



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:24 PM UTC

PDB ID : 1ZOY / pdb_00001zoy
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

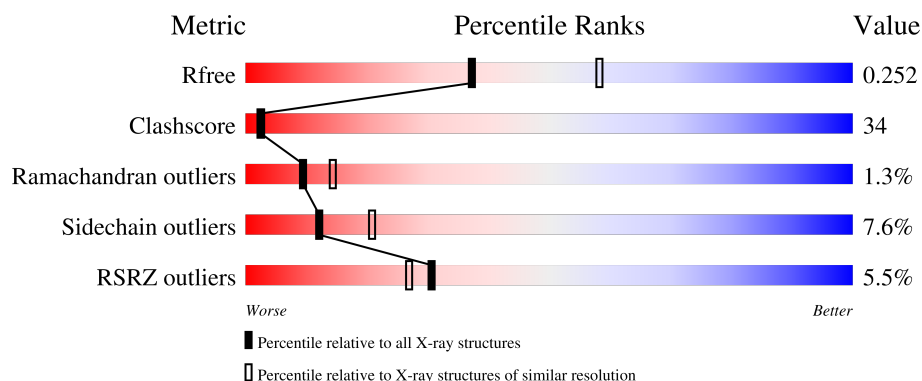
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

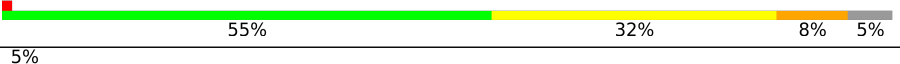
The reported resolution of this entry is 2.40 Å.

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	622	
2	B	252	
3	C	140	
4	D	103	

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
8	F3S	B	304	-	-	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			

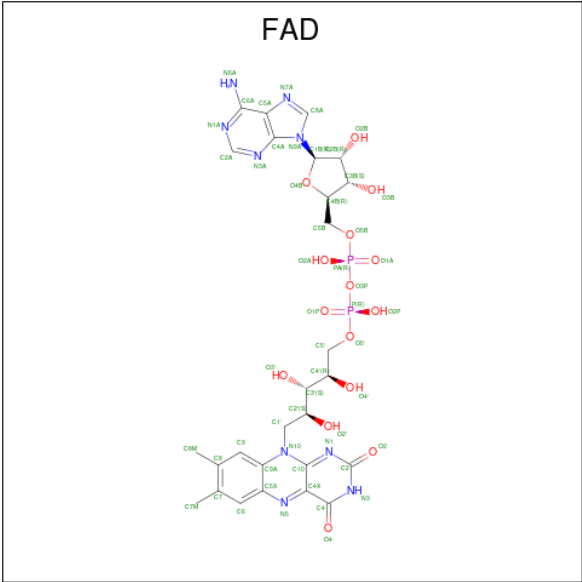
- Molecule 3 is a protein called Large cytochrome binding protein.

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.

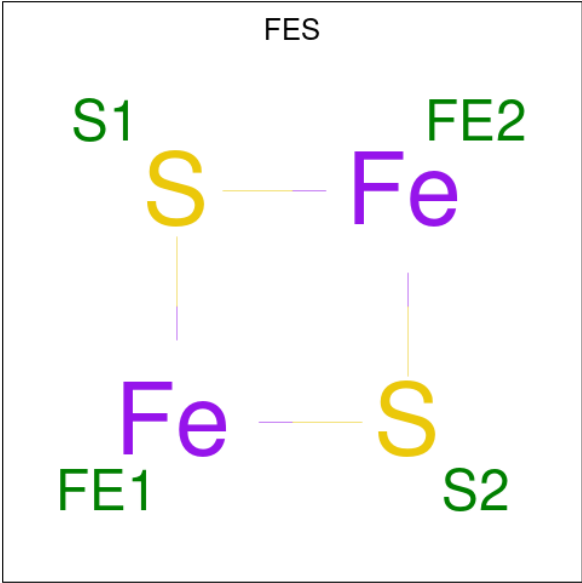
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			765	499	128	133	5			

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



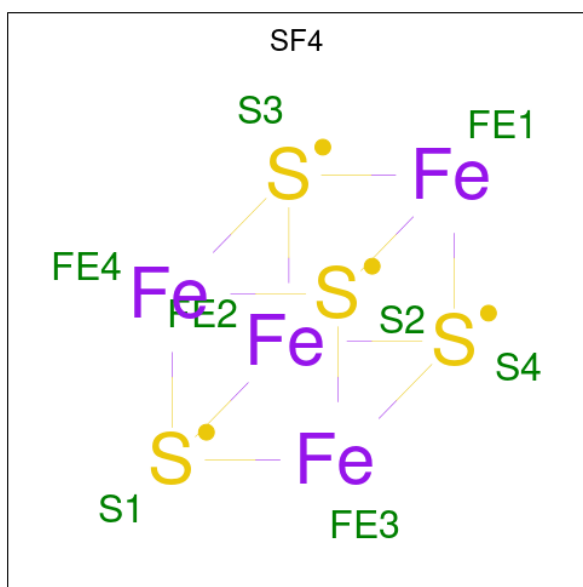
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



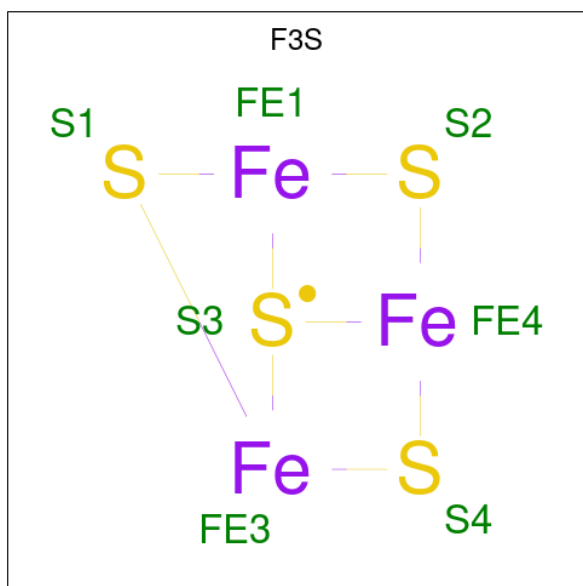
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



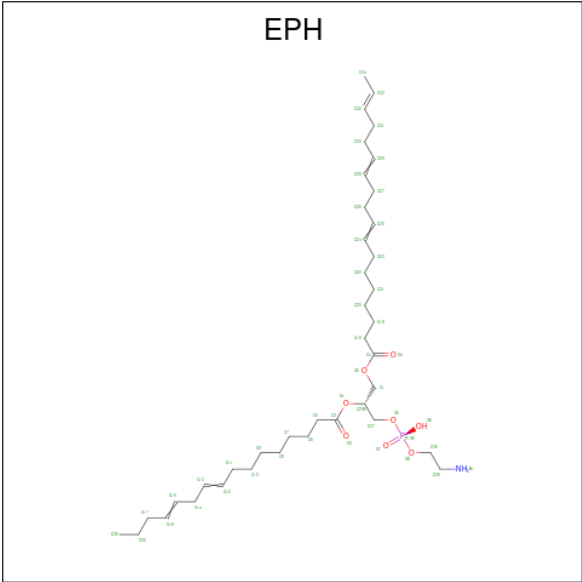
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



