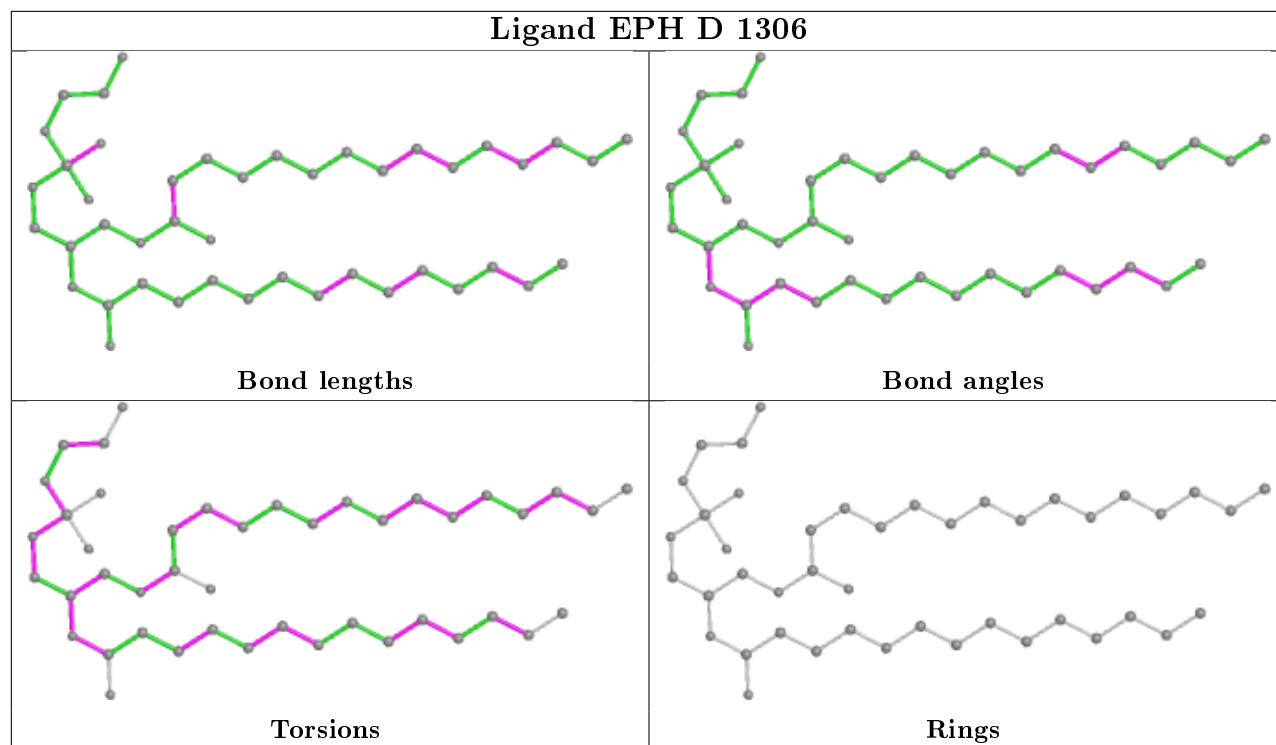
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



