Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 12:23 PM EDT

PDB ID	:	1NU1
Title	:	Crystal Structure of Mitochondrial Cytochrome bc1 Complexed with 2-nonyl -4-hydroxyquinoline N-oxide (NQNO)
Authors	:	Gao, X.; Wen, X.; Esser, L.; Quinn, B.; Yu, L.; Yu, C.-A.; Xia, D.
Deposited on	:	2003-01-30
Resolution	:	3.20 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 (i) 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 (1)) were used in the production of this report:

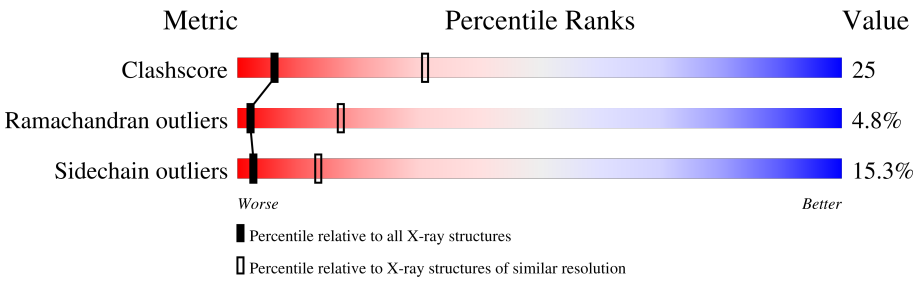
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	54% 38% 7% •
2	B	439	50% 38% 8% •
3	C	379	46% 41% 11% •
4	D	241	38% 49% 12% •
5	E	196	57% 37% 6%
6	F	110	48% 39% 7% • 5%
7	G	81	54% 26% 10% • 7%
8	H	78	54% 29% 5% • 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	57	18% 39% 32% 12%
10	J	62	47% 42% 8%
11	K	56	64% 20% 11% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	QNO	C	383	X	-	-	-
14	FES	E	200	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 16666 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 Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3458	2161	609	668	20	0	0	0

- Molecule 2 is a protein called Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	423	3172	1993	562	610	7	0	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	378	3003	2013	471	501	18	0	0	0

- Molecule 4 is a protein called cytochrome c1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1918	1225	330	348	15	0	0	0

- Molecule 5 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1519	957	263	291	8	0	0	0

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	105	911	576	165	168	2	0	0	0

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	75	628	410	118	99	1	0	0	0

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	70	575	347	102	121	5	0	0	0

- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase 8 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	57	406	253	77	74	2	0	0	0

- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	61	483	316	82	85	0	0	0

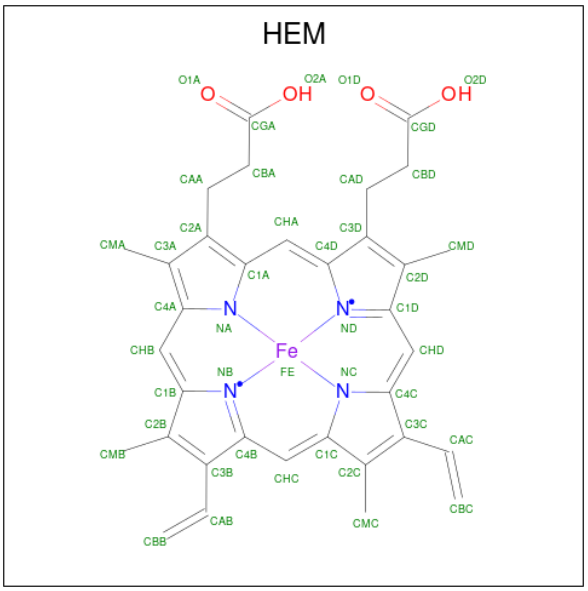
- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase complex 6.4 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	53	437	292	78	66	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

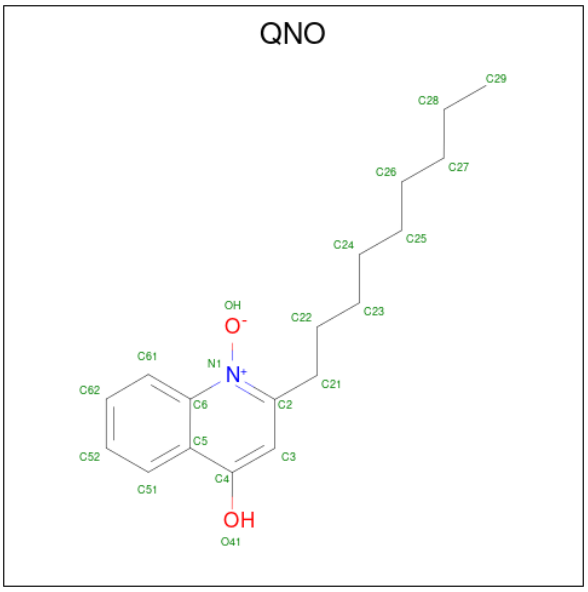
Chain	Residue	Modelled	Actual	Comment	Reference
K	22	GLN	SER	SEE REMARK 999	UNP P07552

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



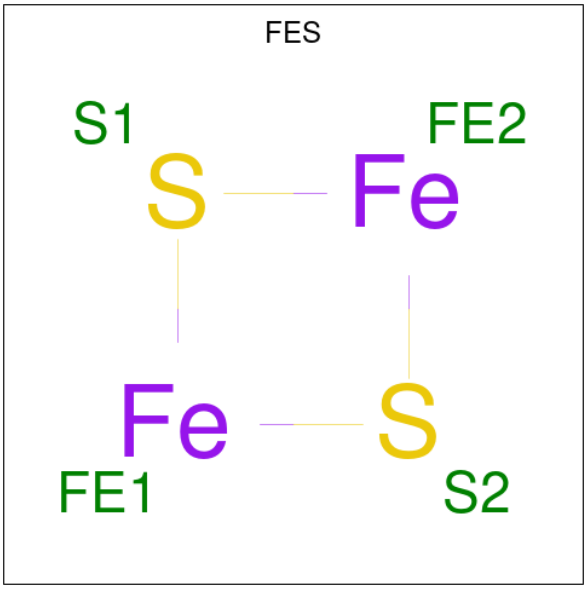
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	D	1	43	34	1	4	4	0	0

- Molecule 13 is 2-NONYL-4-HYDROXYQUINOLINE N-OXIDE (three-letter code: QNO) (formula: $C_{18}H_{25}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	C	1	21	18	1	2	0	0