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

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



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		

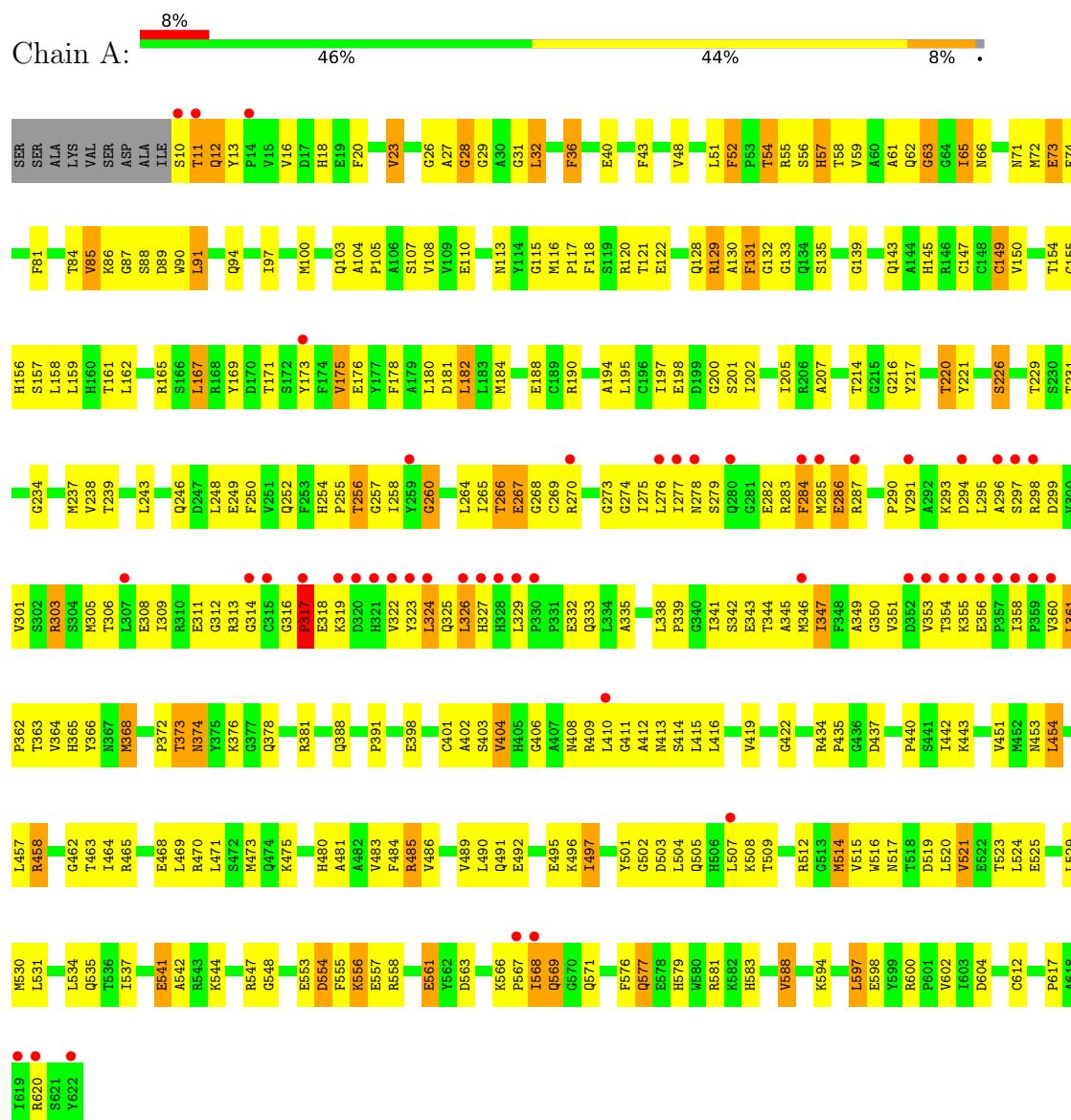
- Molecule 12 is water.

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

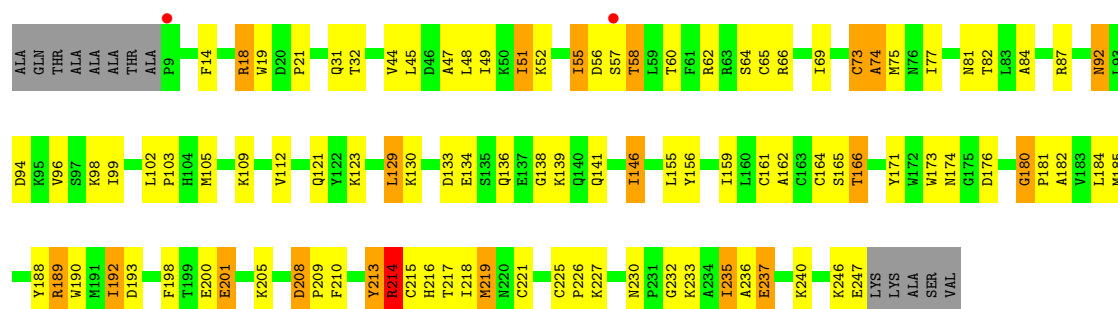
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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, α , β , γ	70.24Å 83.56Å 293.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 82.2 (50.00-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.259 0.205 , 0.252	Depositor DCC
R_{free} test set	5757 reflections (9.58%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPH, SF4, FES, FAD, F3S, HEM, UQ1

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	0.46	0/4828	1.02	21/6531 (0.3%)
2	B	0.47	0/1964	1.03	11/2648 (0.4%)
3	C	0.45	0/1091	0.86	2/1483 (0.1%)
4	D	0.44	0/784	0.91	1/1066 (0.1%)
All	All	0.46	0/8667	1.00	35/11728 (0.3%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	ALA	N-CA-C	-13.33	96.36	112.89
1	A	12	GLN	N-CA-C	-11.62	98.62	113.72
1	A	404	VAL	N-CA-C	-9.17	101.94	113.22
2	B	180	GLY	CA-C-N	8.64	127.96	118.97
2	B	180	GLY	C-N-CA	8.64	127.96	118.97
1	A	422	GLY	N-CA-C	-7.85	103.39	112.50
2	B	73	CYS	N-CA-C	7.69	120.75	111.82
1	A	91	LEU	N-CA-C	-7.18	103.68	113.30
2	B	112	VAL	N-CA-C	6.57	114.63	107.60
1	A	291	VAL	N-CA-C	6.33	116.44	110.30
2	B	58	THR	N-CA-C	-6.22	105.72	113.38
1	A	347	ILE	N-CA-C	6.20	116.94	110.62
1	A	149	CYS	N-CA-C	6.03	118.01	108.79
4	D	97	LEU	N-CA-C	6.00	118.34	111.02
2	B	210	PHE	N-CA-C	5.96	120.85	112.93
2	B	55	ILE	N-CA-C	5.91	116.11	110.74
1	A	28	GLY	N-CA-C	-5.84	102.27	112.55
1	A	267	GLU	N-CA-C	-5.80	106.06	113.01
3	C	113	LEU	N-CA-C	-5.78	106.18	113.18
1	A	94	GLN	N-CA-C	5.71	118.28	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	PHE	N-CA-C	-5.68	101.14	109.50
1	A	256	THR	N-CA-C	5.68	117.99	107.99
1	A	326	LEU	N-CA-C	-5.58	107.73	114.75
2	B	213	TYR	N-CA-C	5.55	122.63	110.80
1	A	485	ARG	N-CA-C	5.48	117.40	109.07
2	B	208	ASP	N-CA-C	-5.41	103.25	108.07
2	B	219	MET	N-CA-C	5.31	120.94	113.56
1	A	120	ARG	N-CA-C	5.31	118.65	110.42
1	A	220	THR	N-CA-C	-5.22	106.17	112.54
1	A	194	ALA	N-CA-C	5.14	117.00	109.24
2	B	214	ARG	N-CA-C	-5.10	107.00	113.18
1	A	226	SER	N-CA-C	5.09	117.42	110.55
1	A	175	VAL	N-CA-C	5.08	115.59	108.89
1	A	57	HIS	N-CA-C	5.06	117.53	111.71
3	C	87	ILE	N-CA-C	-5.00	104.84	111.09

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4729	0	4618	380	0
2	B	1922	0	1900	111	0
3	C	1064	0	1104	69	0
4	D	765	0	773	52	0
5	A	53	0	29	12	0
6	B	4	0	0	0	0
7	B	8	0	0	0	0
8	B	7	0	0	4	0
9	B	18	0	18	1	0
10	C	43	0	30	7	0
11	D	80	0	94	4	0
12	A	195	0	0	52	0
12	B	91	0	0	19	0
12	C	24	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	21	0	0	7	0
All	All	9024	0	8566	593	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 34.