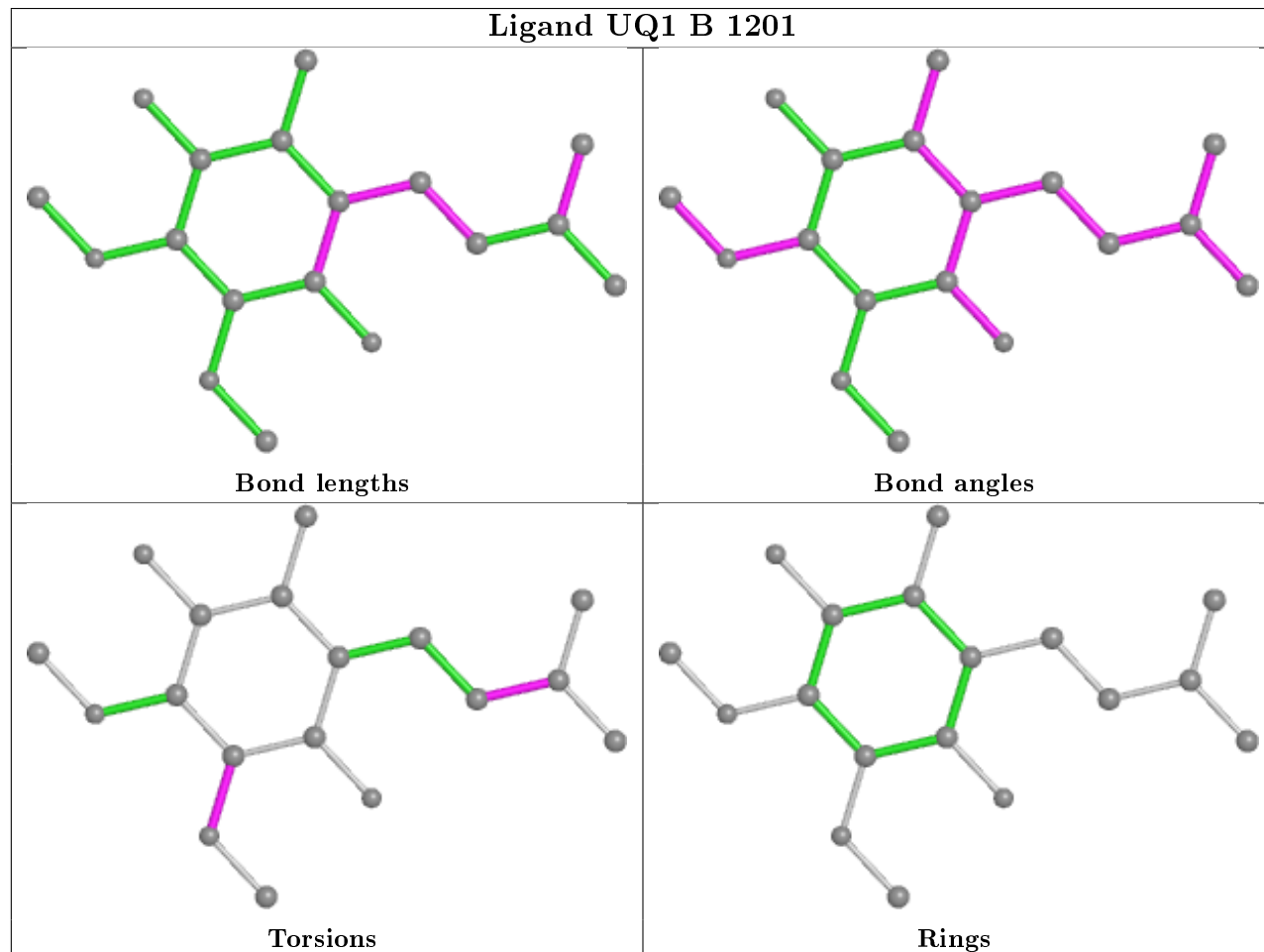
## Ligand HEM C 1305

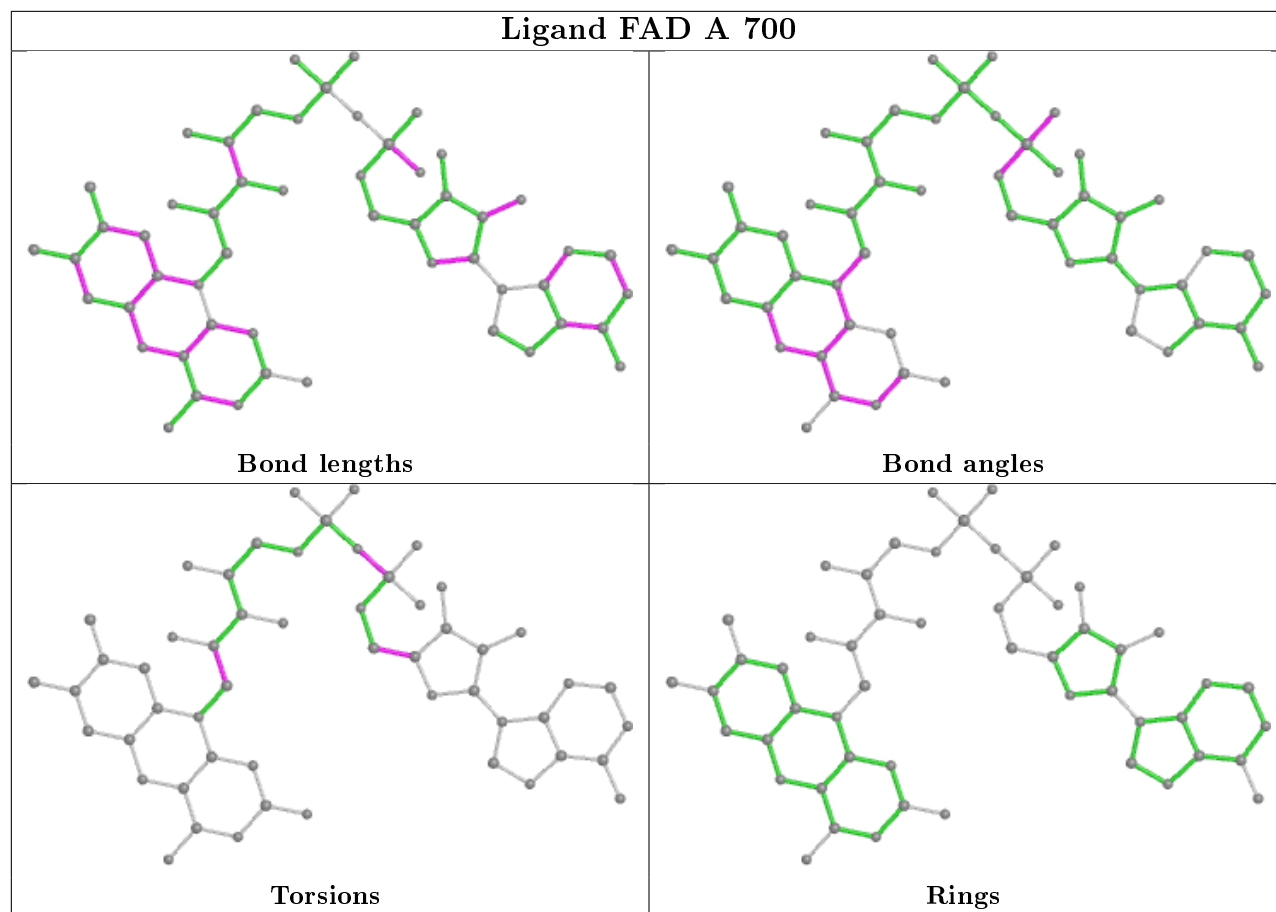


## Ligand EPH D 1306



## Ligand UQ1 B 1201





## 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	613/622 (98%)	0.45	60 (9%) 7 7	39, 64, 108, 123	0
2	B	239/252 (94%)	0.09	14 (5%) 22 21	38, 57, 88, 105	0
3	C	138/140 (98%)	-0.02	5 (3%) 42 42	47, 67, 101, 114	0
4	D	102/103 (99%)	-0.09	4 (3%) 39 38	48, 67, 90, 104	0
All	All	1092/1117 (97%)	0.26	83 (7%) 13 12	38, 63, 104, 123	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	35	SER	6.7
1	A	317	PRO	6.2
1	A	322	VAL	5.8
3	C	143	MET	5.6
3	C	82	LEU	4.6
1	A	328	HIS	4.4
1	A	330	PRO	4.4
1	A	280	GLN	4.3
1	A	332	GLU	4.3
