



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:38 pm BST

PDB ID : 4PD4
Title : Structural analysis of atovaquone-inhibited cytochrome bc1 complex reveals the molecular basis of antimalarial drug action
Authors : Birth, D.; Kao, W.-C.; Hunte, C.
Deposited on : 2014-04-17
Resolution : 3.04 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 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

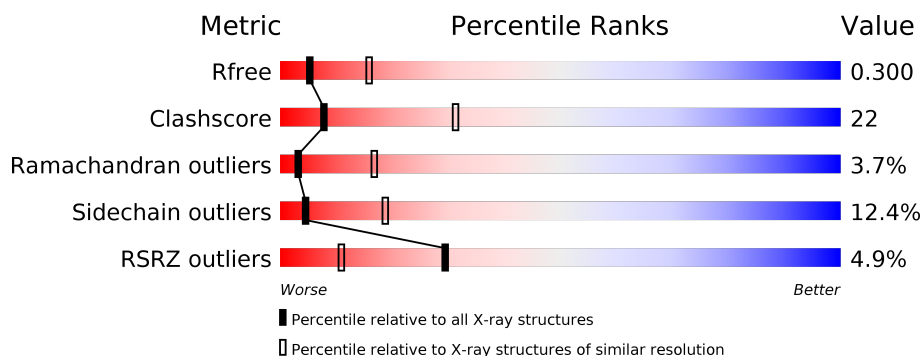
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 ≥ 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	431	<div> <div>9%</div> <div>49%</div> <div>45%</div> <div>6%</div> </div>
2	B	352	<div> <div>9%</div> <div>55%</div> <div>41%</div> <div>• •</div> </div>
3	C	385	<div> <div>48%</div> <div>44%</div> <div>8%</div> <div>•</div> </div>
4	D	248	<div> <div>2%</div> <div>48%</div> <div>46%</div> <div>5%</div> <div>•</div> </div>
5	E	185	<div> <div>4%</div> <div>49%</div> <div>42%</div> <div>9%</div> <div>•</div> </div>
6	F	74	<div> <div>8%</div> <div>59%</div> <div>35%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	126	<div><div></div><div>2%</div><div>52%</div><div>42%</div><div>6%</div></div>
8	H	93	<div><div></div><div>4%</div><div>62%</div><div>30%</div><div>5%</div><div></div></div>
9	I	57	<div><div></div><div>4%</div><div>58%</div><div>40%</div><div></div><div></div></div>
10	J	127	<div><div></div><div>2%</div><div>45%</div><div>42%</div><div>13%</div></div>
11	K	107	<div><div></div><div>7%</div><div>41%</div><div>48%</div><div>11%</div></div>

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 17646 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	115	0	0
			3344	2109	576	653	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	conflict	UNP P07256

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	72	0	0
			2735	1747	453	534	1			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	10	0	0
			3090	2082	484	503	21			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	248	Total	C	N	O	S	5	0	0
			1961	1249	340	363	9			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	27	0	0
			1411	893	242	266	10			

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	126	Total	C	N	O	S	0	0	0
			1019	653	173	191	2			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	98	0	0
			773	510	131	130	2			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	0	0	0
			465	310	77	78			

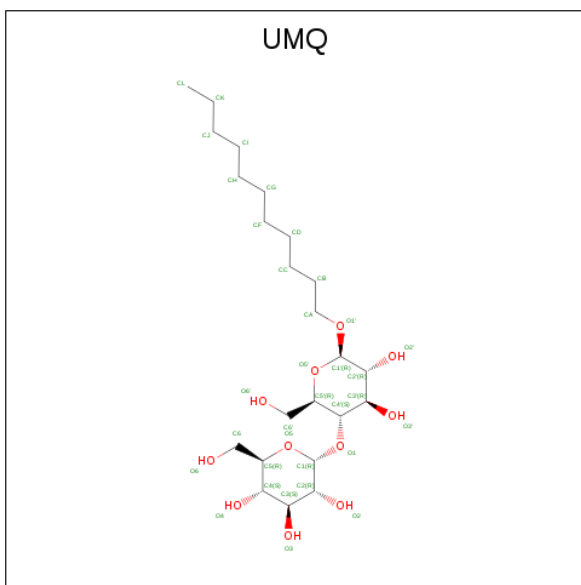
- Molecule 10 is a protein called Igh protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

- Molecule 11 is a protein called Ig kappa chain V-V region HP 124E1.

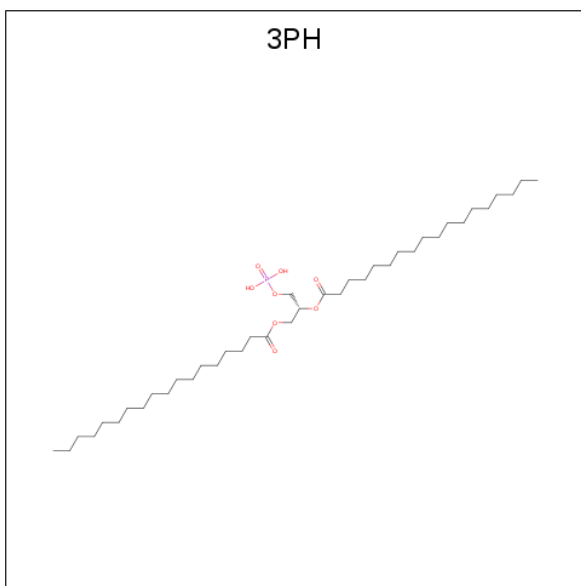
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C₂₃H₄₄O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			34	23	11		

- Molecule 13 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



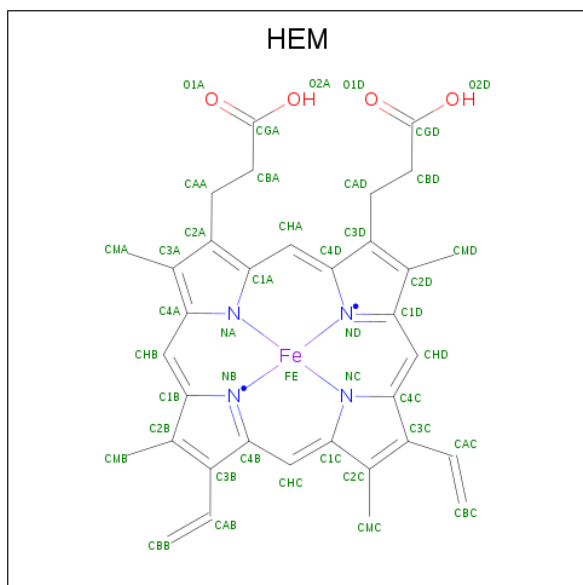
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total 31	C 22	O 8	P 1	0	0
13	C	1	Total 35	C 26	O 8	P 1	0	0

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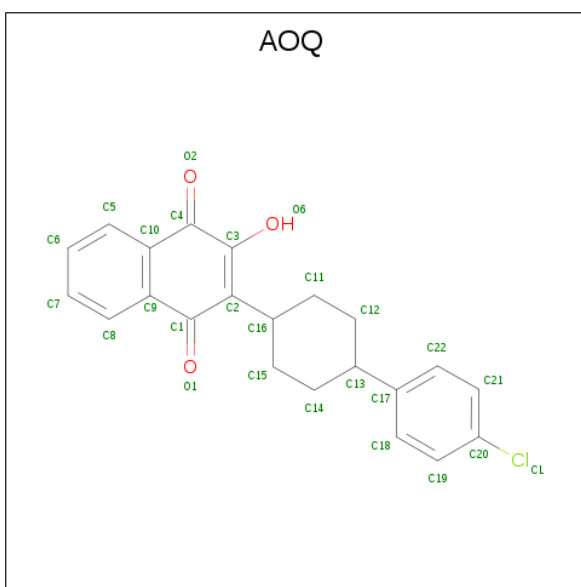
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	E	1	Total	C	O	P	0	0
			38	29	8	1		

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



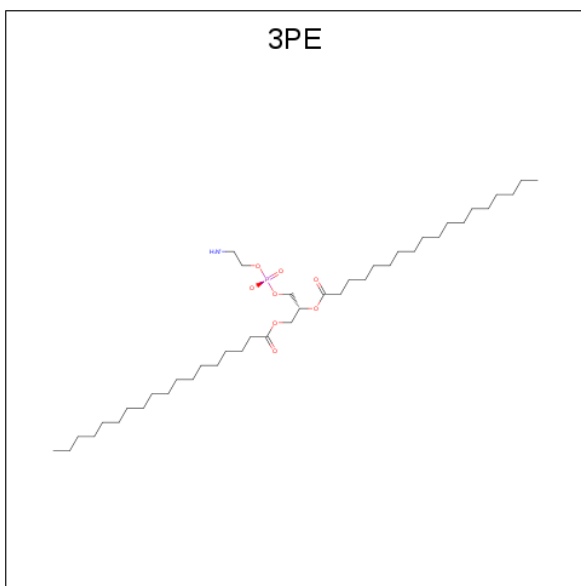
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
14	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
14	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 15 is 2-[trans-4-(4-chlorophenyl)cyclohexyl]-3-hydroxynaphthalene-1,4-dione (three-letter code: AOQ) (formula: $C_{22}H_{19}ClO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	Cl	O	0	0
			26	22	1	3		

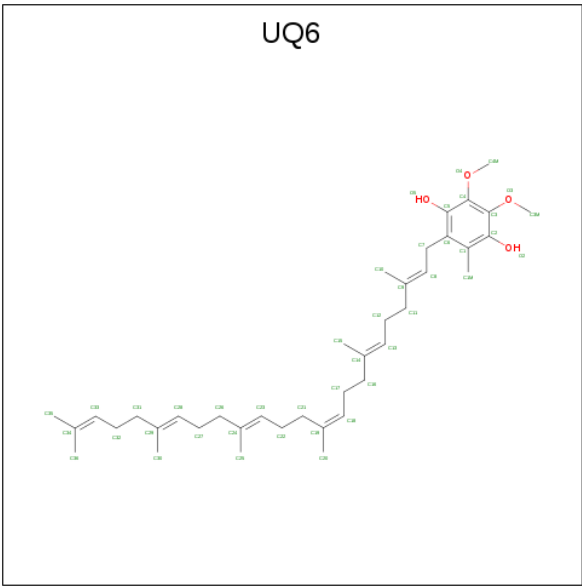
- Molecule 16 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	P	0	0
			27	17	1	8	1		

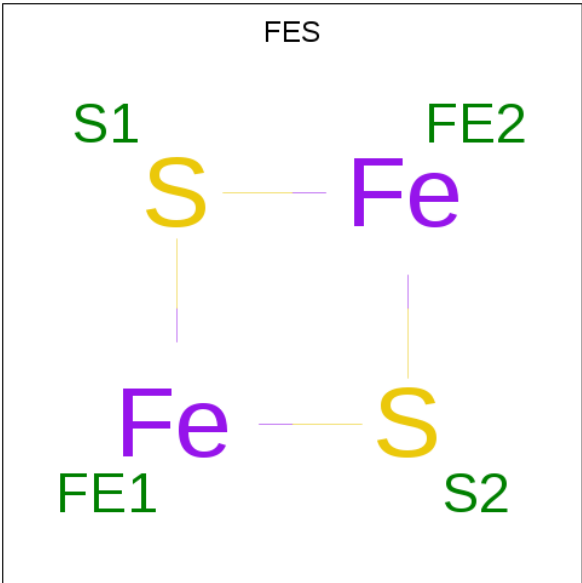
- Molecule 17 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEX AENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6)

(formula: C₃₉H₆₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			43	39	4		

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	E	1	Total	Fe	S	0	0
			4	2	2		

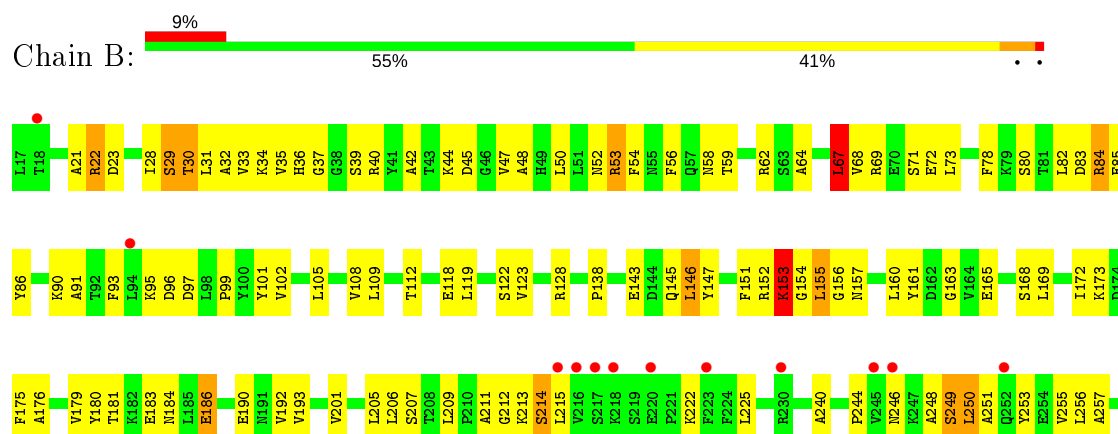
3 Residue-property plots

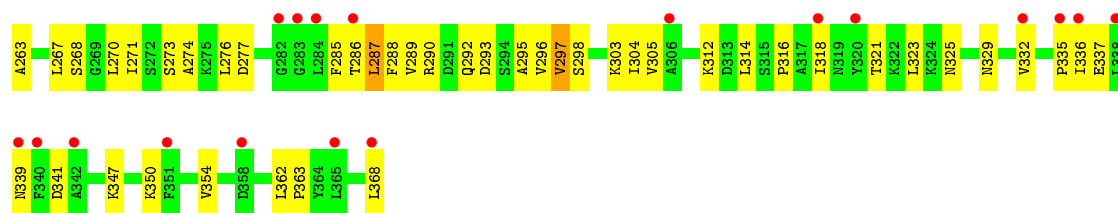
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Cytochrome b-c1 complex subunit 1, mitochondrial



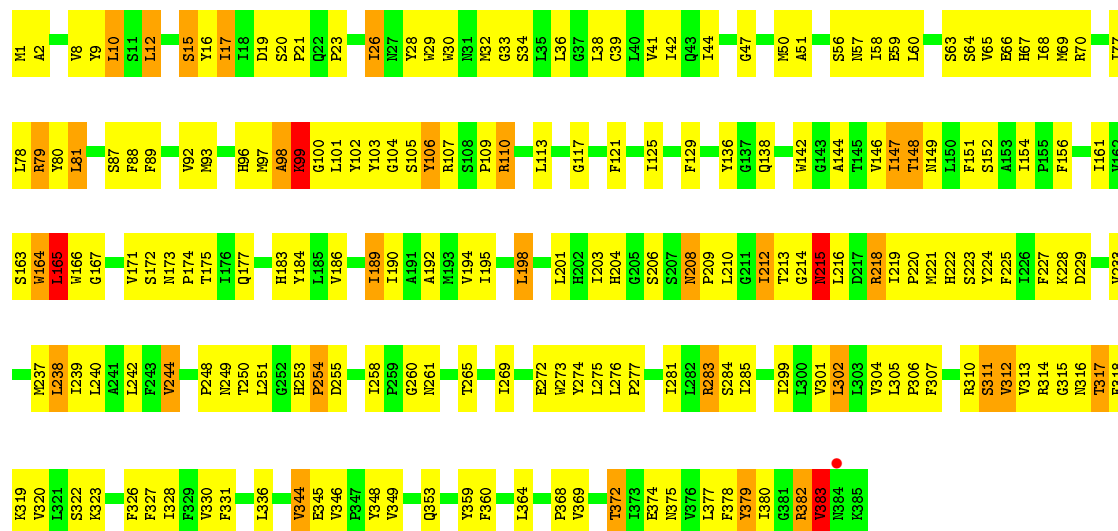
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial





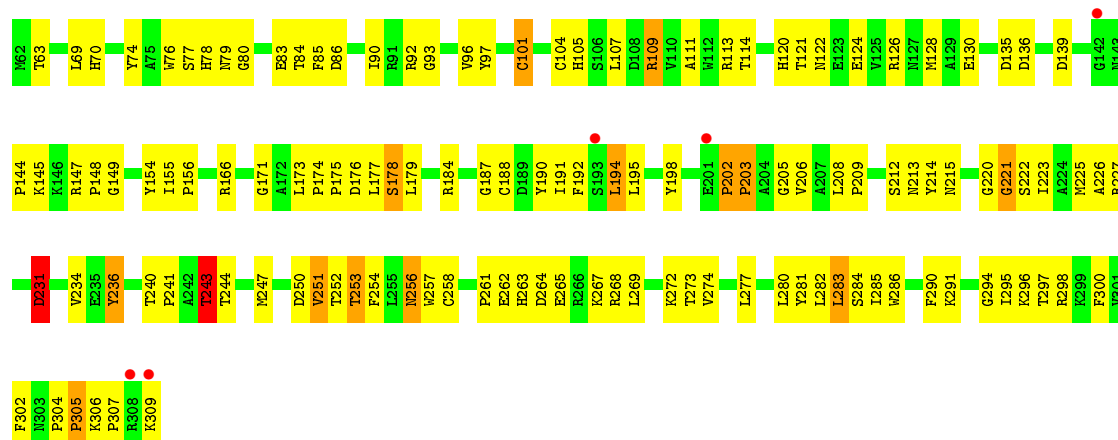
• Molecule 3: Cytochrome b

Chain C: 48% 44% 8%



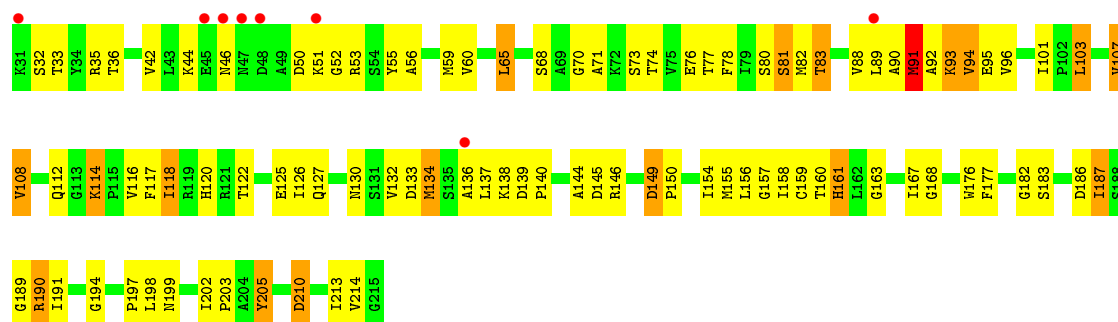
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 48% 46% 5%



• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

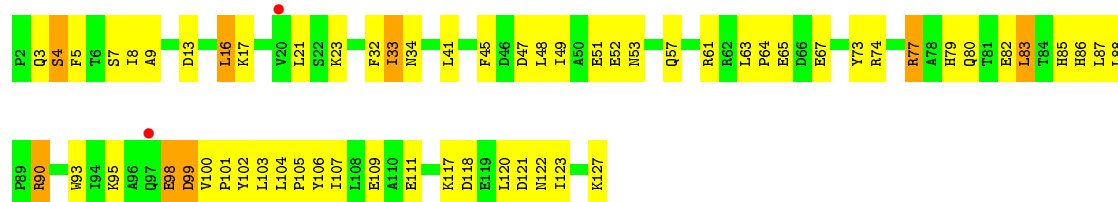
Chain E: 49% 42% 9%



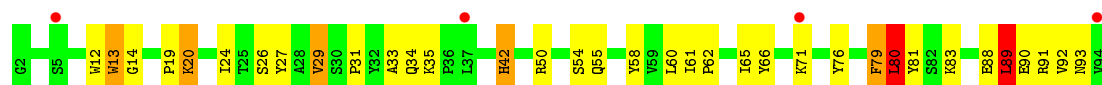
• Molecule 6: Cytochrome b-c1 complex subunit 6



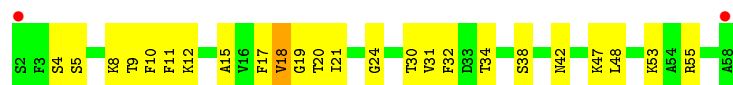
• Molecule 7: Cytochrome b-c1 complex subunit 7