All (593) 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: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:368:MET:HE3	1:A:408:ASN:HA	1.46	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
2:B:219:MET:HE1	2:B:232:GLY:HA3	1.50	0.92
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:72:MET:HE1	1:A:121:THR:HG21	1.61	0.83
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
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
3:C:71:GLU:HG2	4:D:132:MET:HE1	1.60	0.81
1:A:465:ARG:HB3	1:A:468:GLU:HG3	1.63	0.81
1:A:182:LEU:HD23	1:A:184:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:92:ASN:C	2:B:92:ASN:HD22	1.93	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:269:CYS:SG	1:A:341:ILE:HD13	2.28	0.74
1:A:458:ARG:NH2	1:A:514:MET:HE3	2.03	0.73
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:HG3	1:A:512:ARG:HH11	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:155:LEU:HD23	2:B:185:MET:HE2	1.71	0.70
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
1:A:275:ILE:HG22	1:A:276:LEU:H	1.56	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:57:HIS:NE2	5:A:700:FAD:C8	2.52	0.70
1:A:544:LYS:HG2	1:A:555:PHE:CE2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:72:MET:HE1	1:A:121:THR:CG2	2.22	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:252:GLN:CD	1:A:298:ARG:HD2	2.18	0.68
1:A:87:GLY:HA2	1:A:620:ARG:HH12	1.58	0.68
1:A:299:ASP:HB3	1:A:408:ASN:ND2	2.09	0.68
1:A:471:LEU:HD11	1:A:475:LYS:HZ3	1.59	0.68
1:A:486:VAL:CG1	1:A:553:GLU:HB2	2.23	0.68
2:B:219:MET:HE1	2:B:232:GLY:CA	2.24	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:N	1:A:284:PHE:CD2	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:FE3	8:B:304:F3S:S1	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:514:MET:HE2	1:A:514:MET:HA	1.77	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
1:A:516:TRP:HB3	2:B:60:THR:HG21	1.80	0.64
2:B:230:ASN:C	2:B:230:ASN:HD22	2.06	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: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
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:54:THR:O	1:A:59:VAL:HG21	1.99	0.62
1:A:282:GLU:OE1	1:A:287:ARG:HD2	1.98	0.62
1:A:285:MET:HE1	12:A:852:HOH:O	1.98	0.62
2:B:92:ASN:HD22	2:B:94:ASP:H	1.45	0.62
1:A:57:HIS:CE1	1:A:226:SER:HA	2.35	0.62
1:A:458:ARG:HG3	1:A:458:ARG:NH1	2.11	0.62
2:B:176:ASP:CG	4:D:93:ARG:HH22	2.07	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:77:ILE:HD12	2:B:99:ILE:HG13	1.82	0.61
2:B:188:TYR:O	2:B:192:ILE:HD12	1.99	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
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
1:A:59:VAL:CG2	1:A:159:LEU:HD23	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:74:LEU:HD12	4:D:132:MET:HE2	1.84	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:97:ILE:HG12	1:A:404:VAL:HG23	1.84	0.59
1:A:265:ILE:HD12	1:A:360:VAL:HG12	1.84	0.59
1:A:130:ALA:HB2	1:A:145:HIS:CD2	2.38	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:11:THR:HG22	1:A:11:THR:O	2.03	0.59
1:A:117:PRO:HD2	1:A:157:SER:OG	2.02	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:62:GLN:HB2	1:A:266:THR:HB	1.84	0.58
1:A:198:GLU:O	1:A:515:VAL:HG13	2.03	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: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:182:LEU:HD13	1:A:237:MET:HE2	1.85	0.58
1:A:373:THR:HG23	1:A:374:ASN:O	2.03	0.58
1:A:458:ARG:CZ	1:A:514:MET:HE3	2.32	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:66:ARG:HD2	2:B:66:ARG:O	2.04	0.58
1:A:129:ARG:HG3	1:A:129:ARG:NH1	2.16	0.57
1:A:267:GLU:OE1	1:A:298:ARG:NH1	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:531:LEU:O	1:A:535:GLN:HG3	2.05	0.56
12:A:890:HOH:O	2:B:129:LEU:N	2.37	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
1:A:581:ARG:HH22	1:A:604:ASP:CG	2.12	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:61:ALA:HA	5:A:700:FAD:N5	2.20	0.56
1:A:343:GLU:O	1:A:347:ILE:HG13	2.06	0.56
1:A:65:ILE:HD12	1:A:108:VAL:CG2	2.35	0.56
1:A:274:GLY:HA3	1:A:326:LEU:HD23	1.87	0.56
3:C:88:TYR:HB3	12:C:1317:HOH:O	2.06	0.56
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:71:ASN:C	1:A:72:MET:HE2	2.32	0.55
1:A:81:PHE:O	1:A:85:VAL:HG12	2.07	0.55
1:A:541:GLU:HG3	1:A:542:ALA:N	2.21	0.55
1:A:182:LEU:HD23	1:A:184:MET:CE	2.35	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:182:LEU:CD1	1:A:237:MET:HE2	2.37	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
1:A:312:GLY:C	1:A:313:ARG:HG3	2.32	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
1:A:283:ARG:HH21	1:A:294:ASP:CG	2.16	0.54
2:B:198:PHE:HD2	2:B:201:GLU:HG3	1.73	0.54
3:C:99:MET:HE2	3:C:99:MET:HA	1.89	0.54
1:A:264:LEU:HD22	1:A:365:HIS:CE1	2.42	0.54
2:B:105:MET:HE1	12:B:1271:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:73:CYS:O	2:B:74:ALA:C	2.52	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:HD12	1:A:507:LEU:O	2.10	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:87:GLY:CA	1:A:620:ARG:HH12	2.21	0.52
1:A:118:PHE:HA	1:A:150:VAL:HG22	1.91	0.52
1:A:130:ALA:HB2	1:A:145:HIS:HD2	1.75	0.52
1:A:158:LEU:HD23	1:A:415:LEU:HD22	1.92	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
3:C:52:LEU:HB3	10:C:1305:HEM:CAC	2.28	0.52
1:A:10:SER:C	1:A:12:GLN:H	2.18	0.51
1:A:97:ILE:HA	1:A:404:VAL:HG23	1.92	0.51
1:A:278:ASN:OD1	1:A:282:GLU:N	2.43	0.51
1:A:373:THR:HG23	1:A:374:ASN:N	2.26	0.51
2:B:219:MET:HE3	3:C:117:LEU:HD22	1.92	0.51
1:A:10:SER:C	1:A:12:GLN:N	2.67	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:56:ASP:OD1	2:B:58:THR:HB	2.09	0.51
2:B:136:GLN:OE1	2:B:139:LYS:HD2	2.11	0.51
2:B:173:TRP:CD1	9:B:1201:UQ1:HM22	2.46	0.51
3:C:96:PHE:HB3	3:C:97:PRO:CD	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:92:ASN:C	2:B:92:ASN:ND2	2.60	0.51
2:B:219:MET:CE	2:B:232:GLY:HA3	2.31	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:N	1:A:277:ILE:HD12	2.25	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:HD23	1:A:597:LEU:H	1.77	0.50
1:A:36:PHE:CD1	1:A:36:PHE:C	2.88	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:69:ILE:O	2:B:159:ILE:HD12	2.12	0.50
2:B:109:LYS:HE2	12:B:1245:HOH:O	2.11	0.50
1:A:276:LEU:HD23	1:A:305:MET:HE3	1.93	0.50
3:C:35:TRP:HZ3	3:C:43:ILE:HD11	1.77	0.50
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:155:LEU:CD2	2:B:185:MET:HE2	2.41	0.49
3:C:41:MET:HE3	3:C:130:LEU:HD13	1.95	0.49
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:48:THR:O	3:C:52:LEU:HB2	2.12	0.48
3:C:104:ASN:ND2	3:C:107:ARG:HE	2.11	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:65:ILE:HD11	1:A:416:LEU:HD13	1.94	0.48
1:A:84:THR:HA	1:A:410:LEU:HD22	1.95	0.48
1:A:254:HIS:HB2	1:A:365:HIS:CB	2.43	0.48
2:B:51:ILE:HD12	2:B:51:ILE:O	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
1:A:258:ILE:HD12	1:A:258:ILE:N	2.22	0.48
1:A:411:GLY:O	1:A:412:ALA:HB3	2.12	0.48
1:A:454:LEU:CD1	1:A:520:LEU:HD21	2.44	0.48
1:A:497:ILE:CG2	1:A:534:LEU:HD12	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:65:ILE:C	1:A:65:ILE:HD13	2.39	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
2:B:230:ASN:CG	2:B:233:LYS:HB3	2.38	0.48
4:D:89:THR:HG22	4:D:102:LYS:CE	2.44	0.48
1:A:306:THR:HG21	1:A:483:VAL:HG11	1.96	0.47
2:B:66:ARG:HD2	2:B:66:ARG:C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:MET:HG3	2:B:77:ILE:HD11	1.95	0.47
12:A:890:HOH:O	2:B:190:TRP:CZ3	2.66	0.47
2:B:18:ARG:HB3	2:B:18:ARG:HH11	1.78	0.47
2:B:49:ILE:O	2:B:52:LYS:HB3	2.13	0.47
3:C:74:LEU:CD1	4:D:132:MET:HE2	2.45	0.47
1:A:231:THR:HA	1:A:529:LEU:HD21	1.96	0.47
1:A:512:ARG:HG3	1:A:512:ARG:NH1	2.26	0.47
2:B:66:ARG:O	2:B:66:ARG:CD	2.62	0.47
4:D:49:VAL:HG11	4:D:78:LEU:HD13	1.97	0.47
1:A:202:ILE:CD1	1:A:451:VAL:HG22	2.36	0.47
1:A:412:ALA:N	12:A:847:HOH:O	2.47	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
1:A:220:THR:HA	1:A:473:MET:HE3	1.97	0.47
1:A:316:GLY:O	1:A:317:PRO:C	2.57	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:HB	12:B:1257:HOH:O	2.13	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: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
1:A:131:PHE:HE2	1:A:268:GLY:N	2.11	0.47
1:A:258:ILE:H	1:A:258:ILE:CD1	2.21	0.47
1:A:577:GLN:H	1:A:577:GLN:HG2	1.55	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:HD12	2:B:99:ILE:N	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
12:A:830:HOH:O	3:C:6:THR:HG22	2.14	0.46
2:B:65:CYS:O	2:B:66:ARG:HG3	2.15	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:54:THR:HG23	12:A:843:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:MET:O	1:A:309:ILE:HG13	2.16	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:N	1:A:597:LEU:CD2	2.79	0.46
1:A:509:THR:HG23	1:A:512:ARG:HH12	1.79	0.46
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
1:A:276:LEU:C	1:A:277:ILE:HD12	2.40	0.46
2:B:102:LEU:HB3	2:B:166:THR:HG21	1.97	0.46
2:B:146:ILE:O	2:B:146:ILE:HG13	2.11	0.46
2:B:188:TYR:OH	2:B:237:GLU:HG2	2.16	0.46
1:A:197:ILE:HD12	1:A:197:ILE:H	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:501:TYR:HA	1:A:530:MET:HE2	1.97	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:182:LEU:HB3	1:A:184:MET:HE2	1.98	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:23:VAL:HG23	1:A:207:ALA:HB3	1.98	0.45
1:A:176:GLU:O	1:A:197:ILE:HD13	2.16	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
2:B:69:ILE:C	2:B:69:ILE:HD12	2.41	0.45
1:A:73:GLU:HG2	1:A:74:GLU:O	2.17	0.45
1:A:521:VAL:O	1:A:525:GLU:HG3	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:PRO:HG2	12:A:803:HOH:O	2.16	0.45
1:A:556:LYS:HD2	1:A:556:LYS:N	2.32	0.45
1:A:195:LEU:HD22	1:A:454:LEU:HD21	1.99	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:129:ARG:O	1:A:147:CYS:HB3	2.17	0.44
1:A:149:CYS:CB	1:A:154:THR:HG21	2.47	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:OD1	1:A:554:ASP:N	2.39	0.44
2:B:92:ASN:ND2	2:B:94:ASP:HB2	2.30	0.44
2:B:133:ASP:HB3	12:B:1241:HOH:O	2.16	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:HD12	3:C:122:LEU:HA	1.85	0.44
1:A:129:ARG:NH1	1:A:130:ALA:HB3	2.32	0.44
1:A:555:PHE:C	1:A:557:GLU:H	2.26	0.44
3:C:7:THR:HB	12:C:1307:HOH:O	2.17	0.44
3:C:102:THR:OG1	10:C:1305:HEM:HBB2	2.18	0.44
3:C:81:CYS:HA	12:C:1321:HOH:O	2.18	0.44
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
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
4:D:72:LEU:HB3	4:D:126:ILE:HD11	2.00	0.43
1:A:239:THR:HG23	1:A:588:VAL:HG13	2.00	0.43
1:A:512:ARG:HH11	1:A:512:ARG:CG	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:486:VAL:HG12	1:A:554:ASP:OD1	2.18	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:401:CYS:C	1:A:403:SER:N	2.71	0.43
1:A:503:ASP:C	1:A:505:GLN:N	2.76	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:HD22	1:A:374:ASN:HA	1.58	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:HG22	2:B:217:THR:O	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
3:C:46:ARG:O	3:C:47:GLY:C	2.60	0.42
3:C:100:TYR:CD2	3:C:100:TYR:C	2.98	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:409:ARG:HH21	5:A:700:FAD:C2	2.33	0.42
1:A:503:ASP:C	1:A:505:GLN:H	2.28	0.42
2:B:209:PRO:C	12:B:1242:HOH:O	2.62	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:256:THR:CA	1:A:360:VAL:HB	2.45	0.42
1:A:265:ILE:O	1:A:266:THR:C	2.62	0.42
1:A:303:ARG:C	1:A:306:THR:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:57:HIS:HA	12:A:797:HOH:O	2.18	0.42
1:A:351:VAL:HG13	1:A:356:GLU:HB2	2.02	0.42
4:D:72:LEU:HD23	4:D:126:ILE:CD1	2.48	0.42
1:A:40:GLU:HA	1:A:169:TYR:CE2	2.55	0.42
1:A:221:TYR:CD2	1:A:364:VAL:HG21	2.55	0.42
4:D:123:ASP:OD1	4:D:124:VAL:N	2.37	0.42
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
1:A:129:ARG:HD2	1:A:129:ARG:HA	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:376:LYS:C	12:A:794:HOH:O	2.63	0.41
2:B:219:MET:HE2	8:B:304:F3S:S2	2.60	0.41
1:A:72:MET:HE2	1:A:72:MET:N	2.36	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:56:SER:O	1:A:59:VAL:HG23	2.21	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
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:355:LYS:C	1:A:356:GLU:HG2	2.46	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:61:ALA:HA	5:A:700:FAD:C6	2.51	0.41
1:A:327:HIS:ND1	1:A:355:LYS:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ILE:O	1:A:442:ILE:HG23	2.21	0.41
1:A:509:THR:C	1:A:512:ARG:HH12	2.29	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
2:B:98:LYS:C	2:B:99:ILE:HD12	2.45	0.41
3:C:109:LEU:HD13	4:D:51:VAL:HG12	2.02	0.41
1:A:59:VAL:CG2	1:A:159:LEU:CD2	2.99	0.41
1:A:217:TYR:O	1:A:217:TYR:CD1	2.74	0.41
3:C:104:ASN:HD22	3:C:104:ASN:HA	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
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
3:C:98:LEU:HD13	3:C:98:LEU:C	2.46	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:91:LEU:O	1:A:583:HIS:CE1	2.73	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:514:MET:C	12:A:807:HOH:O	2.65	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%)	8	12
2	B	237/252 (94%)	219 (92%)	16 (7%)	2 (1%)	16	25
3	C	136/140 (97%)	125 (92%)	9 (7%)	2 (2%)	8	12
4	D	100/103 (97%)	92 (92%)	7 (7%)	1 (1%)	12	20
All	All	1084/1117 (97%)	977 (90%)	93 (9%)	14 (1%)	9	14