1	A	352	ASP	4.1
1	A	277	ILE	3.9
1	A	327	HIS	3.8
3	C	81	CYS	3.7
1	A	226	SER	3.7
1	A	315	CYS	3.6
1	A	284	PHE	3.5
1	A	622	TYR	3.5
2	B	69	ILE	3.4
1	A	357	PRO	3.4
2	B	68	GLY	3.4
2	B	11	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	263	CYS	3.3
1	A	288	TYR	3.3
1	A	297	SER	3.2
1	A	329	LEU	3.2
1	A	58	THR	3.2
2	B	70	CYS	3.1
1	A	365	HIS	3.1
2	B	64	SER	3.1
1	A	59	VAL	3.1
2	B	73	CYS	3.0
1	A	215	GLY	3.0
2	B	25	GLY	3.0
1	A	355	LYS	2.9
1	A	620	ARG	2.9
1	A	366	TYR	2.9
3	C	80	LEU	2.8
1	A	316	GLY	2.8
3	C	85	THR	2.8
1	A	225	THR	2.8
1	A	323	TYR	2.7
1	A	356	GLU	2.7
1	A	57	HIS	2.7
1	A	56	SER	2.6
1	A	276	LEU	2.6
1	A	279	SER	2.6
1	A	278	ASN	2.6
2	B	72	SER	2.6
1	A	60	ALA	2.5
1	A	214	THR	2.5
1	A	326	LEU	2.5
1	A	154	THR	2.5
2	B	71	GLY	2.5
1	A	10	SER	2.5
1	A	229	THR	2.4
2	B	65	CYS	2.4
1	A	314	GLY	2.4
1	A	28	GLY	2.4
2	B	37	LEU	2.4
1	A	29	GLY	2.3
1	A	359	PRO	2.3
1	A	227	ALA	2.3
1	A	400	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	397	GLY	2.3
1	A	61	ALA	2.3
1	A	399	ALA	2.3
2	B	94	ASP	2.2
1	A	367	ASN	2.2
4	D	65	CYS	2.2
1	A	230	SER	2.2
1	A	157	SER	2.2
1	A	218	GLY	2.2
4	D	62	LEU	2.2
4	D	66	SER	2.2
1	A	216	GLY	2.2
1	A	262	GLY	2.1
1	A	224	CYS	2.1
1	A	217	TYR	2.1
1	A	419	VAL	2.1
2	B	91	THR	2.1
1	A	265	ILE	2.0
1	A	54	THR	2.0
2	B	34	GLU	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 carbohydrates 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.