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O			
15	C	2	2	2		0	0

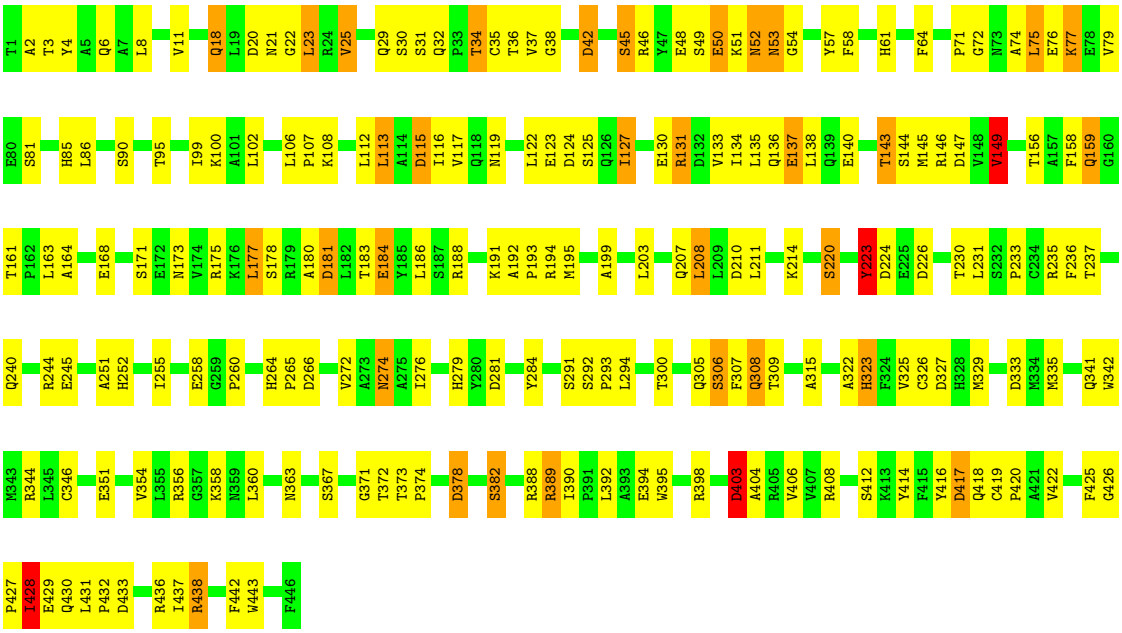
3 Residue-property plots (i)

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

Note EDS was not executed.

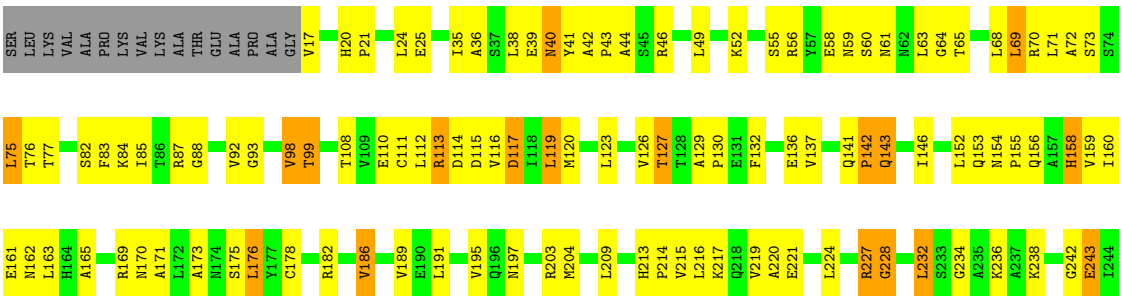
• Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