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	THR
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%)	459 (92%)	40 (8%)	11	19
2	B	214/221 (97%)	199 (93%)	15 (7%)	14	24
3	C	117/118 (99%)	108 (92%)	9 (8%)	12	20
4	D	76/76 (100%)	71 (93%)	5 (7%)	15	26
All	All	906/921 (98%)	837 (92%)	69 (8%)	12	21

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	32	LEU
1	A	36	PHE
1	A	54	THR
1	A	65	ILE
1	A	73	GLU
1	A	85	VAL
1	A	129	ARG
1	A	131	PHE
1	A	165	ARG
1	A	167	LEU
1	A	182	LEU
1	A	284	PHE
1	A	303	ARG
1	A	311	GLU
1	A	317	PRO
1	A	324	LEU
1	A	344	THR
1	A	361	LEU
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	514	MET
1	A	521	VAL
1	A	541	GLU
1	A	554	ASP
1	A	556	LYS
1	A	558	ARG
1	A	561	GLU
1	A	568	ILE
1	A	577	GLN
1	A	588	VAL
1	A	597	LEU
1	A	598	GLU
1	A	602	VAL
2	B	18	ARG
2	B	51	ILE

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Mol	Chain	Res	Type
2	B	92	ASN
2	B	96	VAL
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	201	GLU
2	B	205	LYS
2	B	214	ARG
2	B	235	ILE
2	B	237	GLU
3	C	13	GLU
3	C	29	HIS
3	C	30	ILE
3	C	52	LEU
3	C	72	SER
3	C	108	HIS
3	C	122	LEU
3	C	130	LEU
3	C	143	MET
4	D	52	LEU
4	D	78	LEU
4	D	89	THR
4	D	108	LEU
4	D	134	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	113	ASN
1	A	128	GLN
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

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Mol	Chain	Res	Type
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	38	ASN
2	B	39	ASN
2	B	92	ASN
2	B	121	GLN
2	B	144	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
3	C	104	ASN
4	D	98	GLN
4	D	122	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
10	HEM	C	1305	3,4	50,50,50	1.28	5 (10%)	67,82,82	0.67	1 (1%)
11	EPH	D	1306	-	43,43,48	1.87	9 (20%)	46,48,53	2.31	6 (13%)
11	EPH	D	1307	-	35,35,48	2.00	9 (25%)	38,40,53	2.47	5 (13%)
9	UQ1	B	1201	-	18,18,18	2.84	4 (22%)	24,25,25	2.99	9 (37%)
6	FES	B	302	2	0,4,4	-	-	-	-	-
5	FAD	A	700	1	58,58,58	2.55	15 (25%)	85,89,89	1.01	3 (3%)
8	F3S	B	304	2	0,9,9	-	-	-	-	-
7	SF4	B	303	2	0,12,12	-	-	-	-	-