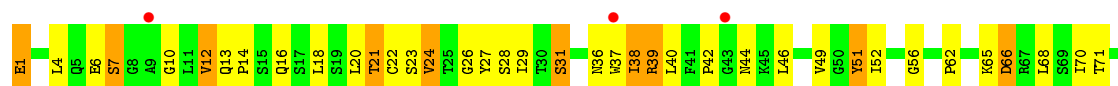
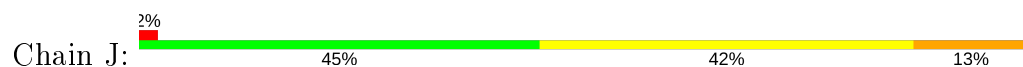
• Molecule 8: Cytochrome b-c1 complex subunit 8

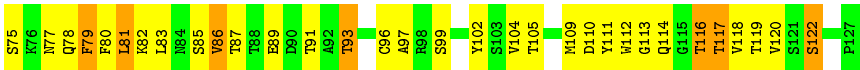


• Molecule 9: Cytochrome b-c1 complex subunit 9

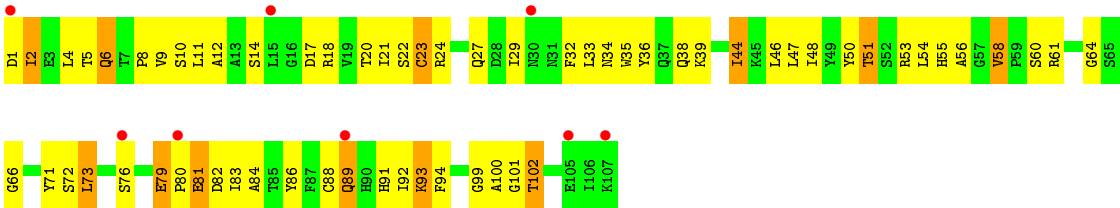


• Molecule 10: Igh protein





• Molecule 11: Ig kappa chain V-V region HP 124E1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	212.26Å 150.88Å 143.09Å 90.00° 115.18° 90.00°	Depositor
Resolution (Å)	24.99 – 3.04 24.99 – 3.04	Depositor EDS
% Data completeness (in resolution range)	98.4 (24.99-3.04) 98.6 (24.99-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.268 , 0.297 0.269 , 0.300	Depositor DCC
R_{free} test set	2008 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	97.2	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17646	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: UMQ, 3PH, FES, AOQ, HEM, 3PE, UQ6

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	0.42	0/3405	0.62	0/4614
2	B	0.37	0/2781	0.58	1/3764 (0.0%)
3	C	0.70	0/3192	0.83	1/4354 (0.0%)
4	D	0.48	0/2022	0.69	0/2751
5	E	0.54	0/1444	0.74	0/1957
6	F	0.40	0/638	0.62	0/858
7	G	0.58	0/1040	0.80	0/1408
8	H	0.55	0/804	0.71	0/1088
9	I	0.43	0/479	0.59	0/646
10	J	0.48	0/1043	0.71	0/1422
11	K	0.38	0/863	0.59	0/1172
All	All	0.51	0/17711	0.69	2/24034 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	67	LEU	CA-CB-CG	5.30	127.50	115.30
3	C	110	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	3344	0	3321	152	0
2	B	2735	0	2774	108	0
3	C	3090	0	3129	167	0
4	D	1961	0	1890	101	0
5	E	1411	0	1386	66	0
6	F	624	0	581	23	0
7	G	1019	0	1034	52	0
8	H	773	0	736	34	0
9	I	465	0	459	18	0
10	J	1015	0	959	57	0
11	K	842	0	820	42	0
12	A	34	0	44	3	0
13	A	31	0	35	2	0
13	C	35	0	46	1	0
13	E	38	0	49	6	0
14	C	86	0	60	15	0
14	D	43	0	30	11	0
15	C	26	0	19	3	0
16	C	27	0	28	1	0
17	C	43	0	58	5	0
18	E	4	0	0	0	0
All	All	17646	0	17458	747	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 22.