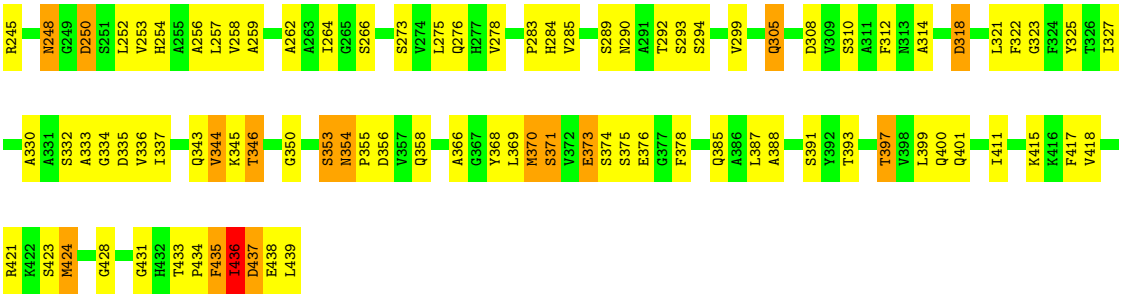
Chain A: 54% 38% 7% •



• Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

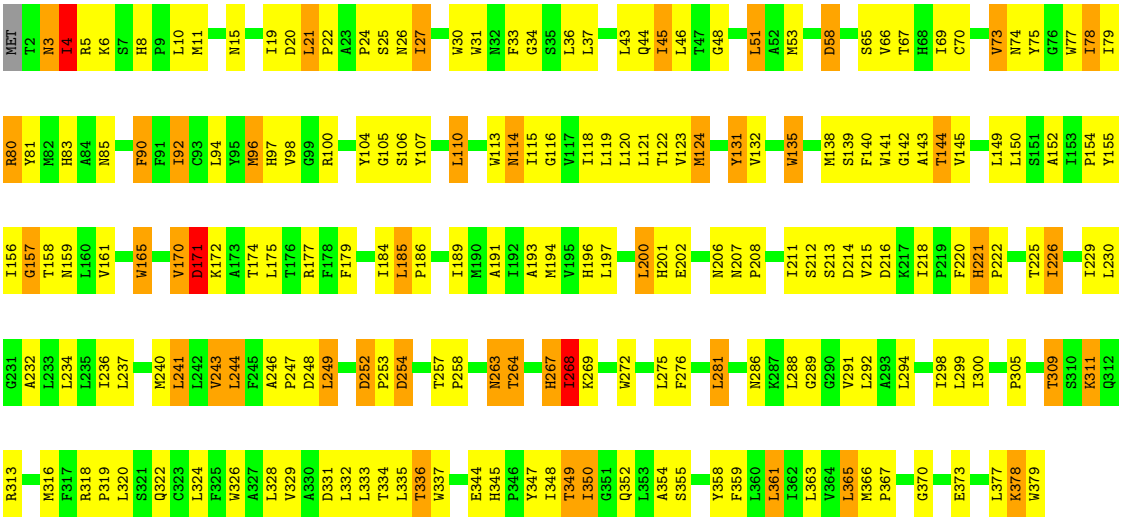
Chain B: 50% 38% 8% •





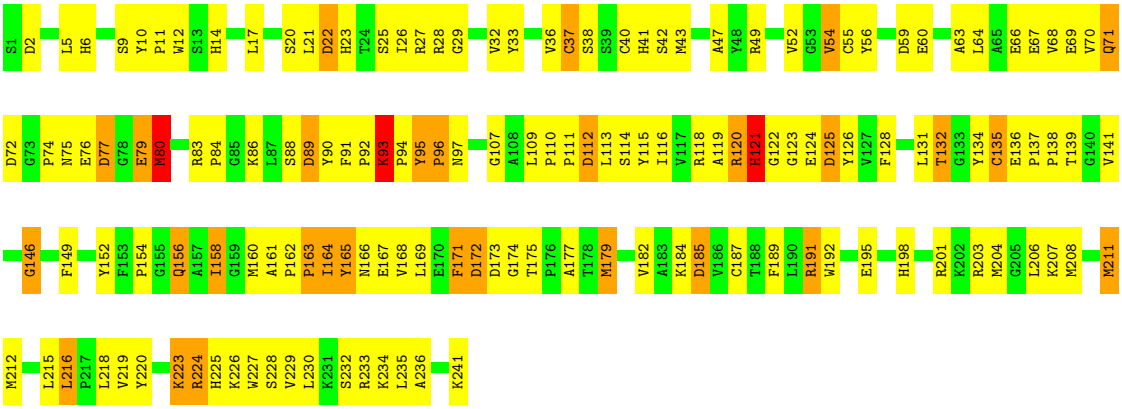
• Molecule 3: Cytochrome b

Chain C: 46% 41% 11%



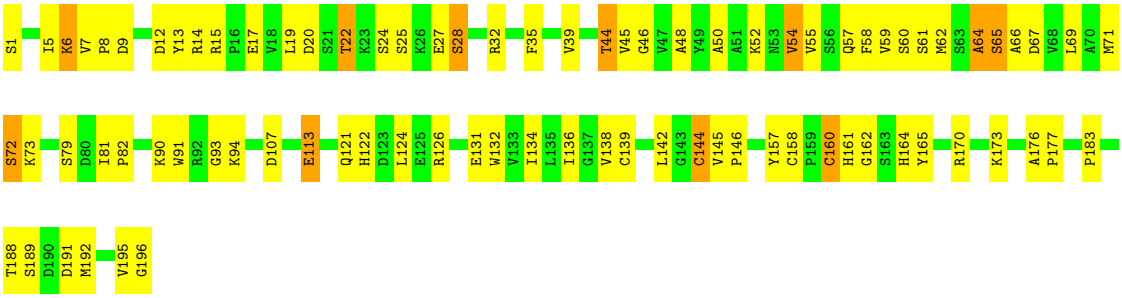
• Molecule 4: cytochrome c1

Chain D: 38% 49% 12%



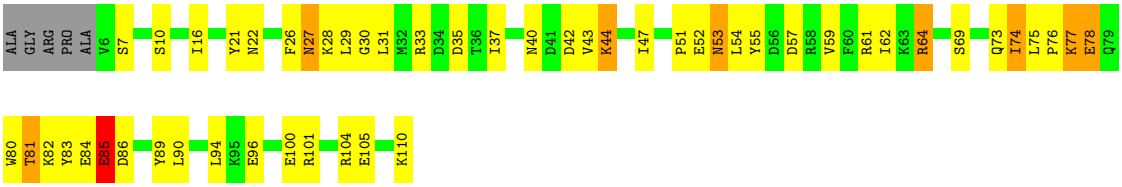
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, mitochondrial

Chain E: 57% 37% 6%



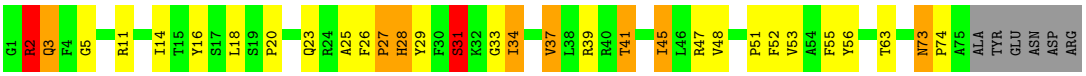
• Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F:



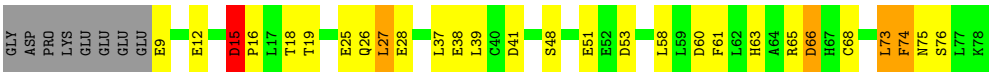
• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain G:



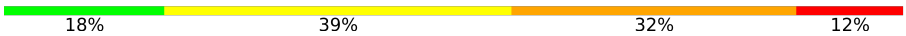
• Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H:



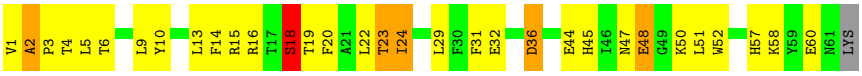
• Molecule 9: Ubiquinol-cytochrome C reductase 8 kDa protein

Chain I:



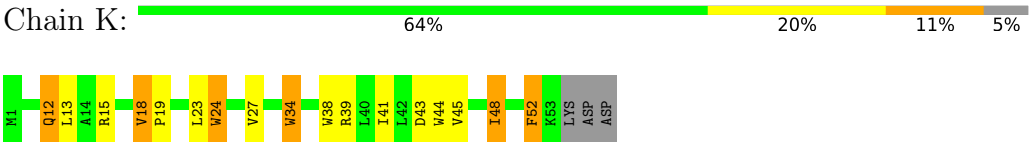
• Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:



• Molecule 11: Ubiquinol-cytochrome C reductase complex 6.4 kDa protein

Chain K:


64%
20%
11%
5%
M1
Q12
L13
A14
R15
V18
P19
L23
W24
V27
W34
W38
R39
L40
T41
L42
D43
W44
V45
T48
F52
K53
LYS
ASP
ASP

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	153.84Å 153.84Å 590.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	99.9 (10.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.215 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16666	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: QNO, HEM, FES