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	1306	-	-	30/47/47/52	-
10	HEM	C	1305	3,4	-	8/14/54/54	-
11	EPH	D	1307	-	-	7/39/39/52	-
9	UQ1	B	1201	-	-	3/9/33/33	0/1/1/1
6	FES	B	302	2	-	-	0/1/1/1
5	FAD	A	700	1	-	3/34/50/50	0/6/6/6
8	F3S	B	304	2	-	-	0/3/3/3
7	SF4	B	303	2	-	-	0/6/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	FAD	C6-C7	11.65	1.55	1.39
9	B	1201	UQ1	C10-C9	7.87	1.71	1.50
9	B	1201	UQ1	C7-C6	7.73	1.65	1.51
11	D	1307	EPH	C29-C28	6.98	1.71	1.31
11	D	1306	EPH	C29-C28	6.83	1.70	1.31
5	A	700	FAD	C9A-N10	5.28	1.50	1.41
5	A	700	FAD	C9-C8	4.94	1.46	1.39
5	A	700	FAD	C4X-N5	4.78	1.41	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	1307	EPH	C25-C24	4.56	1.57	1.31
11	D	1306	EPH	C18-C4	-4.41	1.37	1.50
5	A	700	FAD	C9A-C5X	4.33	1.48	1.41
5	A	700	FAD	C4A-N3A	4.03	1.42	1.34
11	D	1306	EPH	C25-C24	3.87	1.53	1.31
5	A	700	FAD	C9-C9A	3.81	1.45	1.39
10	C	1305	HEM	FE-NA	3.78	2.07	1.95
10	C	1305	HEM	FE-NB	3.76	2.06	1.94
11	D	1306	EPH	C13-C12	3.68	1.52	1.31
11	D	1307	EPH	P1-O7	3.67	1.63	1.50
5	A	700	FAD	C10-N1	3.62	1.40	1.33
5	A	700	FAD	P-O3P	-3.41	1.55	1.59
11	D	1307	EPH	C26-C25	3.41	1.68	1.50
10	C	1305	HEM	FE-NC	3.29	2.06	1.95
11	D	1306	EPH	C27-C28	-3.27	1.32	1.50
11	D	1306	EPH	C15-C16	3.21	1.52	1.29
5	A	700	FAD	C1'-C2'	3.19	1.57	1.52
11	D	1307	EPH	C18-C4	3.13	1.59	1.50
5	A	700	FAD	O2B-C2B	-2.94	1.35	1.43
11	D	1306	EPH	P1-O7	2.86	1.60	1.50
10	C	1305	HEM	FE-ND	2.73	2.03	1.94
11	D	1306	EPH	C26-C25	2.67	1.64	1.50
9	B	1201	UQ1	C7-C8	2.52	1.54	1.50
5	A	700	FAD	C4'-C3'	2.51	1.57	1.53
11	D	1307	EPH	O2-C4	2.41	1.40	1.33
11	D	1307	EPH	C37-C2	2.39	1.58	1.50
11	D	1306	EPH	C10-C11	-2.18	1.43	1.52
9	B	1201	UQ1	C6-C1	2.15	1.52	1.46
5	A	700	FAD	PA-O2A	-2.15	1.45	1.55
5	A	700	FAD	C2A-N1A	2.12	1.37	1.33
11	D	1307	EPH	C5-C3	2.10	1.56	1.50
11	D	1307	EPH	P1-O5	2.08	1.67	1.59
5	A	700	FAD	C6-C5X	2.04	1.43	1.40
10	C	1305	HEM	C4D-ND	-2.04	1.36	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	1307	EPH	C27-C26-C25	13.36	146.29	112.73
11	D	1306	EPH	C27-C26-C25	12.57	144.32	112.73
9	B	1201	UQ1	C8-C7-C6	10.47	137.88	112.08
9	B	1201	UQ1	C10-C9-C8	-6.35	103.59	122.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	1306	EPH	C15-C14-C13	5.56	139.41	112.02
11	D	1307	EPH	C26-C27-C28	3.97	122.72	112.73
9	B	1201	UQ1	C11-C9-C10	-3.83	105.77	114.59
9	B	1201	UQ1	C7-C8-C9	-3.10	118.48	127.25
11	D	1306	EPH	C14-C15-C16	3.02	149.07	123.74
9	B	1201	UQ1	C7-C6-C5	-2.87	119.98	124.89
11	D	1306	EPH	C2-O1-C3	2.68	124.20	117.80
11	D	1307	EPH	C30-C29-C28	-2.57	110.97	126.42
11	D	1306	EPH	C30-C29-C28	-2.47	111.58	126.42
9	B	1201	UQ1	O1-C1-C6	-2.46	117.03	121.79
11	D	1307	EPH	C26-C25-C24	2.38	142.64	124.83
9	B	1201	UQ1	CM5-C5-C6	-2.28	120.69	124.45
5	A	700	FAD	C4'-C3'-C2'	-2.26	109.80	113.57
5	A	700	FAD	O5B-PA-O1A	-2.22	100.15	108.94
10	C	1305	HEM	C4D-ND-C1D	2.19	107.81	105.21
9	B	1201	UQ1	C11-C9-C8	2.14	129.08	122.66
11	D	1306	EPH	C6-C5-C3	-2.09	106.04	113.69
9	B	1201	UQ1	CM3-O3-C3	-2.07	109.21	116.47
11	D	1307	EPH	C37-C2-C1	2.05	116.56	111.78
5	A	700	FAD	C1'-N10-C9A	-2.01	116.72	120.63

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	700	FAD	N10-C1'-C2'-O2'
5	A	700	FAD	N10-C1'-C2'-C3'
10	C	1305	HEM	C2B-C3B-CAB-CBB
10	C	1305	HEM	C4B-C3B-CAB-CBB
10	C	1305	HEM	C2C-C3C-CAC-CBC
10	C	1305	HEM	C4C-C3C-CAC-CBC
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
11	D	1307	EPH	C25-C26-C27-C28
11	D	1307	EPH	O8-C38-C39-N1
9	B	1201	UQ1	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
11	D	1306	EPH	C27-C28-C29-C30
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-C12-C13-C14
11	D	1306	EPH	O4-C4-O2-C1
11	D	1306	EPH	C11-C10-C9-C8
11	D	1306	EPH	C4-C18-C19-C20
11	D	1306	EPH	C21-C22-C23-C24
11	D	1306	EPH	C18-C19-C20-C21
11	D	1306	EPH	O2-C1-C2-O1
11	D	1306	EPH	C7-C8-C9-C10
11	D	1307	EPH	C27-C28-C29-C30
11	D	1306	EPH	O2-C1-C2-C37
11	D	1306	EPH	C12-C13-C14-C15
11	D	1306	EPH	C28-C29-C30-C31
5	A	700	FAD	P-O3P-PA-O1A
11	D	1306	EPH	C38-O8-P1-O5
11	D	1306	EPH	C38-O8-P1-O6
10	C	1305	HEM	CAD-CBD-CGD-O1D
10	C	1305	HEM	CAD-CBD-CGD-O2D
11	D	1306	EPH	C1-C2-O1-C3
11	D	1306	EPH	C37-C2-O1-C3
11	D	1306	EPH	C25-C26-C27-C28
10	C	1305	HEM	CAA-CBA-CGA-O1A
9	B	1201	UQ1	C7-C8-C9-C11
11	D	1306	EPH	C24-C25-C26-C27
10	C	1305	HEM	CAA-CBA-CGA-O2A
11	D	1306	EPH	C5-C6-C7-C8
11	D	1306	EPH	C2-C37-O5-P1
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

There are no ring outliers.

5 monomers are involved in 28 short contacts:

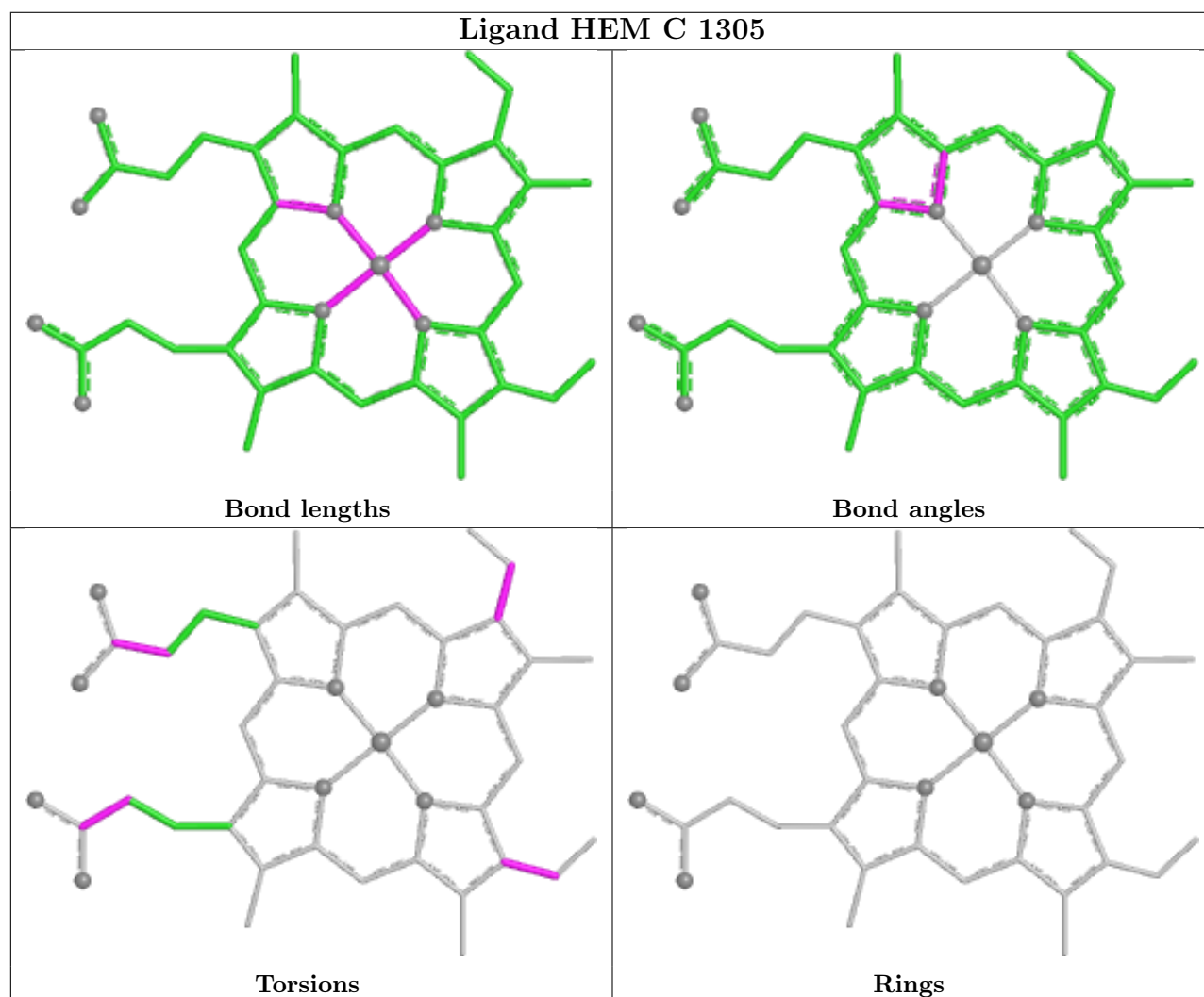
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1305	HEM	7	0
11	D	1306	EPH	4	0
9	B	1201	UQ1	1	0