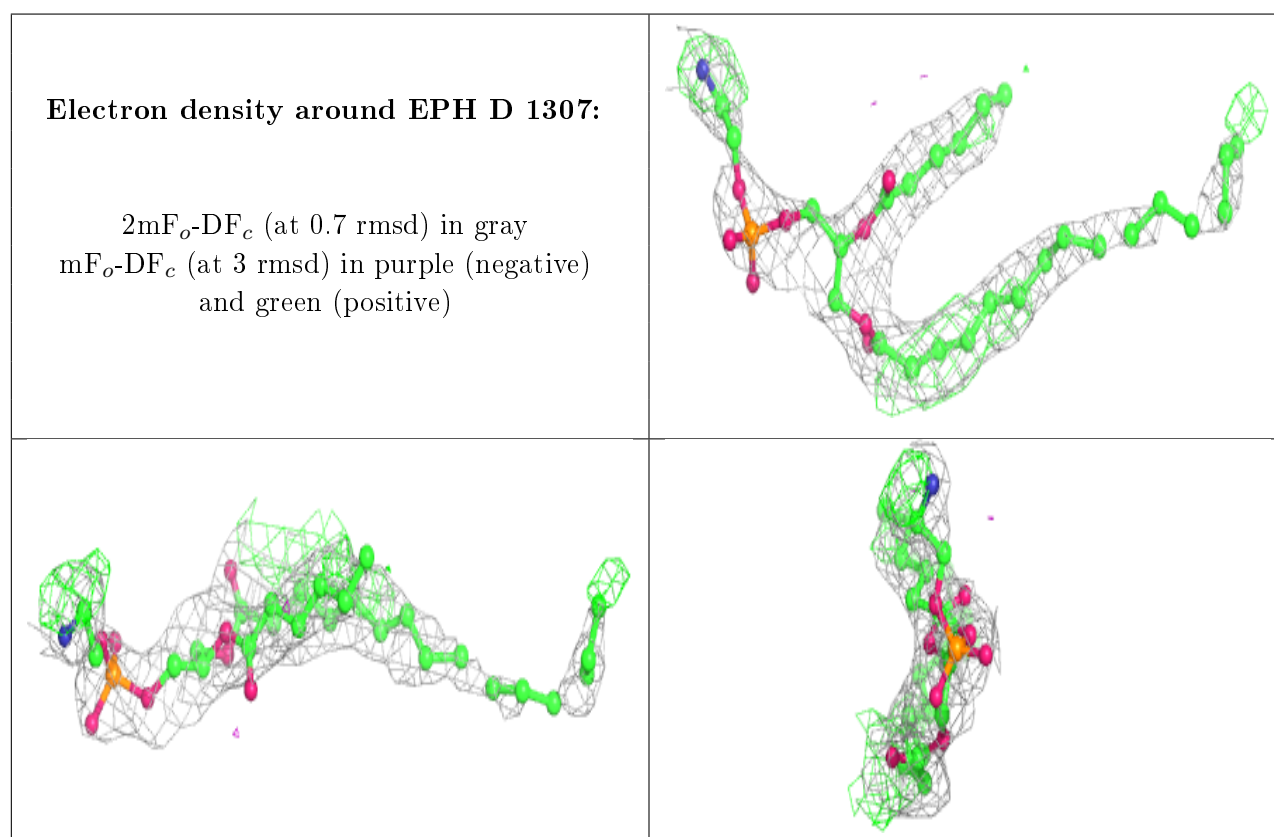
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
11	EPH	D	1307	36/49	0.59	0.29	112,122,143,144	0
9	UQ1	B	1201	18/18	0.71	0.59	67,95,100,102	4
11	EPH	D	1306	44/49	0.86	0.28	73,94,118,123	0

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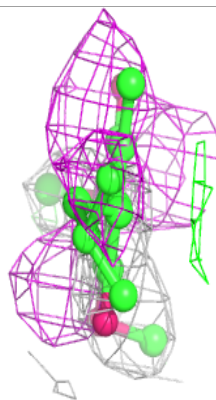
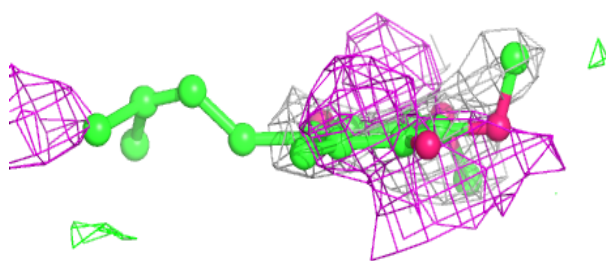
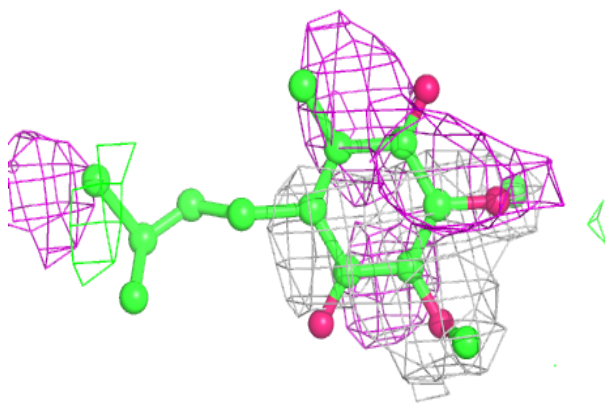
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	HEM	C	1305	43/43	0.97	0.15	53,62,77,80	0
7	SF4	B	303	8/8	0.97	0.21	50,51,54,59	0
5	FAD	A	700	53/53	0.97	0.30	42,52,65,66	0
8	F3S	B	304	7/7	0.98	0.15	45,47,53,54	0
6	FES	B	302	4/4	0.99	0.17	46,50,52,55	0