All (747) 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)
3:C:318:PHE:HD1	7:G:48:LEU:HD21	1.32	0.93
1:A:248:GLU:OE2	1:A:250:ARG:NH2	2.04	0.90
13:A:502:3PH:H321	13:A:502:3PH:H221	1.54	0.89
3:C:32:MET:HE3	3:C:92:VAL:HG13	1.54	0.89
11:K:93:LYS:HD2	11:K:94:PHE:H	1.41	0.83
2:B:33:VAL:HG11	2:B:109:LEU:HD11	1.61	0.83
1:A:99:ARG:HD3	1:A:174:LEU:HD12	1.62	0.80
14:C:4001:HEM:HHD	14:C:4001:HEM:HBC2	1.62	0.79
10:J:38:ILE:HD11	10:J:46:LEU:HD22	1.65	0.79
3:C:144:ALA:O	3:C:148:THR:OG1	1.99	0.79
1:A:443:LEU:HD23	1:A:447:ARG:HG3	1.63	0.79
5:E:118:ILE:HG23	5:E:154:ILE:HG12	1.64	0.79
3:C:310:ARG:HH11	7:G:3:GLN:HA	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:319:LYS:HB3	3:C:322:SER:HB2	1.66	0.78
1:A:71:ASN:O	1:A:75:ASN:ND2	2.16	0.77
3:C:379:TYR:HE2	7:G:9:ALA:HA	1.50	0.77
5:E:126:ILE:O	5:E:130:ASN:ND2	2.18	0.77
10:J:24:VAL:HG21	10:J:29:ILE:HD11	1.67	0.76
3:C:318:PHE:CD1	7:G:48:LEU:HD21	2.18	0.76
4:D:198:TYR:OH	4:D:225:MET:O	2.03	0.75
1:A:300:ILE:HB	1:A:303:LEU:HD12	1.69	0.75
2:B:30:THR:OG1	2:B:31:LEU:N	2.15	0.75
1:A:311:LEU:HB3	1:A:343:LEU:HD23	1.68	0.74
3:C:378:PHE:HA	7:G:33:ILE:HD11	1.67	0.74
7:G:98:GLU:O	7:G:100:VAL:N	2.18	0.74
2:B:40:ARG:HG3	2:B:155:LEU:HG	1.67	0.74
1:A:258:LYS:HG2	1:A:335:ARG:HG3	1.69	0.74
10:J:87:THR:HG22	10:J:89:GLU:H	1.53	0.74
1:A:164:LEU:HD12	1:A:262:SER:HB3	1.71	0.73
2:B:273:SER:HB3	2:B:288:PHE:HB2	1.70	0.73
3:C:30:TRP:NE1	14:C:4002:HEM:O1D	2.21	0.72
4:D:286:TRP:CD2	5:E:59:MET:HG3	2.26	0.71
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.73	0.71
2:B:201:VAL:HG13	2:B:206:LEU:HD23	1.71	0.70
5:E:88:VAL:O	5:E:90:ALA:N	2.23	0.70
10:J:52:ILE:HG12	10:J:56:GLY:HA2	1.73	0.70
2:B:267:LEU:HD22	2:B:304:ILE:HD13	1.74	0.70
4:D:83:GLU:OE2	9:I:47:LYS:NZ	2.24	0.69
3:C:110:ARG:HG2	3:C:113:LEU:HD23	1.74	0.69
4:D:166:ARG:CZ	4:D:173:LEU:HB2	2.21	0.69
3:C:237:MET:HG2	13:E:302:3PH:H282	1.74	0.69
2:B:59:THR:HA	2:B:112:THR:HA	1.75	0.69
1:A:285:PHE:HE2	1:A:354:LEU:HD11	1.56	0.69
7:G:64:PRO:HB2	7:G:67:GLU:HG3	1.75	0.68
3:C:313:VAL:HG22	3:C:319:LYS:HZ2	1.57	0.68
3:C:368:PRO:O	3:C:372:THR:OG1	2.11	0.68
3:C:138:GLN:NE2	3:C:261:ASN:HB3	2.07	0.68
5:E:139:ASP:O	5:E:199:ASN:ND2	2.23	0.68
2:B:145:GLN:HB3	2:B:354:VAL:HG11	1.75	0.68
3:C:138:GLN:HE22	3:C:261:ASN:HB3	1.58	0.68
1:A:129:ALA:HA	1:A:132:LEU:HB2	1.76	0.67
4:D:215:ASN:O	4:D:221:GLY:HA2	1.94	0.67
4:D:175:PRO:HG3	14:D:401:HEM:HAA1	1.76	0.67
3:C:56:SER:OG	3:C:177:GLN:HG2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:5:PHE:HB2	7:G:111:GLU:OE1	1.94	0.67
11:K:21:ILE:HD13	11:K:102:THR:HB	1.77	0.66
5:E:197:PRO:O	5:E:198:LEU:HD23	1.96	0.66
2:B:50:LEU:HD21	2:B:161:TYR:CD1	2.31	0.66
6:F:126:GLU:OE1	8:H:83:LYS:NZ	2.29	0.65
3:C:164:TRP:O	3:C:166:TRP:N	2.29	0.65
1:A:98:SER:OG	1:A:99:ARG:N	2.29	0.65
1:A:365:ARG:NH2	2:B:72:GLU:OE1	2.29	0.65
4:D:101:CYS:HB3	14:D:401:HEM:CHC	2.27	0.65
1:A:80:LYS:NZ	2:B:268:SER:OG	2.28	0.65
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.80	0.64
4:D:176:ASP:OD2	4:D:178:SER:OG	2.14	0.64
5:E:210:ASP:OD1	5:E:210:ASP:N	2.31	0.64
4:D:243:THR:HG21	6:F:76:ASP:HA	1.80	0.64
3:C:28:TYR:HE1	3:C:228:LYS:HG3	1.63	0.63
7:G:87:LEU:H	8:H:50:ARG:HH22	1.47	0.63
3:C:299:ILE:O	3:C:302:LEU:HB2	1.99	0.63
4:D:80:GLY:O	4:D:267:LYS:NZ	2.24	0.63
1:A:40:THR:HG22	1:A:210:GLY:HA3	1.79	0.63
7:G:57:GLN:O	7:G:61:ARG:NH2	2.32	0.63
1:A:258:LYS:HB2	1:A:260:TRP:CH2	2.33	0.63
11:K:5:THR:HB	11:K:24:ARG:HB3	1.81	0.62
3:C:275:LEU:HD22	15:C:4003:AOQ:H8	1.81	0.62
2:B:152:ARG:O	2:B:154:GLY:N	2.33	0.62
1:A:132:LEU:HD22	1:A:190:VAL:HG13	1.82	0.62
5:E:146:ARG:NH1	5:E:189:GLY:O	2.33	0.62
4:D:109:ARG:HG3	4:D:178:SER:HB2	1.80	0.62
5:E:126:ILE:HD13	5:E:150:PRO:HB2	1.82	0.62
11:K:8:PRO:O	11:K:10:SER:N	2.32	0.62
2:B:32:ALA:HA	2:B:90:LYS:HA	1.82	0.61
6:F:143:PHE:CD1	6:F:146:LEU:HD12	2.35	0.61
1:A:38:VAL:HA	1:A:208:VAL:HG13	1.80	0.61
11:K:79:GLU:HG3	11:K:80:PRO:HA	1.82	0.61
3:C:238:LEU:HD21	4:D:274:VAL:HG13	1.82	0.61
5:E:95:GLU:HG2	5:E:213:ILE:HG22	1.82	0.61
1:A:97:ILE:HD12	1:A:102:GLN:HG3	1.81	0.61
2:B:23:ASP:OD2	2:B:95:LYS:NZ	2.34	0.61
2:B:253:TYR:HB2	2:B:276:LEU:HD22	1.83	0.61
10:J:23:SER:HA	10:J:78:GLN:HB3	1.83	0.60
3:C:249:ASN:C	3:C:251:LEU:H	2.05	0.60
3:C:105:SER:C	3:C:107:ARG:H	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:13:GLN:HG2	10:J:122:SER:HA	1.84	0.60
10:J:62:PRO:HA	10:J:65:LYS:HB3	1.83	0.60
1:A:287:SER:HA	1:A:316:ASN:HA	1.82	0.60
2:B:225:LEU:HB3	2:B:350:LYS:HD3	1.83	0.60
2:B:119:LEU:HD12	2:B:123:VAL:HB	1.83	0.60
4:D:208:LEU:HD21	4:D:214:TYR:HB2	1.83	0.60
2:B:36:HIS:NE2	2:B:186:GLU:OE2	2.35	0.60
2:B:295:ALA:O	2:B:298:SER:N	2.34	0.60
3:C:164:TRP:O	3:C:167:GLY:N	2.29	0.59
1:A:292:GLU:OE2	2:B:53:ARG:NH1	2.35	0.59
3:C:117:GLY:HA3	14:C:4002:HEM:C3C	2.37	0.59
4:D:85:PHE:HE1	4:D:257:TRP:HA	1.67	0.59
1:A:133:SER:HB2	1:A:136:ASN:H	1.66	0.59
2:B:257:ALA:HB2	2:B:285:PHE:HE1	1.67	0.59
1:A:80:LYS:HG3	2:B:263:ALA:HB1	1.83	0.59
3:C:10:LEU:HD22	16:C:4004:3PE:H232	1.84	0.59
2:B:271:ILE:HG21	2:B:287:LEU:HD11	1.85	0.59
3:C:301:VAL:O	3:C:304:VAL:HG22	2.03	0.59
2:B:206:LEU:HD12	2:B:209:LEU:HD12	1.85	0.59
3:C:59:GLU:N	3:C:59:GLU:OE2	2.34	0.59
4:D:122:ASN:OD1	4:D:126:ARG:NH2	2.31	0.59
5:E:101:ILE:HG22	5:E:120:HIS:HB2	1.85	0.59
4:D:273:THR:HA	13:E:302:3PH:H32	1.84	0.58
8:H:76:TYR:CZ	8:H:80:LEU:HD21	2.38	0.58
4:D:194:LEU:HD11	4:D:223:ILE:HD12	1.85	0.58
1:A:269:PRO:HG2	1:A:272:SER:HB2	1.84	0.58
2:B:52:ASN:HB2	2:B:82:LEU:HD13	1.84	0.58
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.38	0.58
10:J:91:THR:HG23	10:J:119:THR:HA	1.86	0.58
2:B:101:TYR:O	2:B:105:LEU:HG	2.04	0.58
4:D:195:LEU:HD11	14:D:401:HEM:HMB1	1.86	0.58
11:K:61:ARG:HB2	11:K:76:SER:HB3	1.86	0.58
1:A:72:LEU:HD13	1:A:144:VAL:HG21	1.84	0.58
3:C:379:TYR:CE2	7:G:9:ALA:HA	2.34	0.58
3:C:63:SER:O	3:C:66:GLU:N	2.37	0.58
5:E:186:ASP:OD2	5:E:190:ARG:HD2	2.03	0.57
1:A:252:ARG:NH2	1:A:254:ASP:OD2	2.36	0.57
1:A:300:ILE:HG22	1:A:303:LEU:H	1.68	0.57
3:C:102:TYR:HB2	3:C:326:PHE:CZ	2.39	0.57
5:E:65:LEU:HD21	9:I:24:GLY:HA3	1.85	0.57
2:B:295:ALA:O	2:B:297:VAL:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:ALA:HB2	4:D:154:TYR:CE1	2.40	0.57
10:J:40:LEU:HD21	11:K:38:GLN:HE22	1.69	0.57
3:C:209:PRO:O	3:C:210:LEU:HD23	2.05	0.57
4:D:273:THR:O	4:D:277:LEU:HB2	2.05	0.57
3:C:319:LYS:O	3:C:323:LYS:HG3	2.05	0.56
4:D:220:GLY:O	4:D:222:SER:N	2.33	0.56
1:A:312:CYS:HB3	1:A:343:LEU:HD21	1.88	0.56
3:C:201:LEU:HD21	17:C:4005:UQ6:H3M2	1.87	0.56
1:A:191:ALA:O	1:A:195:SER:OG	2.23	0.56
2:B:42:ALA:HA	2:B:175:PHE:CE1	2.40	0.56
5:E:177:PHE:CE1	5:E:182:GLY:HA2	2.41	0.56
10:J:96:CYS:O	10:J:113:GLY:N	2.26	0.56
2:B:40:ARG:HH11	2:B:85:GLU:HG2	1.70	0.56
11:K:35:TRP:HB2	11:K:48:ILE:HB	1.88	0.56
1:A:169:PHE:O	1:A:175:SER:HB3	2.05	0.56
2:B:246:ASN:H	2:B:249:SER:HB2	1.71	0.55
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.69	0.55
1:A:447:ARG:O	1:A:450:SER:N	2.36	0.55
1:A:365:ARG:HD2	2:B:72:GLU:OE1	2.06	0.55
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.72	0.55
2:B:29:SER:HB2	2:B:95:LYS:HA	1.88	0.55
3:C:117:GLY:O	14:C:4002:HEM:HMC3	2.06	0.55
4:D:124:GLU:O	4:D:128:MET:HG3	2.06	0.55
11:K:14:SER:HB2	11:K:17:ASP:OD2	2.06	0.55
1:A:58:GLY:N	1:A:61:ASN:OD1	2.39	0.55
5:E:103:LEU:HD12	5:E:120:HIS:NE2	2.22	0.55
10:J:99:SER:HB2	10:J:109:MET:HG3	1.89	0.55
8:H:76:TYR:CE2	8:H:80:LEU:HD11	2.42	0.55
3:C:272:GLU:HB2	3:C:275:LEU:HD12	1.88	0.55
3:C:313:VAL:HG22	3:C:319:LYS:NZ	2.22	0.55
3:C:344:VAL:HG12	3:C:349:VAL:HG22	1.87	0.55
1:A:73:TRP:HB3	1:A:104:TYR:OH	2.07	0.55
6:F:96:HIS:O	6:F:99:GLU:N	2.40	0.55
1:A:263:LEU:HD21	1:A:431:ILE:HD12	1.89	0.54
1:A:86:ALA:HB1	1:A:91:LEU:HB2	1.88	0.54
3:C:16:TYR:O	3:C:17:ILE:HG13	2.07	0.54
6:F:144:ASP:OD2	6:F:144:ASP:N	2.38	0.54
2:B:146:LEU:HG	2:B:286:THR:HG22	1.89	0.54
4:D:147:ARG:NH2	4:D:148:PRO:O	2.41	0.54
7:G:3:GLN:NE2	7:G:7:SER:OG	2.38	0.54
11:K:101:GLY:O	11:K:102:THR:OG1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLY:HA3	1:A:430:ASP:HB3	1.90	0.54
3:C:129:PHE:CE1	3:C:147:ILE:HG13	2.41	0.54
4:D:107:LEU:HD11	4:D:258:CYS:SG	2.47	0.54
5:E:94:VAL:HG22	5:E:95:GLU:H	1.72	0.54
1:A:275:TYR:O	1:A:279:LYS:HG3	2.07	0.54
1:A:301:LYS:HD2	1:A:353:ARG:NH2	2.22	0.54
1:A:377:LEU:HD12	1:A:378:TYR:CD2	2.42	0.54
3:C:105:SER:O	3:C:107:ARG:N	2.41	0.54
3:C:360:PHE:O	3:C:364:LEU:HD12	2.07	0.54
4:D:105:HIS:CE1	4:D:174:PRO:HB3	2.43	0.54
11:K:72:SER:OG	11:K:73:LEU:N	2.40	0.54
1:A:302:LEU:HB2	1:A:350:GLN:HG3	1.90	0.54
3:C:229:ASP:O	3:C:233:VAL:HG23	2.07	0.54
10:J:105:THR:HB	11:K:50:TYR:HB2	1.90	0.54
1:A:252:ARG:CZ	1:A:440:GLU:HB2	2.38	0.54
2:B:67:LEU:O	2:B:71:SER:OG	2.19	0.54
4:D:272:LYS:HG2	9:I:32:PHE:CE2	2.43	0.54
1:A:253:ASP:OD1	1:A:255:THR:OG1	2.19	0.54
3:C:208:ASN:OD1	7:G:79:HIS:HE1	1.91	0.54
4:D:101:CYS:SG	14:D:401:HEM:CAB	2.95	0.54
5:E:91:MET:HG3	5:E:112:GLN:NE2	2.23	0.54
7:G:105:PRO:O	7:G:109:GLU:N	2.32	0.54
5:E:73:SER:HB3	13:E:302:3PH:H11	1.89	0.53
4:D:86:ASP:O	4:D:90:ILE:HG13	2.08	0.53
3:C:194:VAL:O	3:C:198:LEU:HD12	2.08	0.53
3:C:8:VAL:HG13	3:C:9:TYR:CD2	2.43	0.53
2:B:147:TYR:OH	2:B:277:ASP:OD2	2.26	0.53
3:C:32:MET:CE	3:C:92:VAL:HG13	2.35	0.53
4:D:166:ARG:HB3	4:D:171:GLY:HA2	1.89	0.53
11:K:4:LEU:HD23	11:K:23:CYS:SG	2.49	0.53
1:A:102:GLN:HE22	1:A:196:PHE:HZ	1.57	0.53
1:A:54:VAL:HG21	1:A:391:GLY:HA3	1.90	0.53
2:B:240:ALA:HB3	2:B:354:VAL:HG23	1.91	0.53
8:H:76:TYR:CE2	8:H:80:LEU:HD21	2.44	0.53
2:B:147:TYR:HB3	2:B:156:GLY:HA2	1.90	0.53
7:G:73:TYR:HD1	8:H:24:ILE:HG12	1.74	0.53
11:K:47:LEU:HA	11:K:58:VAL:HG11	1.89	0.53
4:D:74:TYR:CE2	4:D:192:PHE:HD2	2.27	0.53
3:C:39:CYS:HB2	3:C:89:PHE:CD1	2.44	0.52
1:A:446:MET:O	1:A:450:SER:HB2	2.09	0.52
1:A:67:ASN:HD21	1:A:177:PRO:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ARG:NH2	2:B:157:ASN:O	2.42	0.52
3:C:70:ARG:HH11	4:D:109:ARG:HD3	1.75	0.52
1:A:55:PHE:N	1:A:102:GLN:O	2.42	0.52
5:E:125:GLU:HG2	5:E:187:ILE:HG12	1.91	0.52
1:A:48:THR:HA	1:A:110:PRO:HD3	1.92	0.52
17:C:4005:UQ6:H103	17:C:4005:UQ6:H1M1	1.91	0.52
1:A:244:PHE:CD2	1:A:266:GLU:HB2	2.44	0.52
1:A:280:LEU:HD13	1:A:413:ILE:HG21	1.92	0.52
2:B:48:ALA:HB1	2:B:82:LEU:HD11	1.92	0.52
1:A:172:THR:HG21	1:A:243:ALA:H	1.75	0.52
14:C:4002:HEM:O2A	14:C:4002:HEM:HHA	2.10	0.52
5:E:70:GLY:HA3	13:E:302:3PH:H351	1.91	0.52
11:K:35:TRP:CZ3	11:K:88:CYS:HB3	2.45	0.52
2:B:151:PHE:HD2	2:B:155:LEU:HB2	1.74	0.52
2:B:168:SER:O	2:B:172:ILE:HG13	2.10	0.52
1:A:122:GLN:HA	1:A:126:GLN:HB3	1.92	0.51
1:A:156:HIS:HA	1:A:159:ARG:HB3	1.93	0.51
3:C:277:PRO:O	3:C:281:ILE:HG13	2.10	0.51
7:G:32:PHE:C	7:G:34:ASN:H	2.14	0.51
10:J:93:THR:HG23	10:J:117:THR:HG23	1.92	0.51
3:C:208:ASN:N	3:C:208:ASN:ND2	2.59	0.51
3:C:33:GLY:HA3	14:C:4002:HEM:C3A	2.45	0.51
3:C:98:ALA:O	3:C:100:GLY:N	2.43	0.51
8:H:80:LEU:HD13	8:H:92:VAL:HG21	1.93	0.51
4:D:203:PRO:O	4:D:206:VAL:HG23	2.11	0.51
7:G:118:ASP:O	7:G:122:ASN:ND2	2.43	0.51
7:G:90:ARG:HA	7:G:93:TRP:NE1	2.25	0.51
11:K:32:PHE:HD2	11:K:92:ILE:HG13	1.75	0.51
1:A:195:SER:O	1:A:199:ASN:ND2	2.43	0.51
3:C:88:PHE:CZ	3:C:239:ILE:HG22	2.45	0.51
5:E:156:LEU:HD21	5:E:203:PRO:HB3	1.93	0.51
7:G:4:SER:O	7:G:8:ILE:HG13	2.11	0.51
2:B:33:VAL:O	2:B:35:VAL:HG23	2.11	0.51
3:C:377:LEU:HD23	7:G:32:PHE:CG	2.46	0.51
2:B:22:ARG:HH11	2:B:332:VAL:HG12	1.76	0.50
3:C:64:SER:O	3:C:67:HIS:HB3	2.11	0.50
7:G:64:PRO:O	7:G:67:GLU:HB2	2.11	0.50
1:A:285:PHE:CE2	1:A:354:LEU:HD11	2.43	0.50
1:A:428:ASP:OD2	5:E:53:ARG:NH2	2.43	0.50
3:C:314:ARG:NH1	7:G:52:GLU:OE2	2.43	0.50
10:J:1:GLU:O	10:J:26:GLY:HA3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:18:LEU:HB3	10:J:83:LEU:HB3	1.93	0.50
1:A:80:LYS:HE2	2:B:263:ALA:HA	1.92	0.50
10:J:81:LEU:HD12	10:J:82:LYS:H	1.75	0.50
2:B:29:SER:HB3	2:B:93:PHE:CE1	2.46	0.50
3:C:149:ASN:O	3:C:152:SER:OG	2.29	0.50
8:H:89:LEU:O	8:H:91:ARG:N	2.45	0.50
2:B:257:ALA:HB2	2:B:285:PHE:CE1	2.46	0.50
2:B:225:LEU:HD21	2:B:244:PRO:HD2	1.93	0.50
3:C:328:ILE:HD12	8:H:66:TYR:HE1	1.76	0.50
1:A:170:GLN:HB2	5:E:36:THR:HG21	1.93	0.50
3:C:249:ASN:C	3:C:251:LEU:N	2.64	0.50
1:A:91:LEU:HD23	1:A:106:VAL:HG11	1.94	0.50
3:C:215:ASN:OD1	3:C:215:ASN:N	2.45	0.50
5:E:149:ASP:HB2	10:J:104:VAL:HG11	1.93	0.50
10:J:38:ILE:HG12	10:J:112:TRP:CZ3	2.47	0.50
1:A:315:PHE:CE1	1:A:317:HIS:CE1	2.99	0.50
4:D:263:HIS:CE1	4:D:267:LYS:HE2	2.47	0.50
1:A:86:ALA:HB2	1:A:119:PHE:CZ	2.47	0.49
3:C:214:GLY:O	3:C:216:LEU:N	2.45	0.49
1:A:167:THR:O	1:A:247:SER:OG	2.29	0.49
2:B:325:ASN:O	2:B:329:ASN:ND2	2.46	0.49
4:D:85:PHE:HE1	4:D:257:TRP:CA	2.25	0.49
1:A:141:LYS:HA	1:A:144:VAL:HG22	1.95	0.49
1:A:156:HIS:O	1:A:160:VAL:HG23	2.12	0.49
4:D:90:ILE:HG23	4:D:254:PHE:HA	1.94	0.49
1:A:375:GLY:HA3	2:B:28:ILE:HG13	1.95	0.49
1:A:431:ILE:CD1	1:A:448:ILE:HG22	2.43	0.49
14:D:401:HEM:HBD1	14:D:401:HEM:HHA	1.95	0.49
4:D:297:THR:HG21	5:E:42:VAL:HG11	1.94	0.49
4:D:300:PHE:HE1	7:G:80:GLN:OE1	1.96	0.49
10:J:24:VAL:HG23	10:J:77:ASN:O	2.13	0.49
11:K:2:ILE:HD12	11:K:2:ILE:H	1.76	0.49
1:A:348:LEU:O	1:A:352:ASN:ND2	2.46	0.49
7:G:117:LYS:NZ	7:G:121:ASP:OD2	2.45	0.49
3:C:29:TRP:HB3	3:C:99:LYS:HG3	1.94	0.49
4:D:101:CYS:HB3	14:D:401:HEM:HHC	1.95	0.49
6:F:77:GLN:O	6:F:81:LEU:HD12	2.12	0.49
1:A:441:GLY:HA2	8:H:13:TRP:HB3	1.95	0.49
1:A:349:LYS:HA	1:A:352:ASN:OD1	2.13	0.49
2:B:34:LYS:HB3	2:B:86:TYR:CE1	2.48	0.49
3:C:240:LEU:O	3:C:244:VAL:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:105:HIS:CD2	4:D:177:LEU:HD11	2.48	0.49
4:D:294:GLY:O	4:D:298:ARG:HB2	2.13	0.49
4:D:93:GLY:O	4:D:97:TYR:N	2.43	0.49
10:J:14:PRO:HD3	10:J:120:VAL:HG12	1.95	0.49
10:J:40:LEU:HD21	11:K:38:GLN:NE2	2.28	0.49
3:C:77:ILE:O	3:C:81:LEU:HB2	2.12	0.48
3:C:96:HIS:HE1	14:C:4002:HEM:C1A	2.31	0.48
11:K:35:TRP:CD2	11:K:73:LEU:HG	2.46	0.48
1:A:63:ASN:HB2	1:A:64:PRO:HD2	1.94	0.48
3:C:29:TRP:CZ2	13:C:4006:3PH:H322	2.49	0.48
12:A:501:UMQ:HB1	9:I:18:VAL:HG13	1.94	0.48
3:C:326:PHE:O	3:C:330:VAL:HG23	2.13	0.48
1:A:125:ILE:HG12	1:A:230:LEU:HD23	1.94	0.48
2:B:44:LYS:HE2	2:B:165:GLU:HG2	1.95	0.48
2:B:64:ALA:O	2:B:68:VAL:HG23	2.13	0.48
3:C:208:ASN:N	3:C:208:ASN:HD22	2.09	0.48
3:C:29:TRP:O	3:C:32:MET:HG2	2.13	0.48
3:C:65:VAL:O	3:C:69:MET:HG2	2.13	0.48
10:J:6:GLU:H	10:J:114:GLN:HE22	1.62	0.48
6:F:78:LEU:O	6:F:82:ARG:HG3	2.12	0.48
7:G:61:ARG:HH21	7:G:61:ARG:HB2	1.79	0.48
10:J:87:THR:O	10:J:120:VAL:HG21	2.13	0.48
1:A:258:LYS:HB2	1:A:260:TRP:CZ2	2.49	0.48
3:C:21:PRO:HB2	3:C:218:ARG:HG3	1.96	0.48
4:D:69:LEU:HD22	4:D:70:HIS:H	1.79	0.48
5:E:55:TYR:O	5:E:59:MET:HG2	2.13	0.48
5:E:65:LEU:HA	9:I:21:ILE:HG23	1.96	0.48
1:A:141:LYS:HE3	1:A:186:GLU:HA	1.94	0.48
2:B:48:ALA:O	2:B:52:ASN:N	2.35	0.48
3:C:360:PHE:HB3	3:C:364:LEU:HD12	1.96	0.48
3:C:79:ARG:NH2	14:C:4001:HEM:O1A	2.45	0.48
1:A:245:LEU:HD11	8:H:33:ALA:HB1	1.95	0.47
1:A:392:ALA:O	1:A:396:ILE:HG13	2.14	0.47
1:A:289:ASN:O	1:A:291:PHE:N	2.47	0.47
1:A:375:GLY:O	1:A:378:TYR:N	2.47	0.47
3:C:317:THR:HG22	3:C:318:PHE:CD2	2.49	0.47
17:C:4005:UQ6:H171	17:C:4005:UQ6:H151	1.49	0.47
6:F:104:ARG:O	6:F:108:GLN:HG3	2.14	0.47
1:A:415:VAL:O	1:A:418:VAL:N	2.47	0.47
2:B:99:PRO:HA	2:B:102:VAL:HB	1.96	0.47
5:E:80:SER:HA	5:E:83:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ASN:HB3	1:A:427:TRP:HZ3	1.78	0.47
3:C:26:ILE:HA	3:C:209:PRO:HD3	1.96	0.47
5:E:183:SER:HA	5:E:194:GLY:HA3	1.96	0.47
1:A:200:HIS:HD2	1:A:236:PRO:HB2	1.78	0.47
3:C:225:PHE:HA	3:C:228:LYS:HB3	1.96	0.47
4:D:202:PRO:HA	4:D:203:PRO:HD2	1.59	0.47
4:D:304:PRO:HA	4:D:305:PRO:HD3	1.68	0.47
2:B:181:THR:HB	2:B:211:ALA:O	2.15	0.47
2:B:21:ALA:HB1	2:B:192:VAL:HB	1.95	0.47
3:C:208:ASN:C	3:C:210:LEU:H	2.18	0.47
7:G:13:ASP:HB3	7:G:17:LYS:NZ	2.29	0.47
2:B:255:VAL:HG23	2:B:314:LEU:HB3	1.97	0.47
3:C:213:THR:HB	7:G:51:GLU:OE2	2.14	0.47
1:A:263:LEU:O	1:A:329:GLY:HA3	2.15	0.47
3:C:96:HIS:CD2	14:C:4002:HEM:C1C	3.03	0.47
4:D:120:HIS:HB3	4:D:124:GLU:HB3	1.96	0.47
5:E:74:THR:O	5:E:77:THR:HB	2.15	0.47
6:F:104:ARG:HA	6:F:107:ILE:HD12	1.96	0.47
4:D:265:GLU:O	4:D:268:ARG:HB3	2.15	0.47
5:E:44:LYS:HB3	8:H:35:LYS:HG3	1.95	0.47
5:E:51:LYS:HG2	9:I:4:SER:HB2	1.97	0.47
1:A:168:ALA:HB1	1:A:244:PHE:CE1	2.49	0.47
2:B:184:ASN:HD21	2:B:215:LEU:HD12	1.80	0.47
3:C:223:SER:O	3:C:227:PHE:HD1	1.97	0.47
2:B:36:HIS:HB2	2:B:184:ASN:OD1	2.15	0.47
3:C:253:HIS:HA	3:C:254:PRO:HD2	1.79	0.47
5:E:155:MET:HB3	5:E:202:ILE:HD13	1.96	0.47
10:J:39:ARG:HD2	10:J:49:VAL:HG22	1.96	0.47
11:K:34:ASN:OD1	11:K:91:HIS:NE2	2.48	0.47
11:K:54:LEU:HD23	11:K:58:VAL:O	2.15	0.47
1:A:285:PHE:CE1	1:A:350:GLN:HB3	2.50	0.46
2:B:138:PRO:HD2	2:B:290:ARG:NH2	2.30	0.46
4:D:286:TRP:CG	5:E:59:MET:HG3	2.49	0.46
10:J:29:ILE:HA	10:J:29:ILE:HD13	1.67	0.46
1:A:332:THR:HG21	1:A:343:LEU:HD11	1.97	0.46
5:E:107:VAL:HG12	5:E:118:ILE:HG13	1.97	0.46
3:C:283:ARG:O	3:C:285:ILE:N	2.49	0.46
3:C:311:SER:OG	3:C:312:VAL:N	2.49	0.46