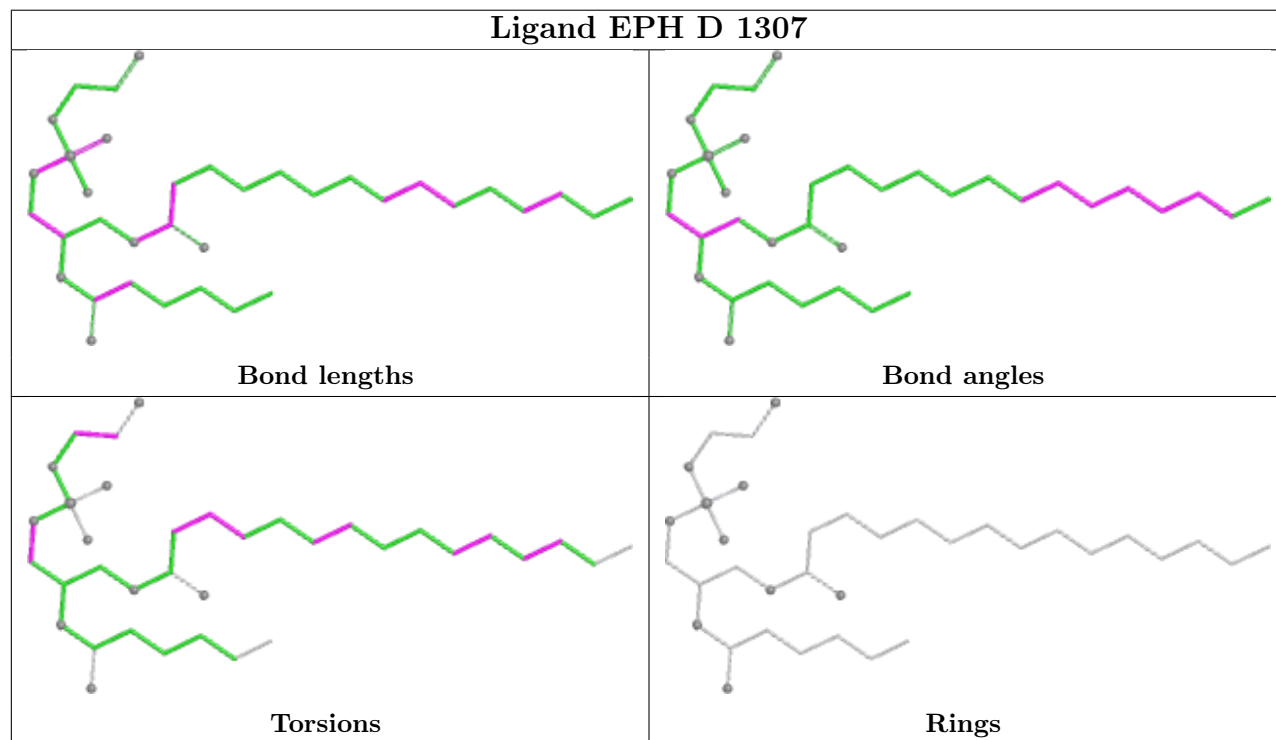
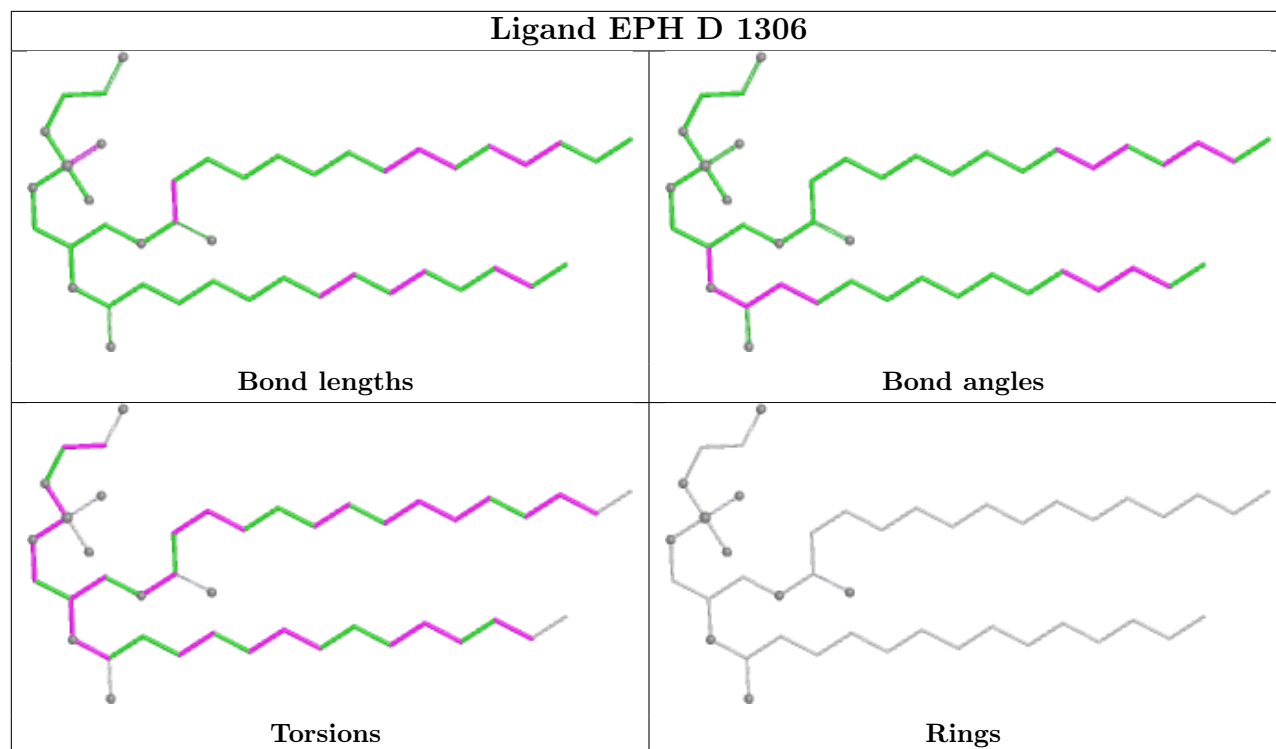
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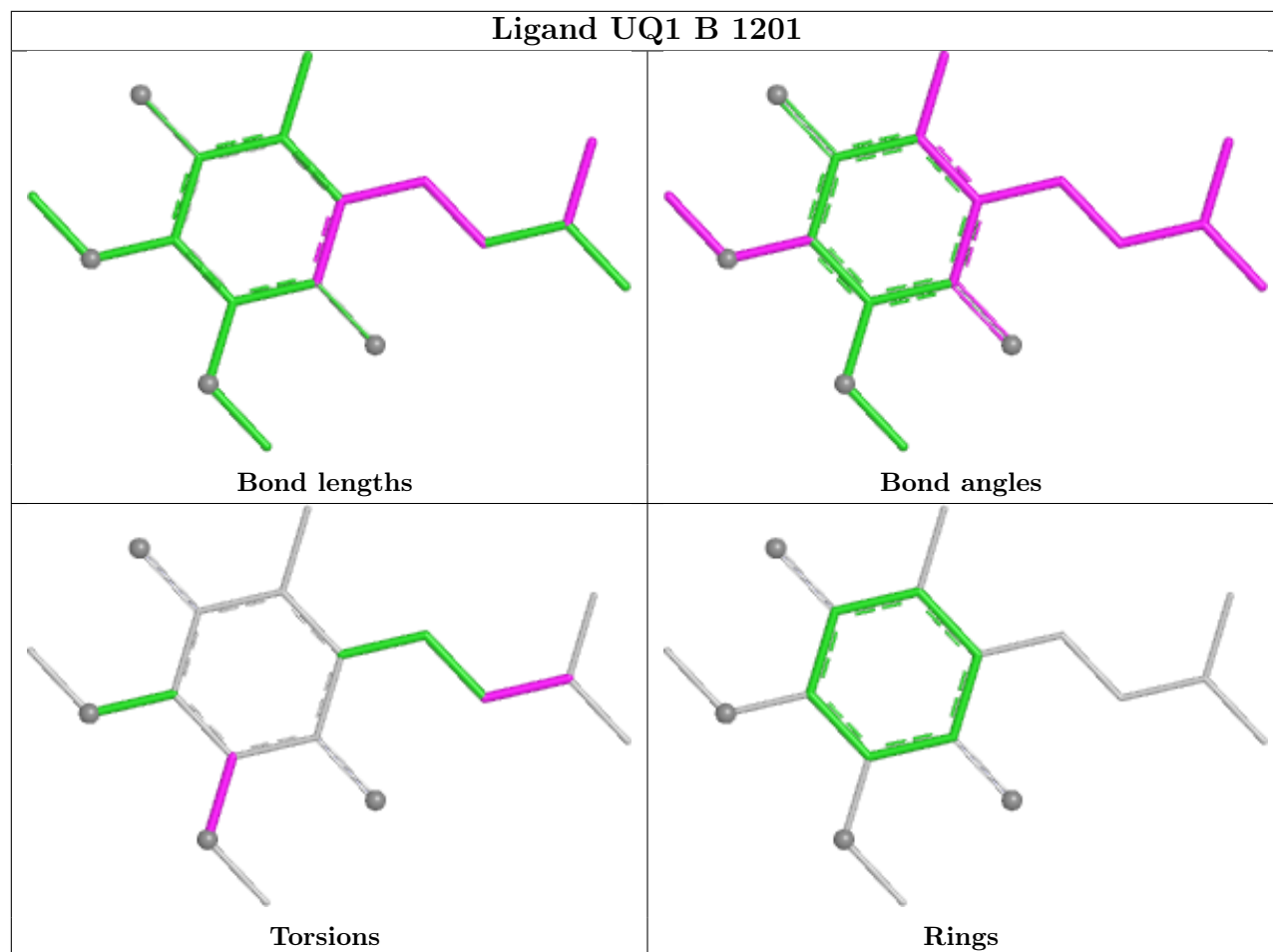
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	700	FAD	12	0
8	B	304	F3S	4	0