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	0.83	1/3531 (0.0%)	0.96	14/4792 (0.3%)
2	B	1.11	5/3232 (0.2%)	1.04	8/4386 (0.2%)
3	C	0.79	0/3100	0.92	10/4242 (0.2%)
4	D	0.66	0/1977	0.98	12/2684 (0.4%)
5	E	0.60	0/1553	0.89	5/2100 (0.2%)
6	F	0.97	0/930	1.03	2/1246 (0.2%)
7	G	0.83	0/649	0.87	0/878
8	H	0.55	0/580	0.96	6/777 (0.8%)
9	I	1.00	0/411	1.48	5/558 (0.9%)
10	J	0.67	0/495	0.86	0/672
11	K	0.67	0/453	0.87	1/621 (0.2%)
All	All	0.85	6/16911 (0.0%)	0.97	63/22956 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	2	0
3	C	2	0
4	D	2	0
7	G	1	0
8	H	1	0
9	I	2	0
All	All	10	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	437	ASP	CB-CG	-6.05	1.39	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	VAL	CB-CG2	-5.79	1.40	1.52
2	B	159	VAL	CB-CG2	-5.26	1.41	1.52
2	B	262	ALA	CA-CB	-5.22	1.41	1.52
2	B	137	VAL	CB-CG2	-5.18	1.42	1.52
2	B	344	VAL	CB-CG2	-5.16	1.42	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	122	GLY	N-CA-C	-7.87	93.42	113.10
2	B	250	ASP	CB-CG-OD2	7.34	124.91	118.30
6	F	85	GLU	N-CA-C	-7.32	91.25	111.00
2	B	318	ASP	CB-CG-OD2	7.16	124.75	118.30
5	E	67	ASP	CB-CG-OD2	6.75	124.37	118.30
9	I	44	ASP	CB-CG-OD2	6.73	124.36	118.30
2	B	437	ASP	N-CA-CB	-6.69	98.56	110.60
2	B	234	GLY	N-CA-C	6.52	129.41	113.10
9	I	29	LEU	N-CA-C	-6.47	93.52	111.00
2	B	114	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	42	ASP	CB-CG-OD2	6.35	124.01	118.30
2	B	117	ASP	CB-CG-OD2	6.30	123.97	118.30
4	D	185	ASP	CB-CG-OD2	6.26	123.93	118.30
2	B	119	LEU	CA-CB-CG	-6.16	101.14	115.30
1	A	333	ASP	CB-CG-OD2	6.15	123.83	118.30
6	F	57	ASP	CB-CG-OD2	6.05	123.75	118.30
5	E	12	ASP	CB-CG-OD2	6.04	123.73	118.30
1	A	115	ASP	CB-CG-OD2	6.00	123.70	118.30
3	C	252	ASP	CB-CG-OD2	5.97	123.67	118.30
4	D	93	LYS	N-CA-C	5.94	127.04	111.00
2	B	335	ASP	CB-CG-OD2	5.90	123.61	118.30
8	H	27	LEU	N-CA-C	5.89	126.91	111.00
1	A	327	ASP	CB-CG-OD2	5.84	123.56	118.30
9	I	27	ARG	N-CA-C	-5.83	95.26	111.00
9	I	15	LEU	CA-CB-CG	-5.80	101.96	115.30
3	C	222	PRO	N-CD-CG	-5.80	94.50	103.20
1	A	266	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	433	ASP	CB-CG-OD2	5.74	123.47	118.30
11	K	43	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	181	ASP	CB-CG-OD2	5.67	123.41	118.30
3	C	254	ASP	CB-CG-OD2	5.67	123.41	118.30
8	H	60	ASP	CB-CG-OD2	5.61	123.35	118.30
4	D	125	ASP	CB-CG-OD2	5.60	123.34	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	417	ASP	CB-CG-OD2	5.53	123.28	118.30
4	D	59	ASP	CB-CG-OD2	5.52	123.27	118.30
3	C	361	LEU	CA-CB-CG	5.51	127.98	115.30
3	C	331	ASP	CB-CG-OD2	5.46	123.21	118.30
3	C	58	ASP	CB-CG-OD2	5.45	123.20	118.30
8	H	53	ASP	N-CA-C	5.44	125.69	111.00
1	A	403	ASP	CB-CG-OD2	5.42	123.18	118.30
4	D	2	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	378	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	147	ASP	CB-CG-OD2	5.38	123.14	118.30
3	C	248	ASP	CB-CG-OD2	5.33	123.10	118.30
4	D	173	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	210	ASP	CB-CG-OD2	5.31	123.08	118.30
4	D	72	ASP	CB-CG-OD2	5.29	123.06	118.30
4	D	22	ASP	CB-CG-OD2	5.28	123.06	118.30
5	E	191	ASP	CB-CG-OD2	5.24	123.02	118.30
4	D	89	ASP	CB-CG-OD2	5.24	123.01	118.30
4	D	77	ASP	CB-CG-OD2	5.23	123.01	118.30
9	I	46	LYS	N-CA-C	5.20	125.03	111.00
3	C	171	ASP	CB-CG-OD2	5.20	122.97	118.30
1	A	20	ASP	CB-CG-OD2	5.19	122.97	118.30
3	C	200	LEU	CA-CB-CG	-5.19	103.36	115.30
8	H	53	ASP	CB-CG-OD2	5.16	122.94	118.30
8	H	66	ASP	CB-CG-OD2	5.14	122.93	118.30
8	H	15	ASP	CB-CG-OD2	5.13	122.92	118.30
5	E	107	ASP	CB-CG-OD2	5.12	122.91	118.30
3	C	268	ILE	N-CA-C	5.11	124.79	111.00
5	E	9	ASP	CB-CG-OD2	5.08	122.87	118.30
4	D	146	GLY	N-CA-C	-5.03	100.53	113.10
1	A	226	ASP	CB-CG-OD2	5.00	122.80	118.30

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	197	ASN	CA
2	B	305	GLN	CA
3	C	221	HIS	CA
3	C	345	HIS	CA
4	D	145	GLU	CA
4	D	169	LEU	CA
7	G	2	ARG	CA
8	H	12	GLU	CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
9	I	25	ALA	CA
9	I	42	VAL	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	150	0
2	B	3172	0	3152	160	1
3	C	3003	0	3065	184	0
4	D	1918	0	1870	138	0
5	E	1519	0	1503	66	0
6	F	911	0	904	37	0
7	G	628	0	636	31	0
8	H	575	0	550	13	0
9	I	406	0	437	99	0
10	J	483	0	465	40	0
11	K	437	0	439	17	0
12	C	86	0	60	21	0
12	D	43	0	30	5	0
13	C	21	0	24	6	0
14	E	4	0	0	2	0
15	C	2	0	0	5	0
All	All	16666	0	16491	814	1

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 25.