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.

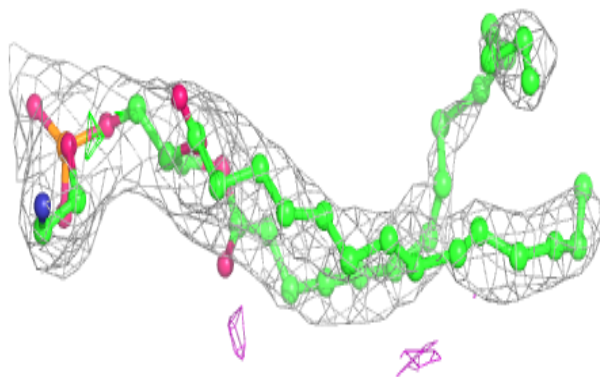
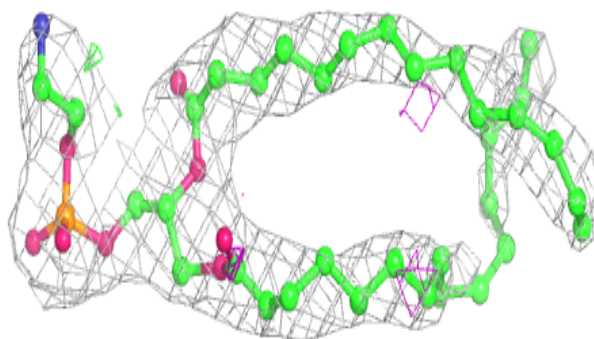


**Electron density around UQ1 B 1201:**

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

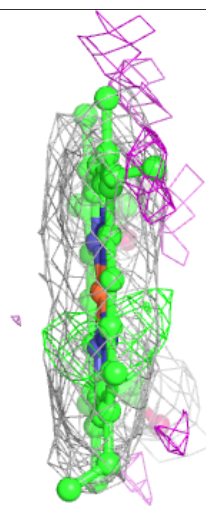
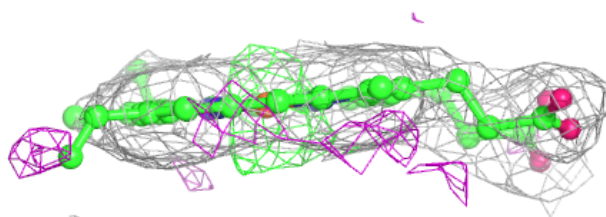
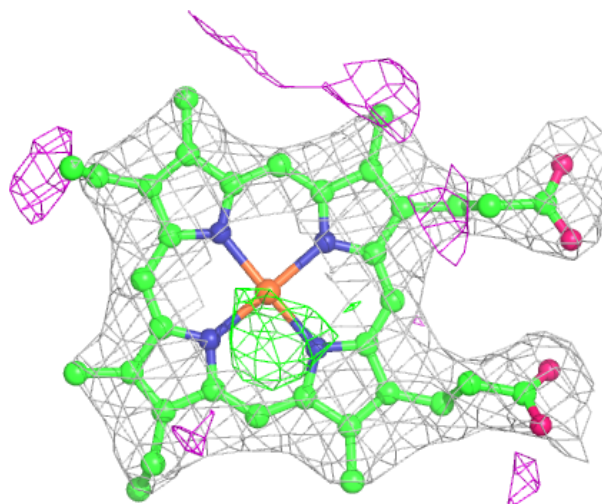
**Electron density around EPH D 1306:**