5:E:213:ILE:HG13	5:E:213:ILE:O	2.15	0.46
4:D:205:GLY:HA3	6:F:122:ASP:HB3	1.97	0.46
10:J:7:SER:O	10:J:21:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:TYR:C	3:C:17:ILE:HG13	2.36	0.46
3:C:320:VAL:HG13	8:H:58:TYR:HE2	1.80	0.46
1:A:445:TYR:O	1:A:449:ARG:HB3	2.15	0.46
3:C:1:MET:HG3	3:C:2:ALA:O	2.16	0.46
15:C:4003:AOQ:H7	15:C:4003:AOQ:O1	2.15	0.46
11:K:54:LEU:HD21	11:K:60:SER:HA	1.98	0.46
11:K:66:GLY:HA3	11:K:71:TYR:HA	1.97	0.46
1:A:110:PRO:HB3	1:A:213:ASN:HB3	1.96	0.46
2:B:255:VAL:HG12	2:B:321:THR:HG21	1.98	0.46
3:C:194:VAL:HG22	14:C:4002:HEM:HBB2	1.96	0.46
5:E:93:LYS:HB2	5:E:93:LYS:NZ	2.31	0.46
7:G:74:ARG:HG2	7:G:77:ARG:HH22	1.81	0.46
10:J:81:LEU:HD12	10:J:82:LYS:N	2.31	0.46
1:A:390:LEU:HD23	1:A:400:LYS:HD2	1.97	0.46
11:K:6:GLN:HG3	11:K:99:GLY:HA3	1.96	0.46
1:A:52:GLY:HA3	1:A:105:ILE:HA	1.98	0.46
1:A:73:TRP:HA	1:A:73:TRP:CE3	2.50	0.46
2:B:30:THR:HG23	2:B:190:GLU:HB3	1.98	0.46
2:B:39:SER:OG	2:B:84:ARG:NH2	2.44	0.46
3:C:166:TRP:NE1	3:C:171:VAL:HG23	2.31	0.46
3:C:23:PRO:HB2	3:C:26:ILE:HG23	1.98	0.46
8:H:12:TRP:CD1	8:H:13:TRP:HD1	2.34	0.46
7:G:87:LEU:HD12	8:H:50:ARG:CZ	2.46	0.46
10:J:27:TYR:CE2	10:J:31:SER:HB2	2.51	0.46
10:J:38:ILE:HG12	10:J:112:TRP:CH2	2.51	0.46
10:J:6:GLU:H	10:J:114:GLN:NE2	2.14	0.46
1:A:359:THR:O	1:A:362:GLU:HB2	2.16	0.46
1:A:363:VAL:O	1:A:366:ALA:HB3	2.15	0.46
3:C:249:ASN:O	3:C:251:LEU:N	2.48	0.46
4:D:101:CYS:SG	14:D:401:HEM:CBB	3.04	0.46
1:A:301:LYS:HD2	1:A:353:ARG:HH22	1.81	0.45
3:C:79:ARG:HG2	14:C:4001:HEM:O2D	2.16	0.45
5:E:78:PHE:O	5:E:81:SER:HB3	2.16	0.45
6:F:98:TYR:HE1	6:F:123:CYS:HB2	1.81	0.45
4:D:203:PRO:HG3	6:F:127:PHE:CD2	2.51	0.45
10:J:4:LEU:HG	10:J:24:VAL:HG13	1.98	0.45
10:J:21:THR:HB	10:J:80:PHE:CD2	2.51	0.45
1:A:288:TYR:HB3	1:A:315:PHE:CD2	2.50	0.45
4:D:261:PRO:C	4:D:263:HIS:H	2.20	0.45
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.97	0.45
5:E:33:THR:O	8:H:27:TYR:OH	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:36:ASN:OD1	10:J:51:TYR:HB3	2.16	0.45
1:A:158:ASN:O	1:A:162:GLU:N	2.42	0.45
1:A:117:LEU:HD11	1:A:223:ILE:HG13	1.99	0.45
1:A:250:ARG:NH1	1:A:443:LEU:O	2.41	0.45
3:C:44:ILE:HG12	14:C:4001:HEM:HMC2	1.98	0.45
10:J:10:GLY:O	10:J:118:VAL:HA	2.17	0.45
1:A:140:THR:O	1:A:144:VAL:HG13	2.17	0.45
2:B:155:LEU:HD12	2:B:155:LEU:H	1.82	0.45
2:B:270:LEU:HD22	2:B:303:LYS:HD3	1.99	0.45
2:B:271:ILE:HA	2:B:289:VAL:HG22	1.99	0.45
3:C:166:TRP:HE1	3:C:171:VAL:HG23	1.81	0.45
3:C:186:VAL:HA	3:C:189:ILE:HG13	1.99	0.45
12:A:501:UMQ:O2'	9:I:17:PHE:HA	2.17	0.45
1:A:318:PHE:HE2	1:A:331:SER:OG	2.00	0.45
4:D:121:THR:HG22	9:I:53:LYS:HE3	1.97	0.45
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.98	0.45
1:A:268:GLU:OE1	1:A:269:PRO:HD2	2.16	0.45
1:A:349:LYS:HE2	1:A:451:ASP:OD2	2.17	0.45
2:B:271:ILE:HG22	2:B:287:LEU:HD21	1.99	0.45
3:C:265:THR:CG2	3:C:269:ILE:HD11	2.47	0.45
3:C:320:VAL:HG13	8:H:58:TYR:CE2	2.51	0.45
4:D:283:LEU:HA	4:D:283:LEU:HD12	1.74	0.45
6:F:143:PHE:HD1	6:F:146:LEU:HD12	1.82	0.45
9:I:8:LYS:O	9:I:12:LYS:HD3	2.17	0.45
1:A:397:LYS:NZ	1:A:401:LEU:HB2	2.31	0.45
3:C:121:PHE:CZ	3:C:125:ILE:HD11	2.52	0.45
4:D:273:THR:HG22	4:D:277:LEU:HD12	1.99	0.45
1:A:450:SER:OG	13:A:502:3PH:O14	2.32	0.45
3:C:316:ASN:HA	3:C:319:LYS:HB2	1.98	0.45
3:C:328:ILE:HG23	8:H:66:TYR:HE1	1.82	0.45
10:J:20:LEU:HD22	10:J:116:THR:HG21	1.97	0.45
10:J:6:GLU:N	10:J:114:GLN:HE22	2.15	0.45
11:K:39:LYS:NZ	11:K:81:GLU:O	2.50	0.45
2:B:119:LEU:HA	2:B:123:VAL:HB	1.98	0.45
4:D:92:ARG:HD2	4:D:250:ASP:OD2	2.16	0.45
6:F:105:VAL:O	6:F:109:GLN:HG3	2.17	0.45
4:D:243:THR:HG21	6:F:77:GLN:OE1	2.17	0.45
10:J:112:TRP:CZ2	11:K:44:ILE:HD11	2.52	0.45
3:C:109:PRO:HB2	3:C:204:HIS:CE1	2.52	0.45
3:C:222:HIS:HA	3:C:223:SER:HA	1.58	0.45
3:C:377:LEU:HB3	7:G:32:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:HA	1:A:147:GLN:HB3	1.99	0.44
2:B:44:LYS:O	2:B:47:VAL:HG23	2.17	0.44
4:D:231:ASP:OD2	4:D:243:THR:HG22	2.17	0.44
4:D:69:LEU:HD22	4:D:70:HIS:N	2.32	0.44
5:E:159:CYS:O	5:E:161:HIS:N	2.49	0.44
9:I:10:PHE:HB2	9:I:11:PHE:CD2	2.52	0.44
10:J:65:LYS:HG3	10:J:66:ASP:N	2.31	0.44
4:D:261:PRO:O	4:D:263:HIS:N	2.50	0.44
5:E:122:THR:O	5:E:126:ILE:HG13	2.17	0.44
3:C:323:LYS:NZ	8:H:55:GLN:OE1	2.36	0.44
8:H:79:PHE:O	8:H:81:TYR:N	2.49	0.44
11:K:64:GLY:HA2	11:K:73:LEU:HA	1.99	0.44
3:C:345:GLU:O	3:C:348:TYR:HB2	2.18	0.44
5:E:155:MET:HA	5:E:203:PRO:HD2	1.99	0.44
2:B:90:LYS:HG3	2:B:91:ALA:N	2.32	0.44
3:C:375:ASN:HB3	7:G:8:ILE:HD13	2.00	0.44
3:C:88:PHE:HZ	3:C:239:ILE:HG22	1.82	0.44
4:D:101:CYS:HB3	14:D:401:HEM:C4B	2.52	0.44
4:D:286:TRP:CZ3	4:D:290:PHE:HB2	2.52	0.44
1:A:205:ASN:CG	1:A:236:PRO:HG3	2.38	0.44
1:A:268:GLU:O	1:A:321:SER:OG	2.19	0.44
2:B:305:VAL:HG21	2:B:368:LEU:HD22	1.98	0.44
3:C:105:SER:C	3:C:107:ARG:N	2.70	0.44
3:C:50:MET:CG	3:C:78:LEU:HB3	2.47	0.44
7:G:47:ASP:OD1	7:G:102:TYR:OH	2.20	0.44
11:K:36:TYR:CE2	11:K:89:GLN:HG2	2.50	0.44
3:C:318:PHE:CE1	7:G:48:LEU:HD11	2.52	0.44
5:E:56:ALA:O	5:E:60:VAL:HG23	2.18	0.44
3:C:192:ALA:O	3:C:195:ILE:HB	2.18	0.44
5:E:205:TYR:N	5:E:205:TYR:CD1	2.86	0.44
9:I:30:THR:O	9:I:34:THR:OG1	2.25	0.44
11:K:29:ILE:HA	11:K:92:ILE:HD12	1.98	0.44
1:A:43:ASN:ND2	1:A:46:ALA:HB2	2.33	0.44
3:C:142:TRP:O	3:C:146:VAL:HG23	2.18	0.44
3:C:183:HIS:HE1	14:C:4001:HEM:NB	2.11	0.44
3:C:315:GLY:O	3:C:319:LYS:HD2	2.18	0.44
17:C:4005:UQ6:H321	17:C:4005:UQ6:H301	1.58	0.44
3:C:60:LEU:HA	3:C:60:LEU:HD13	1.76	0.44
4:D:265:GLU:OE2	4:D:268:ARG:HD3	2.18	0.44
1:A:112:SER:HB3	1:A:115:LYS:HB2	2.00	0.44
1:A:315:PHE:CE1	1:A:317:HIS:HE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:TYR:HA	2:B:256:LEU:HB3	1.99	0.44
10:J:110:ASP:HB2	11:K:55:HIS:NE2	2.32	0.44
10:J:97:ALA:HA	10:J:111:TYR:O	2.17	0.44
10:J:39:ARG:O	10:J:39:ARG:HG2	2.18	0.44
10:J:38:ILE:HA	10:J:49:VAL:HG23	1.99	0.44
1:A:288:TYR:CE1	1:A:306:ILE:HD11	2.52	0.43
3:C:208:ASN:H	3:C:208:ASN:HD22	1.66	0.43
3:C:307:PHE:N	3:C:307:PHE:CD1	2.85	0.43
4:D:113:ARG:HG3	4:D:114:THR:N	2.33	0.43
4:D:213:ASN:ND2	4:D:226:ALA:HA	2.33	0.43
5:E:44:LYS:NZ	5:E:52:GLY:H	2.16	0.43
7:G:51:GLU:O	7:G:53:ASN:N	2.48	0.43
9:I:5:SER:O	9:I:9:THR:HG23	2.18	0.43
5:E:96:VAL:HG21	5:E:118:ILE:HD11	2.00	0.43
3:C:328:ILE:HD13	8:H:62:PRO:HB3	2.00	0.43
11:K:29:ILE:C	11:K:92:ILE:HD12	2.39	0.43
1:A:80:LYS:HB2	1:A:80:LYS:HE3	1.85	0.43
2:B:255:VAL:HA	2:B:321:THR:OG1	2.18	0.43
3:C:222:HIS:CE1	3:C:223:SER:HB3	2.54	0.43
5:E:205:TYR:N	5:E:205:TYR:HD1	2.17	0.43
6:F:101:CYS:O	6:F:105:VAL:HG23	2.18	0.43
1:A:183:GLU:N	1:A:183:GLU:OE1	2.51	0.43
3:C:151:PHE:O	3:C:154:ILE:HG13	2.18	0.43
3:C:64:SER:O	3:C:68:ILE:HG13	2.18	0.43
7:G:16:LEU:HD12	7:G:16:LEU:HA	1.70	0.43
1:A:382:ASN:OD1	1:A:384:VAL:HG22	2.18	0.43
1:A:413:ILE:HG23	1:A:417:ASP:CB	2.49	0.43
3:C:161:ILE:O	3:C:165:LEU:HB2	2.18	0.43
4:D:202:PRO:HB3	4:D:208:LEU:HD22	2.00	0.43
4:D:198:TYR:CD2	4:D:227:ARG:HB2	2.53	0.43
4:D:243:THR:O	4:D:247:MET:HB2	2.18	0.43
4:D:76:TRP:CH2	4:D:252:THR:HB	2.53	0.43
6:F:143:PHE:HA	6:F:143:PHE:HD1	1.65	0.43
10:J:36:ASN:HD21	10:J:99:SER:HB2	1.84	0.43
1:A:88:LYS:HD3	2:B:316:PRO:HB3	2.01	0.43
4:D:191:ILE:HA	4:D:191:ILE:HD13	1.62	0.43
4:D:203:PRO:HG3	6:F:127:PHE:HD2	1.84	0.43
4:D:208:LEU:HA	4:D:209:PRO:HD3	1.78	0.43
4:D:269:LEU:HA	4:D:269:LEU:HD23	1.82	0.43
5:E:187:ILE:HA	5:E:187:ILE:HD12	1.83	0.43
4:D:290:PHE:O	8:H:31:PRO:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ALA:HA	1:A:426:LEU:HB2	2.00	0.43
3:C:218:ARG:HA	3:C:218:ARG:HD2	1.44	0.43
3:C:237:MET:CG	13:E:302:3PH:H282	2.46	0.43
7:G:100:VAL:HA	7:G:101:PRO:HD3	1.89	0.43
10:J:52:ILE:HD12	10:J:71:THR:HA	2.00	0.43
1:A:115:LYS:N	1:A:115:LYS:HD2	2.33	0.43
1:A:313:ASP:OD1	1:A:335:ARG:HD3	2.19	0.43
2:B:73:LEU:HA	2:B:73:LEU:HD13	1.91	0.43
4:D:272:LYS:HG2	9:I:32:PHE:CD2	2.54	0.43
4:D:78:HIS:O	4:D:83:GLU:HB2	2.18	0.43
8:H:20:LYS:NZ	8:H:20:LYS:HB3	2.34	0.43
5:E:144:ALA:HA	10:J:102:TYR:CE1	2.53	0.43
10:J:10:GLY:HA2	10:J:118:VAL:HG12	2.00	0.43
10:J:36:ASN:HD21	10:J:99:SER:CB	2.32	0.43
3:C:210:LEU:HD13	3:C:212:ILE:HD11	2.01	0.43
5:E:158:ILE:HG22	5:E:163:GLY:HA2	2.00	0.43
1:A:359:THR:HG23	1:A:362:GLU:OE1	2.18	0.43
1:A:444:ASP:OD2	3:C:224:TYR:OH	2.17	0.43
1:A:94:SER:HB2	1:A:105:ILE:HG22	1.99	0.43
2:B:151:PHE:CD2	2:B:155:LEU:HB2	2.53	0.43
3:C:12:LEU:HA	3:C:12:LEU:HD22	1.86	0.43
4:D:136:ASP:HB2	4:D:147:ARG:HG2	1.99	0.43
4:D:306:LYS:HA	4:D:307:PRO:HD3	1.80	0.43
10:J:12:VAL:HG21	10:J:86:VAL:HG21	2.00	0.43
11:K:6:GLN:HB2	11:K:100:ALA:HB3	1.99	0.43
2:B:183:GLU:HG2	2:B:211:ALA:O	2.19	0.42
3:C:172:SER:OG	3:C:174:PRO:HD2	2.18	0.42
3:C:147:ILE:HD11	15:C:4003:AOQ:H13	2.01	0.42
3:C:93:MET:O	3:C:97:MET:HG3	2.19	0.42
4:D:130:GLU:HA	4:D:149:GLY:H	1.83	0.42
5:E:136:ALA:O	5:E:137:LEU:HD23	2.19	0.42
3:C:216:LEU:HD11	8:H:19:PRO:HD2	2.01	0.42
1:A:285:PHE:HB2	1:A:317:HIS:NE2	2.34	0.42
1:A:280:LEU:HD11	1:A:367:LYS:HG3	2.01	0.42
2:B:143:GLU:HB2	2:B:288:PHE:HZ	1.83	0.42
3:C:104:GLY:HA2	3:C:106:TYR:CE2	2.53	0.42
3:C:106:TYR:HD1	3:C:306:PRO:HG3	1.84	0.42
4:D:109:ARG:HG3	4:D:178:SER:CB	2.48	0.42
1:A:248:GLU:CD	1:A:250:ARG:HH21	2.22	0.42
1:A:288:TYR:HE1	1:A:306:ILE:HD11	1.84	0.42
1:A:440:GLU:HG2	8:H:14:GLY:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:TYR:CE2	3:C:209:PRO:HA	2.53	0.42
3:C:20:SER:O	3:C:220:PRO:HA	2.19	0.42
10:J:85:SER:OG	10:J:85:SER:O	2.34	0.42
1:A:176:LEU:HA	1:A:177:PRO:HD2	1.94	0.42
2:B:35:VAL:CG1	2:B:179:VAL:HG12	2.49	0.42
2:B:248:ALA:C	2:B:250:LEU:H	2.23	0.42
2:B:274:ALA:HB2	2:B:287:LEU:HD12	2.01	0.42
3:C:269:ILE:HG22	3:C:269:ILE:O	2.19	0.42
3:C:276:LEU:HB2	3:C:277:PRO:HD3	2.01	0.42
3:C:379:TYR:O	3:C:383:VAL:HG23	2.19	0.42
4:D:244:THR:OG1	6:F:76:ASP:OD1	2.35	0.42
7:G:95:LYS:HB2	7:G:98:GLU:OE1	2.20	0.42
5:E:127:GLN:NE2	11:K:56:ALA:HB3	2.34	0.42
2:B:298:SER:OG	2:B:363:PRO:HD3	2.19	0.42
3:C:208:ASN:OD1	7:G:79:HIS:CE1	2.72	0.42
8:H:76:TYR:O	8:H:80:LEU:HG	2.19	0.42
11:K:18:ARG:NH2	11:K:20:THR:OG1	2.53	0.42
11:K:21:ILE:HG22	11:K:22:SER:N	2.34	0.42
11:K:46:LEU:HD23	11:K:55:HIS:CD2	2.54	0.42
1:A:49:ALA:HB2	1:A:213:ASN:H	1.85	0.42
3:C:15:SER:O	3:C:15:SER:OG	2.37	0.42
3:C:190:ILE:O	3:C:194:VAL:HG23	2.19	0.42
4:D:236:TYR:HD2	4:D:236:TYR:HA	1.67	0.42
8:H:71:LYS:HB3	8:H:71:LYS:HE3	1.91	0.42
11:K:84:ALA:HB3	11:K:86:TYR:HE1	1.84	0.42
1:A:36:ILE:O	1:A:38:VAL:HG23	2.20	0.42
3:C:210:LEU:HD21	7:G:82:GLU:OE2	2.19	0.42
4:D:282:LEU:HA	4:D:285:ILE:HD12	2.01	0.42
10:J:22:CYS:HB3	10:J:79:PHE:CE2	2.55	0.42
1:A:374:LEU:HA	1:A:374:LEU:HD12	1.89	0.42
14:D:401:HEM:HMB1	14:D:401:HEM:HBB2	2.01	0.42
1:A:421:TRP:O	1:A:425:ARG:HB2	2.20	0.42
2:B:153:LYS:HG3	2:B:153:LYS:O	2.20	0.42
2:B:183:GLU:O	2:B:214:SER:OG	2.25	0.42
2:B:52:ASN:OD1	2:B:80:SER:OG	2.35	0.42
3:C:242:LEU:HA	3:C:242:LEU:HD23	1.73	0.42
3:C:102:TYR:HD1	3:C:326:PHE:CD2	2.38	0.42
3:C:32:MET:O	3:C:36:LEU:N	2.53	0.42
6:F:126:GLU:O	6:F:129:HIS:N	2.47	0.42
7:G:64:PRO:HG2	7:G:67:GLU:OE1	2.18	0.42
1:A:252:ARG:NH1	1:A:440:GLU:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:ASN:C	3:C:175:THR:N	2.73	0.42
4:D:126:ARG:HB2	4:D:126:ARG:NH2	2.34	0.42
4:D:155:ILE:HA	4:D:156:PRO:HD3	1.78	0.42
4:D:179:LEU:HD23	4:D:179:LEU:HA	1.71	0.42
6:F:109:GLN:HG2	6:F:114:TYR:CZ	2.55	0.42
4:D:296:LYS:NZ	7:G:83:LEU:O	2.44	0.42
1:A:290:ALA:HB1	1:A:310:GLN:HE22	1.84	0.41
2:B:108:VAL:HA	2:B:112:THR:HG23	2.01	0.41
3:C:38:LEU:O	3:C:42:ILE:HG13	2.20	0.41
4:D:101:CYS:HA	14:D:401:HEM:HMC3	2.01	0.41
5:E:112:GLN:CB	5:E:114:LYS:HE2	2.50	0.41
5:E:71:ALA:N	13:E:302:3PH:H362	2.35	0.41
5:E:90:ALA:O	5:E:92:ALA:N	2.53	0.41
11:K:82:ASP:HB3	11:K:86:TYR:OH	2.20	0.41
1:A:181:THR:O	1:A:185:LEU:HB2	2.20	0.41
1:A:197:ALA:O	1:A:201:PHE:HB2	2.20	0.41
1:A:68:GLY:HA3	1:A:185:LEU:HD13	2.01	0.41
2:B:169:LEU:HD13	2:B:173:LYS:HE2	2.02	0.41
3:C:219:ILE:HD12	3:C:224:TYR:CD1	2.56	0.41
4:D:203:PRO:HG2	4:D:206:VAL:HG21	2.01	0.41
3:C:378:PHE:CG	7:G:45:PHE:CE1	3.08	0.41
1:A:115:LYS:HD2	1:A:115:LYS:H	1.85	0.41
2:B:58:ASN:OD1	2:B:64:ALA:N	2.34	0.41
4:D:111:ALA:HB3	4:D:114:THR:HG23	2.01	0.41
4:D:256:ASN:C	4:D:256:ASN:HD22	2.23	0.41
5:E:74:THR:HG22	5:E:78:PHE:HE2	1.85	0.41
5:E:80:SER:C	5:E:82:MET:H	2.23	0.41
11:K:86:TYR:CD1	11:K:86:TYR:N	2.88	0.41
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.20	0.41
1:A:299:GLY:HA2	2:B:69:ARG:CZ	2.51	0.41
2:B:251:ALA:O	2:B:255:VAL:HG13	2.20	0.41
3:C:109:PRO:HB2	3:C:204:HIS:NE2	2.35	0.41
3:C:47:GLY:HA3	14:C:4001:HEM:C3C	2.56	0.41
4:D:250:ASP:O	4:D:253:THR:N	2.53	0.41
7:G:103:LEU:O	7:G:106:TYR:HD1	2.03	0.41
3:C:320:VAL:HG22	8:H:58:TYR:OH	2.20	0.41
10:J:16:GLN:O	10:J:85:SER:N	2.54	0.41
10:J:37:TRP:CZ3	10:J:96:CYS:HB3	2.55	0.41
1:A:424:LYS:HZ2	1:A:425:ARG:HD2	1.85	0.41
12:A:501:UMQ:HH2	5:E:68:SER:OG	2.21	0.41
2:B:93:PHE:HB3	2:B:101:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:84:THR:O	9:I:47:LYS:HE3	2.20	0.41
5:E:138:LYS:O	5:E:140:PRO:HD3	2.20	0.41
5:E:191:ILE:HG22	5:E:199:ASN:OD1	2.20	0.41
6:F:82:ARG:HG2	6:F:138:THR:HG21	2.01	0.41
10:J:12:VAL:CG2	10:J:86:VAL:HG21	2.50	0.41
2:B:168:SER:OG	2:B:169:LEU:N	2.53	0.41
3:C:258:ILE:HD11	4:D:184:ARG:HH22	1.86	0.41
7:G:74:ARG:HG2	7:G:77:ARG:NH2	2.35	0.41
8:H:88:GLU:HG3	8:H:91:ARG:NH1	2.36	0.41
9:I:17:PHE:O	9:I:19:GLY:N	2.54	0.41
9:I:9:THR:O	9:I:12:LYS:NZ	2.40	0.41
1:A:424:LYS:HD3	1:A:425:ARG:HD3	2.03	0.41
2:B:270:LEU:CD2	2:B:303:LYS:HD3	2.51	0.41
2:B:273:SER:OG	2:B:288:PHE:HD1	2.03	0.41
2:B:62:ARG:NH2	2:B:67:LEU:HD13	2.36	0.41
5:E:156:LEU:O	5:E:158:ILE:N	2.48	0.41
8:H:89:LEU:HD23	8:H:93:ASN:HB2	2.02	0.41
10:J:27:TYR:CD2	10:J:28:SER:N	2.88	0.41
10:J:42:PRO:C	10:J:44:ASN:H	2.24	0.41
1:A:305:ASN:O	1:A:307:GLN:N	2.53	0.41
2:B:267:LEU:HB2	2:B:304:ILE:HD11	2.02	0.41
3:C:138:GLN:HB2	3:C:255:ASP:O	2.20	0.41
7:G:5:PHE:CD1	7:G:107:ILE:HG21	2.56	0.41
1:A:157:PRO:O	1:A:161:LEU:HB2	2.21	0.41
2:B:176:ALA:O	2:B:180:TYR:HB2	2.21	0.41
2:B:212:GLY:O	2:B:213:LYS:HG3	2.20	0.41
2:B:143:GLU:HB2	2:B:288:PHE:CZ	2.55	0.41
1:A:369:LEU:HD11	2:B:72:GLU:HG2	2.03	0.41
4:D:190:TYR:OH	14:D:401:HEM:O2A	2.27	0.41
7:G:33:ILE:HG22	7:G:33:ILE:O	2.19	0.41
7:G:63:LEU:HA	7:G:64:PRO:HD2	1.77	0.41
3:C:382:ARG:HD2	7:G:99:ASP:OD2	2.21	0.41
11:K:86:TYR:HD1	11:K:86:TYR:N	2.19	0.41
2:B:62:ARG:HH22	2:B:67:LEU:HD13	1.85	0.41
7:G:61:ARG:HB2	7:G:61:ARG:NH2	2.36	0.41
5:E:149:ASP:HB2	10:J:104:VAL:HG21	2.03	0.41
1:A:289:ASN:C	1:A:291:PHE:H	2.24	0.41
2:B:58:ASN:HB2	2:B:118:GLU:OE2	2.20	0.41
3:C:216:LEU:HD11	8:H:19:PRO:CD	2.51	0.41
3:C:323:LYS:O	3:C:326:PHE:HB3	2.21	0.41
3:C:327:PHE:O	3:C:331:PHE:HD1	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51:ALA:HB2	14:C:4001:HEM:CBC	2.51	0.41
1:A:286:GLY:O	1:A:317:HIS:N	2.53	0.40
1:A:302:LEU:HD13	1:A:347:THR:HA	2.03	0.40
1:A:285:PHE:HE1	1:A:350:GLN:HB3	1.87	0.40
2:B:56:PHE:CE2	2:B:78:PHE:HB3	2.56	0.40
4:D:76:TRP:H	4:D:79:ASN:ND2	2.19	0.40
6:F:126:GLU:O	6:F:127:PHE:C	2.58	0.40
7:G:120:LEU:HD23	7:G:123:ILE:HD13	2.02	0.40
8:H:29:VAL:HG12	8:H:34:GLN:HE21	1.86	0.40
1:A:117:LEU:HD21	1:A:223:ILE:HG12	2.03	0.40
2:B:152:ARG:HB3	2:B:153:LYS:H	1.77	0.40
3:C:58:ILE:HD11	3:C:136:TYR:CZ	2.56	0.40
3:C:129:PHE:CZ	3:C:147:ILE:HD11	2.56	0.40
3:C:273:TRP:CD2	3:C:274:TYR:N	2.89	0.40
4:D:126:ARG:HB2	4:D:126:ARG:CZ	2.51	0.40
5:E:108:VAL:HG13	5:E:117:PHE:CD2	2.56	0.40
3:C:147:ILE:HG12	3:C:147:ILE:H	1.61	0.40
3:C:58:ILE:CG2	3:C:173:ASN:HB2	2.52	0.40
3:C:221:MET:HB2	3:C:221:MET:HE2	1.87	0.40
3:C:16:TYR:O	17:C:4005:UQ6:H1M2	2.21	0.40
4:D:281:TYR:CZ	4:D:285:ILE:HD11	2.56	0.40
5:E:32:SER:HB3	5:E:35:ARG:HG3	2.03	0.40
5:E:80:SER:O	5:E:83:THR:HG23	2.20	0.40
8:H:88:GLU:HG3	8:H:91:ARG:CZ	2.52	0.40
1:A:148:VAL:HG12	1:A:148:VAL:O	2.22	0.40
1:A:230:LEU:O	1:A:230:LEU:HD12	2.22	0.40
3:C:80:TYR:CD2	3:C:248:PRO:HB3	2.56	0.40
4:D:295:ILE:O	4:D:298:ARG:HB3	2.22	0.40
11:K:4:LEU:HB3	11:K:23:CYS:SG	2.62	0.40
1:A:148:VAL:HG11	1:A:180:GLY:O	2.22	0.40
2:B:222:LYS:HE2	2:B:222:LYS:HB3	1.72	0.40
2:B:318:ILE:HA	2:B:318:ILE:HD12	1.92	0.40
2:B:97:ASP:HB2	2:B:101:TYR:HE1	1.86	0.40
4:D:302:PHE:HB2	7:G:73:TYR:CD1	2.57	0.40
9:I:31:VAL:O	9:I:34:THR:HB	2.22	0.40
4:D:86:ASP:HA	9:I:47:LYS:HG2	2.03	0.40
10:J:52:ILE:HB	10:J:70:ILE:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	349 (81%)	67 (16%)	13 (3%)	4	21
2	B	350/352 (99%)	284 (81%)	56 (16%)	10 (3%)	4	22
3	C	383/385 (100%)	318 (83%)	49 (13%)	16 (4%)	3	14
4	D	246/248 (99%)	199 (81%)	36 (15%)	11 (4%)	2	13
5	E	183/185 (99%)	142 (78%)	33 (18%)	8 (4%)	2	13
6	F	72/74 (97%)	60 (83%)	10 (14%)	2 (3%)	5	23
7	G	124/126 (98%)	102 (82%)	16 (13%)	6 (5%)	2	12
8	H	91/93 (98%)	61 (67%)	23 (25%)	7 (8%)	1	4
9	I	55/57 (96%)	41 (74%)	13 (24%)	1 (2%)	8	34
10	J	125/127 (98%)	115 (92%)	9 (7%)	1 (1%)	19	54
11	K	105/107 (98%)	76 (72%)	23 (22%)	6 (6%)	1	9
All	All	2163/2185 (99%)	1747 (81%)	335 (16%)	81 (4%)	3	17