All (814) 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:11:MET:SD	3:C:11:MET:CE	2.05	1.45
10:J:18:SER:HA	11:K:24:TRP:CZ3	1.76	1.21
10:J:18:SER:HA	11:K:24:TRP:HZ3	0.94	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:20:ARG:HG3	9:I:51:CYS:HB2	1.28	1.08
2:B:76:THR:HG22	2:B:82:SER:H	1.19	1.05
6:F:31:LEU:O	6:F:81:THR:HG21	1.57	1.02
9:I:46:LYS:HG2	9:I:47:ARG:H	1.20	1.02
4:D:37:CYS:SG	12:D:242:HEM:HAB	2.02	0.99
1:A:146:ARG:H	9:I:42:VAL:HG12	1.27	0.98
9:I:34:VAL:HB	9:I:35:PRO:HD3	1.43	0.98
2:B:325:TYR:HD2	9:I:28:PRO:HD2	1.25	0.98
3:C:221:HIS:CG	3:C:221:HIS:O	2.12	0.97
3:C:214:ASP:OD2	7:G:2:ARG:NH2	1.98	0.96
2:B:325:TYR:CD2	9:I:28:PRO:HD2	2.00	0.96
3:C:319:PRO:HG3	7:G:47:ARG:HH12	1.34	0.92
9:I:44:ASP:O	9:I:46:LYS:HB2	1.71	0.91
7:G:73:ASN:HB3	7:G:74:PRO:HD3	1.51	0.91
2:B:35:ILE:HD11	2:B:220:ALA:CB	2.03	0.88
2:B:99:THR:HB	9:I:14:VAL:HG22	1.53	0.88
5:E:6:LYS:H	5:E:6:LYS:HD3	1.39	0.88
9:I:41:PRO:O	9:I:42:VAL:HG23	1.73	0.87
2:B:388:ALA:HB3	9:I:2:LEU:HD13	1.56	0.87
2:B:111:CYS:SG	2:B:119:LEU:HD12	2.14	0.87
2:B:176:LEU:HG	9:I:13:PRO:HG2	1.56	0.87
2:B:283:PRO:HG3	9:I:31:GLN:HG3	1.58	0.86
4:D:27:ARG:NH1	10:J:57:HIS:NE2	2.23	0.85
7:G:28:HIS:HB3	7:G:31:SER:HB2	1.58	0.85
6:F:27:ASN:HA	6:F:81:THR:HG23	1.59	0.85
2:B:49:LEU:HD23	2:B:127:THR:HG21	1.61	0.83
1:A:378:ASP:OD2	1:A:389:ARG:NH1	2.12	0.82
10:J:18:SER:CA	11:K:24:TRP:HZ3	1.87	0.82
3:C:131:TYR:HA	12:C:381:HEM:HAD2	1.61	0.82
4:D:120:ARG:O	4:D:121:HIS:HB2	1.78	0.81
3:C:309:THR:HG21	3:C:367:PRO:O	1.81	0.81
4:D:167:GLU:HG3	4:D:177:ALA:HB3	1.61	0.81
12:C:382:HEM:HHA	12:C:382:HEM:HBA1	1.62	0.81
2:B:353:SER:HB3	2:B:356:ASP:HB2	1.61	0.81
3:C:361:LEU:HA	3:C:365:LEU:HB2	1.63	0.81
3:C:106:SER:HB3	12:C:382:HEM:HBD2	1.64	0.80
3:C:114:ASN:N	3:C:114:ASN:HD22	1.80	0.80
4:D:171:PHE:HE1	4:D:177:ALA:HB2	1.47	0.80
3:C:165:TRP:O	3:C:174:THR:OG1	1.99	0.80
2:B:215:VAL:O	2:B:219:VAL:HG23	1.81	0.80
2:B:39:GLU:OE2	2:B:113:ARG:NH2	2.15	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:37:CYS:SG	12:D:242:HEM:CAB	2.70	0.79
10:J:50:LYS:O	10:J:52:TRP:HD1	1.65	0.79
1:A:144:SER:HA	9:I:42:VAL:HB	1.65	0.78
1:A:388:ARG:NH2	1:A:394:GLU:OE2	2.16	0.77
3:C:221:HIS:O	3:C:221:HIS:ND1	2.15	0.77
2:B:71:LEU:CD2	9:I:15:LEU:HG	2.13	0.77
3:C:272:TRP:HA	3:C:275:LEU:HG	1.66	0.77
6:F:42:ASP:OD2	6:F:101:ARG:NH2	2.17	0.77
6:F:64:ARG:HH11	6:F:64:ARG:HB3	1.49	0.77
2:B:156:GLN:NE2	9:I:28:PRO:O	2.18	0.77
9:I:34:VAL:HB	9:I:35:PRO:CD	2.14	0.76
3:C:119:LEU:HD13	12:C:382:HEM:HBB2	1.66	0.76
2:B:435:PHE:O	2:B:436:ILE:HB	1.86	0.76
5:E:15:ARG:HD2	5:E:32:ARG:HD2	1.68	0.76
1:A:325:VAL:HG21	9:I:43:LEU:HD12	1.68	0.76
3:C:226:ILE:HG23	4:D:223:LYS:HB2	1.68	0.76
4:D:212:MET:HG3	4:D:216:LEU:HD12	1.67	0.76
4:D:211:MET:CE	10:J:31:PHE:HE2	2.00	0.75
2:B:294:SER:HB3	2:B:343:GLN:HE21	1.52	0.75
5:E:6:LYS:H	5:E:6:LYS:CD	2.00	0.74
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.68	0.74
3:C:15:ASN:HA	3:C:19:ILE:HG12	1.71	0.73
4:D:224:ARG:HB3	7:G:25:ALA:HB1	1.71	0.73
3:C:319:PRO:HG3	7:G:47:ARG:NH1	2.04	0.73
9:I:29:LEU:O	9:I:32:ALA:HB3	1.89	0.73
3:C:214:ASP:CG	7:G:2:ARG:HH22	1.92	0.72
4:D:165:TYR:HE1	8:H:15:ASP:OD1	1.72	0.72
3:C:113:TRP:HA	12:C:382:HEM:HHD	1.71	0.72
7:G:27:PRO:O	7:G:29:TYR:N	2.23	0.72
4:D:28:ARG:O	4:D:32:VAL:HG23	1.90	0.72
1:A:417:ASP:OD1	1:A:438:ARG:NH2	2.23	0.72
1:A:251:ALA:HB2	1:A:427:PRO:HD2	1.72	0.72
3:C:216:ASP:OD2	4:D:233:ARG:NH2	2.23	0.72
9:I:11:PHE:HZ	9:I:27:ARG:NH2	1.88	0.72
2:B:156:GLN:O	2:B:160:ILE:HG13	1.89	0.71
4:D:28:ARG:HD2	4:D:185:ASP:OD2	1.91	0.70
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.73	0.70
4:D:26:ILE:HG23	4:D:189:PHE:HA	1.74	0.70
4:D:91:PHE:O	4:D:93:LYS:HG2	1.91	0.70
3:C:349:THR:HA	3:C:352:GLN:HE21	1.56	0.70
3:C:30:TRP:HZ3	3:C:96:MET:HG2	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:MET:O	1:A:149:VAL:HG23	1.92	0.70
9:I:20:ARG:NH1	9:I:48:SER:OG	2.25	0.70
3:C:201:HIS:NE2	15:C:1010:HOH:O	2.24	0.69
5:E:44:THR:HB	10:J:24:ILE:HD12	1.73	0.69
2:B:343:GLN:O	2:B:346:THR:HG22	1.92	0.69
