



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:48 PM UTC

PDB ID : 4PD4 / pdb_00004pd4
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 types of validation reports are described at

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

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

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

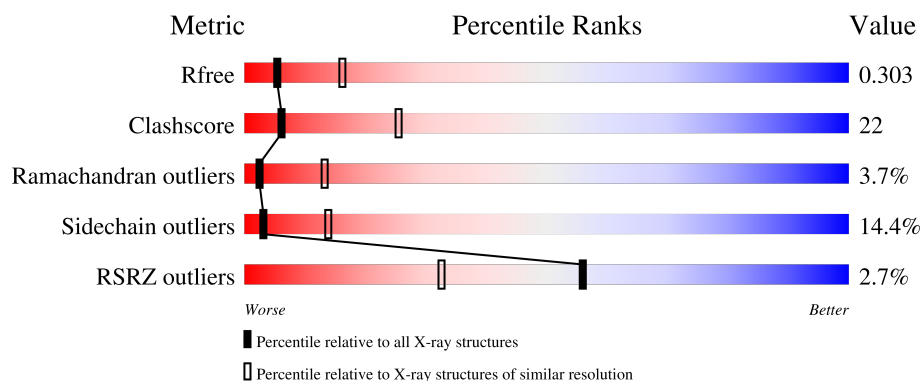
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (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 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	431	6% 47% 46% 6%
2	B	352	6% 53% 42% .
3	C	385	44% 45% 8% .
4	D	248	47% 44% 8% .
5	E	185	% 45% 43% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	74	% 61% 35% .
7	G	126	48% 43% 10%
8	H	93	3% 56% 34% 8% .
9	I	57	2% 56% 42% .
10	J	127	42% 43% 15%
11	K	107	4% 41% 48% 11%

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			

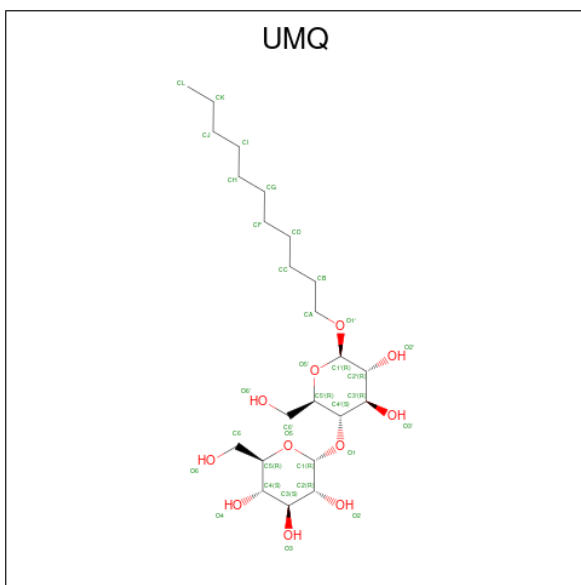
- Molecule 10 is a protein called Igh protein.

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.

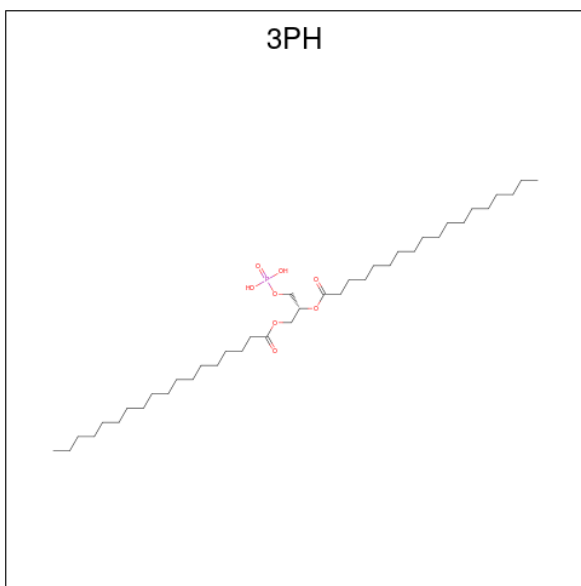
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is UNDECYL-MALTOSIDE (CCD ID: 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 (CCD ID: 3PH) (formula: $\text{C}_{39}\text{H}_{77}\text{O}_8\text{P}$).



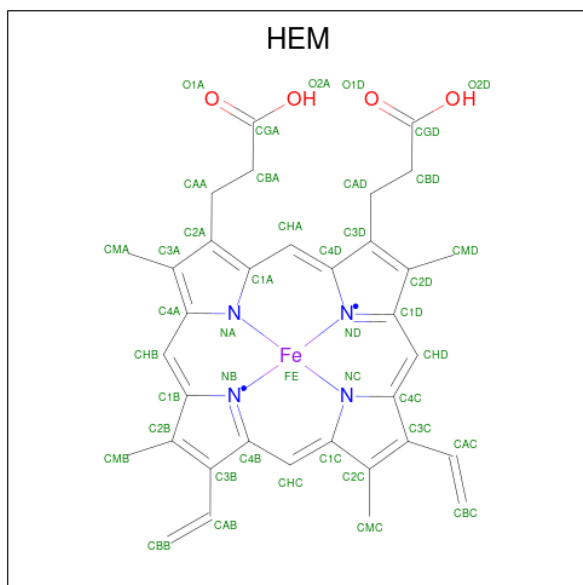
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total 31	C 22	O 8	P 1	0	0
13	C	1	Total 35	C 26	O 8	P 1	0	0

Continued on next page...

Continued from previous page...

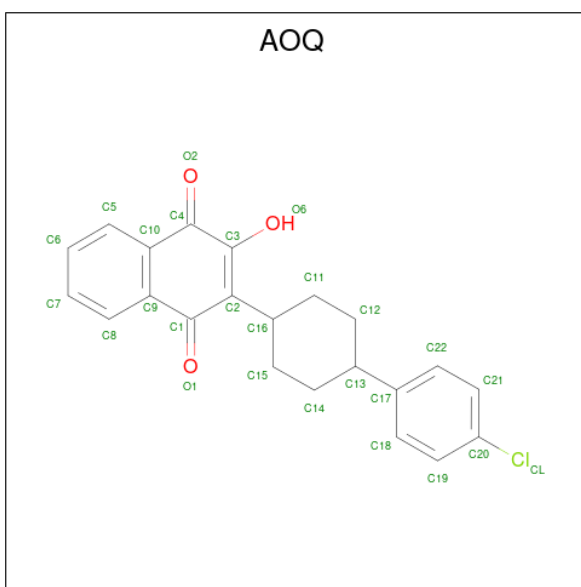
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	E	1	Total	C	O	P	0	0
			38	29	8	1		

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



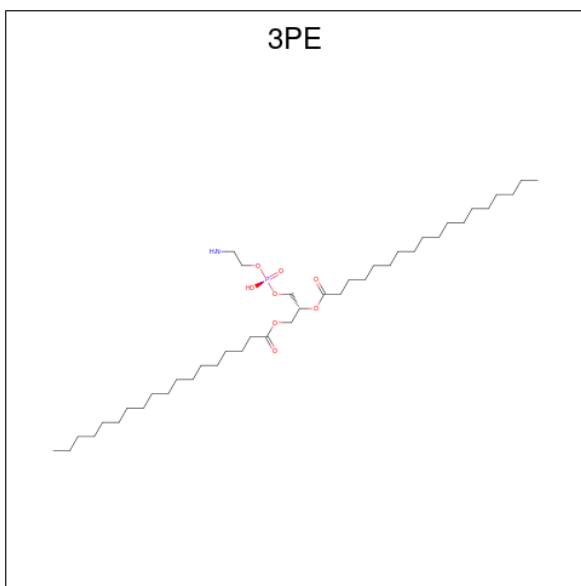
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
14	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
14	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 15 is 2-[trans-4-(4-chlorophenyl)cyclohexyl]-3-hydroxynaphthalene-1,4-dione (CCD ID: 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		

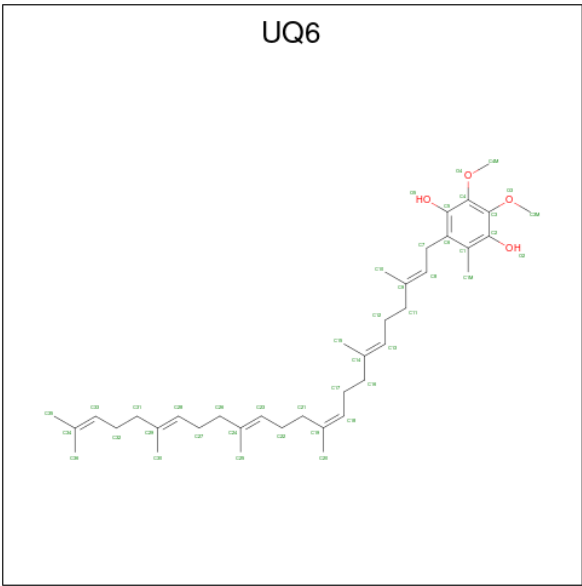
- Molecule 16 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



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

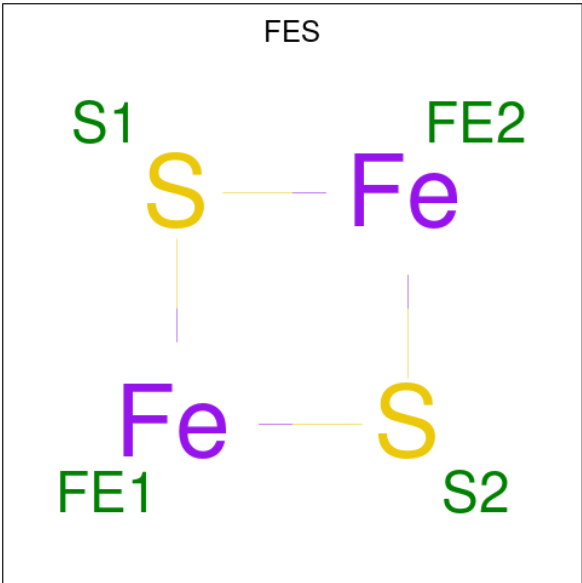
- Molecule 17 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula: $C_{41}H_{82}NO_8P$).

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 (CCD ID: FES) (formula: Fe₂S₂).

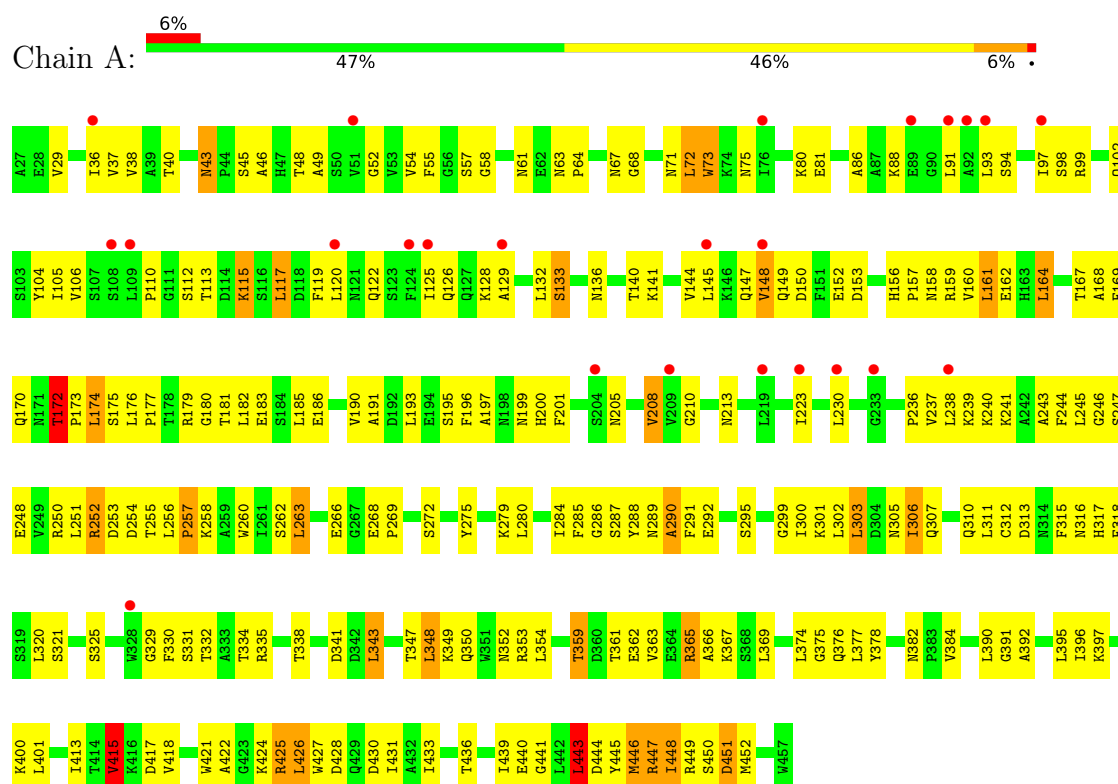


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	E	1	Total	Fe	S	0	0
			4	2	2		

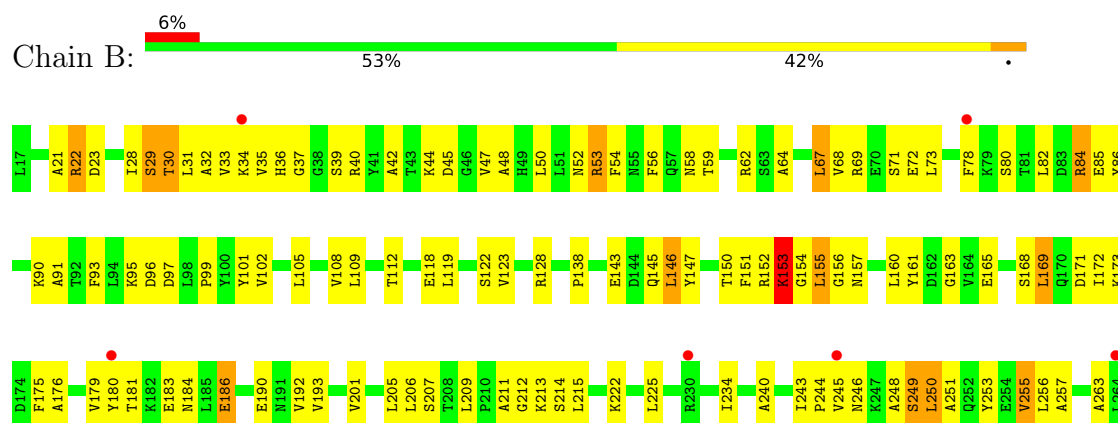
3 Residue-property plots

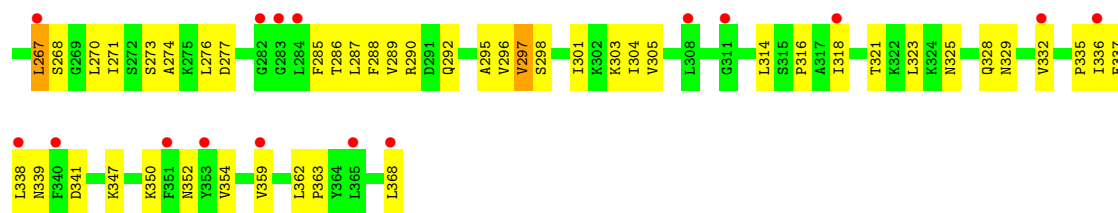
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