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	PRO
2	B	153	LYS
3	C	99	LYS
3	C	164	TRP
3	C	165	LEU
3	C	311	SER
4	D	221	GLY
5	E	89	LEU
7	G	99	ASP
10	J	31	SER
1	A	29	VAL
1	A	290	ALA
1	A	448	ILE

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Mol	Chain	Res	Type
2	B	296	VAL
2	B	336	ILE
2	B	339	ASN
3	C	106	TYR
3	C	215	ASN
3	C	250	THR
3	C	284	SER
4	D	203	PRO
4	D	243	THR
4	D	262	GLU
5	E	91	MET
5	E	160	THR
7	G	33	ILE
8	H	79	PHE
8	H	90	GLU
11	K	2	ILE
11	K	9	VAL
1	A	376	GLN
2	B	163	GLY
2	B	249	SER
3	C	359	TYR
4	D	139	ASP
4	D	241	PRO
4	D	305	PRO
5	E	134	MET
5	E	157	GLY
8	H	13	TRP
8	H	42	HIS
8	H	80	LEU
9	I	15	ALA
1	A	451	ASP
2	B	45	ASP
2	B	96	ASP
3	C	98	ALA
3	C	156	PHE
3	C	254	PRO
5	E	46	ASN
5	E	161	HIS
6	F	127	PHE
11	K	51	THR
1	A	81	GLU
1	A	182	LEU

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Mol	Chain	Res	Type
1	A	443	LEU
2	B	337	GLU
3	C	369	VAL
6	F	139	ALA
7	G	65	GLU
7	G	90	ARG
8	H	89	LEU
11	K	12	ALA
11	K	102	THR
1	A	343	LEU
1	A	447	ARG
3	C	17	ILE
4	D	144	PRO
4	D	231	ASP
1	A	173	PRO
4	D	187	GLY
4	D	202	PRO
7	G	49	ILE
11	K	83	ILE
1	A	148	VAL
3	C	260	GLY
3	C	383	VAL
2	B	335	PRO
7	G	104	LEU
8	H	65	ILE
5	E	214	VAL

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	370/370 (100%)	324 (88%)	46 (12%)	4	19
2	B	301/301 (100%)	272 (90%)	29 (10%)	8	29
3	C	338/338 (100%)	295 (87%)	43 (13%)	4	18
4	D	206/206 (100%)	181 (88%)	25 (12%)	5	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	151/151 (100%)	127 (84%)	24 (16%)	2	11
6	F	67/67 (100%)	59 (88%)	8 (12%)	5	20
7	G	110/110 (100%)	99 (90%)	11 (10%)	7	27
8	H	77/77 (100%)	69 (90%)	8 (10%)	7	25
9	I	47/47 (100%)	41 (87%)	6 (13%)	4	18
10	J	112/112 (100%)	94 (84%)	18 (16%)	2	11
11	K	93/93 (100%)	78 (84%)	15 (16%)	2	11
All	All	1872/1872 (100%)	1639 (88%)	233 (12%)	4	19

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	73	TRP
1	A	93	LEU
1	A	113	THR
1	A	115	LYS
1	A	117	LEU
1	A	120	LEU
1	A	128	LYS
1	A	133	SER
1	A	145	LEU
1	A	149	GLN
1	A	152	GLU
1	A	153	ASP
1	A	161	LEU
1	A	164	LEU
1	A	172	THR
1	A	179	ARG
1	A	208	VAL
1	A	237	VAL
1	A	238	LEU
1	A	239	LYS
1	A	240	LYS
1	A	241	LYS
1	A	252	ARG
1	A	263	LEU
1	A	295	SER
1	A	303	LEU
1	A	306	ILE

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Mol	Chain	Res	Type
1	A	320	LEU
1	A	324	ASP
1	A	325	SER
1	A	330	PHE
1	A	334	THR
1	A	338	THR
1	A	341	ASP
1	A	359	THR
1	A	361	THR
1	A	365	ARG
1	A	395	LEU
1	A	415	VAL
1	A	417	ASP
1	A	425	ARG
1	A	426	LEU
1	A	439	ILE
1	A	446	MET
1	A	452	MET
2	B	22	ARG
2	B	29	SER
2	B	30	THR
2	B	53	ARG
2	B	54	PHE
2	B	67	LEU
2	B	83	ASP
2	B	84	ARG
2	B	122	SER
2	B	128	ARG
2	B	146	LEU
2	B	153	LYS
2	B	155	LEU
2	B	160	LEU
2	B	186	GLU
2	B	193	VAL
2	B	205	LEU
2	B	207	SER
2	B	214	SER
2	B	250	LEU
2	B	287	LEU
2	B	292	GLN
2	B	293	ASP
2	B	297	VAL

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Mol	Chain	Res	Type
2	B	312	LYS
2	B	323	LEU
2	B	341	ASP
2	B	347	LYS
2	B	362	LEU
3	C	10	LEU
3	C	12	LEU
3	C	15	SER
3	C	19	ASP
3	C	26	ILE
3	C	34	SER
3	C	41	VAL
3	C	57	ASN
3	C	79	ARG
3	C	81	LEU
3	C	87	SER
3	C	99	LYS
3	C	101	LEU
3	C	147	ILE
3	C	148	THR
3	C	163	SER
3	C	165	LEU
3	C	184	TYR
3	C	189	ILE
3	C	198	LEU
3	C	203	ILE
3	C	206	SER
3	C	208	ASN
3	C	212	ILE
3	C	215	ASN
3	C	218	ARG
3	C	238	LEU
3	C	244	VAL
3	C	283	ARG
3	C	302	LEU
3	C	305	LEU
3	C	312	VAL
3	C	317	THR
3	C	336	LEU
3	C	344	VAL
3	C	346	VAL
3	C	353	GLN

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Mol	Chain	Res	Type
3	C	372	THR
3	C	374	GLU
3	C	379	TYR
3	C	380	ILE
3	C	382	ARG
3	C	383	VAL
4	D	63	THR
4	D	77	SER
4	D	101	CYS
4	D	104	CYS
4	D	109	ARG
4	D	135	ASP
4	D	145	LYS
4	D	178	SER
4	D	188	CYS
4	D	194	LEU
4	D	212	SER
4	D	231	ASP
4	D	234	VAL
4	D	236	TYR
4	D	240	THR
4	D	243	THR
4	D	251	VAL
4	D	253	THR
4	D	256	ASN
4	D	264	ASP
4	D	280	LEU
4	D	283	LEU
4	D	284	SER
4	D	291	LYS
4	D	309	LYS
5	E	50	ASP
5	E	65	LEU
5	E	76	GLU
5	E	81	SER
5	E	83	THR
5	E	91	MET
5	E	93	LYS
5	E	94	VAL
5	E	103	LEU
5	E	107	VAL
5	E	108	VAL

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Mol	Chain	Res	Type
5	E	114	LYS
5	E	116	VAL
5	E	118	ILE
5	E	132	VAL
5	E	133	ASP
5	E	134	MET
5	E	145	ASP
5	E	149	ASP
5	E	167	ILE
5	E	187	ILE
5	E	190	ARG
5	E	205	TYR
5	E	210	ASP
6	F	81	LEU
6	F	89	GLU
6	F	97	HIS
6	F	120	LYS
6	F	130	LEU
6	F	142	LEU
6	F	143	PHE
6	F	144	ASP
7	G	4	SER
7	G	16	LEU
7	G	21	LEU
7	G	23	LYS
7	G	41	LEU
7	G	77	ARG
7	G	83	LEU
7	G	85	HIS
7	G	86	HIS
7	G	98	GLU
7	G	127	LYS
8	H	20	LYS
8	H	26	SER
8	H	29	VAL
8	H	42	HIS
8	H	54	SER
8	H	60	LEU
8	H	80	LEU
8	H	89	LEU
9	I	18	VAL
9	I	20	THR

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Mol	Chain	Res	Type
9	I	38	SER
9	I	42	ASN
9	I	48	LEU
9	I	55	ARG
10	J	1	GLU
10	J	7	SER
10	J	12	VAL
10	J	21	THR
10	J	24	VAL
10	J	38	ILE
10	J	39	ARG
10	J	51	TYR
10	J	66	ASP
10	J	68	LEU
10	J	75	SER
10	J	79	PHE
10	J	81	LEU
10	J	86	VAL
10	J	93	THR
10	J	116	THR
10	J	117	THR
10	J	122	SER
11	K	1	ASP
11	K	6	GLN
11	K	11	LEU
11	K	23	CYS
11	K	27	GLN
11	K	33	LEU
11	K	44	ILE
11	K	51	THR
11	K	53	ARG
11	K	58	VAL
11	K	73	LEU
11	K	79	GLU
11	K	81	GLU
11	K	89	GLN
11	K	93	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN

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Mol	Chain	Res	Type
3	C	22	GLN
3	C	141	HIS
4	D	79	ASN
5	E	127	GLN
7	G	79	HIS
11	K	38	GLN
11	K	89	GLN

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 ⓘ

11 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
13	3PH	C	4006	-	34,34,47	1.17	2 (5%)	38,39,52	1.66	8 (21%)
17	UQ6	C	4005	-	43,43,43	1.19	3 (6%)	51,55,55	2.25	20 (39%)
13	3PH	E	302	-	37,37,47	1.10	2 (5%)	41,42,52	1.27	2 (4%)
14	HEM	D	401	4	27,50,50	2.18	5 (18%)	17,82,82	2.06	6 (35%)
12	UMQ	A	501	-	35,35,35	0.47	0	46,46,46	1.19	4 (8%)
18	FES	E	301	5	0,4,4	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEM	C	4002	3	27,50,50	1.97	5 (18%)	17,82,82	2.44	7 (41%)
14	HEM	C	4001	3	27,50,50	2.15	10 (37%)	17,82,82	2.06	6 (35%)
13	3PH	A	502	-	30,30,47	1.23	2 (6%)	34,35,52	1.14	3 (8%)
16	3PE	C	4004	-	26,26,50	1.37	2 (7%)	29,31,55	1.42	5 (17%)
15	AOQ	C	4003	-	29,29,29	1.76	7 (24%)	40,42,42	1.61	9 (22%)

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
13	3PH	C	4006	-	-	13/36/36/49	-
17	UQ6	C	4005	-	-	14/39/39/39	0/1/1/1
13	3PH	E	302	-	-	19/39/39/49	-
14	HEM	D	401	4	-	0/6/54/54	-
12	UMQ	A	501	-	-	3/20/60/60	0/2/2/2
18	FES	E	301	5	-	-	0/1/1/1
14	HEM	C	4002	3	-	0/6/54/54	-
14	HEM	C	4001	3	-	0/6/54/54	-
13	3PH	A	502	-	-	14/32/32/49	-
16	3PE	C	4004	-	-	16/30/30/54	-
15	AOQ	C	4003	-	-	4/8/38/38	0/4/4/4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	401	HEM	C3D-C2D	5.67	1.54	1.37
14	C	4001	HEM	C3D-C2D	5.64	1.54	1.37
14	D	401	HEM	C3B-C2B	-4.97	1.33	1.40
14	C	4002	HEM	C3D-C2D	4.96	1.52	1.37
15	C	4003	AOQ	C9-C1	-4.64	1.39	1.48
16	C	4004	3PE	O21-C21	4.50	1.47	1.34
17	C	4005	UQ6	O5-C5	-4.50	1.26	1.37
13	C	4006	3PH	O31-C31	4.49	1.46	1.33
13	A	502	3PH	O31-C31	4.49	1.46	1.33
13	E	302	3PH	O31-C31	4.43	1.46	1.33
15	C	4003	AOQ	C10-C4	-4.37	1.39	1.48
16	C	4004	3PE	O31-C31	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	4006	3PH	O21-C21	4.27	1.46	1.34
13	E	302	3PH	O21-C21	4.25	1.46	1.34
13	A	502	3PH	O21-C21	4.22	1.46	1.34
17	C	4005	UQ6	O2-C2	-4.20	1.27	1.37
14	D	401	HEM	C3B-CAB	3.89	1.55	1.47
14	D	401	HEM	C3C-C2C	-3.81	1.35	1.40
14	C	4001	HEM	C3C-C2C	-3.79	1.35	1.40
14	C	4002	HEM	C3C-C2C	-3.77	1.35	1.40
14	C	4002	HEM	C3B-CAB	3.68	1.55	1.47
14	C	4002	HEM	C3C-CAC	3.60	1.55	1.47
15	C	4003	AOQ	C3-C4	-3.48	1.37	1.46
14	C	4002	HEM	C3B-C2B	-3.43	1.35	1.40
14	C	4001	HEM	C3C-CAC	3.38	1.54	1.47
14	C	4001	HEM	C3B-CAB	3.32	1.54	1.47
14	D	401	HEM	C3C-CAC	3.12	1.54	1.47
14	C	4001	HEM	CMD-C2D	2.83	1.57	1.51
15	C	4003	AOQ	C3-C2	2.72	1.39	1.35
14	C	4001	HEM	C4A-NA	2.58	1.41	1.36
15	C	4003	AOQ	C2-C1	-2.49	1.41	1.47
14	C	4001	HEM	C3B-C2B	-2.41	1.37	1.40
15	C	4003	AOQ	C17-C13	-2.39	1.47	1.52
14	C	4001	HEM	CAD-C3D	2.17	1.56	1.52
17	C	4005	UQ6	C7-C6	2.12	1.54	1.51
14	C	4001	HEM	CMC-C2C	2.09	1.56	1.51
14	C	4001	HEM	C1C-C2C	2.05	1.47	1.42
15	C	4003	AOQ	C20-CL	2.03	1.78	1.74