4:D:14:HIS:NE2	4:D:124:GLU:OE1	2.17	0.69
2:B:153:GLN:HE22	9:I:46:LYS:HD2	1.58	0.69
9:I:46:LYS:HG2	9:I:47:ARG:N	2.03	0.69
9:I:47:ARG:HD2	9:I:48:SER:H	1.56	0.69
1:A:42:ASP:O	1:A:194:ARG:NH2	2.25	0.69
1:A:146:ARG:H	9:I:42:VAL:CG1	2.06	0.69
3:C:3:ASN:HD22	3:C:6:LYS:HG3	1.57	0.68
5:E:17:GLU:HB3	5:E:28:SER:HB3	1.75	0.68
3:C:243:VAL:O	3:C:247:PRO:HG3	1.94	0.68
4:D:211:MET:HE1	10:J:31:PHE:HE2	1.59	0.68
2:B:385:GLN:HE22	2:B:393:THR:H	1.42	0.68
4:D:14:HIS:CD2	4:D:191:ARG:HD3	2.29	0.68
4:D:71:GLN:HE21	4:D:80:MET:HG3	1.58	0.67
6:F:27:ASN:HA	6:F:81:THR:CG2	2.24	0.67
9:I:47:ARG:CD	9:I:48:SER:H	2.07	0.67
4:D:225:HIS:O	4:D:228:SER:HB3	1.94	0.67
3:C:26:ASN:HD21	6:F:69:SER:HB3	1.60	0.67
3:C:24:PRO:C	3:C:26:ASN:H	1.95	0.67
9:I:20:ARG:HG3	9:I:51:CYS:CB	2.15	0.67
3:C:33:PHE:HA	3:C:36:LEU:HB2	1.77	0.67
13:C:383:QNO:C3	15:C:1010:HOH:O	2.42	0.67
3:C:370:GLY:HA2	3:C:373:GLU:OE2	1.96	0.66
3:C:45:ILE:HA	12:C:381:HEM:HAB	1.76	0.66
5:E:121:GLN:O	5:E:170:ARG:NH1	2.24	0.66
8:H:25:GLU:HG3	8:H:61:PHE:HZ	1.61	0.66
2:B:436:ILE:HG22	2:B:437:ASP:N	2.09	0.66
3:C:241:LEU:HD13	4:D:208:MET:HE1	1.78	0.66
3:C:267:HIS:CE1	3:C:269:LYS:HG2	2.31	0.66
4:D:112:ASP:OD1	4:D:112:ASP:N	2.27	0.66
3:C:257:THR:HG22	4:D:115:TYR:HE1	1.60	0.66
6:F:53:ASN:N	6:F:53:ASN:HD22	1.92	0.66
5:E:121:GLN:OE1	5:E:126:ARG:NH1	2.29	0.65
3:C:90:PHE:HD1	3:C:90:PHE:O	1.80	0.65
2:B:245:ARG:NH2	2:B:433:THR:O	2.30	0.65
1:A:252:HIS:CE1	9:I:42:VAL:O	2.49	0.65
4:D:79:GLU:O	4:D:80:MET:HB2	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:ASN:HA	3:C:19:ILE:CG1	2.26	0.65
9:I:46:LYS:CG	9:I:47:ARG:H	1.91	0.65
2:B:49:LEU:HD11	2:B:204:MET:HE2	1.80	0.64
3:C:138:MET:O	3:C:142:GLY:N	2.28	0.64
10:J:50:LYS:O	10:J:52:TRP:N	2.30	0.64
2:B:46:ARG:HG3	2:B:46:ARG:HH11	1.62	0.64
4:D:211:MET:HE1	10:J:31:PHE:CE2	2.33	0.64
3:C:267:HIS:HE1	3:C:269:LYS:HG2	1.62	0.64
4:D:165:TYR:HD2	4:D:165:TYR:O	1.79	0.64
2:B:129:ALA:N	2:B:130:PRO:HD3	2.14	0.63
2:B:71:LEU:HD23	9:I:15:LEU:HG	1.80	0.63
7:G:29:TYR:O	7:G:33:GLY:HA3	1.98	0.63
3:C:131:TYR:CA	12:C:381:HEM:HAD2	2.29	0.63
4:D:184:LYS:HB2	8:H:74:PHE:HE2	1.63	0.63
1:A:281:ASP:OD1	9:I:47:ARG:HG2	1.99	0.63
3:C:220:PHE:HE2	13:C:383:QNO:C61	2.12	0.63
1:A:371:GLY:O	1:A:374:PRO:HD2	1.98	0.63
3:C:51:LEU:HD21	3:C:80:ARG:HA	1.80	0.63
9:I:39:GLU:O	9:I:40:SER:HB3	1.98	0.63
1:A:416:TYR:CE1	1:A:442:PHE:HA	2.33	0.63
2:B:68:LEU:HD23	2:B:186:VAL:HG22	1.80	0.62
10:J:2:ALA:HB3	10:J:3:PRO:HD3	1.80	0.62
1:A:37:VAL:HG21	1:A:106:LEU:CD1	2.29	0.62
1:A:23:LEU:HD23	1:A:195:MET:O	2.00	0.62
2:B:99:THR:CB	9:I:14:VAL:HG22	2.28	0.62
3:C:85:ASN:HB2	3:C:243:VAL:HG12	1.81	0.62
4:D:60:GLU:O	4:D:64:LEU:HG	1.98	0.62
4:D:124:GLU:HB3	4:D:187:CYS:HB3	1.81	0.62
1:A:138:LEU:HB3	5:E:1:SER:H1	1.64	0.62
1:A:255:ILE:HD12	1:A:335:MET:CE	2.29	0.62
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.81	0.62
4:D:215:LEU:HD21	5:E:46:GLY:HA3	1.81	0.62
4:D:54:VAL:HG21	4:D:192:TRP:CZ2	2.35	0.62
9:I:49:VAL:HG12	9:I:50:LEU:N	2.14	0.61
1:A:341:GLN:HE22	1:A:344:ARG:HH21	1.48	0.61
3:C:234:LEU:HD21	4:D:216:LEU:HD21	1.83	0.61
3:C:241:LEU:HD13	4:D:208:MET:CE	2.30	0.61
1:A:11:VAL:HG21	1:A:392:LEU:HD12	1.81	0.61
2:B:153:GLN:HE22	9:I:46:LYS:CD	2.12	0.61
5:E:52:LYS:HD2	11:K:34:TRP:CZ2	2.36	0.61
3:C:8:HIS:HD2	3:C:11:MET:H	1.49	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:267:HIS:ND1	3:C:267:HIS:C	2.53	0.61
5:E:144:CYS:HB3	5:E:158:CYS:SG	2.40	0.61
3:C:116:GLY:HA3	12:C:382:HEM:C3C	2.35	0.61
10:J:22:LEU:HA	11:K:27:VAL:HG22	1.82	0.61
3:C:106:SER:CB	12:C:382:HEM:HBD2	2.30	0.61
1:A:255:ILE:HD12	1:A:335:MET:HE1	1.81	0.61
1:A:373:THR:HB	1:A:374:PRO:HD3	1.81	0.61
2:B:35:ILE:HD11	2:B:220:ALA:HB2	1.81	0.61
5:E:55:VAL:O	5:E:59:VAL:HG23	2.00	0.61
1:A:354:VAL:O	1:A:358:LYS:HG3	2.00	0.60
3:C:140:PHE:O	3:C:144:THR:OG1	2.19	0.60
8:H:25:GLU:HG3	8:H:61:PHE:CZ	2.36	0.60
3:C:51:LEU:HD13	3:C:79:ILE:HG22	1.81	0.60
7:G:41:THR:O	7:G:45:ILE:HG12	2.00	0.60
10:J:14:PHE:HD1	10:J:20:PHE:HD1	1.49	0.60
5:E:50:ALA:O	5:E:54:VAL:HG23	2.00	0.60