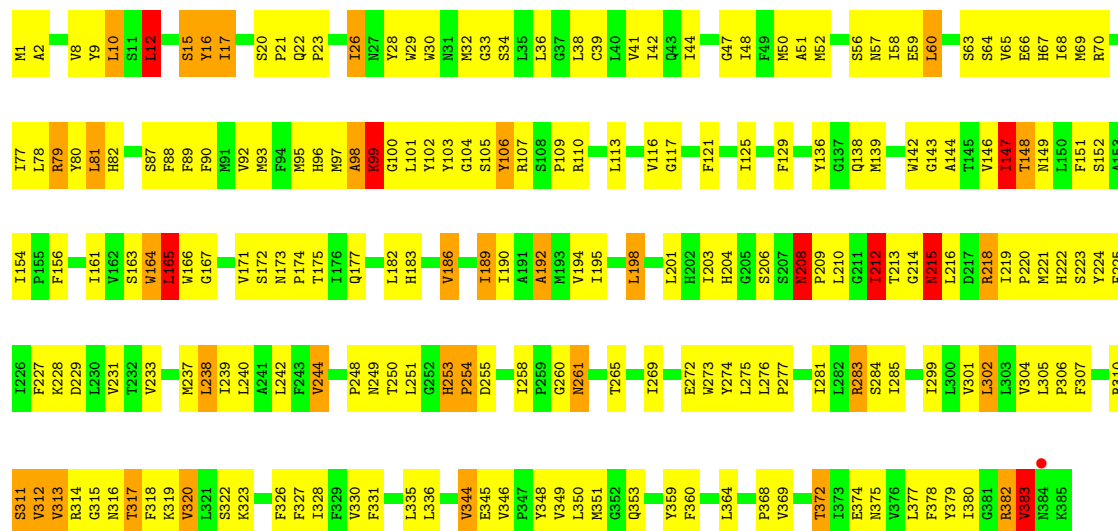
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial





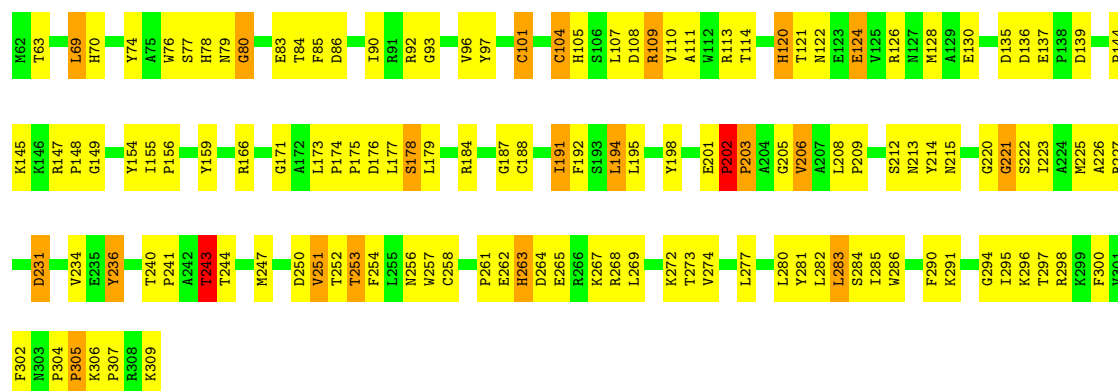
• Molecule 3: Cytochrome b

Chain C: 44% 45% 8% •



• Molecule 4: Cytochrome c1, heme protein, mitochondrial

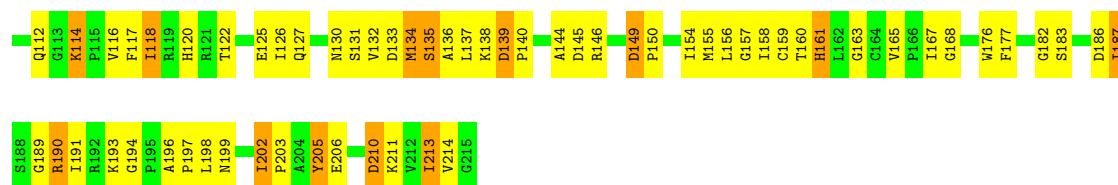
Chain D: 47% 44% 8% •



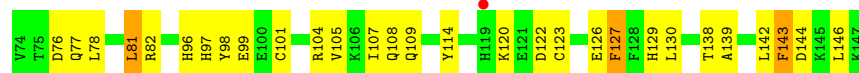
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E: 45% 43% 12% •

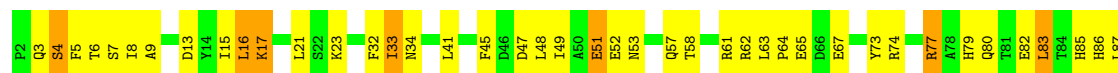




• Molecule 6: Cytochrome b-c1 complex subunit 6



• Molecule 7: Cytochrome b-c1 complex subunit 7



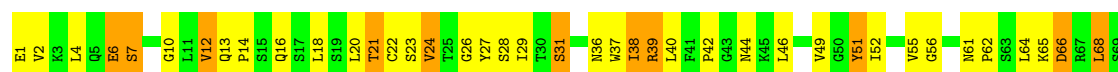
• Molecule 8: Cytochrome b-c1 complex subunit 8

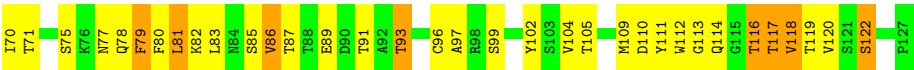


• Molecule 9: Cytochrome b-c1 complex subunit 9

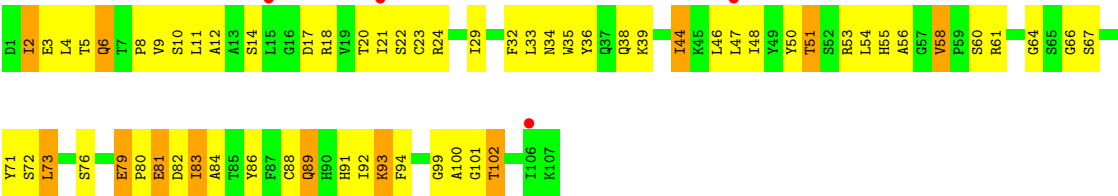


• Molecule 10: Igh protein





● 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) 98.4 (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 0.270 , 0.303	Depositor DCC
R_{free} test set	2008 reflections (2.56%)	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 , 31.7	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	0.93	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, UQ6, 3PE, FES, HEM, 3PH, AOQ

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	0.51	0/3405	0.96	8/4614 (0.2%)
2	B	0.50	0/2781	0.91	3/3764 (0.1%)
3	C	0.90	1/3192 (0.0%)	1.22	15/4354 (0.3%)
4	D	0.60	0/2022	1.11	9/2751 (0.3%)
5	E	0.71	1/1444 (0.1%)	1.20	8/1957 (0.4%)
6	F	0.46	0/638	0.94	0/858
7	G	0.73	0/1040	1.18	1/1408 (0.1%)
8	H	0.65	0/804	1.06	2/1088 (0.2%)
9	I	0.48	0/479	0.89	0/646
10	J	0.58	0/1043	1.01	2/1422 (0.1%)
11	K	0.51	0/863	0.87	0/1172
All	All	0.64	2/17711 (0.0%)	1.06	48/24034 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	147	ILE	CA-CB	-6.56	1.46	1.54
5	E	213	ILE	CA-CB	5.87	1.59	1.53

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	202	PRO	CA-C-N	9.37	131.55	119.84
4	D	202	PRO	C-N-CA	9.37	131.55	119.84
5	E	135	SER	N-CA-C	-8.72	103.76	114.75
3	C	261	ASN	CA-C-N	7.83	128.01	119.87
3	C	261	ASN	C-N-CA	7.83	128.01	119.87
1	A	150	ASP	N-CA-C	-7.67	104.82	114.56
1	A	256	LEU	CA-C-N	7.47	129.18	119.84
1	A	256	LEU	C-N-CA	7.47	129.18	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	165	VAL	CA-C-N	7.45	127.90	119.93
5	E	165	VAL	C-N-CA	7.45	127.90	119.93
8	H	21	GLN	N-CA-C	7.35	121.04	110.24
8	H	49	PHE	N-CA-C	-7.29	105.57	114.75
3	C	253	HIS	CA-C-N	7.12	128.74	119.84
3	C	253	HIS	C-N-CA	7.12	128.74	119.84
1	A	172	THR	CA-C-N	7.05	128.66	119.84
1	A	172	THR	C-N-CA	7.05	128.66	119.84
3	C	90	PHE	N-CA-C	6.98	118.54	111.07
7	G	58	THR	N-CA-C	-6.64	105.00	113.23
5	E	139	ASP	CA-C-N	6.37	126.59	119.90
5	E	139	ASP	C-N-CA	6.37	126.59	119.90
5	E	202	ILE	N-CA-C	6.25	113.25	107.56
3	C	208	ASN	N-CA-C	6.14	115.37	108.25
10	J	68	LEU	N-CA-C	6.07	117.80	109.18
4	D	80	GLY	CA-C-N	6.03	126.14	119.87
4	D	80	GLY	C-N-CA	6.03	126.14	119.87
4	D	108	ASP	N-CA-C	5.93	118.70	111.82
5	E	196	ALA	CA-C-N	-5.92	114.13	120.47
5	E	196	ALA	C-N-CA	-5.92	114.13	120.47
3	C	82	HIS	N-CA-C	-5.86	104.81	111.14
4	D	263	HIS	N-CA-C	5.78	118.04	111.11
3	C	16	TYR	N-CA-C	-5.58	105.91	114.16
4	D	201	GLU	CA-C-N	5.55	126.10	120.38
4	D	201	GLU	C-N-CA	5.55	126.10	120.38
2	B	54	PHE	N-CA-C	-5.48	106.45	114.39
2	B	243	ILE	CA-C-N	5.48	126.69	119.84
2	B	243	ILE	C-N-CA	5.48	126.69	119.84
3	C	143	GLY	N-CA-C	-5.47	106.02	112.64
4	D	120	HIS	N-CA-C	5.33	115.43	108.07
1	A	415	VAL	N-CA-C	-5.33	105.65	110.82
3	C	186	VAL	N-CA-CB	5.21	113.78	110.50
3	C	192	ALA	N-CA-C	-5.20	104.87	111.11
1	A	43	ASN	CA-C-N	5.09	125.16	119.87
1	A	43	ASN	C-N-CA	5.09	125.16	119.87
3	C	320	VAL	CB-CA-C	-5.05	105.24	112.22
3	C	12	LEU	N-CA-C	-5.04	105.43	111.03
3	C	212	ILE	CB-CA-C	-5.02	103.06	111.29
10	J	61	ASN	N-CA-C	-5.00	103.73	109.93
3	C	231	VAL	CB-CA-C	-5.00	105.47	112.02