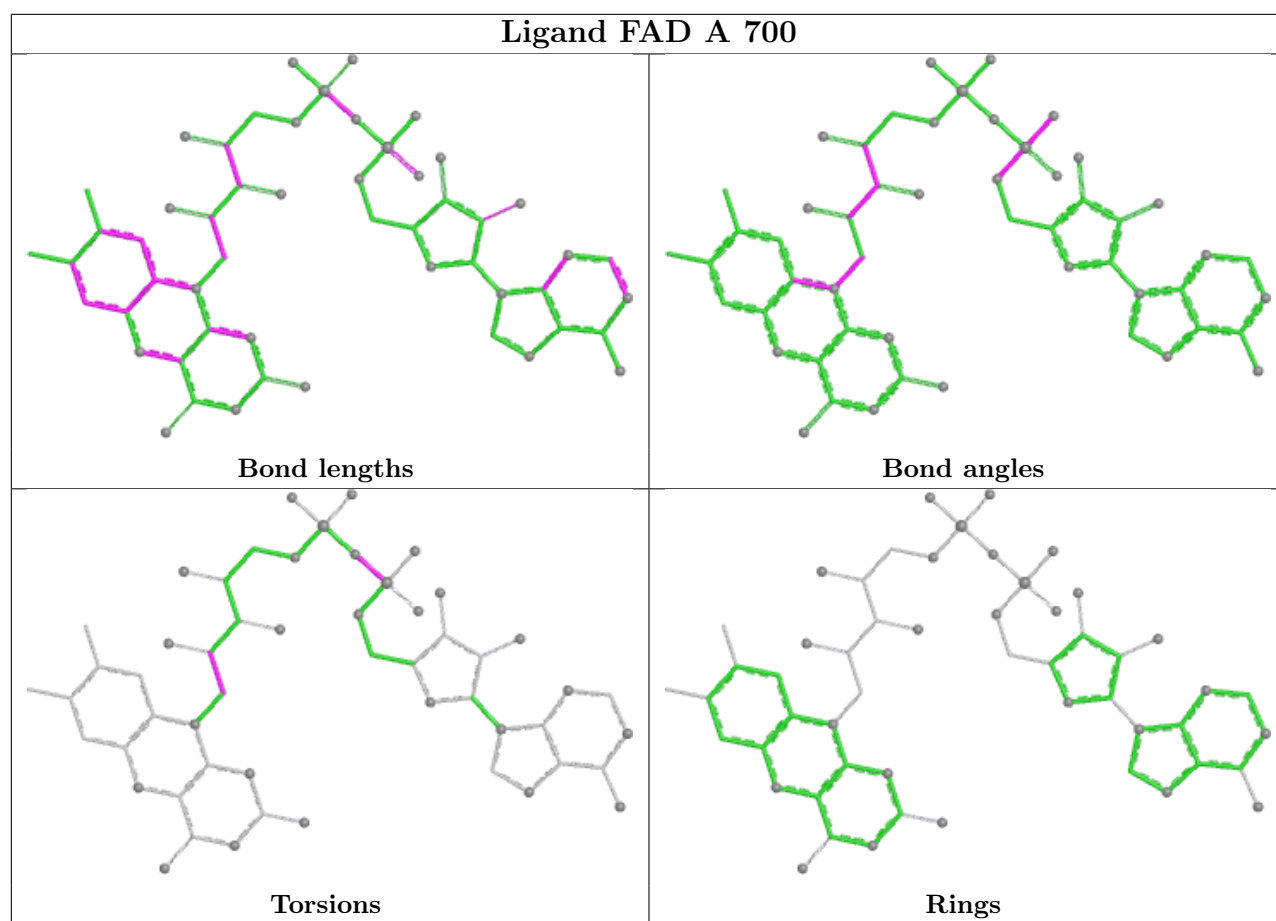
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	613/622 (98%)	0.45	50 (8%) 17 14	39, 64, 108, 123	0
2	B	239/252 (94%)	0.09	2 (0%) 82 80	38, 57, 88, 105	0
3	C	138/140 (98%)	0.51	7 (5%) 33 30	47, 67, 101, 114	0
4	D	102/103 (99%)	0.36	1 (0%) 79 76	48, 67, 90, 104	0
All	All	1092/1117 (97%)	0.37	60 (5%) 30 27	38, 63, 104, 123	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	VAL	5.9
1	A	297	SER	4.8
2	B	9	PRO	4.3
1	A	277	ILE	4.2
1	A	324	LEU	4.2
1	A	276	LEU	3.6
1	A	359	PRO	3.6
1	A	620	ARG	3.5
1	A	327	HIS	3.5
3	C	35	TRP	3.4
1	A	317	PRO	3.4
1	A	352	ASP	3.2
4	D	35	SER	3.2
3	C	143	MET	3.2
1	A	357	PRO	3.2
1	A	14	PRO	3.1
3	C	82	LEU	3.1
1	A	326	LEU	3.0
3	C	84	PRO	3.0
1	A	319	LYS	2.9
1	A	330	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	315	CYS	2.9
1	A	358	ILE	2.9
1	A	259	TYR	2.9
1	A	298	ARG	2.8
1	A	622	TYR	2.8
1	A	568	ILE	2.7
1	A	173	TYR	2.7
1	A	329	LEU	2.7
1	A	356	GLU	2.7
1	A	284	PHE	2.6
1	A	507	LEU	2.6
1	A	278	ASN	2.6
1	A	314	GLY	2.5
1	A	567	PRO	2.5
1	A	320	ASP	2.4
1	A	355	LYS	2.4
1	A	285	MET	2.4
1	A	321	HIS	2.4
1	A	291	VAL	2.4
1	A	307	LEU	2.3
1	A	328	HIS	2.3
1	A	296	ALA	2.3
1	A	353	VAL	2.3
1	A	410	LEU	2.2
1	A	354	THR	2.2
1	A	11	THR	2.1
1	A	323	TYR	2.1
1	A	346	MET	2.1
3	C	85	THR	2.1
3	C	88	TYR	2.1
1	A	294	ASP	2.1
1	A	287	ARG	2.1
1	A	280	GLN	2.0
1	A	270	ARG	2.0
3	C	83	GLY	2.0
1	A	619	ILE	2.0
2	B	57	SER	2.0
1	A	360	VAL	2.0
1	A	10	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