1:A:260:PRO:HD3	1:A:414:TYR:CE2	2.37	0.60
2:B:153:GLN:HE22	9:I:46:LYS:HG3	1.66	0.60
3:C:116:GLY:HA3	12:C:382:HEM:C4C	2.36	0.60
1:A:252:HIS:HE1	9:I:43:LEU:HB2	1.67	0.60
1:A:131:ARG:NH2	1:A:177:LEU:O	2.29	0.60
2:B:294:SER:CB	2:B:343:GLN:HE21	2.13	0.60
3:C:226:ILE:CG2	4:D:223:LYS:HB2	2.32	0.60
3:C:377:LEU:O	3:C:378:LYS:HB2	2.02	0.60
9:I:9:GLY:CA	9:I:26:LEU:H	2.15	0.59
3:C:3:ASN:CG	3:C:4:ILE:H	2.04	0.59
3:C:30:TRP:O	3:C:100:ARG:HG3	2.01	0.59
9:I:11:PHE:CZ	9:I:27:ARG:NH2	2.69	0.59
9:I:43:LEU:HA	9:I:46:LYS:HD3	1.84	0.59
4:D:229:VAL:HG23	7:G:20:PRO:HD3	1.83	0.59
3:C:26:ASN:OD1	3:C:207:ASN:OD1	2.19	0.59
5:E:72:SER:CB	5:E:91:TRP:HD1	2.15	0.59
9:I:42:VAL:O	9:I:43:LEU:HB2	2.02	0.59
4:D:171:PHE:O	4:D:174:GLY:N	2.35	0.59
2:B:436:ILE:CG2	2:B:437:ASP:N	2.65	0.59
5:E:64:ALA:O	5:E:65:SER:CB	2.50	0.59
3:C:21:LEU:HD13	3:C:201:HIS:CD2	2.38	0.59
4:D:165:TYR:O	4:D:167:GLU:N	2.35	0.59
9:I:11:PHE:HZ	9:I:27:ARG:CZ	2.15	0.59
2:B:70:ARG:HG3	2:B:98:VAL:HG22	1.85	0.59
7:G:34:ILE:HA	7:G:37:VAL:HG13	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:90:TYR:C	4:D:92:PRO:HD3	2.23	0.59
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.38	0.58
1:A:351:GLU:H	11:K:12:GLN:HE21	1.51	0.58
2:B:40:ASN:O	2:B:40:ASN:ND2	2.32	0.58
2:B:126:VAL:O	2:B:130:PRO:HG3	2.04	0.58
2:B:344:VAL:HG11	2:B:417:PHE:CD2	2.38	0.58
3:C:81:TYR:OH	4:D:118:ARG:NH2	2.36	0.58
3:C:105:GLY:HA2	3:C:107:TYR:CE1	2.38	0.58
1:A:57:TYR:HE2	1:A:134:ILE:HG23	1.69	0.58
3:C:152:ALA:CB	3:C:291:VAL:HG11	2.32	0.58
4:D:75:ASN:O	4:D:77:ASP:N	2.37	0.58
3:C:114:ASN:HD22	3:C:114:ASN:H	1.52	0.58
5:E:72:SER:HB2	5:E:91:TRP:CD1	2.38	0.58
9:I:16:SER:HB3	9:I:19:SER:O	2.03	0.58
1:A:136:GLN:NE2	9:I:37:THR:OG1	2.36	0.58
1:A:146:ARG:N	9:I:42:VAL:HG12	2.10	0.58
6:F:28:LYS:HB2	6:F:74:ILE:HG12	1.86	0.58
4:D:20:SER:HB3	10:J:47:ASN:CG	2.24	0.58
10:J:29:LEU:HD13	11:K:34:TRP:HD1	1.68	0.58
1:A:237:THR:OG1	5:E:14:ARG:NH2	2.36	0.58
2:B:314:ALA:HA	9:I:10:PRO:HG3	1.83	0.58
3:C:201:HIS:CE1	15:C:1010:HOH:O	2.56	0.58
9:I:4:VAL:O	9:I:7:ARG:HB3	2.04	0.58
2:B:253:VAL:HG23	2:B:330:ALA:HA	1.86	0.58
7:G:53:VAL:HA	7:G:56:TYR:HB3	1.86	0.58
7:G:73:ASN:CB	7:G:74:PRO:HD3	2.27	0.58
9:I:52:ARG:O	9:I:53:GLU:HB2	2.03	0.58
12:C:382:HEM:HBC2	12:C:382:HEM:CMC	2.34	0.57
3:C:30:TRP:CZ3	3:C:96:MET:HG2	2.37	0.57
3:C:206:ASN:HB2	3:C:313:ARG:NH2	2.19	0.57
5:E:72:SER:HB3	5:E:91:TRP:HD1	1.68	0.57
8:H:73:LEU:O	8:H:75:ASN:N	2.36	0.57
2:B:248:ASN:HB3	2:B:428:GLY:HA2	1.85	0.57
4:D:165:TYR:O	4:D:165:TYR:CD2	2.57	0.57
4:D:12:TRP:HH2	4:D:128:PHE:HB2	1.69	0.57
4:D:184:LYS:HB2	8:H:74:PHE:CE2	2.39	0.57
7:G:48:VAL:O	7:G:51:PRO:HD2	2.05	0.57
3:C:268:ILE:HG23	3:C:268:ILE:O	2.05	0.57
1:A:378:ASP:O	1:A:382:SER:HB2	2.05	0.57
2:B:254:HIS:CE1	2:B:327:ILE:CD1	2.87	0.57
1:A:260:PRO:HG3	1:A:414:TYR:OH	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:291:VAL:HG13	3:C:292:LEU:N	2.20	0.57
1:A:146:ARG:HH12	1:A:308:GLN:NE2	2.02	0.57
2:B:44:ALA:HA	2:B:112:LEU:HA	1.85	0.57
2:B:76:THR:HG22	2:B:82:SER:N	2.04	0.57
2:B:111:CYS:SG	2:B:119:LEU:CD1	2.92	0.57
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.40	0.57
10:J:14:PHE:HD1	10:J:20:PHE:CD1	2.23	0.57
2:B:369:LEU:HD11	2:B:399:LEU:HD11	1.85	0.56
3:C:114:ASN:N	3:C:114:ASN:ND2	2.53	0.56
3:C:150:LEU:O	3:C:157:GLY:HA2	2.04	0.56
4:D:83:ARG:NH2	4:D:89:ASP:OD1	2.38	0.56
7:G:56:TYR:C	7:G:56:TYR:CD1	2.78	0.56
9:I:2:LEU:O	9:I:3:SER:CB	2.53	0.56
9:I:46:LYS:CG	9:I:47:ARG:N	2.64	0.56
6:F:75:LEU:HD23	6:F:76:PRO:HD2	1.86	0.56
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.86	0.56
2:B:256:ALA:HB2	2:B:325:TYR:CD1	2.41	0.56
3:C:44:GLN:NE2	12:C:381:HEM:HBC2	2.20	0.56
5:E:28:SER:HB2	5:E:32:ARG:HH11	1.69	0.56
1:A:146:ARG:HH22	1:A:308:GLN:HE22	1.53	0.56
4:D:22:ASP:HB3	4:D:25:SER:HB3	1.86	0.56
4:D:165:TYR:CE1	8:H:15:ASP:OD1	2.57	0.56
1:A:124:ASP:HA	1:A:127:ILE:CG2	2.36	0.56
4:D:63:ALA:O	4:D:67:GLU:HG3	2.06	0.56
2:B:56:ARG:HB2	2:B:171:ALA:HB1	1.88	0.56
4:D:109:LEU:O	4:D:111:PRO:HD3	2.05	0.56
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.41	0.56