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	159	0
2	B	2735	0	2774	109	0
3	C	3090	0	3129	173	0
4	D	1961	0	1890	104	0
5	E	1411	0	1386	70	0
6	F	624	0	581	23	0
7	G	1019	0	1034	54	0
8	H	773	0	736	39	0
9	I	465	0	459	19	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	10	0
15	C	26	0	19	3	0
16	C	27	0	28	1	0
17	C	43	0	58	4	0
18	E	4	0	0	0	0
All	All	17646	0	17458	773	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 (773) 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:32:MET:HE3	3:C:92:VAL:HG13	1.41	1.00
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:502:3PH:H321	13:A:502:3PH:H221	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:HBC2	14:C:4001:HEM:HHD	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:C:249:ASN:C	3:C:251:LEU:H	2.05	0.65
1:A:365:ARG:NH2	2:B:72:GLU:OE1	2.29	0.65
3:C:105:SER:C	3:C:107:ARG:H	2.05	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:C:351:MET:HE3	8:H:69:TRP:CD1	2.37	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:80:LYS:HG3	2:B:263:ALA:HB1	1.83	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:268:GLU:O	1:A:321:SER:OG	2.19	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:98:SER:OG	1:A:99:ARG:N	2.29	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
7:G:32:PHE:C	7:G:34:ASN:H	2.14	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
3:C:249:ASN:C	3:C:251:LEU:N	2.64	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:47:ASP:OD1	7:G:102:TYR:OH	2.20	0.55
6:F:96:HIS:O	6:F:99:GLU:N	2.40	0.55
1:A:86:ALA:HB1	1:A:91:LEU:HB2	1.88	0.54
1:A:263:LEU:HD21	1:A:431:ILE:HD12	1.89	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
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:8:VAL:HG13	3:C:9:TYR:CD2	2.43	0.53
3:C:194:VAL:O	3:C:198:LEU:HD12	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:TYR:OH	2:B:277:ASP:OD2	2.26	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:54:VAL:HG21	1:A:391:GLY:HA3	1.90	0.53
1:A:102:GLN:HE22	1:A:196:PHE:HZ	1.57	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
1:A:444:ASP:OD2	3:C:224:TYR:OH	2.17	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
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
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
3:C:208:ASN:C	3:C:210:LEU:H	2.18	0.51
10:J:93:THR:HG23	10:J:117:THR:HG23	1.92	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
4:D:120:HIS:CE1	4:D:128:MET:HE1	2.45	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:90:ARG:HA	7:G:93:TRP:NE1	2.25	0.51
7:G:118:ASP:O	7:G:122:ASN:ND2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:16:TYR:C	3:C:17:ILE:HG13	2.36	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
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
4:D:261:PRO:C	4:D:263:HIS:H	2.20	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
1:A:170:GLN:HB2	5:E:36:THR:HG21	1.93	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
4:D:296:LYS:NZ	7:G:83:LEU:O	2.44	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
3:C:139:MET:HA	3:C:139:MET:HE2	1.93	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
14:D:401:HEM:HBD1	14:D:401:HEM:HHA	1.95	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
1:A:441:GLY:HA2	8:H:13:TRP:HB3	1.95	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:205:ASN:CG	1:A:236:PRO:HG3	2.38	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
4:D:93:GLY:O	4:D:97:TYR:N	2.43	0.49
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
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
12:A:501:UMQ:HB1	9:I:18:VAL:HG13	1.94	0.48
3:C:29:TRP:CZ2	13:C:4006:3PH:H322	2.49	0.48
3:C:326:PHE:O	3:C:330:VAL:HG23	2.13	0.48
4:D:286:TRP:CD1	5:E:59:MET:HE3	2.48	0.48
11:K:29:ILE:C	11:K:92:ILE:HD12	2.39	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: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
3:C:208:ASN:HD22	3:C:208:ASN:N	2.09	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:HB2	7:G:61:ARG:HH21	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:79:ARG:NH2	14:C:4001:HEM:O1A	2.45	0.48
3:C:360:PHE:HB3	3:C:364:LEU:HD12	1.96	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
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
2:B:248:ALA:C	2:B:250:LEU:H	2.23	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
1:A:248:GLU:CD	1:A:250:ARG:HH21	2.22	0.47
2:B:21:ALA:HB1	2:B:192:VAL:HB	1.95	0.47
2:B:181:THR:HB	2:B:211:ALA:O	2.15	0.47
7:G:13:ASP:HB3	7:G:17:LYS:NZ	2.29	0.47
1:A:263:LEU:O	1:A:329:GLY:HA3	2.15	0.47
2:B:255:VAL:HG23	2:B:314:LEU:HB3	1.97	0.47
3:C:32:MET:HE2	3:C:95:MET:HE2	1.97	0.47
3:C:96:HIS:CD2	14:C:4002:HEM:C1C	3.03	0.47
3:C:213:THR:HB	7:G:51:GLU:OE2	2.14	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:I:9:THR:O	9:I:12:LYS:NZ	2.40	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:HD13	10:J:29:ILE:HA	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
4:D:111:ALA:O	4:D:114:THR:OG1	2.28	0.46
4:D:205:GLY:HA3	6:F:122:ASP:HB3	1.97	0.46
5:E:213:ILE:O	5:E:213:ILE:HG13	2.15	0.46
10:J:7:SER:O	10:J:21:THR:HG23	2.15	0.46
3:C:320:VAL:HG13	8:H:58:TYR:HE2	1.80	0.46
5:E:80:SER:C	5:E:82:MET:H	2.23	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:O1	15:C:4003:AOQ:H7	2.15	0.46
4:D:256:ASN:C	4:D:256:ASN:HD22	2.23	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
3:C:208:ASN:N	3:C:208:ASN:ND2	2.59	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:23:PRO:HB2	3:C:26:ILE:HG23	1.98	0.46
3:C:166:TRP:NE1	3:C:171:VAL:HG23	2.31	0.46
3:C:173:ASN:C	3:C:175:THR:N	2.73	0.46
7:G:87:LEU:HD12	8:H:50:ARG:CZ	2.46	0.46
8:H:12:TRP:CD1	8:H:13:TRP:HD1	2.34	0.46
10:J:6:GLU:H	10:J:114:GLN:NE2	2.14	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:42:PRO:C	10:J:44:ASN:H	2.24	0.46
1:A:289:ASN:C	1:A:291:PHE:H	2.24	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
4:D:203:PRO:HG3	6:F:127:PHE:CD2	2.51	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
7:G:93:TRP:H	7:G:93:TRP:CD1	2.33	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: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
10:J:36:ASN:OD1	10:J:51:TYR:HB3	2.16	0.45
1:A:117:LEU:HD11	1:A:223:ILE:HG13	1.99	0.45
1:A:158:ASN:O	1:A:162:GLU:N	2.42	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
12:A:501:UMQ:O2'	9:I:17:PHE:HA	2.17	0.45
2:B:155:LEU:H	2:B:155:LEU:HD12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:VAL:HA	3:C:189:ILE:HG13	1.99	0.45
6:F:126:GLU:O	6:F:127:PHE:C	2.58	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:HD12	4:D:283:LEU:HA	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:6:GLU:N	10:J:114:GLN:HE22	2.15	0.45
10:J:20:LEU:HD22	10:J:116:THR:HG21	1.97	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
4:D:243:THR:HG21	6:F:77:GLN:OE1	2.17	0.45
6:F:105:VAL:O	6:F:109:GLN:HG3	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
5:E:127:GLN:O	5:E:131:SER:OG	2.32	0.45
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:69:LEU:HD22	4:D:70:HIS:N	2.32	0.44
4:D:231:ASP:OD2	4:D:243:THR:HG22	2.17	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
3:C:323:LYS:NZ	8:H:55:GLN:OE1	2.36	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:447:ARG:O	1:A:448:ILE:C	2.60	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:88:PHE:HZ	3:C:239:ILE:HG22	1.82	0.44
3:C:375:ASN:HB3	7:G:8:ILE:HD13	2.00	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:67:ASN:CG	1:A:176:LEU:HD12	2.43	0.44
2:B:305:VAL:HG21	2:B:368:LEU:HD22	1.98	0.44
3:C:50:MET:CG	3:C:78:LEU:HB3	2.47	0.44
11:K:36:TYR:CE2	11:K:89:GLN:HG2	2.50	0.44
3:C:22:GLN:HE21	3:C:221:MET:HE2	1.82	0.44
3:C:318:PHE:CE1	7:G:48:LEU:HD11	2.52	0.44
3:C:351:MET:HE3	8:H:69:TRP:NE1	2.33	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:CD1	5:E:205:TYR:N	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:60:LEU:HD13	3:C:60:LEU:HA	1.76	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
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
2:B:253:TYR:HA	2:B:256:LEU:HB3	1.99	0.44
3:C:164:TRP:C	3:C:166:TRP:H	2.26	0.44
10:J:38:ILE:HA	10:J:49:VAL:HG23	1.99	0.44
10:J:39:ARG:O	10:J:39:ARG:HG2	2.18	0.44
10:J:97:ALA:HA	10:J:111:TYR:O	2.17	0.44
10:J:110:ASP:HB2	11:K:55:HIS:NE2	2.32	0.44
1:A:288:TYR:CE1	1:A:306:ILE:HD11	2.52	0.43
3:C:208:ASN:HD22	3:C:208:ASN:H	1.66	0.43
3:C:307:PHE:N	3:C:307:PHE:CD1	2.85	0.43
4:D:213:ASN:ND2	4:D:226:ALA:HA	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:328:ILE:HD13	8:H:62:PRO:HB3	2.00	0.43
5:E:96:VAL:HG21	5:E:118:ILE:HD11	2.00	0.43
1:A:80:LYS:HE3	1:A:80:LYS:HB2	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:OE1	1:A:183:GLU:N	2.51	0.43
3:C:64:SER:O	3:C:68:ILE:HG13	2.18	0.43
3:C:151:PHE:O	3:C:154:ILE:HG13	2.18	0.43
4:D:104:CYS:HG	4:D:159:TYR:HH	1.65	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:76:TRP:CH2	4:D:252:THR:HB	2.53	0.43
4:D:198:TYR:CD2	4:D:227:ARG:HB2	2.53	0.43
4:D:202:PRO:HB3	4:D:208:LEU:HD22	2.00	0.43
4:D:243:THR:O	4:D:247:MET:HB2	2.18	0.43
6:F:143:PHE:HD1	6:F:143:PHE:HA	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
1:A:424:LYS:HZ1	1:A:425:ARG:NH2	2.16	0.43
4:D:191:ILE:HD13	4:D:191:ILE:HA	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:HD23	4:D:269:LEU:HA	1.82	0.43
4:D:290:PHE:O	8:H:31:PRO:HB3	2.19	0.43
5:E:187:ILE:HD12	5:E:187:ILE:HA	1.83	0.43
1:A:422:ALA:HA	1:A:426:LEU:HB2	2.00	0.43
3:C:218:ARG:HD2	3:C:218:ARG:HA	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:HD2	1:A:115:LYS:N	2.33	0.43
1:A:313:ASP:OD1	1:A:335:ARG:HD3	2.19	0.43
2:B:73:LEU:HD13	2:B:73:LEU:HA	1.91	0.43
4:D:78:HIS:O	4:D:83:GLU:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:272:LYS:HG2	9:I:32:PHE:CD2	2.54	0.43
5:E:144:ALA:HA	10:J:102:TYR:CE1	2.53	0.43
8:H:20:LYS:NZ	8:H:20:LYS:HB3	2.34	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:94:SER:HB2	1:A:105:ILE:HG22	1.99	0.43
1:A:359:THR:HG23	1:A:362:GLU:OE1	2.18	0.43
2:B:151:PHE:CD2	2:B:155:LEU:HB2	2.53	0.43
3:C:12:LEU:HD22	3:C:12:LEU:HA	1.86	0.43
4:D:113:ARG:HG3	4:D:114:THR:N	2.33	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:93:MET:O	3:C:97:MET:HG3	2.19	0.42
3:C:147:ILE:HD11	15:C:4003:AOQ:H13	2.01	0.42
3:C:172:SER:OG	3:C:174:PRO:HD2	2.18	0.42
3:C:216:LEU:HD11	8:H:19:PRO:HD2	2.01	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
1:A:280:LEU:HD11	1:A:367:LYS:HG3	2.01	0.42
1:A:285:PHE:HB2	1:A:317:HIS:NE2	2.34	0.42
2:B:143:GLU:HB2	2:B:288:PHE:HZ	1.83	0.42
2:B:150:THR:HG22	2:B:352:ASN:CG	2.44	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: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
3:C:20:SER:O	3:C:220:PRO:HA	2.19	0.42
3:C:103:TYR:CE2	3:C:209:PRO:HA	2.53	0.42
10:J:85:SER:O	10:J:85:SER:OG	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:244:THR:OG1	6:F:76:ASP:OD1	2.35	0.42
5:E:127:GLN:NE2	11:K:56:ALA:HB3	2.34	0.42
7:G:95:LYS:HB2	7:G:98:GLU:OE1	2.20	0.42
1:A:183:GLU:C	1:A:185:LEU:H	2.28	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:13:TRP:CD1	8:H:13:TRP:H	2.36	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
5:E:149:ASP:OD1	5:E:149:ASP:C	2.63	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:HD12	1:A:374:LEU:HA	1.89	0.42
14:D:401:HEM:HMB1	14:D:401:HEM:HBB2	2.01	0.42
8:H:64:GLY:O	8:H:65:ILE:C	2.63	0.42
1:A:421:TRP:O	1:A:425:ARG:HB2	2.20	0.42
2:B:52:ASN:OD1	2:B:80:SER:OG	2.35	0.42
2:B:153:LYS:O	2:B:153:LYS:HG3	2.20	0.42
3:C:32:MET:O	3:C:36:LEU:N	2.53	0.42
3:C:102:TYR:HD1	3:C:326:PHE:CD2	2.38	0.42
3:C:242:LEU:HD23	3:C:242:LEU:HA	1.73	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
4:D:126:ARG:NH2	4:D:126:ARG:HB2	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:101:CYS:HA	14:D:401:HEM:HMC3	2.01	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
5:E:112:GLN:CB	5:E:114:LYS:HE2	2.50	0.41
11:K:82:ASP:HB3	11:K:86:TYR:OH	2.20	0.41
1:A:68:GLY:HA3	1:A:185:LEU:HD13	2.01	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
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
3:C:378:PHE:CG	7:G:45:PHE:CE1	3.08	0.41
4:D:203:PRO:HG2	4:D:206:VAL:HG21	2.01	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
5:E:74:THR:HG22	5:E:78:PHE:HE2	1.85	0.41
11:K:86:TYR:N	11:K:86:TYR:CD1	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:47:GLY:HA3	14:C:4001:HEM:C3C	2.56	0.41
3:C:109:PRO:HB2	3:C:204:HIS:NE2	2.35	0.41
3:C:320:VAL:HG22	8:H:58:TYR:OH	2.20	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
8:H:59:VAL:C	8:H:62:PRO:HD2	2.45	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:67:ASN:CG	1:A:180:GLY:HA2	2.46	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:HD3	1:A:425:ARG:HD3	2.03	0.41
2:B:62:ARG:NH2	2:B:67:LEU:HD13	2.36	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
3:C:98:ALA:C	3:C:100:GLY:N	2.79	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
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
3:C:173:ASN:C	3:C:175:THR:H	2.27	0.41
7:G:5:PHE:CD1	7:G:107:ILE:HG21	2.56	0.41
1:A:55:PHE:C	1:A:57:SER:H	2.28	0.41
1:A:157:PRO:O	1:A:161:LEU:HB2	2.21	0.41
1:A:369:LEU:HD11	2:B:72:GLU:HG2	2.03	0.41
2:B:62:ARG:HH22	2:B:67:LEU:HD13	1.85	0.41
2:B:143:GLU:HB2	2:B:288:PHE:CZ	2.55	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
3:C:98:ALA:C	3:C:100:GLY:H	2.28	0.41
3:C:164:TRP:C	3:C:166:TRP:N	2.79	0.41
3:C:382:ARG:HD2	7:G:99:ASP:OD2	2.21	0.41
5:E:149:ASP:HB2	10:J:104:VAL:HG21	2.03	0.41
7:G:33:ILE:HG22	7:G:33:ILE:O	2.19	0.41
7:G:61:ARG:NH2	7:G:61:ARG:HB2	2.36	0.41
7:G:63:LEU:HA	7:G:64:PRO:HD2	1.77	0.41
11:K:86:TYR:N	11:K:86:TYR:HD1	2.19	0.41
2:B:58:ASN:HB2	2:B:118:GLU:OE2	2.20	0.41
3:C:51:ALA:HB2	14:C:4001:HEM:CBC	2.51	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
9:I:17:PHE:O	9:I:18:VAL:C	2.63	0.41
1:A:285:PHE:HE1	1:A:350:GLN:HB3	1.87	0.40
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
2:B:56:PHE:CE2	2:B:78:PHE:HB3	2.56	0.40
2:B:95:LYS:C	2:B:97:ASP:H	2.29	0.40
4:D:76:TRP:H	4:D:79:ASN:ND2	2.19	0.40
7:G:32:PHE:C	7:G:34:ASN:N	2.78	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:251:LEU:O	1:A:436:THR:OG1	2.36	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
17:C:4005:UQ6:H1M3	17:C:4005:UQ6:H1O3	2.04	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
5:E:135:SER:C	5:E:137:LEU:H	2.29	0.40
3:C:58:ILE:CG2	3:C:173:ASN:HB2	2.52	0.40
3:C:147:ILE:H	3:C:147:ILE:HG12	1.61	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:HD12	1:A:230:LEU:O	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
1:A:397:LYS:HZ1	1:A:401:LEU:HB2	1.86	0.40
2:B:97:ASP:HB2	2:B:101:TYR:HE1	1.86	0.40
2:B:222:LYS:HE2	2:B:222:LYS:HB3	1.72	0.40
2:B:318:ILE:HD12	2:B:318:ILE:HA	1.92	0.40
4:D:86:ASP:HA	9:I:47:LYS:HG2	2.03	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
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%)	3	17
2	B	350/352 (99%)	284 (81%)	56 (16%)	10 (3%)	3	17
3	C	383/385 (100%)	318 (83%)	49 (13%)	16 (4%)	2	11
4	D	246/248 (99%)	199 (81%)	36 (15%)	11 (4%)	2	10
5	E	183/185 (99%)	142 (78%)	33 (18%)	8 (4%)	2	10
6	F	72/74 (97%)	60 (83%)	10 (14%)	2 (3%)	4	18
7	G	124/126 (98%)	102 (82%)	16 (13%)	6 (5%)	2	9
8	H	91/93 (98%)	61 (67%)	23 (25%)	7 (8%)	1	3
9	I	55/57 (96%)	41 (74%)	13 (24%)	1 (2%)	6	28
10	J	125/127 (98%)	115 (92%)	9 (7%)	1 (1%)	16	46
11	K	105/107 (98%)	76 (72%)	23 (22%)	6 (6%)	1	7
All	All	2163/2185 (99%)	1747 (81%)	335 (16%)	81 (4%)	2	13