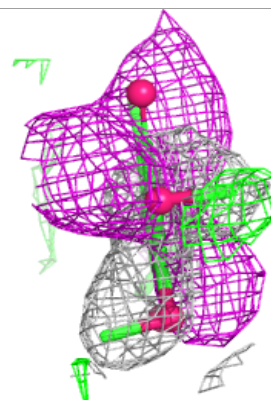
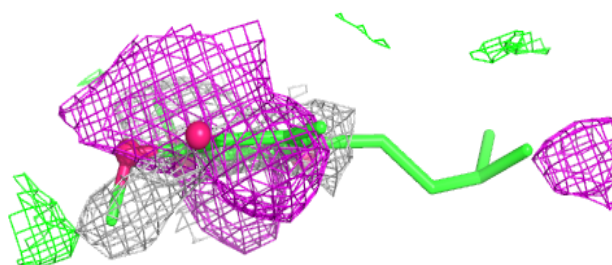
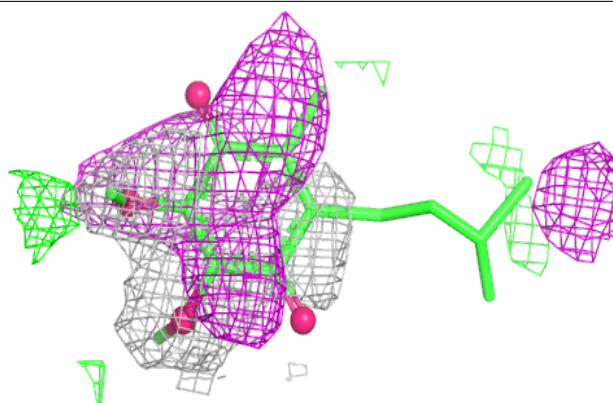
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	UQ1	B	1201	18/18	0.67	0.32	67,95,100,102	4
11	EPH	D	1307	36/49	0.69	0.28	112,122,143,144	0
11	EPH	D	1306	44/49	0.89	0.16	73,94,118,123	0
7	SF4	B	303	8/8	0.95	0.17	50,51,54,59	0
10	HEM	C	1305	43/43	0.96	0.14	53,62,77,80	0
8	F3S	B	304	7/7	0.96	0.12	45,47,53,54	0
5	FAD	A	700	53/53	0.96	0.09	42,52,65,66	0
6	FES	B	302	4/4	0.97	0.09	46,50,52,55	0

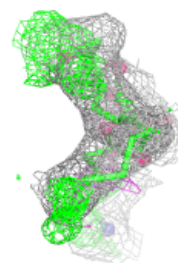
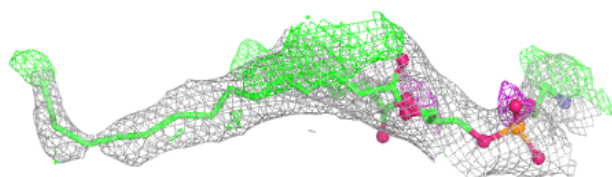
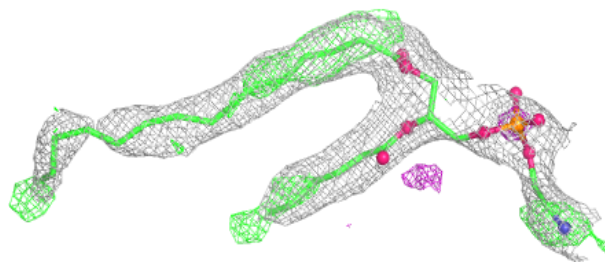
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

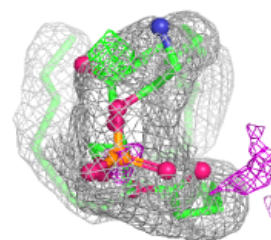
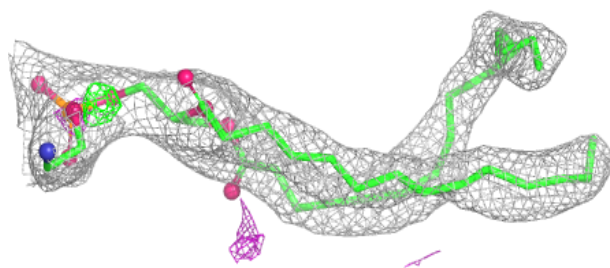
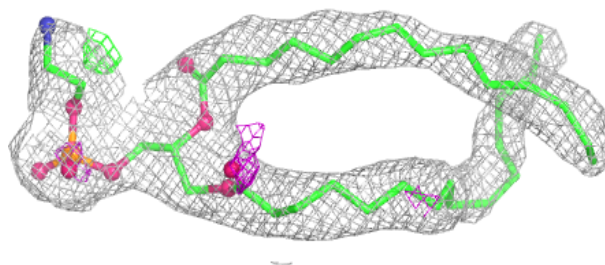
**Electron density around EPH D 1307:**

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



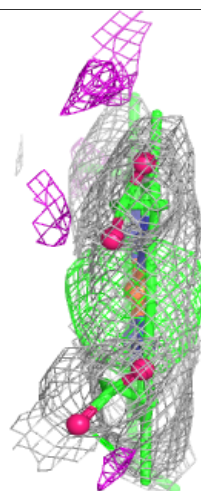
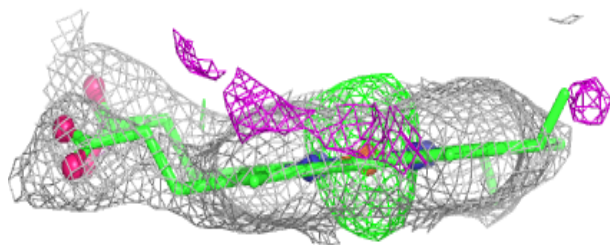
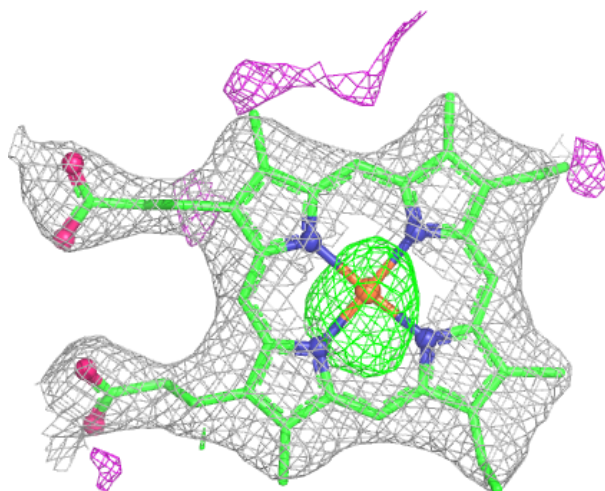
Electron density around EPH D 1306:

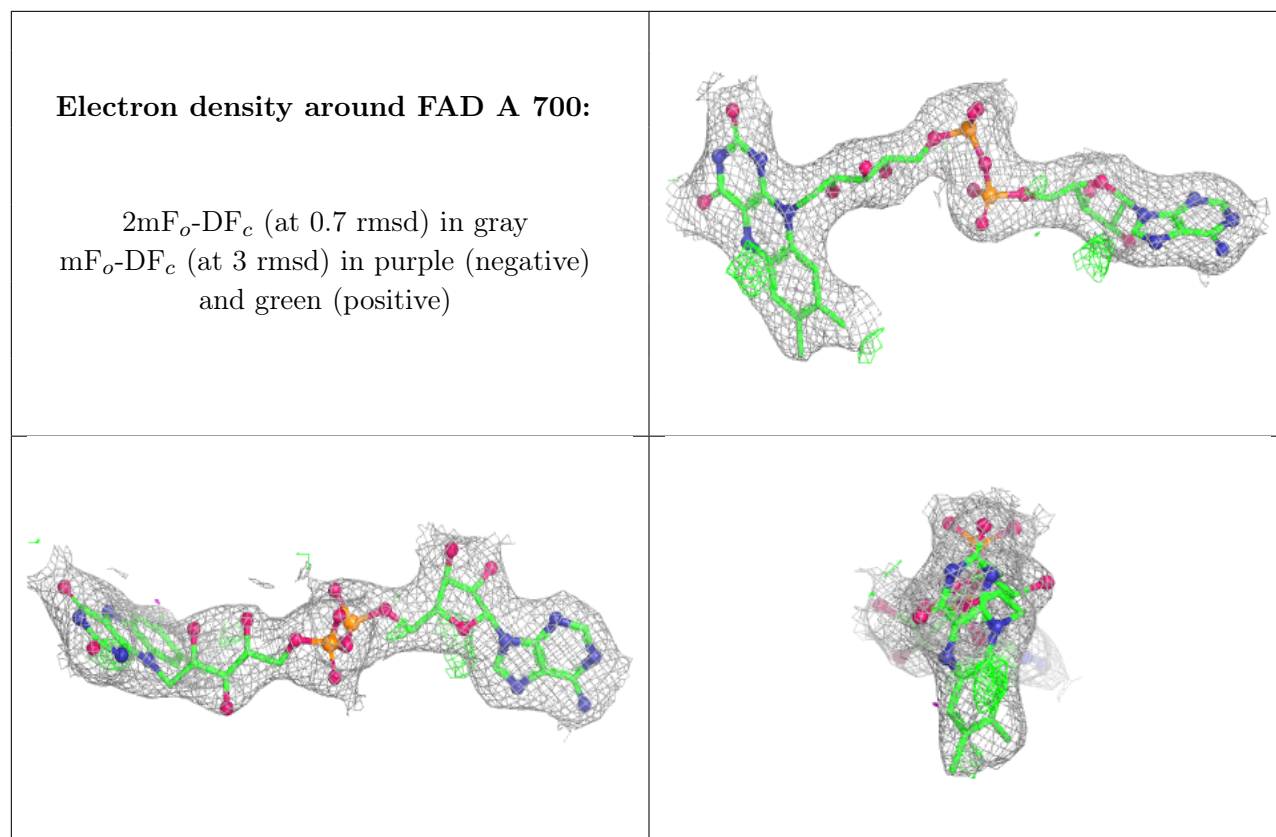
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



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.