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	4001	HEM	CBA-CAA-C2A	-5.16	102.97	112.49
14	C	4002	HEM	CAA-CBA-CGA	-5.01	104.27	112.67
17	C	4005	UQ6	C10-C9-C11	4.74	123.25	115.27
14	C	4002	HEM	CMC-C2C-C3C	4.65	133.38	124.68
16	C	4004	3PE	O21-C21-C22	4.47	121.13	111.50
13	C	4006	3PH	O21-C21-C22	4.45	121.08	111.50
17	C	4005	UQ6	C3M-O3-C3	4.37	126.75	114.78
17	C	4005	UQ6	C17-C18-C19	-4.30	117.30	127.66
14	C	4002	HEM	CBD-CAD-C3D	-4.27	104.61	112.48
13	E	302	3PH	O21-C21-C22	4.20	120.56	111.50
14	D	401	HEM	CAA-CBA-CGA	-4.08	105.83	112.67
15	C	4003	AOQ	C15-C16-C2	-3.95	105.13	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	4005	UQ6	C12-C13-C14	-3.91	118.24	127.66
17	C	4005	UQ6	C6-C7-C8	-3.75	106.22	112.17
17	C	4005	UQ6	C27-C28-C29	-3.67	118.82	127.66
15	C	4003	AOQ	C2-C3-C4	-3.64	119.50	123.34
14	C	4002	HEM	CBA-CAA-C2A	-3.52	106.00	112.49
13	C	4006	3PH	O14-P-O11	-3.48	97.47	106.73
17	C	4005	UQ6	C20-C19-C21	3.47	121.11	115.27
14	D	401	HEM	CBA-CAA-C2A	3.39	118.74	112.49
13	C	4006	3PH	C3E-C3D-C3C	-3.37	97.33	114.42
17	C	4005	UQ6	C1M-C1-C2	-3.36	114.81	120.50
17	C	4005	UQ6	C4M-O4-C4	3.23	123.62	114.78
14	C	4001	HEM	C1D-C2D-C3D	-3.20	104.77	107.00
15	C	4003	AOQ	C22-C17-C18	3.13	122.19	118.29
15	C	4003	AOQ	C19-C18-C17	-3.10	118.08	121.20
14	C	4001	HEM	C4C-C3C-C2C	3.03	109.01	106.90
16	C	4004	3PE	O31-C31-C32	3.00	121.34	111.91
17	C	4005	UQ6	O2-C2-C3	2.98	126.41	119.85
17	C	4005	UQ6	C7-C8-C9	-2.94	122.68	127.24
12	A	501	UMQ	C1'-C2'-C3'	2.92	116.08	110.00
17	C	4005	UQ6	C1M-C1-C6	2.91	124.64	120.42
15	C	4003	AOQ	C15-C14-C13	-2.88	105.09	110.52
13	A	502	3PH	O21-C21-C22	2.86	117.67	111.50
13	C	4006	3PH	O14-P-O13	2.84	118.49	107.64
14	D	401	HEM	C4A-C3A-C2A	2.82	108.95	107.00
15	C	4003	AOQ	O1-C1-C9	-2.80	117.03	121.56
17	C	4005	UQ6	C25-C24-C26	2.71	119.83	115.27
17	C	4005	UQ6	C30-C29-C31	2.69	119.80	115.27
17	C	4005	UQ6	O5-C5-C4	-2.64	114.03	119.85
13	A	502	3PH	O31-C31-C32	2.61	120.11	111.91
14	C	4001	HEM	CAD-CBD-CGD	-2.61	108.29	112.67
13	C	4006	3PH	O31-C31-C32	2.55	119.91	111.91
17	C	4005	UQ6	O5-C5-C6	2.54	125.58	118.13
16	C	4004	3PE	C3-C2-C1	-2.51	105.84	111.79
15	C	4003	AOQ	C10-C4-C3	2.47	120.93	117.06
15	C	4003	AOQ	C15-C16-C11	2.44	115.13	109.97
17	C	4005	UQ6	C20-C19-C18	-2.39	117.54	123.68
14	C	4002	HEM	CAA-C2A-C3A	-2.39	120.38	127.25
17	C	4005	UQ6	C26-C24-C23	-2.38	116.30	121.12
13	C	4006	3PH	C3-C2-C1	-2.38	106.16	111.79
17	C	4005	UQ6	C21-C22-C23	-2.35	104.16	111.88
13	C	4006	3PH	O21-C21-O22	-2.33	118.06	123.70
13	C	4006	3PH	C2-O21-C21	-2.32	112.07	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	502	3PH	O11-P-O12	-2.30	100.03	106.47
14	D	401	HEM	CAA-C2A-C3A	-2.28	120.69	127.25
14	D	401	HEM	CMC-C2C-C3C	2.27	128.93	124.68
14	C	4001	HEM	CBD-CAD-C3D	-2.22	108.39	112.48
12	A	501	UMQ	O3'-C3'-C2'	-2.18	105.30	110.35
14	C	4002	HEM	CMB-C2B-C3B	2.17	128.75	124.68
12	A	501	UMQ	C1-O5-C5	-2.17	109.42	113.69
16	C	4004	3PE	C2-O21-C21	-2.15	112.49	117.79
16	C	4004	3PE	O31-C31-O32	-2.15	118.17	123.59
14	D	401	HEM	C1D-C2D-C3D	-2.14	105.51	107.00
15	C	4003	AOQ	O1-C1-C2	2.12	124.03	120.78
14	C	4001	HEM	CMA-C3A-C4A	-2.08	125.27	128.46
17	C	4005	UQ6	O4-C4-C3	2.05	125.12	120.39
13	E	302	3PH	C3-C2-C1	-2.04	106.96	111.79
14	C	4002	HEM	CMA-C3A-C4A	-2.01	125.37	128.46
12	A	501	UMQ	C2'-C3'-C4'	2.00	114.25	109.68

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	C	4005	UQ6	C12-C11-C9-C8
17	C	4005	UQ6	C12-C11-C9-C10
17	C	4005	UQ6	C13-C14-C16-C17
17	C	4005	UQ6	C15-C14-C16-C17
17	C	4005	UQ6	C30-C29-C31-C32
17	C	4005	UQ6	C29-C31-C32-C33
13	E	302	3PH	C1-O11-P-O13
13	E	302	3PH	C1-O11-P-O14
13	E	302	3PH	C1-O11-P-O12
13	A	502	3PH	C22-C21-O21-C2
16	C	4004	3PE	C11-O13-P-O14
16	C	4004	3PE	O13-C11-C12-N
15	C	4003	AOQ	C11-C16-C2-C1
13	A	502	3PH	O22-C21-O21-C2
17	C	4005	UQ6	C28-C29-C31-C32
17	C	4005	UQ6	C4-C3-O3-C3M
17	C	4005	UQ6	C14-C16-C17-C18
17	C	4005	UQ6	C19-C21-C22-C23
17	C	4005	UQ6	C24-C26-C27-C28
13	E	302	3PH	O32-C31-O31-C3
13	E	302	3PH	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
13	A	502	3PH	C32-C31-O31-C3
13	C	4006	3PH	C31-C32-C33-C34
13	A	502	3PH	O32-C31-O31-C3
17	C	4005	UQ6	C2-C3-O3-C3M
13	E	302	3PH	C26-C27-C28-C29
13	C	4006	3PH	C39-C3A-C3B-C3C
12	A	501	UMQ	C2'-C1'-O1'-CA
13	A	502	3PH	C39-C3A-C3B-C3C
13	A	502	3PH	C21-C22-C23-C24
12	A	501	UMQ	O5'-C1'-O1'-CA
13	C	4006	3PH	C38-C39-C3A-C3B
13	E	302	3PH	C38-C39-C3A-C3B
13	C	4006	3PH	C33-C34-C35-C36
13	E	302	3PH	C28-C29-C2A-C2B
16	C	4004	3PE	C23-C24-C25-C26
16	C	4004	3PE	C21-C22-C23-C24
13	E	302	3PH	C32-C33-C34-C35
13	A	502	3PH	O21-C2-C3-O31
17	C	4005	UQ6	C20-C19-C21-C22
13	A	502	3PH	C23-C24-C25-C26
13	C	4006	3PH	C32-C33-C34-C35
13	C	4006	3PH	C22-C21-O21-C2
16	C	4004	3PE	C32-C31-O31-C3
13	E	302	3PH	O11-C1-C2-C3
13	C	4006	3PH	C3D-C3E-C3F-C3G
16	C	4004	3PE	C1-C2-C3-O31
17	C	4005	UQ6	C18-C19-C21-C22
16	C	4004	3PE	C22-C23-C24-C25
13	E	302	3PH	C29-C2A-C2B-C2C
15	C	4003	AOQ	C11-C16-C2-C3
13	C	4006	3PH	O22-C21-O21-C2
13	E	302	3PH	C2A-C2B-C2C-C2D
13	E	302	3PH	C31-C32-C33-C34
13	C	4006	3PH	O11-C1-C2-C3
13	E	302	3PH	O11-C1-C2-O21
13	C	4006	3PH	O21-C2-C3-O31
16	C	4004	3PE	O32-C31-O31-C3
12	A	501	UMQ	CF-CG-CH-CI
13	A	502	3PH	O11-C1-C2-C3
16	C	4004	3PE	C12-C11-O13-P
13	A	502	3PH	C31-C32-C33-C34
13	C	4006	3PH	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
13	A	502	3PH	O11-C1-C2-O21
16	C	4004	3PE	C11-O13-P-O11
13	A	502	3PH	C1-C2-C3-O31
16	C	4004	3PE	O31-C31-C32-C33
15	C	4003	AOQ	C12-C13-C17-C22
16	C	4004	3PE	C2-C1-O11-P
13	E	302	3PH	C25-C26-C27-C28
15	C	4003	AOQ	C12-C13-C17-C18
16	C	4004	3PE	O21-C2-C3-O31
13	A	502	3PH	C22-C23-C24-C25
13	A	502	3PH	C33-C34-C35-C36
16	C	4004	3PE	C1-O11-P-O13
13	C	4006	3PH	C35-C36-C37-C38
16	C	4004	3PE	C24-C25-C26-C27
13	C	4006	3PH	C3E-C3F-C3G-C3H
13	E	302	3PH	C34-C35-C36-C37
13	E	302	3PH	O21-C21-C22-C23
13	E	302	3PH	O21-C2-C3-O31
13	E	302	3PH	O22-C21-C22-C23
16	C	4004	3PE	C1-O11-P-O14

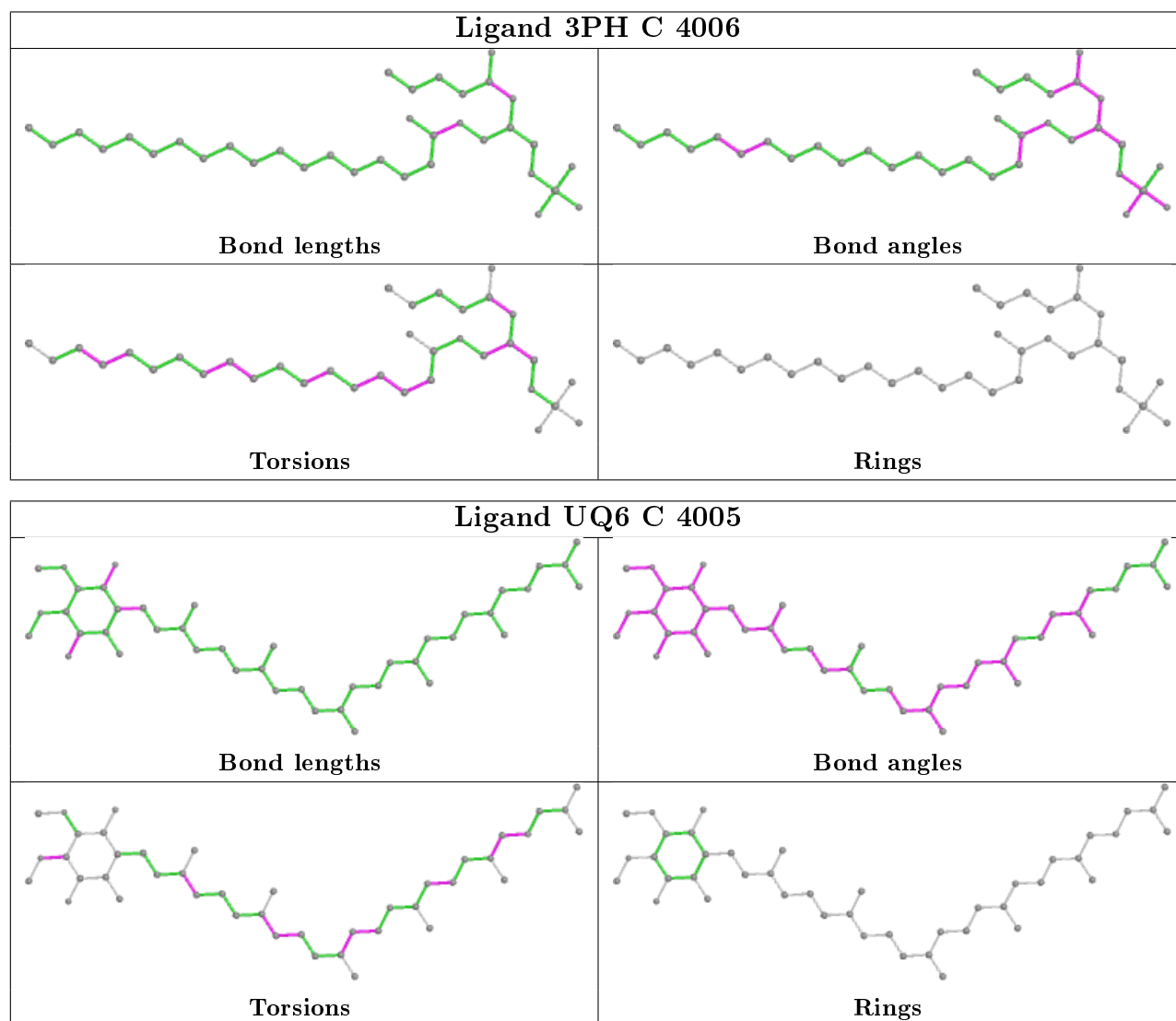
There are no ring outliers.

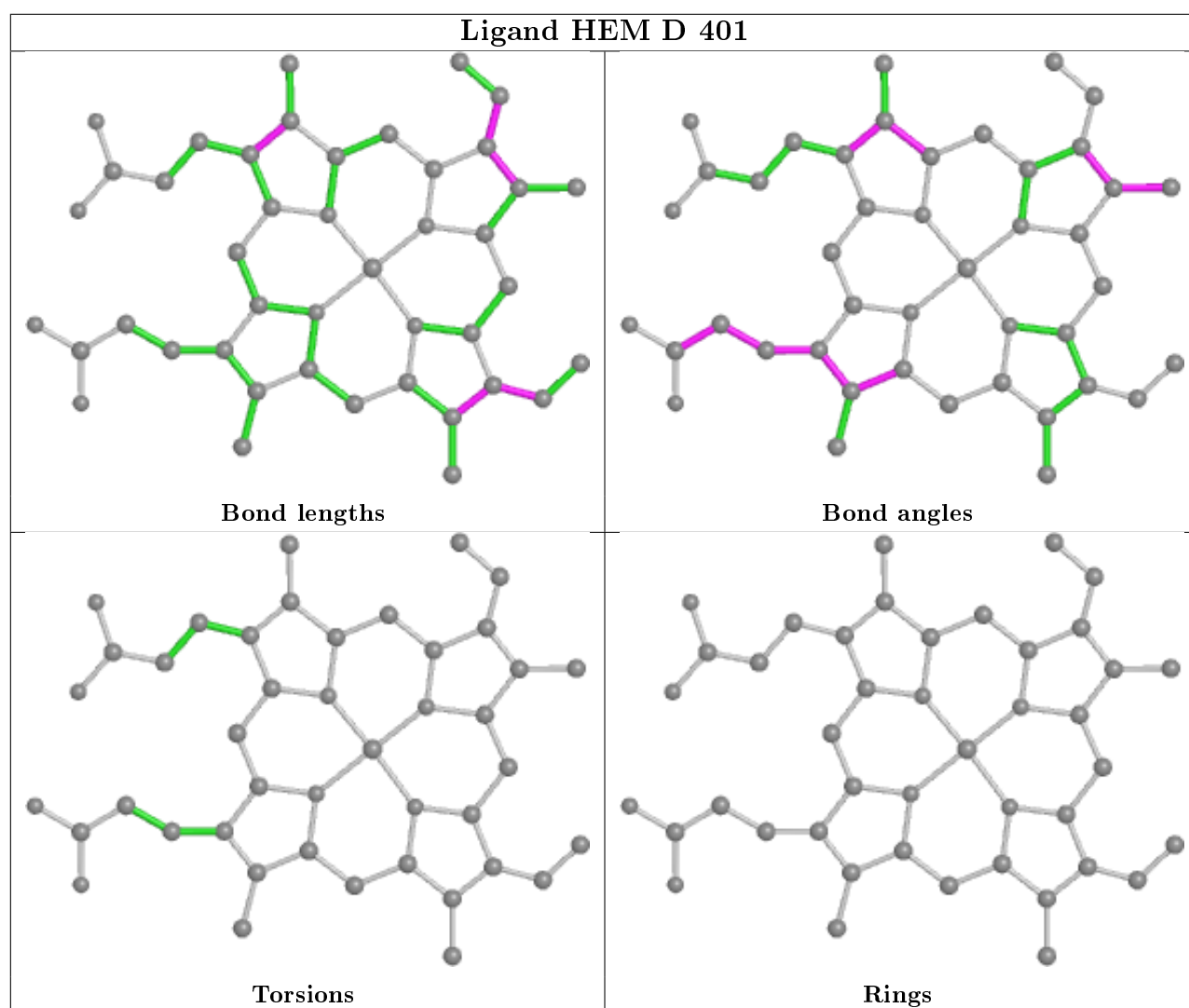
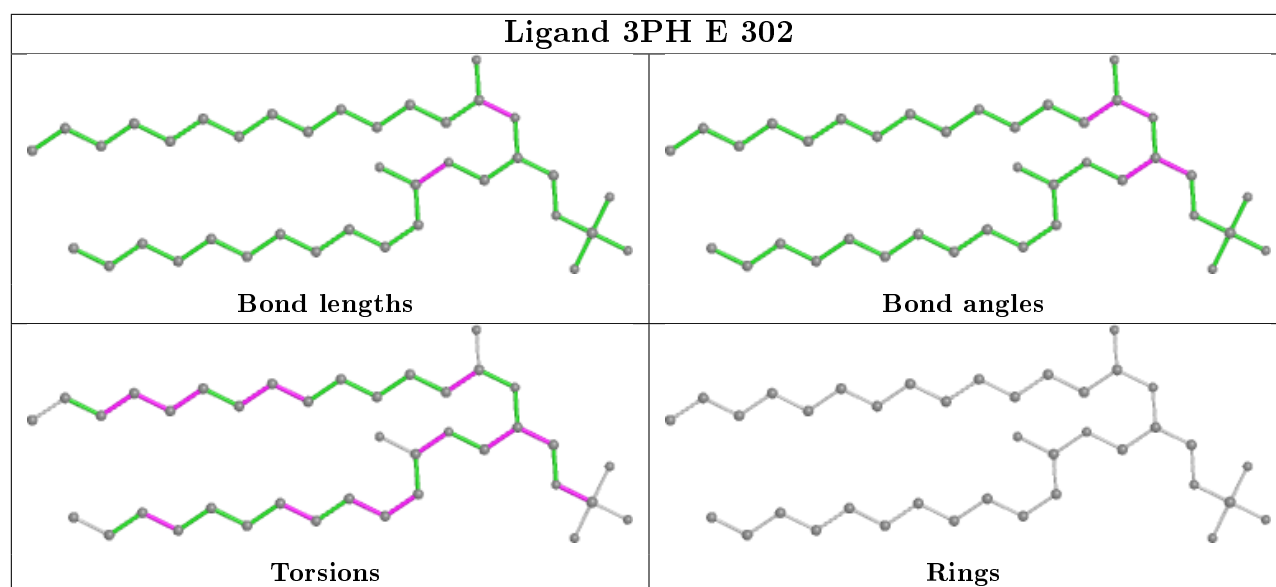
10 monomers are involved in 47 short contacts:

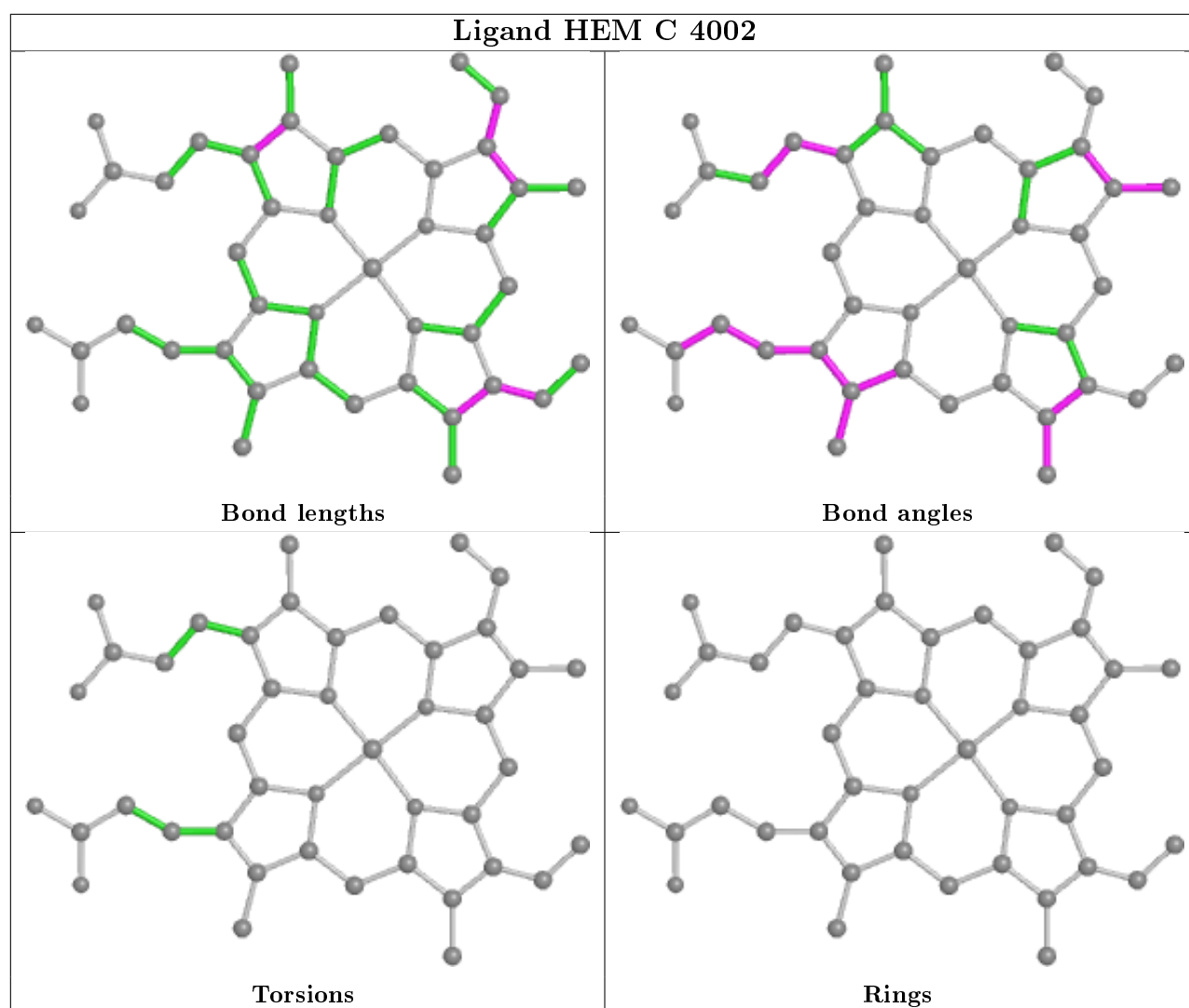
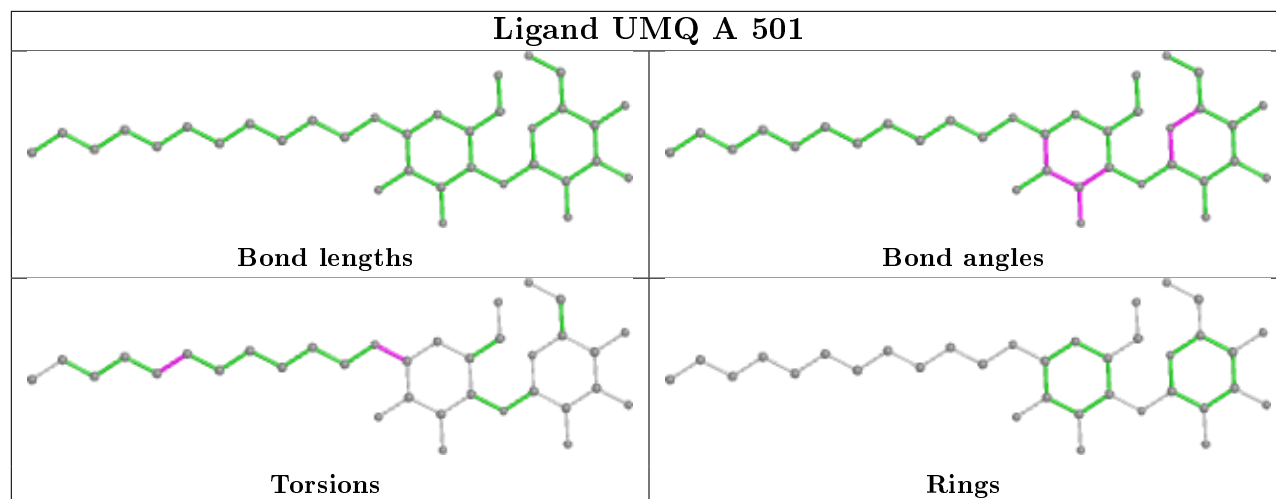
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	4006	3PH	1	0
17	C	4005	UQ6	5	0
13	E	302	3PH	6	0
14	D	401	HEM	11	0
12	A	501	UMQ	3	0
14	C	4002	HEM	8	0
14	C	4001	HEM	7	0
13	A	502	3PH	2	0
16	C	4004	3PE	1	0
15	C	4003	AOQ	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

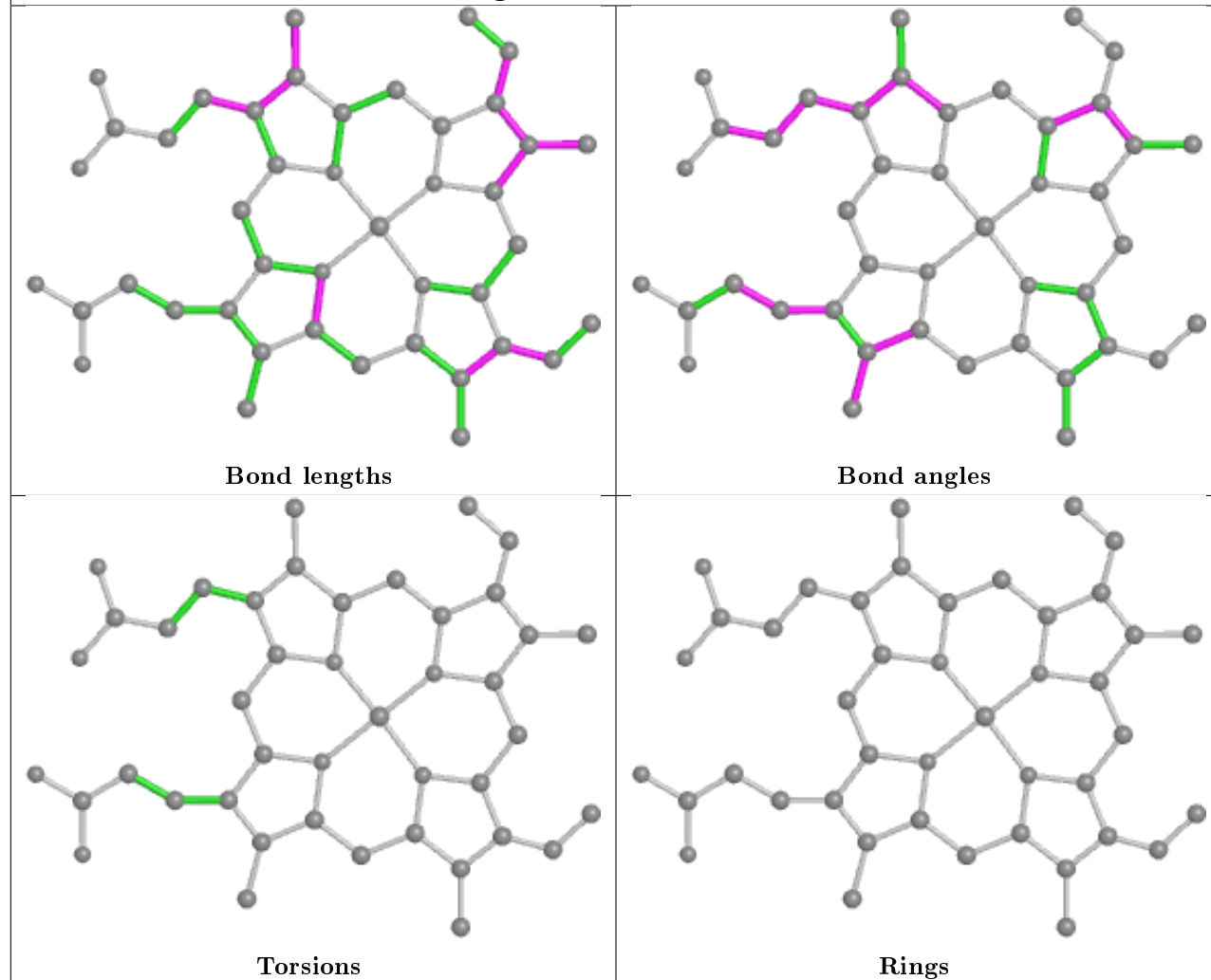
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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



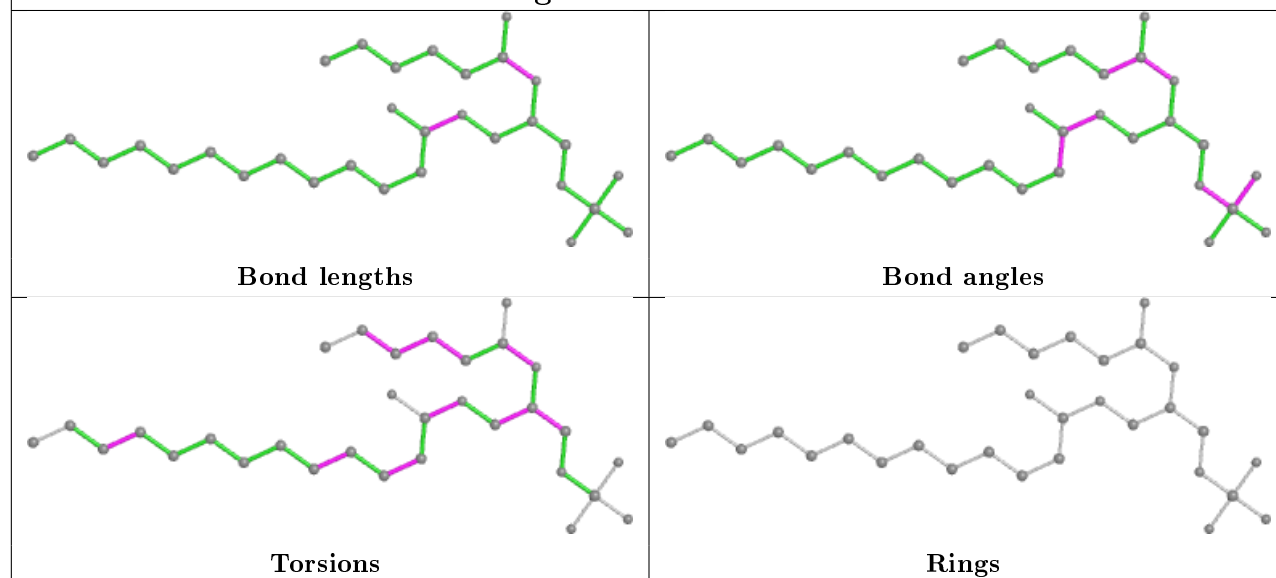


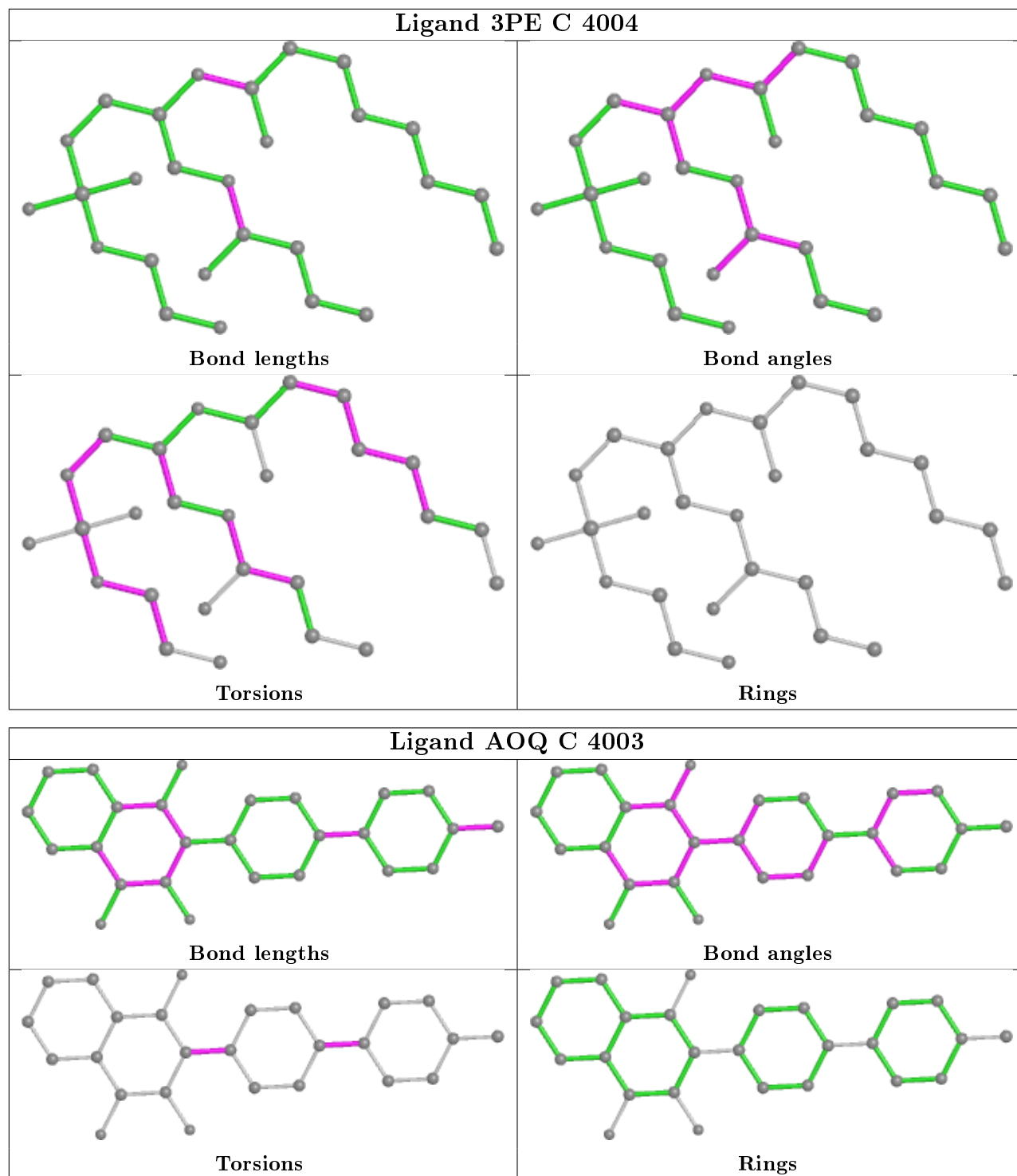


Ligand HEM C 4001



Ligand 3PH A 502





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	417/431 (96%)	0.42	37 (8%) 9 3	17, 69, 116, 122	0
2	B	344/352 (97%)	0.55	30 (8%) 10 3	29, 71, 104, 127	0
3	C	384/385 (99%)	-0.25	1 (0%) 94 83	0, 7, 18, 69	0
4	D	248/248 (100%)	0.14	5 (2%) 65 36	16, 40, 63, 83	1 (0%)
5	E	182/185 (98%)	0.03	8 (4%) 34 13	4, 26, 70, 112	0
6	F	74/74 (100%)	0.35	6 (8%) 12 3	38, 61, 92, 94	0
7	G	126/126 (100%)	-0.19	2 (1%) 72 44	6, 27, 48, 67	0
8	H	82/93 (88%)	0.21	4 (4%) 29 11	7, 29, 67, 88	1 (1%)
9	I	57/57 (100%)	0.02	2 (3%) 44 19	24, 45, 78, 102	0
10	J	127/127 (100%)	0.14	3 (2%) 59 30	27, 44, 63, 68	0
11	K	107/107 (100%)	0.38	8 (7%) 14 4	36, 67, 105, 116	0
All	All	2148/2185 (98%)	0.18	106 (4%) 29 11	0, 42, 102, 127	2 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ALA	8.9
3	C	384	ASN	7.9
9	I	58	ALA	7.7
2	B	282	GLY	5.7
6	F	119	HIS	5.5
6	F	74	VAL	5.4
1	A	52	GLY	5.1
1	A	35	GLY	5.0
11	K	15	LEU	4.4
2	B	252	GLN	4.3
2	B	230	ARG	4.3
8	H	37	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	339	ASN	3.9
1	A	91	LEU	3.9
5	E	51	LYS	3.8
1	A	32	LEU	3.8
6	F	118	GLU	3.8
1	A	34	ASN	3.8
1	A	53	VAL	3.8
2	B	351	PHE	3.7
2	B	216	VAL	3.7
2	B	340	PHE	3.7
5	E	46	ASN	3.6
1	A	204	SER	3.6
2	B	286	THR	3.6
5	E	47	ASN	3.5
11	K	76	SER	3.5
2	B	365	LEU	3.5
1	A	134	SER	3.5
2	B	217	SER	3.4
2	B	368	LEU	3.4
2	B	335	PRO	3.3
2	B	358	ASP	3.3
2	B	223	PHE	3.3
1	A	127	GLN	3.3
2	B	318	ILE	3.2
5	E	48	ASP	3.2
8	H	94	VAL	3.2
1	A	88	LYS	3.1
9	I	2	SER	3.1
1	A	31	GLN	3.1
1	A	33	SER	3.0
2	B	342	ALA	3.0
5	E	45	GLU	3.0
1	A	103	SER	3.0
1	A	90	GLY	2.9
2	B	283	GLY	2.9
1	A	136	ASN	2.9
1	A	198	ASN	2.9
1	A	456	ARG	2.8
1	A	243	ALA	2.8
1	A	129	ALA	2.7
1	A	223	ILE	2.7
2	B	284	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	65	TYR	2.7
1	A	238	LEU	2.7
1	A	210	GLY	2.6
2	B	215	LEU	2.6
2	B	338	LEU	2.6
4	D	309	LYS	2.6
4	D	308	ARG	2.6
10	J	43	GLY	2.5
8	H	5	SER	2.5
2	B	320	TYR	2.5
11	K	30	ASN	2.5
2	B	336	ILE	2.5
11	K	105	GLU	2.5
1	A	244	PHE	2.4
6	F	117	LEU	2.4
1	A	108	SER	2.4
5	E	136	ALA	2.4
1	A	36	ILE	2.4
2	B	306	ALA	2.4
11	K	1	ASP	2.4
11	K	89	GLN	2.4
5	E	89	LEU	2.4
1	A	92	ALA	2.4
10	J	9	ALA	2.3
1	A	380	SER	2.3
4	D	142	GLY	2.3
1	A	173	PRO	2.3
1	A	205	ASN	2.2
11	K	107	LYS	2.2
1	A	217	GLU	2.2
1	A	236	PRO	2.2
1	A	235	LYS	2.2
1	A	70	SER	2.2
2	B	246	ASN	2.1
2	B	218	LYS	2.1
6	F	80	ASP	2.1
6	F	147	LYS	2.1
5	E	31	LYS	2.1
8	H	71	LYS	2.1
7	G	20	VAL	2.1
2	B	94	LEU	2.1
7	G	97	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	332	VAL	2.1
10	J	37	TRP	2.1
1	A	71	ASN	2.0
2	B	18	THR	2.0
4	D	193	SER	2.0
2	B	245	VAL	2.0
1	A	399	SER	2.0
11	K	80	PRO	2.0
2	B	220	GLU	2.0
4	D	201	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.