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
2	B	296	VAL
2	B	336	ILE
2	B	339	ASN
3	C	106	TYR
3	C	215	ASN
3	C	250	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	A	443	LEU
2	B	337	GLU
3	C	369	VAL
6	F	139	ALA
7	G	65	GLU
7	G	90	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	317 (86%)	53 (14%)	3	14
2	B	301/301 (100%)	267 (89%)	34 (11%)	5	22
3	C	338/338 (100%)	290 (86%)	48 (14%)	3	14
4	D	206/206 (100%)	177 (86%)	29 (14%)	3	14
5	E	151/151 (100%)	124 (82%)	27 (18%)	2	9
6	F	67/67 (100%)	61 (91%)	6 (9%)	9	31
7	G	110/110 (100%)	91 (83%)	19 (17%)	2	9
8	H	77/77 (100%)	67 (87%)	10 (13%)	4	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	47/47 (100%)	40 (85%)	7 (15%)	3	13
10	J	112/112 (100%)	90 (80%)	22 (20%)	1	7
11	K	93/93 (100%)	78 (84%)	15 (16%)	2	11
All	All	1872/1872 (100%)	1602 (86%)	270 (14%)	3	14

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	45	SER
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	174	LEU
1	A	179	ARG
1	A	193	LEU
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	257	PRO
1	A	263	LEU
1	A	284	ILE
1	A	295	SER
1	A	303	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	306	ILE
1	A	320	LEU
1	A	325	SER
1	A	330	PHE
1	A	334	THR
1	A	338	THR
1	A	341	ASP
1	A	348	LEU
1	A	359	THR
1	A	361	THR
1	A	365	ARG
1	A	395	LEU
1	A	415	VAL
1	A	425	ARG
1	A	426	LEU
1	A	433	ILE
1	A	439	ILE
1	A	443	LEU
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	67	LEU
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	169	LEU
2	B	171	ASP
2	B	186	GLU
2	B	193	VAL
2	B	205	LEU
2	B	207	SER
2	B	214	SER
2	B	234	ILE
2	B	245	VAL
2	B	250	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	255	VAL
2	B	267	LEU
2	B	292	GLN
2	B	297	VAL
2	B	301	ILE
2	B	323	LEU
2	B	328	GLN
2	B	338	LEU
2	B	341	ASP
2	B	347	LYS
2	B	359	VAL
2	B	362	LEU
3	C	10	LEU
3	C	12	LEU
3	C	15	SER
3	C	26	ILE
3	C	34	SER
3	C	41	VAL
3	C	48	ILE
3	C	52	MET
3	C	57	ASN
3	C	60	LEU
3	C	79	ARG
3	C	81	LEU
3	C	87	SER
3	C	99	LYS
3	C	101	LEU
3	C	116	VAL
3	C	147	ILE
3	C	148	THR
3	C	163	SER
3	C	165	LEU
3	C	182	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	244	VAL
3	C	283	ARG
3	C	302	LEU
3	C	305	LEU
3	C	312	VAL
3	C	313	VAL
3	C	317	THR
3	C	335	LEU
3	C	336	LEU
3	C	344	VAL
3	C	346	VAL
3	C	350	LEU
3	C	353	GLN
3	C	372	THR
3	C	374	GLU
3	C	380	ILE
3	C	382	ARG
3	C	383	VAL
4	D	63	THR
4	D	69	LEU
4	D	77	SER
4	D	101	CYS
4	D	104	CYS
4	D	109	ARG
4	D	110	VAL
4	D	124	GLU
4	D	135	ASP
4	D	137	GLU
4	D	145	LYS
4	D	178	SER
4	D	188	CYS
4	D	191	ILE
4	D	194	LEU
4	D	206	VAL
4	D	212	SER
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	264	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	51	LYS
5	E	65	LEU
5	E	76	GLU
5	E	81	SER
5	E	83	THR
5	E	93	LYS
5	E	94	VAL
5	E	103	LEU
5	E	107	VAL
5	E	108	VAL
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	193	LYS
5	E	205	TYR
5	E	206	GLU
5	E	210	ASP
5	E	211	LYS
6	F	81	LEU
6	F	97	HIS
6	F	120	LYS
6	F	130	LEU
6	F	142	LEU
6	F	143	PHE
7	G	4	SER
7	G	6	THR
7	G	15	ILE
7	G	16	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	17	LYS
7	G	21	LEU
7	G	23	LYS
7	G	41	LEU
7	G	51	GLU
7	G	62	ARG
7	G	77	ARG
7	G	83	LEU
7	G	85	HIS
7	G	86	HIS
7	G	97	GLN
7	G	98	GLU
7	G	100	VAL
7	G	123	ILE
7	G	127	LYS
8	H	15	HIS
8	H	20	LYS
8	H	24	ILE
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
9	I	27	VAL
9	I	29	GLN
9	I	38	SER
9	I	42	ASN
9	I	48	LEU
10	J	2	VAL
10	J	6	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	55	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	64	LEU
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	118	VAL
10	J	122	SER
11	K	3	GLU
11	K	6	GLN
11	K	11	LEU
11	K	33	LEU
11	K	44	ILE
11	K	51	THR
11	K	53	ARG
11	K	58	VAL
11	K	67	SER
11	K	73	LEU
11	K	79	GLU
11	K	81	GLU
11	K	83	ILE
11	K	89	GLN
11	K	93	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	102	GLN
1	A	170	GLN
1	A	388	ASN
2	B	328	GLN
3	C	22	GLN
3	C	84	ASN
3	C	141	HIS
3	C	149	ASN
3	C	343	HIS
4	D	79	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	143	ASN
4	D	185	HIS
5	E	127	GLN
7	G	79	HIS
7	G	80	GLN
7	G	97	GLN
8	H	34	GLN
8	H	47	ASN
9	I	43	HIS
10	J	78	GLN
11	K	38	GLN
11	K	77	ASN
11	K	89	GLN
11	K	90	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](#)

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	A	502	-	30,30,47	1.24	2 (6%)	33,35,52	1.16	3 (9%)
13	3PH	C	4006	-	34,34,47	1.17	2 (5%)	37,39,52	1.70	8 (21%)
13	3PH	E	302	-	37,37,47	1.10	2 (5%)	40,42,52	1.25	2 (5%)
14	HEM	C	4002	3	50,50,50	1.70	8 (16%)	67,82,82	1.63	12 (17%)
14	HEM	C	4001	3	50,50,50	2.00	9 (18%)	67,82,82	1.46	10 (14%)
18	FES	E	301	5	0,4,4	-	-	-	-	-
12	UMQ	A	501	-	35,35,35	0.47	0	46,46,46	1.20	7 (15%)
16	3PE	C	4004	-	26,26,50	1.37	2 (7%)	29,31,55	1.44	5 (17%)
17	UQ6	C	4005	-	43,43,43	1.20	3 (6%)	54,55,55	2.20	20 (37%)
14	HEM	D	401	4	50,50,50	2.02	9 (18%)	67,82,82	1.65	11 (16%)
15	AOQ	C	4003	-	29,29,29	1.73	7 (24%)	41,42,42	1.80	9 (21%)

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

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	401	HEM	C3D-C2D	8.21	1.54	1.36
14	C	4001	HEM	C3D-C2D	8.16	1.54	1.36
14	C	4002	HEM	C3D-C2D	7.23	1.52	1.36
14	C	4001	HEM	FE-NA	5.79	2.14	1.95
14	D	401	HEM	FE-NA	5.61	2.13	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	401	HEM	FE-NB	5.51	2.11	1.94
17	C	4005	UQ6	O5-C5	-4.53	1.26	1.36
15	C	4003	AOQ	C9-C1	-4.53	1.39	1.48
16	C	4004	3PE	O21-C21	4.50	1.47	1.34
13	C	4006	3PH	O31-C31	4.50	1.46	1.33
13	A	502	3PH	O31-C31	4.50	1.46	1.33
13	E	302	3PH	O31-C31	4.44	1.46	1.33
16	C	4004	3PE	O31-C31	4.33	1.46	1.33
13	C	4006	3PH	O21-C21	4.27	1.46	1.34
15	C	4003	AOQ	C10-C4	-4.26	1.39	1.48
13	E	302	3PH	O21-C21	4.25	1.46	1.34
17	C	4005	UQ6	O2-C2	-4.23	1.27	1.36
13	A	502	3PH	O21-C21	4.22	1.46	1.34
14	C	4001	HEM	FE-ND	3.69	2.06	1.94
14	C	4002	HEM	FE-NC	3.57	2.06	1.95
15	C	4003	AOQ	C3-C4	-3.37	1.37	1.46
14	C	4001	HEM	CMD-C2D	3.30	1.57	1.50
14	C	4001	HEM	FE-NB	3.23	2.04	1.94
14	D	401	HEM	CAB-C3B	3.17	1.55	1.47
14	C	4002	HEM	FE-ND	3.08	2.04	1.94
14	C	4002	HEM	CAB-C3B	3.01	1.55	1.47
14	C	4002	HEM	CAC-C3C	2.92	1.55	1.47
14	C	4002	HEM	FE-NB	2.92	2.03	1.94
14	C	4001	HEM	CMC-C2C	2.82	1.56	1.50
14	C	4001	HEM	CAC-C3C	2.75	1.54	1.47
14	C	4001	HEM	CAB-C3B	2.74	1.54	1.47
14	D	401	HEM	CAC-C3C	2.55	1.54	1.47
15	C	4003	AOQ	C2-C1	-2.53	1.41	1.46
14	D	401	HEM	FE-NC	2.49	2.03	1.95
15	C	4003	AOQ	C3-C2	2.47	1.39	1.35
14	C	4002	HEM	CMB-C2B	2.45	1.55	1.50
15	C	4003	AOQ	C17-C13	-2.45	1.47	1.52
14	C	4002	HEM	C2A-C3A	-2.33	1.32	1.38
14	D	401	HEM	C2A-C3A	-2.32	1.32	1.38
14	D	401	HEM	FE-ND	2.27	2.01	1.94
14	D	401	HEM	CMD-C2D	2.14	1.55	1.50
17	C	4005	UQ6	C7-C6	2.11	1.54	1.51
14	C	4001	HEM	C1B-NB	2.04	1.43	1.40
15	C	4003	AOQ	O1-C1	2.01	1.27	1.23