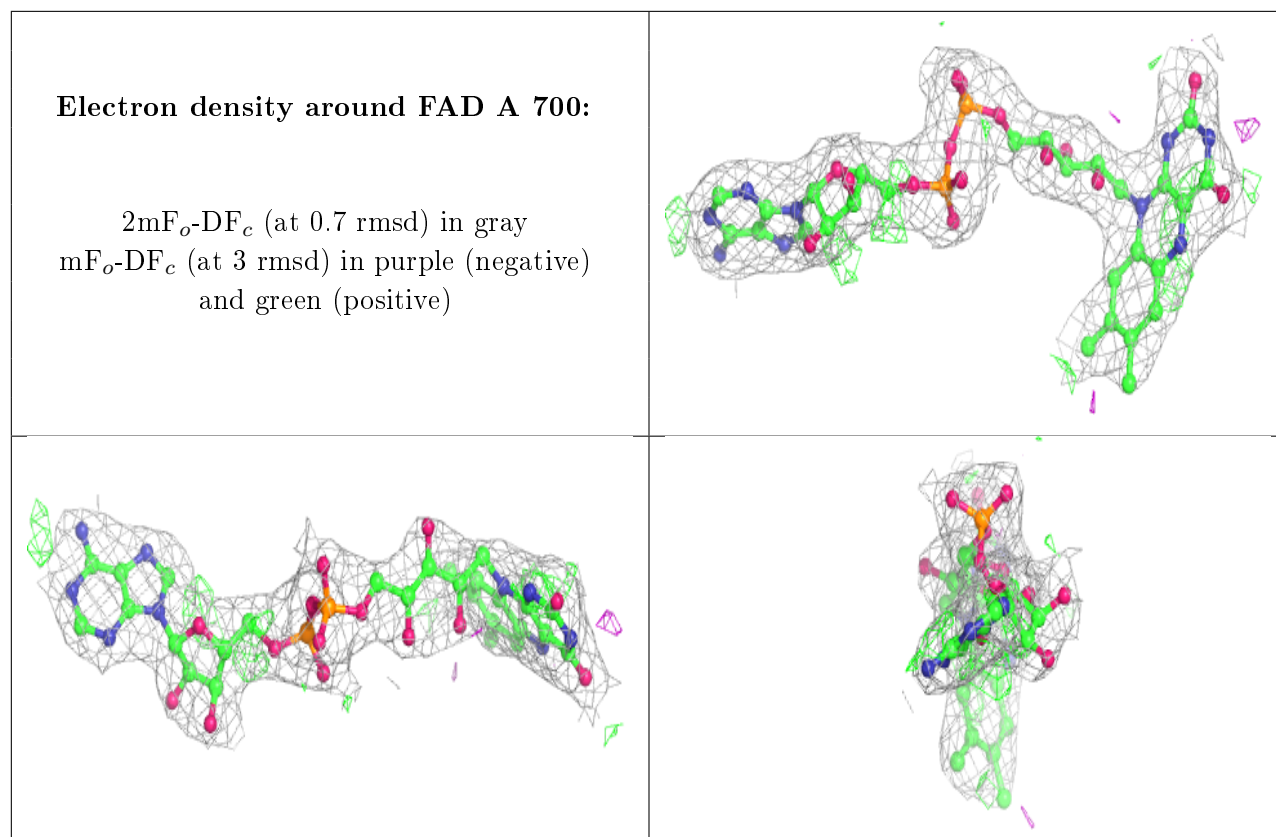
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 1305:**

$2mF_o-DF_c$  (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.