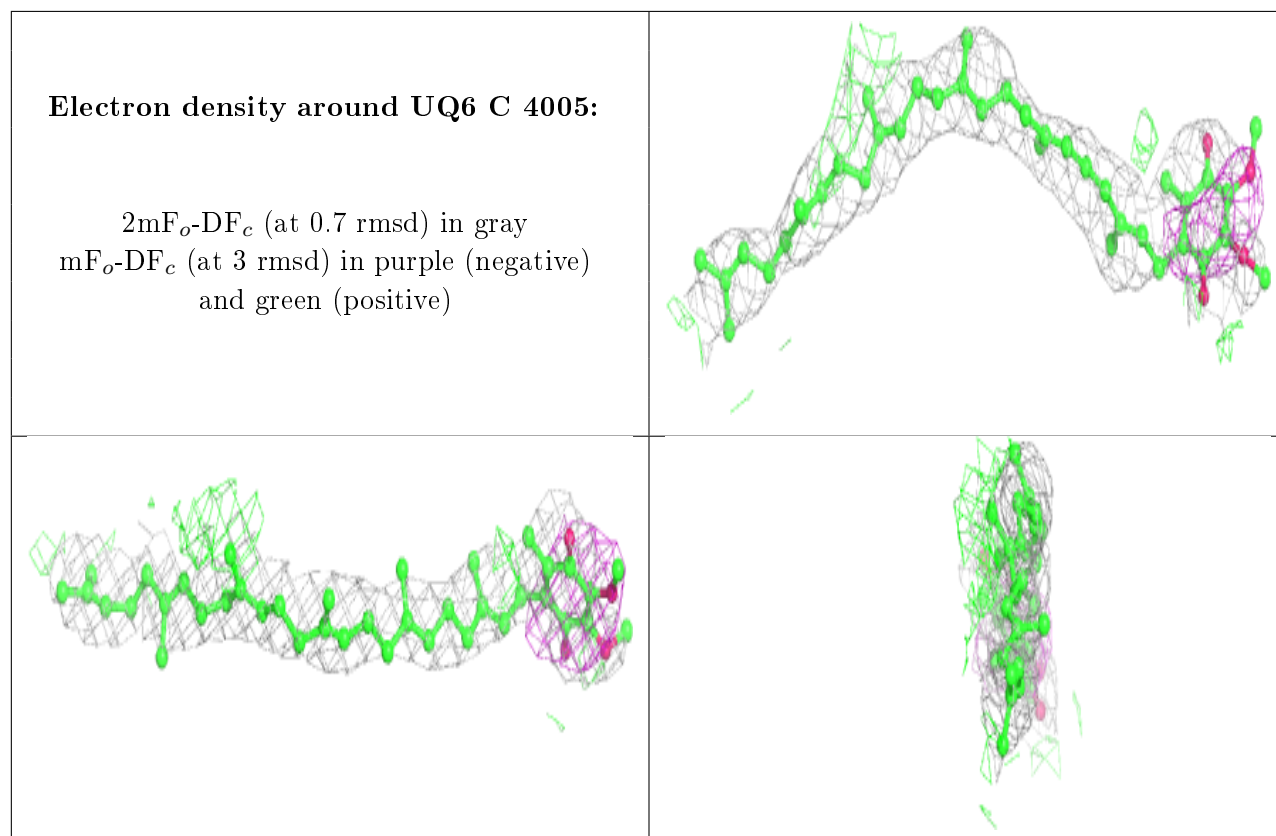
6.4 Ligands [i](#)

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, 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(\AA^2)	Q<0.9
17	UQ6	C	4005	43/43	0.83	0.35	6,12,21,24	0
13	3PH	C	4006	35/48	0.88	0.25	3,17,29,39	0
12	UMQ	A	501	34/34	0.89	0.24	13,31,43,48	0
13	3PH	E	302	38/48	0.91	0.26	7,15,21,23	0
13	3PH	A	502	31/48	0.91	0.22	13,20,33,38	0
16	3PE	C	4004	27/51	0.93	0.27	4,8,12,14	0
14	HEM	D	401	43/43	0.94	0.25	22,31,37,43	0
15	AOQ	C	4003	26/26	0.96	0.17	7,12,16,22	0
14	HEM	C	4001	43/43	0.98	0.25	0,2,7,20	0
14	HEM	C	4002	43/43	0.98	0.27	2,5,10,11	0
18	FES	E	301	4/4	0.99	0.18	6,7,7,13	0

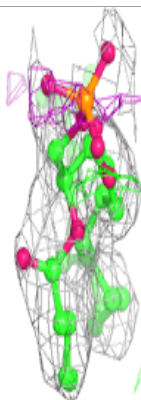
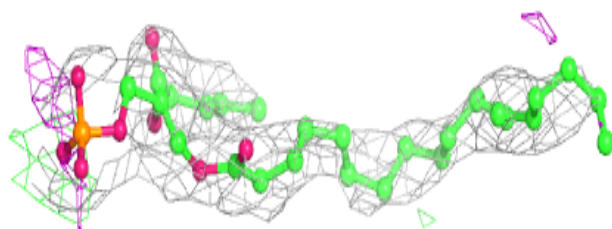
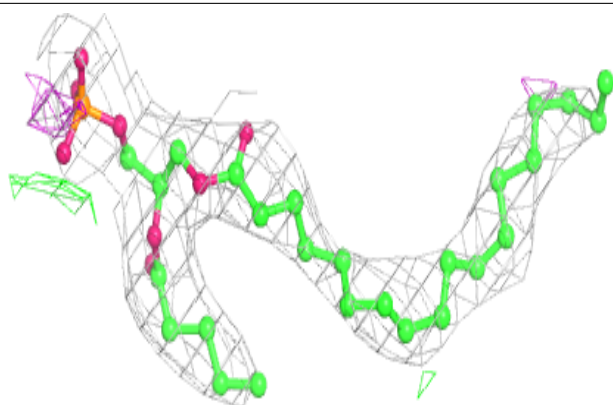
The following is a graphical depiction of the model fit to experimental electron density of all

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.

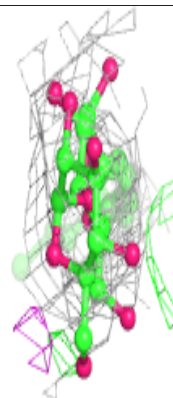
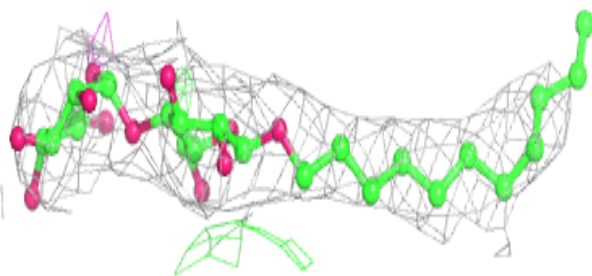
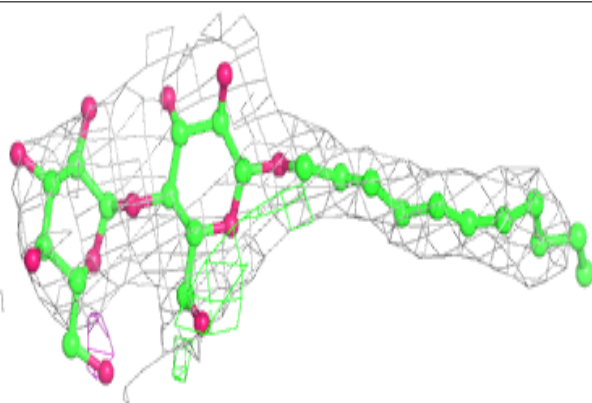


Electron density around 3PH C 4006:

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

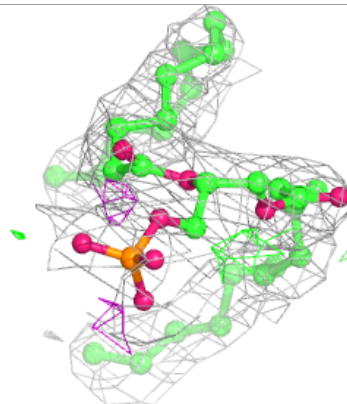
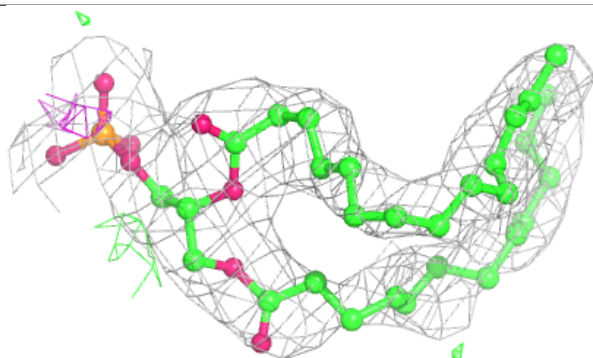
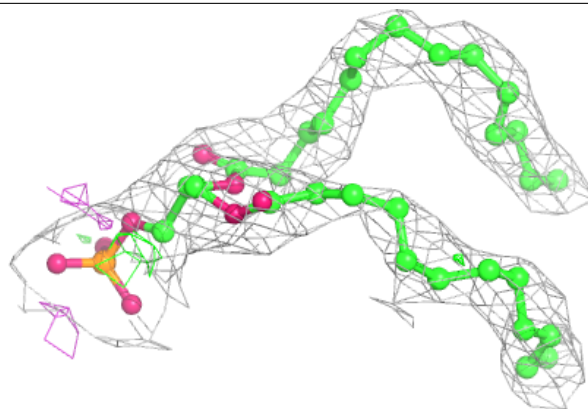
**Electron density around UMQ A 501:**

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

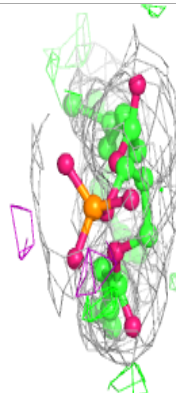
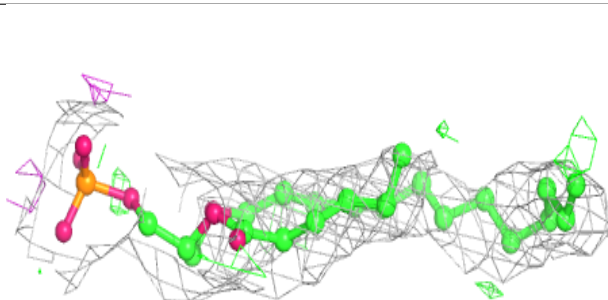
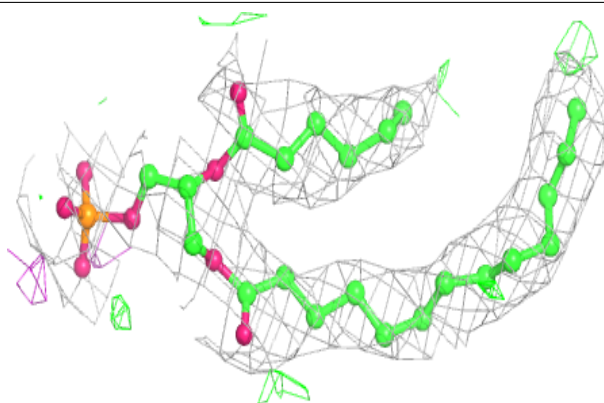


Electron density around 3PH E 302:

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

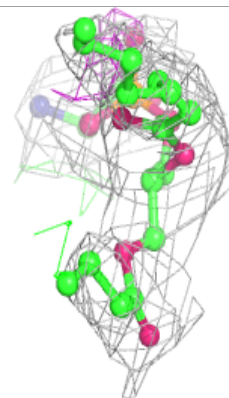
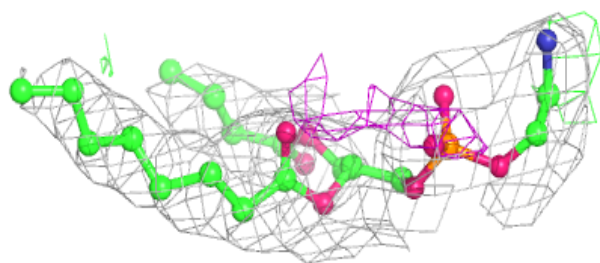
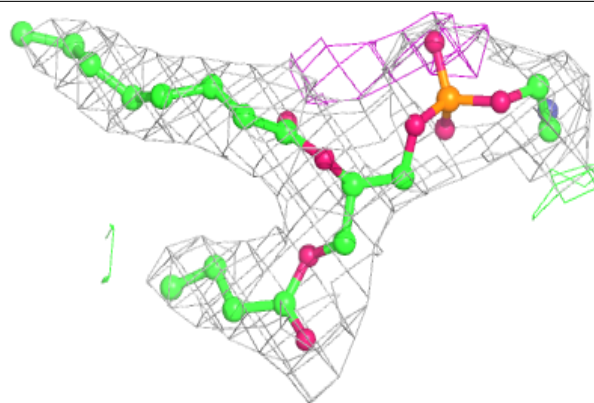
**Electron density around 3PH A 502:**

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



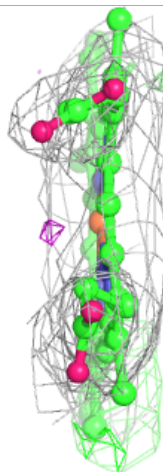
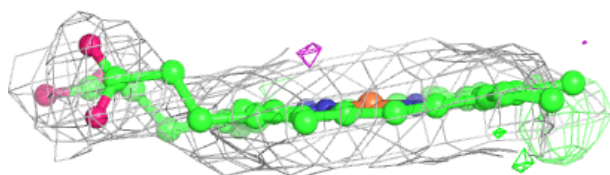
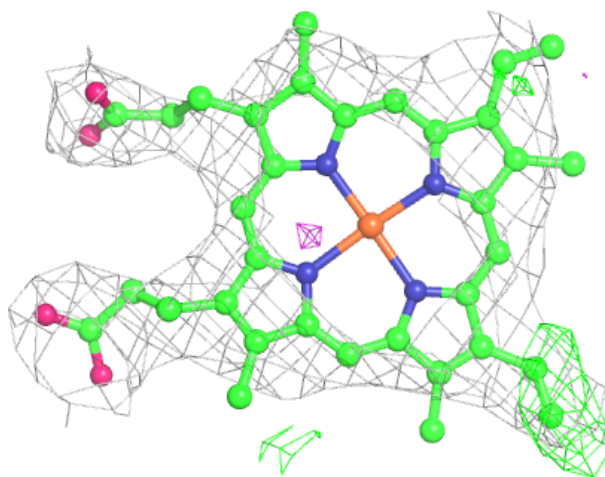
Electron density around 3PE C 4004:

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



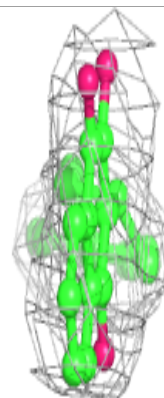
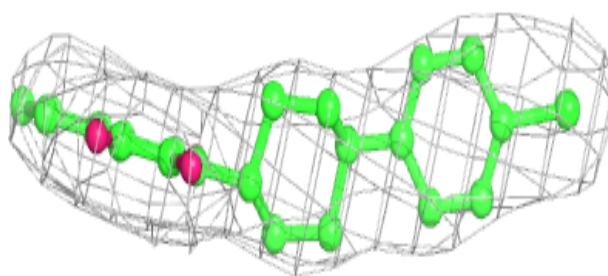
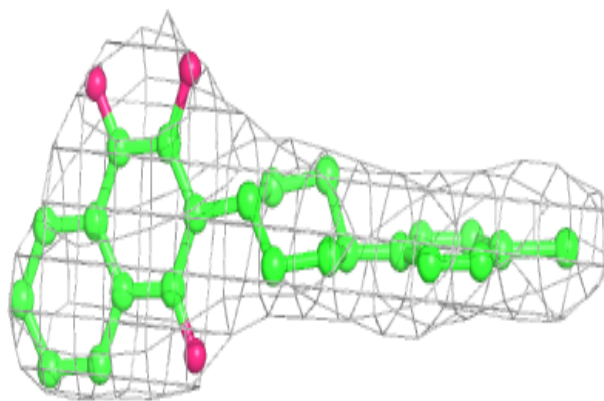
Electron density around HEM D 401:

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



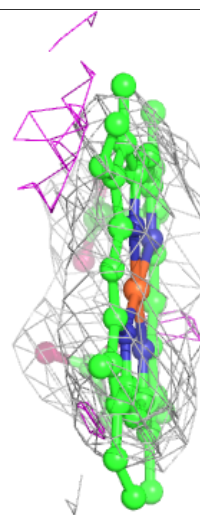
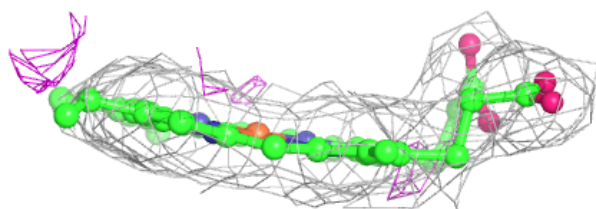
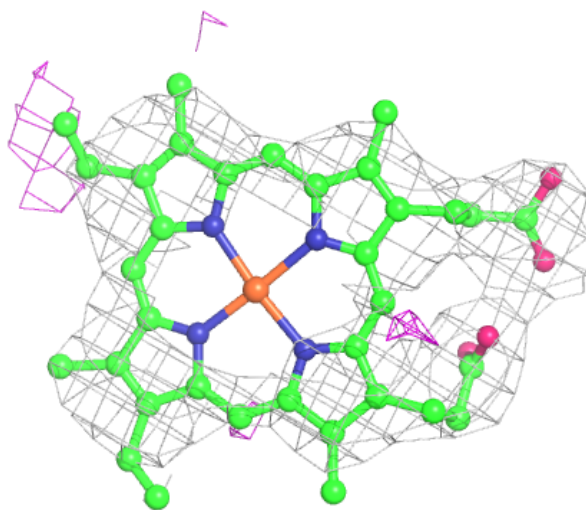
Electron density around AOQ C 4003:

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



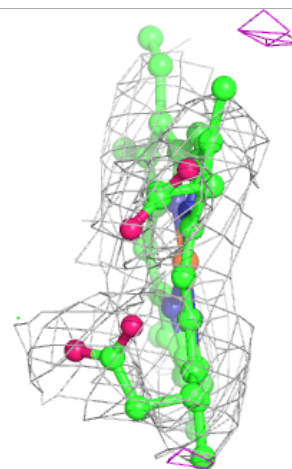
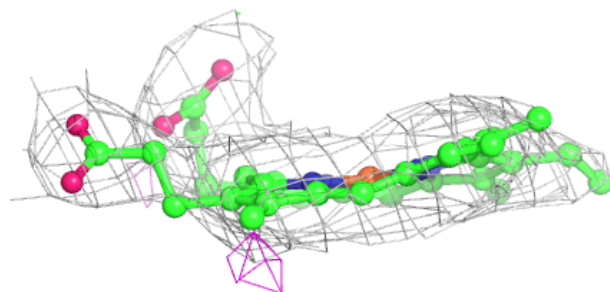
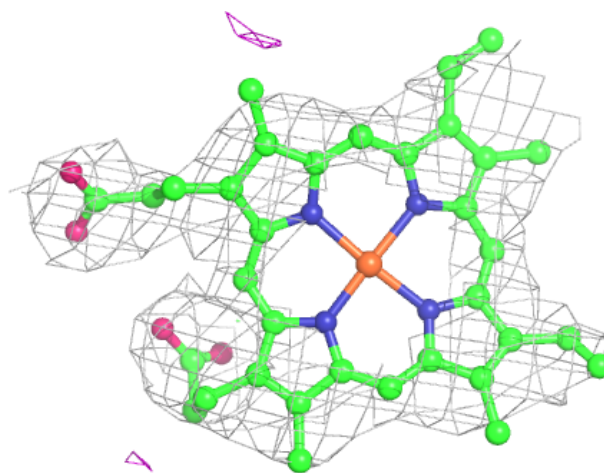
Electron density around HEM C 4001:

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



Electron density around HEM C 4002:

$2mF_o-DF_c$ (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.