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	4002	HEM	C4D-ND-C1D	6.22	112.58	105.21
14	D	401	HEM	C4D-ND-C1D	5.99	112.30	105.21
15	C	4003	AOQ	C16-C2-C1	4.90	125.20	119.11
14	C	4001	HEM	C4D-ND-C1D	4.80	110.89	105.21
17	C	4005	UQ6	C10-C9-C11	4.62	123.25	115.23
17	C	4005	UQ6	C17-C18-C19	-4.51	117.30	127.62
16	C	4004	3PE	O21-C21-C22	4.46	121.13	111.48
13	C	4006	3PH	O21-C21-C22	4.44	121.08	111.48
17	C	4005	UQ6	C3M-O3-C3	4.43	126.75	114.74
13	E	302	3PH	O21-C21-C22	4.20	120.56	111.48
17	C	4005	UQ6	C12-C13-C14	-4.10	118.24	127.62
15	C	4003	AOQ	C15-C16-C2	-4.09	105.13	113.81
15	C	4003	AOQ	C2-C3-C4	-4.06	119.50	123.40
17	C	4005	UQ6	C27-C28-C29	-3.85	118.82	127.62
14	D	401	HEM	C3B-C2B-C1B	3.81	109.27	106.41
14	C	4001	HEM	O2D-CGD-CBD	3.75	125.86	114.00
14	D	401	HEM	CAA-C2A-C1A	3.62	132.01	124.94
14	C	4001	HEM	CHC-C4B-NB	3.55	128.24	124.42
14	C	4002	HEM	CAA-CBA-CGA	-3.54	104.27	113.67
13	C	4006	3PH	O14-P-O11	-3.53	97.47	106.67
14	C	4001	HEM	CBA-CAA-C2A	-3.46	102.97	112.53
17	C	4005	UQ6	C1M-C1-C2	-3.43	114.81	120.52
17	C	4005	UQ6	C6-C7-C8	-3.42	106.22	112.06
17	C	4005	UQ6	C20-C19-C21	3.39	121.11	115.23
13	C	4006	3PH	C3E-C3D-C3C	-3.37	97.33	114.37
17	C	4005	UQ6	C7-C8-C9	-3.31	122.68	127.42
17	C	4005	UQ6	C4M-O4-C4	3.27	123.62	114.74
15	C	4003	AOQ	C22-C17-C18	3.14	122.19	118.30
16	C	4004	3PE	O31-C31-C32	3.12	121.34	111.83
15	C	4003	AOQ	C19-C18-C17	-3.11	118.08	121.18
14	C	4002	HEM	CAA-C2A-C1A	3.10	131.00	124.94
14	C	4002	HEM	CMC-C2C-C1C	-3.01	119.43	124.73
15	C	4003	AOQ	C15-C14-C13	-3.00	105.09	110.61
14	C	4002	HEM	CAA-C2A-C3A	-2.98	120.38	127.07
14	D	401	HEM	CAA-CBA-CGA	-2.95	105.83	113.67
17	C	4005	UQ6	C1M-C1-C6	2.92	124.64	120.43
17	C	4005	UQ6	O2-C2-C3	2.91	126.41	119.86
14	D	401	HEM	CHB-C1B-NB	2.89	127.94	124.37
12	A	501	UMQ	C1'-C2'-C3'	2.88	116.08	110.01
14	D	401	HEM	CHA-C4D-ND	2.87	127.91	124.37
14	C	4002	HEM	CBD-CAD-C3D	-2.87	104.61	112.53
13	A	502	3PH	O21-C21-C22	2.86	117.67	111.48
13	C	4006	3PH	O14-P-O13	2.85	118.49	107.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	D	401	HEM	CAA-C2A-C3A	-2.84	120.69	127.07
15	C	4003	AOQ	O1-C1-C9	-2.84	117.03	121.57
13	A	502	3PH	O31-C31-C32	2.72	120.11	111.83
14	C	4002	HEM	C2A-C1A-NA	-2.68	107.18	110.15
17	C	4005	UQ6	C25-C24-C26	2.65	119.83	115.23
13	C	4006	3PH	O31-C31-C32	2.65	119.91	111.83
17	C	4005	UQ6	C30-C29-C31	2.63	119.80	115.23
14	D	401	HEM	CHD-C1D-ND	2.59	127.21	124.42
17	C	4005	UQ6	O5-C5-C4	-2.59	114.03	119.86
17	C	4005	UQ6	O5-C5-C6	2.55	125.58	118.18
16	C	4004	3PE	C3-C2-C1	-2.55	105.84	111.78
14	C	4001	HEM	C4C-C3C-C2C	2.54	109.01	106.81
14	D	401	HEM	CHC-C1C-NC	2.50	127.18	124.45
14	C	4001	HEM	O1D-CGD-CBD	-2.49	115.19	123.09
15	C	4003	AOQ	C10-C4-C3	2.47	120.93	117.12
15	C	4003	AOQ	C15-C16-C11	2.43	115.13	110.00
13	C	4006	3PH	C3-C2-C1	-2.41	106.16	111.78
13	C	4006	3PH	O21-C21-O22	-2.41	118.06	123.70
13	C	4006	3PH	C2-O21-C21	-2.39	112.07	117.80
13	A	502	3PH	O11-P-O12	-2.37	100.03	106.44
17	C	4005	UQ6	C20-C19-C18	-2.37	117.54	123.63
14	C	4002	HEM	C3D-C4D-ND	-2.37	107.57	110.17
14	C	4002	HEM	CBA-CAA-C2A	-2.36	106.00	112.53
14	C	4002	HEM	CHC-C1C-NC	2.35	127.01	124.45
17	C	4005	UQ6	C7-C6-C1	-2.35	117.21	120.79
14	D	401	HEM	CBA-CAA-C2A	2.25	118.74	112.53
14	C	4002	HEM	CHA-C1A-C2A	2.23	130.18	125.30
16	C	4004	3PE	C2-O21-C21	-2.22	112.49	117.80
12	A	501	UMQ	C1-O5-C5	-2.20	109.42	113.72
14	D	401	HEM	C2A-C1A-NA	-2.19	107.72	110.15
16	C	4004	3PE	O31-C31-O32	-2.18	118.17	123.63
17	C	4005	UQ6	C26-C24-C23	-2.17	116.30	121.17
12	A	501	UMQ	O3'-C3'-C2'	-2.15	105.30	110.38
14	C	4001	HEM	CAD-C3D-C4D	2.11	128.38	124.70
14	C	4001	HEM	C1D-C2D-C3D	-2.10	104.77	106.98
17	C	4005	UQ6	O4-C4-C3	2.09	125.12	120.35
13	E	302	3PH	C3-C2-C1	-2.07	106.96	111.78
14	C	4002	HEM	CMC-C2C-C3C	2.05	133.38	128.43
12	A	501	UMQ	O1-C1-C2	2.04	113.11	108.09
14	C	4001	HEM	CAD-CBD-CGD	-2.03	108.29	113.67
12	A	501	UMQ	C1'-O5'-C5'	-2.03	109.76	113.72
14	C	4001	HEM	CHD-C1D-ND	2.02	126.60	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	501	UMQ	C1-O1-C4'	-2.02	113.19	117.98
12	A	501	UMQ	C2'-C3'-C4'	2.01	114.25	109.68

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	502	3PH	C22-C21-O21-C2
13	E	302	3PH	C1-O11-P-O13
13	E	302	3PH	C1-O11-P-O14
13	E	302	3PH	C1-O11-P-O12
15	C	4003	AOQ	C11-C16-C2-C1
15	C	4003	AOQ	C15-C16-C2-C1
16	C	4004	3PE	C11-O13-P-O14
16	C	4004	3PE	O13-C11-C12-N
13	A	502	3PH	O22-C21-O21-C2
17	C	4005	UQ6	C12-C11-C9-C10
17	C	4005	UQ6	C15-C14-C16-C17
17	C	4005	UQ6	C30-C29-C31-C32
17	C	4005	UQ6	C12-C11-C9-C8
17	C	4005	UQ6	C13-C14-C16-C17
17	C	4005	UQ6	C4-C3-O3-C3M
17	C	4005	UQ6	C28-C29-C31-C32
17	C	4005	UQ6	C14-C16-C17-C18
17	C	4005	UQ6	C19-C21-C22-C23
17	C	4005	UQ6	C24-C26-C27-C28
17	C	4005	UQ6	C29-C31-C32-C33
13	E	302	3PH	O32-C31-O31-C3
13	A	502	3PH	C32-C31-O31-C3
13	E	302	3PH	C32-C31-O31-C3
13	C	4006	3PH	C31-C32-C33-C34
13	A	502	3PH	O32-C31-O31-C3
12	A	501	UMQ	C2'-C1'-O1'-CA
17	C	4005	UQ6	C2-C3-O3-C3M
12	A	501	UMQ	O5'-C1'-O1'-CA
13	E	302	3PH	C26-C27-C28-C29
13	A	502	3PH	C39-C3A-C3B-C3C
13	A	502	3PH	C21-C22-C23-C24
13	C	4006	3PH	C39-C3A-C3B-C3C
13	C	4006	3PH	C33-C34-C35-C36
13	E	302	3PH	C28-C29-C2A-C2B
13	C	4006	3PH	C38-C39-C3A-C3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	C	4004	3PE	C21-C22-C23-C24
13	E	302	3PH	C32-C33-C34-C35
13	E	302	3PH	C38-C39-C3A-C3B
13	A	502	3PH	O21-C2-C3-O31
17	C	4005	UQ6	C20-C19-C21-C22
16	C	4004	3PE	C23-C24-C25-C26
16	C	4004	3PE	C32-C31-O31-C3
13	A	502	3PH	C23-C24-C25-C26
13	C	4006	3PH	C22-C21-O21-C2
13	E	302	3PH	O11-C1-C2-C3
15	C	4003	AOQ	C11-C16-C2-C3
17	C	4005	UQ6	C18-C19-C21-C22
13	C	4006	3PH	C32-C33-C34-C35
13	C	4006	3PH	C3D-C3E-C3F-C3G
16	C	4004	3PE	C22-C23-C24-C25
13	E	302	3PH	C29-C2A-C2B-C2C
13	C	4006	3PH	O11-C1-C2-C3
13	E	302	3PH	C2A-C2B-C2C-C2D
14	D	401	HEM	C2A-CAA-CBA-CGA
13	C	4006	3PH	O22-C21-O21-C2
16	C	4004	3PE	O32-C31-O31-C3
13	E	302	3PH	O11-C1-C2-O21
16	C	4004	3PE	C1-C2-C3-O31
16	C	4004	3PE	C12-C11-O13-P
13	C	4006	3PH	O21-C2-C3-O31
13	E	302	3PH	C31-C32-C33-C34
12	A	501	UMQ	CF-CG-CH-CI
13	A	502	3PH	O11-C1-C2-C3
13	A	502	3PH	O11-C1-C2-O21
13	C	4006	3PH	O11-C1-C2-O21
16	C	4004	3PE	C1-O11-P-O13
13	A	502	3PH	C31-C32-C33-C34
13	A	502	3PH	C1-C2-C3-O31
15	C	4003	AOQ	C12-C13-C17-C22
16	C	4004	3PE	O31-C31-C32-C33
15	C	4003	AOQ	C12-C13-C17-C18
13	E	302	3PH	C25-C26-C27-C28
16	C	4004	3PE	O21-C2-C3-O31
14	C	4001	HEM	CAA-CBA-CGA-O1A
14	C	4001	HEM	CAA-CBA-CGA-O2A
13	A	502	3PH	C22-C23-C24-C25
16	C	4004	3PE	C2-C1-O11-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	C	4002	HEM	CAA-CBA-CGA-O1A
13	A	502	3PH	C33-C34-C35-C36
14	D	401	HEM	CAA-CBA-CGA-O1A
14	D	401	HEM	CAA-CBA-CGA-O2A
14	C	4002	HEM	CAA-CBA-CGA-O2A
13	E	302	3PH	O21-C2-C3-O31
13	C	4006	3PH	C35-C36-C37-C38
13	C	4006	3PH	C3E-C3F-C3G-C3H
13	E	302	3PH	C34-C35-C36-C37
16	C	4004	3PE	C24-C25-C26-C27
14	C	4001	HEM	C4C-C3C-CAC-CBC
13	E	302	3PH	O21-C21-C22-C23
14	D	401	HEM	C4D-C3D-CAD-CBD
14	C	4002	HEM	CAD-CBD-CGD-O1D
14	C	4002	HEM	CAD-CBD-CGD-O2D
13	E	302	3PH	O22-C21-C22-C23

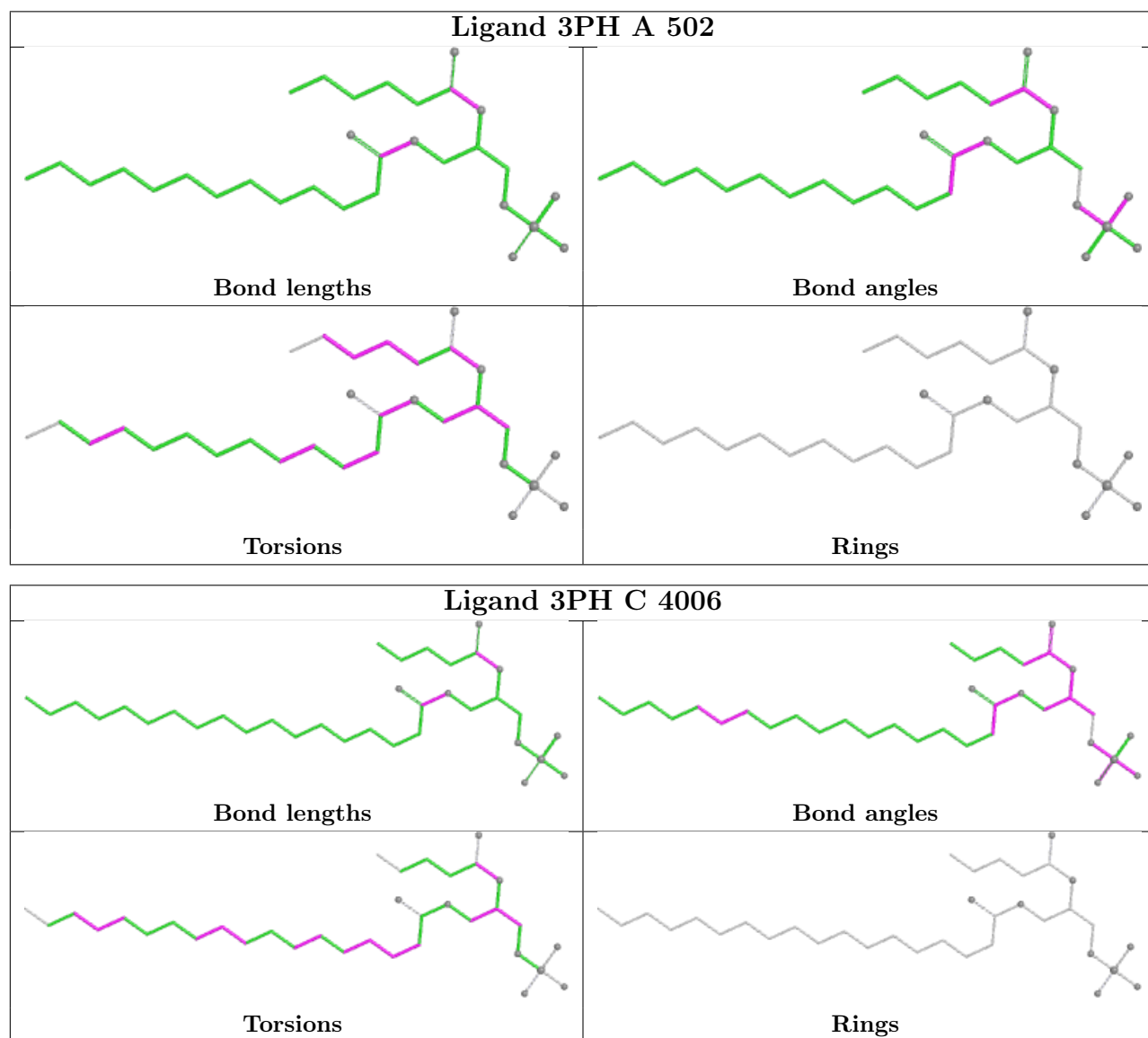
There are no ring outliers.

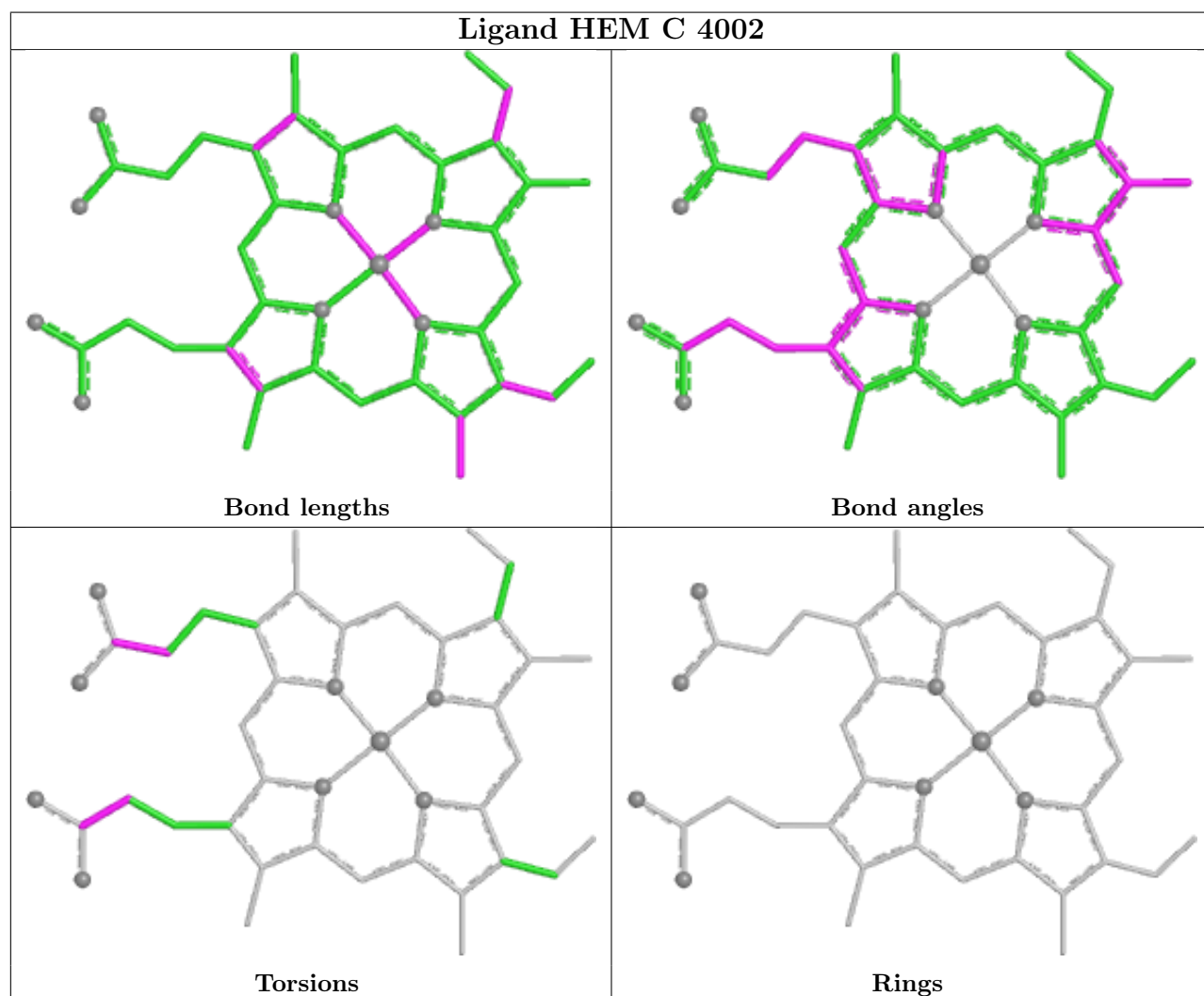
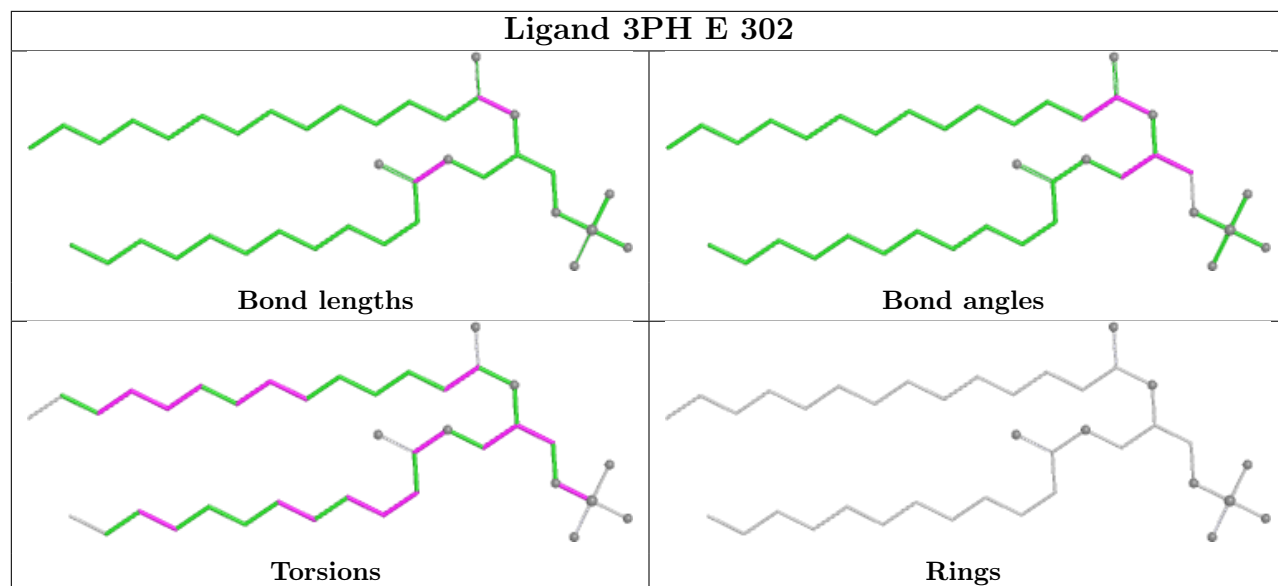
10 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	502	3PH	2	0
13	C	4006	3PH	1	0
13	E	302	3PH	6	0
14	C	4002	HEM	8	0
14	C	4001	HEM	7	0
12	A	501	UMQ	3	0
16	C	4004	3PE	1	0
17	C	4005	UQ6	4	0
14	D	401	HEM	10	0
15	C	4003	AOQ	3	0

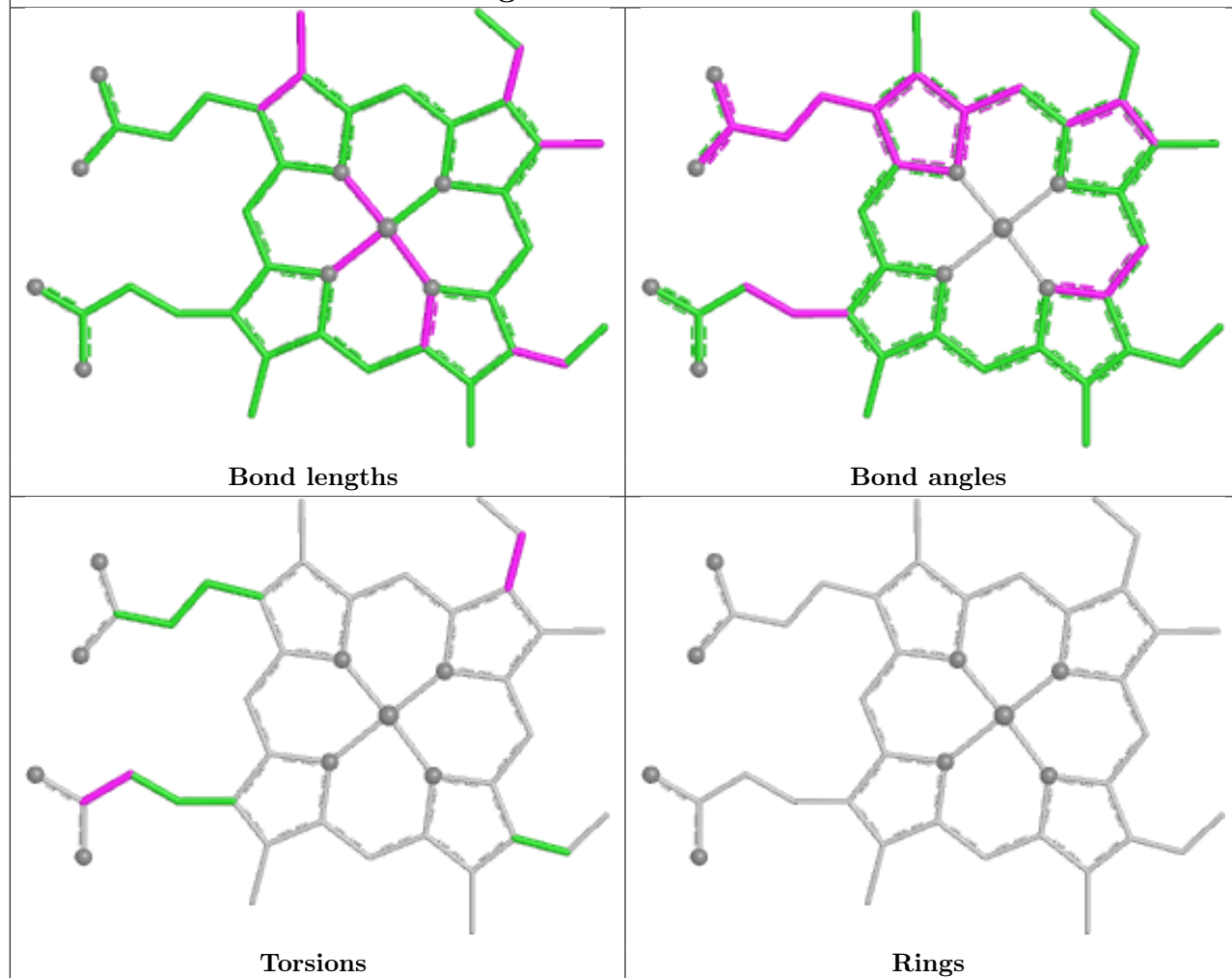
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

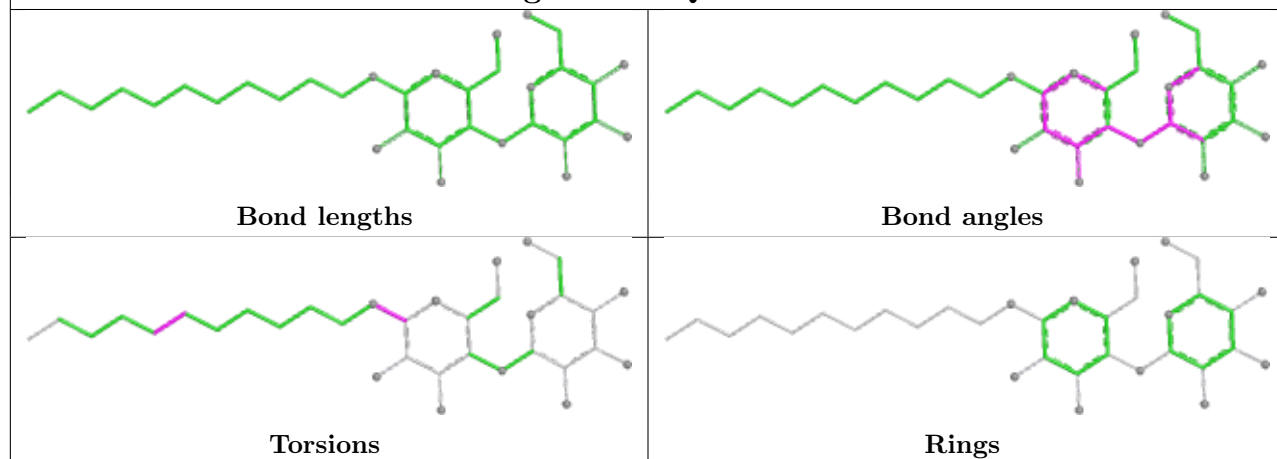


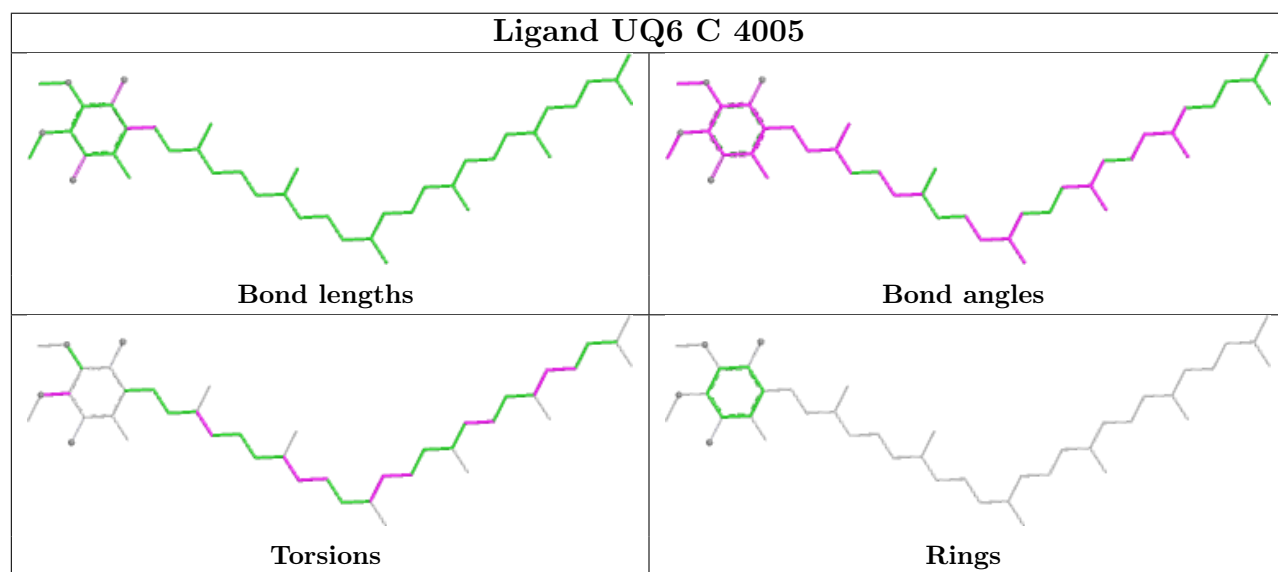
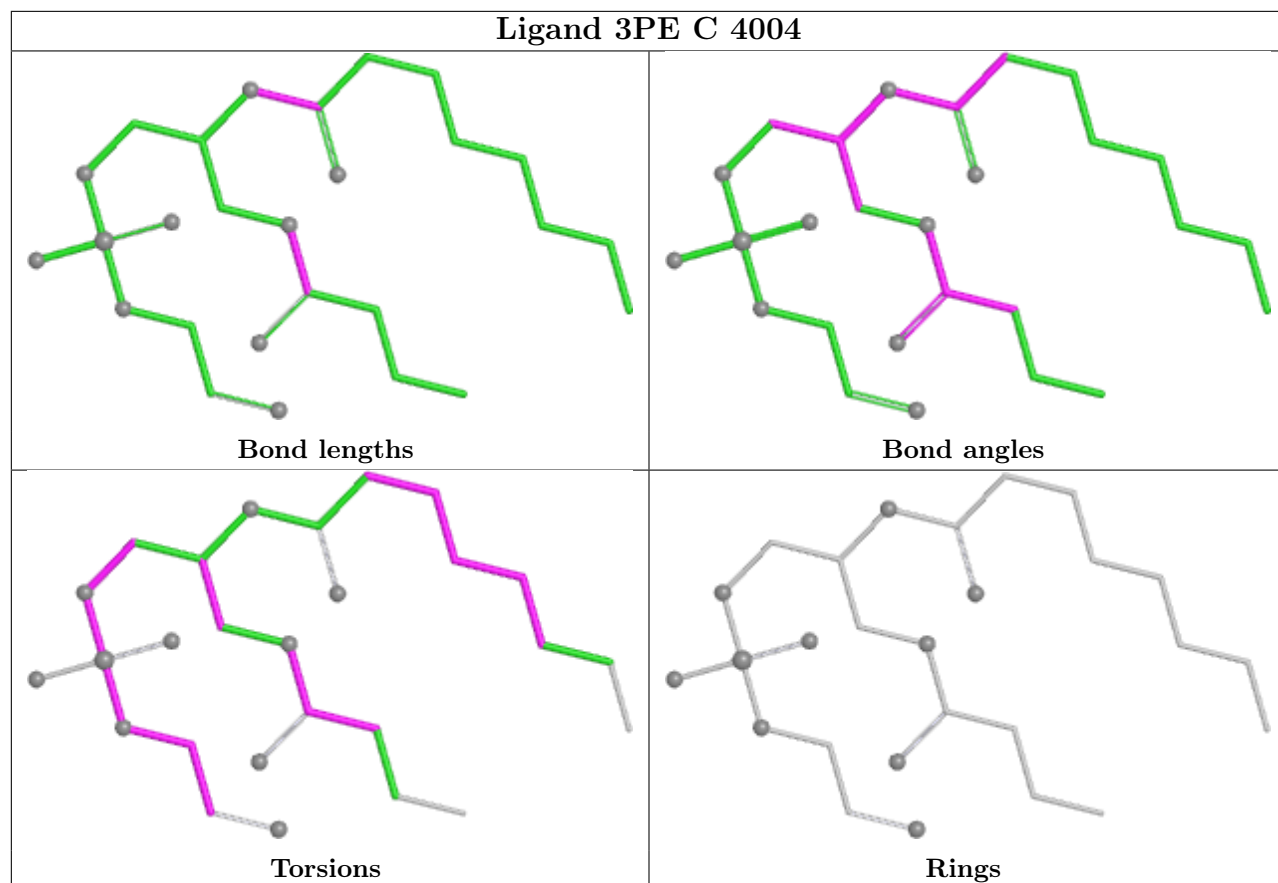


Ligand HEM C 4001

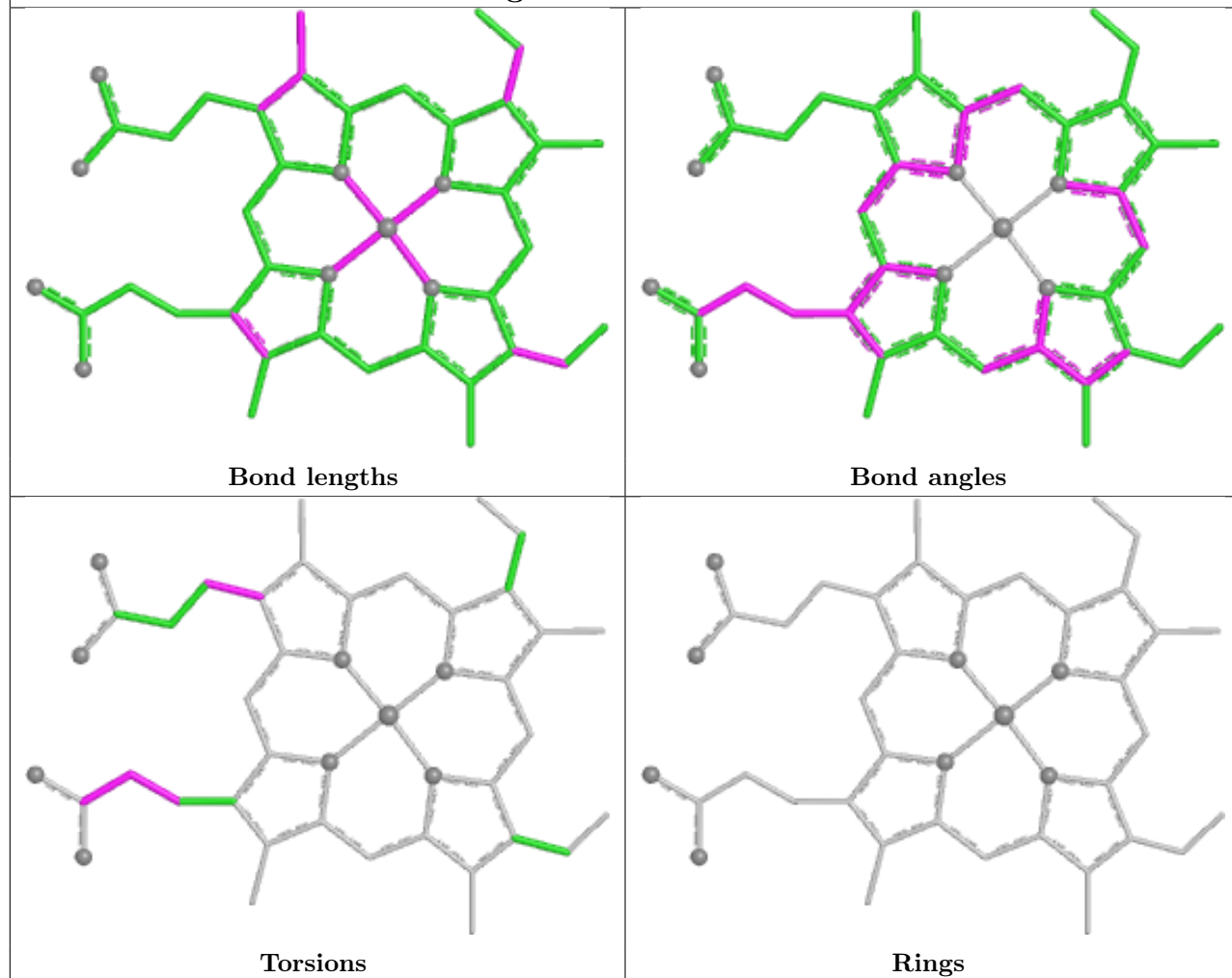


Ligand UMQ A 501

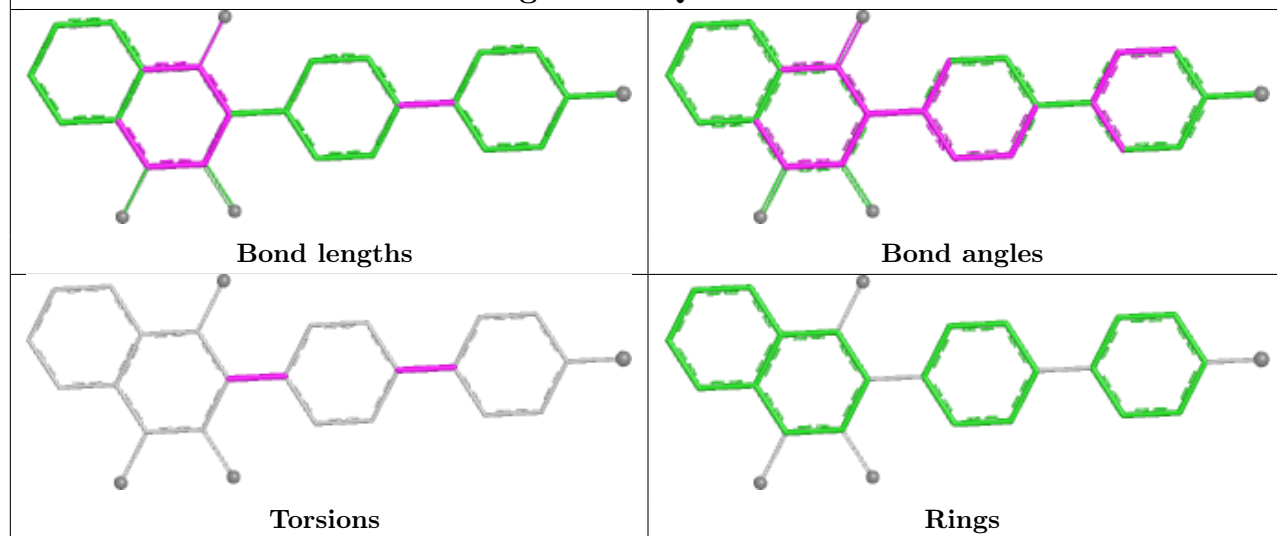




Ligand HEM D 401



Ligand AOQ C 4003



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	417/431 (96%)	0.42	24 (5%) 29 14	17, 69, 116, 122	0
2	B	344/352 (97%)	0.52	22 (6%) 25 13	29, 71, 104, 127	0
3	C	384/385 (99%)	-0.40	1 (0%) 90 79	0, 7, 18, 69	0
4	D	248/248 (100%)	-0.00	0 100 100	16, 40, 63, 83	1 (0%)
5	E	182/185 (98%)	-0.20	2 (1%) 78 56	4, 26, 70, 112	0
6	F	74/74 (100%)	0.30	1 (1%) 73 50	38, 61, 92, 94	0
7	G	126/126 (100%)	-0.39	0 100 100	6, 27, 48, 67	0
8	H	82/93 (88%)	-0.00	3 (3%) 45 25	7, 29, 67, 88	1 (1%)
9	I	57/57 (100%)	0.04	1 (1%) 67 43	24, 45, 78, 102	0
10	J	127/127 (100%)	-0.05	0 100 100	27, 44, 63, 68	0
11	K	107/107 (100%)	0.32	4 (3%) 45 25	36, 67, 105, 116	0
All	All	2148/2185 (98%)	0.08	58 (2%) 56 32	0, 42, 102, 127	2 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	LEU	4.7
3	C	384	ASN	4.5
8	H	45	VAL	4.2
2	B	230	ARG	4.2
11	K	15	LEU	4.1
1	A	92	ALA	3.7
1	A	230	LEU	3.5
2	B	282	GLY	3.5
1	A	108	SER	3.4
2	B	338	LEU	3.2
1	A	223	ILE	3.1
1	A	129	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	233	GLY	2.9
2	B	336	ILE	2.8
11	K	47	LEU	2.7
11	K	21	ILE	2.7
11	K	106	ILE	2.7
2	B	351	PHE	2.7
6	F	119	HIS	2.7
2	B	340	PHE	2.6
8	H	37	LEU	2.6
1	A	328	TRP	2.5
2	B	245	VAL	2.5
2	B	332	VAL	2.5
2	B	353	TYR	2.5
1	A	76	ILE	2.5
2	B	180	TYR	2.4
2	B	283	GLY	2.4
1	A	125	ILE	2.4
1	A	93	LEU	2.4
1	A	109	LEU	2.4
1	A	36	ILE	2.4
2	B	78	PHE	2.4
2	B	365	LEU	2.3
1	A	124	PHE	2.3
1	A	145	LEU	2.3
2	B	284	LEU	2.3
1	A	89	GLU	2.2
9	I	58	ALA	2.2
2	B	359	VAL	2.2
1	A	97	ILE	2.2
5	E	51	LYS	2.2
2	B	318	ILE	2.2
1	A	219	LEU	2.2
2	B	267	LEU	2.1
1	A	204	SER	2.1
2	B	34	LYS	2.1
1	A	209	VAL	2.1
1	A	238	LEU	2.1
5	E	49	ALA	2.1
1	A	51	VAL	2.1
8	H	94	VAL	2.1
2	B	368	LEU	2.1
2	B	264	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	148	VAL	2.0
1	A	120	LEU	2.0
2	B	311	GLY	2.0
2	B	308	LEU	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](#)

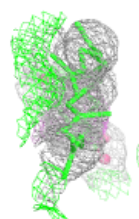
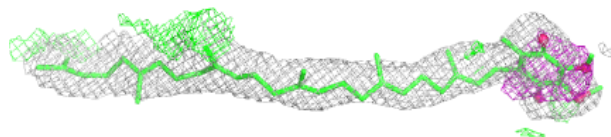
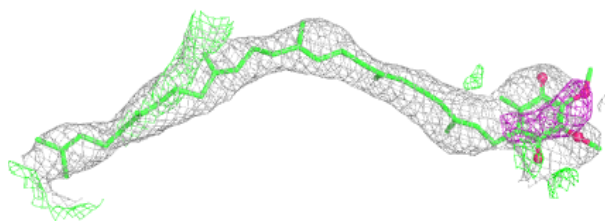
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	UQ6	C	4005	43/43	0.76	0.16	6,12,21,24	0
13	3PH	C	4006	35/48	0.88	0.12	3,17,29,39	0
12	UMQ	A	501	34/34	0.89	0.10	13,31,43,48	0
13	3PH	A	502	31/48	0.90	0.10	13,20,33,38	0
13	3PH	E	302	38/48	0.92	0.11	7,15,21,23	0
15	AOQ	C	4003	26/26	0.94	0.08	7,12,16,22	0
16	3PE	C	4004	27/51	0.95	0.07	4,8,12,14	0
14	HEM	D	401	43/43	0.95	0.10	22,31,37,43	0
14	HEM	C	4001	43/43	0.98	0.10	0,2,7,20	0
14	HEM	C	4002	43/43	0.98	0.09	2,5,10,11	0
18	FES	E	301	4/4	0.99	0.03	6,7,7,13	0

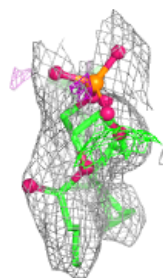
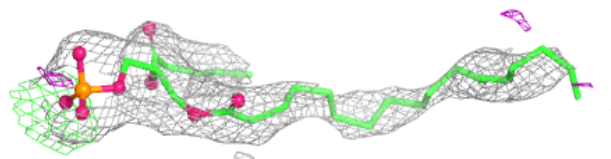
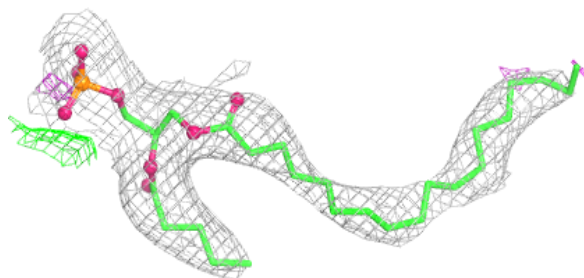
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UQ6 C 4005:

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

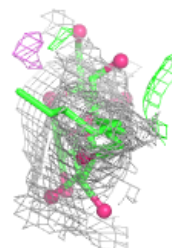
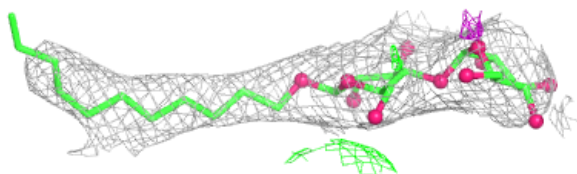
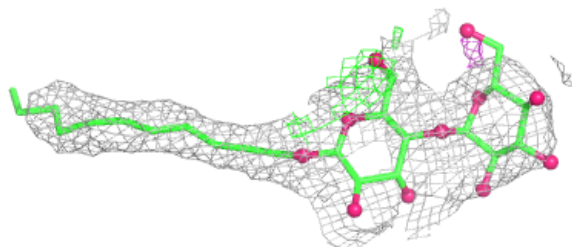
**Electron density around 3PH C 4006:**

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

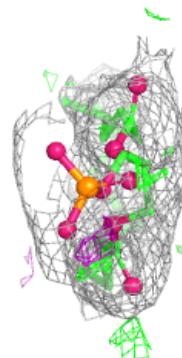
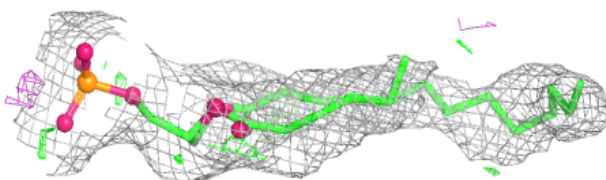
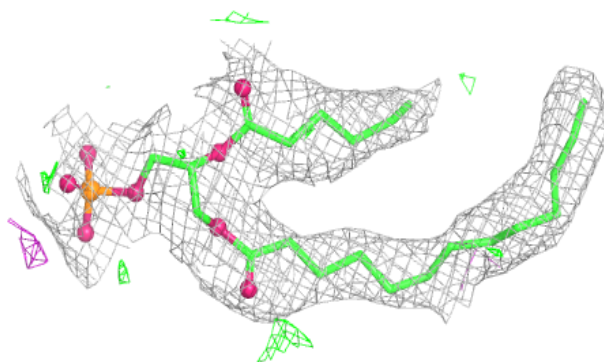


Electron density around UMQ A 501:

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

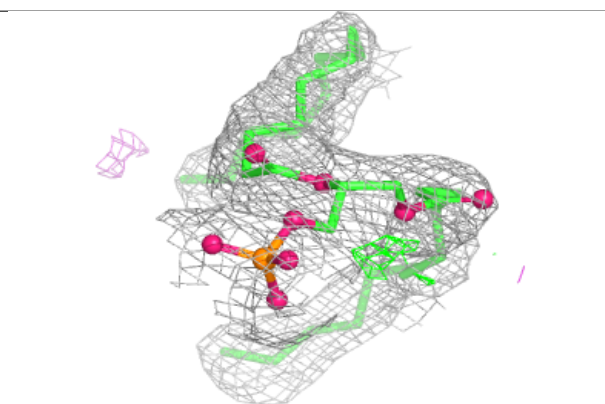
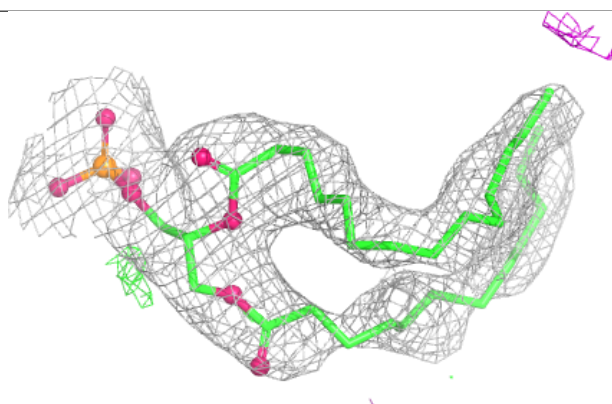
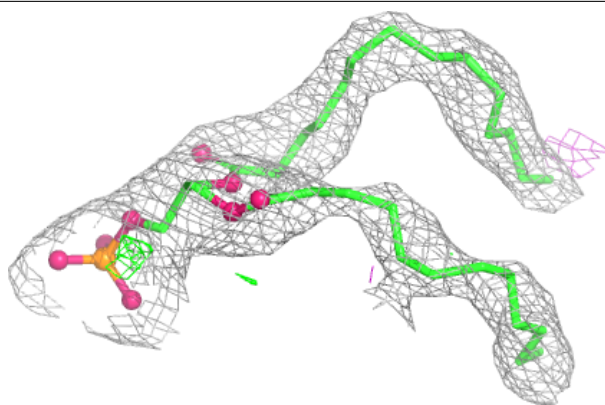
**Electron density around 3PH A 502:**

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

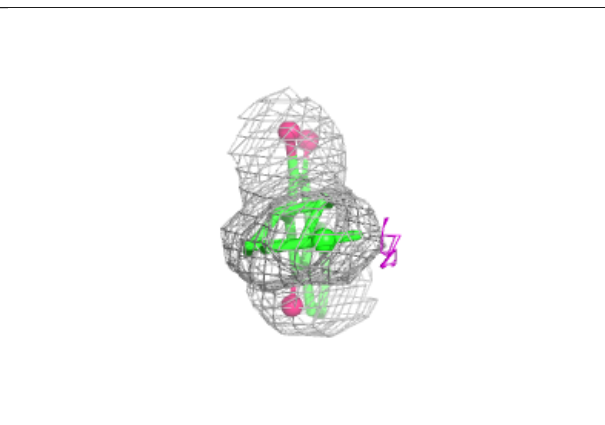
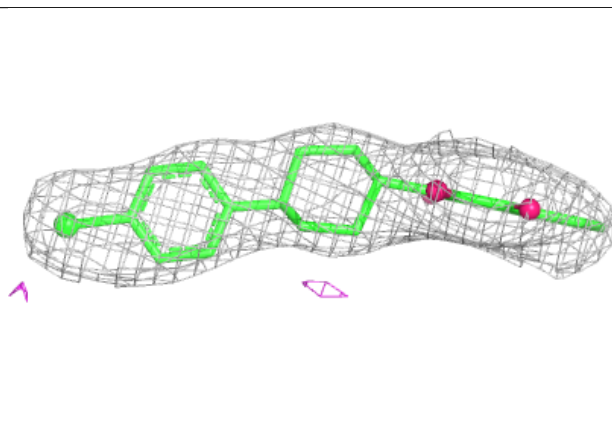
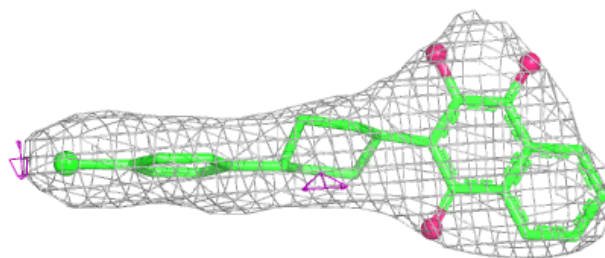


Electron density around 3PH E 302:

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

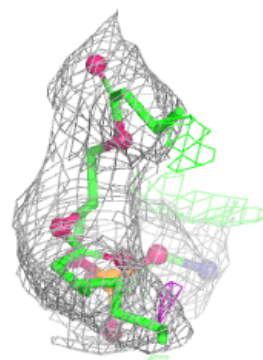
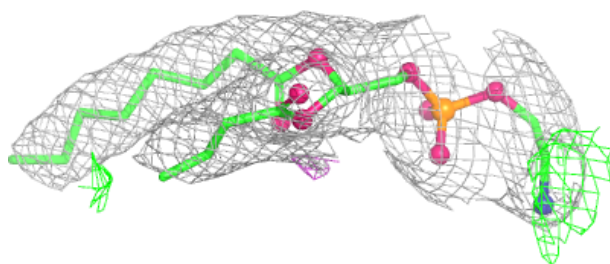
**Electron density around AOQ C 4003:**

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



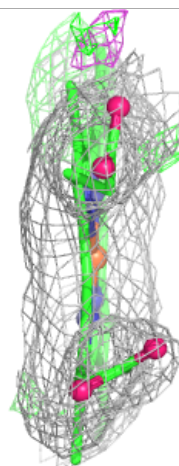
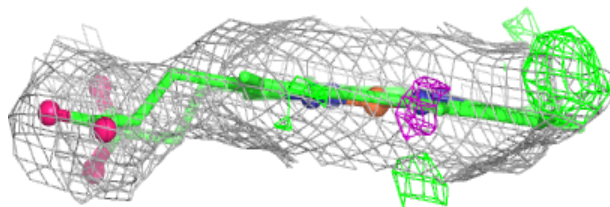
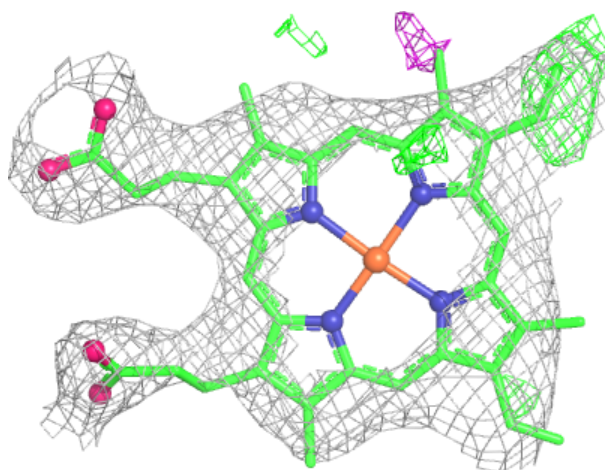
Electron density around 3PE C 4004:

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



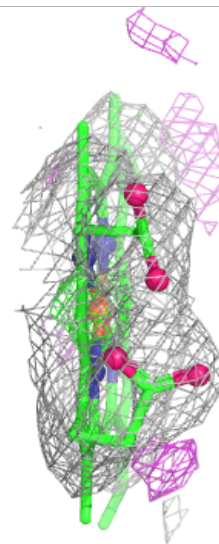
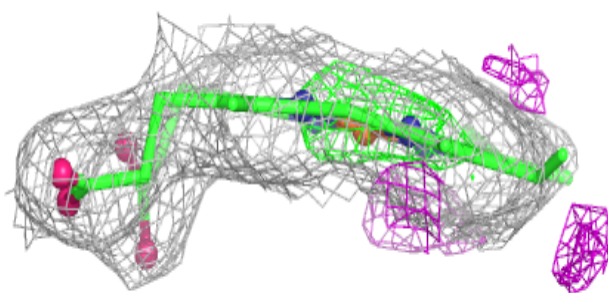
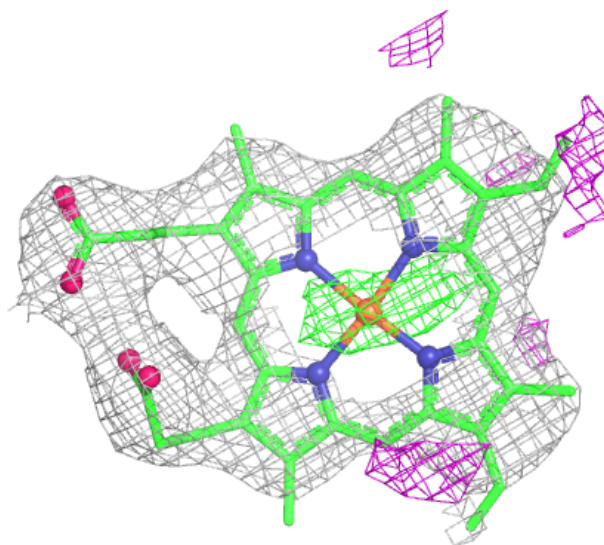
Electron density around HEM D 401:

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



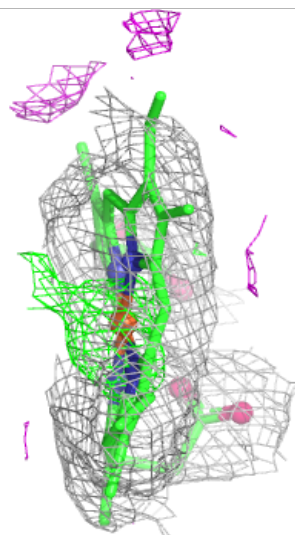
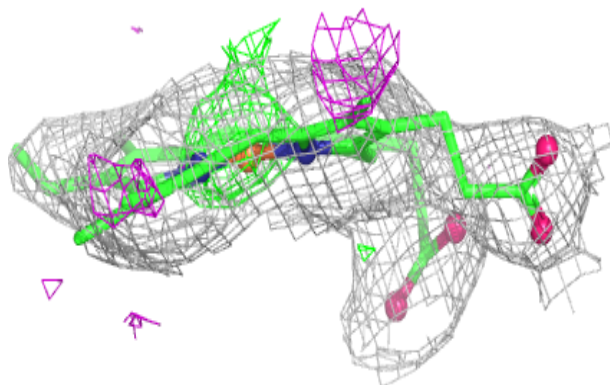
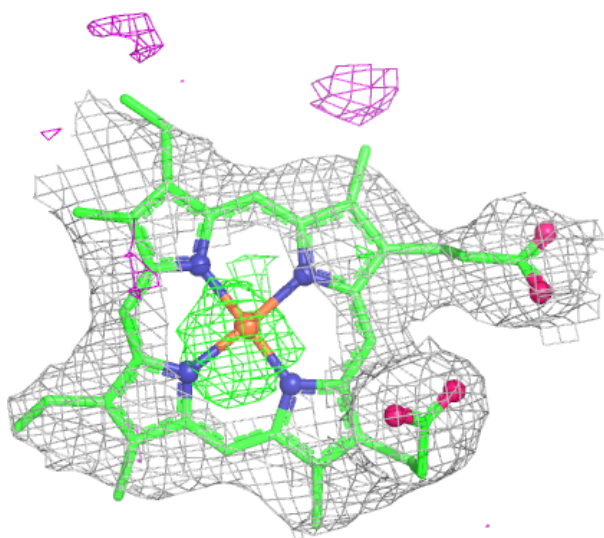
Electron density around HEM C 4001:

$2mF_o-DF_c$ (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.