10:J:50:LYS:O	10:J:52:TRP:CD1	2.54	0.56
9:I:20:ARG:CG	9:I:51:CYS:HB2	2.19	0.56
1:A:76:GLU:O	1:A:77:LYS:C	2.45	0.55
1:A:284:TYR:HE1	9:I:20:ARG:HG2	1.71	0.55
3:C:229:ILE:O	3:C:232:ALA:N	2.39	0.55
3:C:332:LEU:HD21	3:C:358:TYR:CE1	2.41	0.55
10:J:32:GLU:O	10:J:36:ASP:HB2	2.06	0.55
3:C:230:LEU:HD13	4:D:219:VAL:HG12	1.89	0.55
4:D:112:ASP:O	4:D:116:ILE:HG12	2.05	0.55
6:F:26:PHE:HB2	6:F:31:LEU:HB2	1.89	0.55
11:K:18:VAL:HG12	11:K:19:PRO:HD3	1.87	0.55
1:A:130:GLU:O	1:A:134:ILE:HG13	2.06	0.55
4:D:21:LEU:HD21	4:D:191:ARG:HG2	1.87	0.55
6:F:28:LYS:CB	6:F:74:ILE:HG12	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:MET:O	1:A:149:VAL:CG2	2.54	0.55
1:A:220:SER:HA	1:A:223:TYR:HB3	1.89	0.55
3:C:211:ILE:HG21	6:F:62:ILE:HD13	1.88	0.55
9:I:9:GLY:HA2	9:I:26:LEU:CA	2.37	0.55
1:A:45:SER:HA	1:A:48:GLU:HG2	1.88	0.55
10:J:58:LYS:C	10:J:60:GLU:H	2.09	0.55
4:D:69:GLU:HA	4:D:83:ARG:O	2.07	0.55
1:A:2:ALA:O	2:B:113:ARG:HD3	2.06	0.54
1:A:178:SER:O	1:A:181:ASP:HB2	2.06	0.54
2:B:385:GLN:HA	9:I:2:LEU:HD12	1.88	0.54
3:C:25:SER:HA	3:C:218:ILE:CD1	2.37	0.54
5:E:139:CYS:SG	5:E:165:TYR:OH	2.65	0.54
4:D:28:ARG:HD3	4:D:171:PHE:CE2	2.43	0.54
5:E:20:ASP:OD2	5:E:22:THR:HB	2.07	0.54
2:B:308:ASP:OD1	9:I:28:PRO:HB3	2.07	0.54
9:I:11:PHE:CE2	9:I:25:ALA:N	2.65	0.54
2:B:65:THR:O	2:B:69:LEU:HB2	2.07	0.54
3:C:154:PRO:O	3:C:155:TYR:HB3	2.08	0.54
9:I:39:GLU:O	9:I:40:SER:CB	2.56	0.54
10:J:29:LEU:HG	11:K:48:ILE:HD13	1.89	0.54
3:C:218:ILE:HG21	4:D:230:LEU:HD11	1.90	0.54
1:A:442:PHE:C	1:A:442:PHE:CD2	2.81	0.54
3:C:44:GLN:HE21	12:C:381:HEM:HBC2	1.73	0.54
3:C:200:LEU:HD22	12:C:382:HEM:HAA1	1.90	0.54
5:E:35:PHE:O	5:E:39:VAL:HG23	2.07	0.54
1:A:255:ILE:HG23	1:A:342:TRP:HH2	1.73	0.54
2:B:153:GLN:HE22	9:I:46:LYS:CG	2.21	0.54
2:B:254:HIS:CE1	2:B:327:ILE:HD11	2.43	0.54
4:D:120:ARG:O	4:D:121:HIS:CB	2.54	0.54
9:I:18:THR:HG23	9:I:19:SER:H	1.73	0.54
1:A:61:HIS:NE2	1:A:137:GLU:OE2	2.41	0.54
4:D:204:MET:HA	4:D:207:LYS:HD2	1.90	0.54
1:A:75:LEU:CD1	1:A:112:LEU:HD22	2.38	0.53
1:A:233:PRO:HB2	5:E:22:THR:O	2.08	0.53
3:C:332:LEU:HD21	3:C:358:TYR:HE1	1.73	0.53
8:H:38:GLU:O	8:H:41:ASP:HB2	2.08	0.53
12:C:382:HEM:HBC2	12:C:382:HEM:HMC1	1.89	0.53
1:A:294:LEU:HG	1:A:307:PHE:CE1	2.44	0.53
6:F:53:ASN:ND2	6:F:54:LEU:H	2.07	0.53
1:A:252:HIS:CE1	9:I:43:LEU:HB2	2.43	0.53
3:C:116:GLY:O	12:C:382:HEM:HMC3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:PHE:O	1:A:164:ALA:HB2	2.08	0.53
9:I:49:VAL:CG1	9:I:50:LEU:N	2.72	0.53
2:B:258:VAL:HG11	2:B:321:LEU:HB3	1.90	0.53
5:E:28:SER:HB2	5:E:32:ARG:NH1	2.24	0.53
3:C:85:ASN:HD22	3:C:243:VAL:HG12	1.74	0.53
2:B:436:ILE:HG22	2:B:437:ASP:H	1.73	0.53
4:D:158:ILE:HG13	4:D:160:MET:H	1.73	0.53
4:D:211:MET:HE3	10:J:31:PHE:HE2	1.71	0.53
9:I:49:VAL:CG1	9:I:50:LEU:H	2.21	0.53
1:A:143:THR:HG21	9:I:39:GLU:HG2	1.91	0.53
3:C:329:VAL:CG1	7:G:52:PHE:HZ	2.22	0.53
1:A:53:ASN:HD22	1:A:54:GLY:H	1.57	0.52
3:C:211:ILE:CG2	6:F:62:ILE:HD13	2.39	0.52
5:E:58:PHE:O	5:E:61:SER:OG	2.27	0.52
3:C:65:SER:O	3:C:69:ILE:HG13	2.09	0.52
5:E:71:MET:O	5:E:73:LYS:N	2.43	0.52
1:A:75:LEU:HD13	1:A:112:LEU:HD22	1.91	0.52
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.92	0.52
3:C:77:TRP:O	3:C:80:ARG:N	2.42	0.52
3:C:349:THR:HA	3:C:352:GLN:NE2	2.22	0.52
4:D:33:TYR:CD1	4:D:37:CYS:HB2	2.44	0.52
1:A:25:VAL:HG23	1:A:208:LEU:HD13	1.92	0.52
2:B:256:ALA:HB2	2:B:325:TYR:HD1	1.75	0.52
4:D:23:HIS:CD2	10:J:50:LYS:HA	2.44	0.52
10:J:44:GLU:CG	10:J:52:TRP:HZ2	2.23	0.52
2:B:20:HIS:CD2	2:B:21:PRO:HD2	2.45	0.52
2:B:191:LEU:O	2:B:195:VAL:HG23	2.10	0.52
4:D:33:TYR:HA	4:D:37:CYS:SG	2.49	0.52
3:C:179:PHE:CE2	12:C:381:HEM:HMA3	2.45	0.52
9:I:11:PHE:HZ	9:I:27:ARG:HH21	1.55	0.52
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.92	0.52
2:B:250:ASP:C	2:B:252:LEU:H	2.14	0.52
4:D:28:ARG:HD3	4:D:171:PHE:HE2	1.74	0.52
9:I:9:GLY:HA2	9:I:26:LEU:H	1.74	0.52
1:A:53:ASN:HD22	1:A:54:GLY:N	2.08	0.51
4:D:131:LEU:HD13	4:D:164:ILE:HD11	1.92	0.51
4:D:167:GLU:HG3	4:D:177:ALA:CB	2.35	0.51
2:B:437:ASP:HB3	2:B:438:GLU:HG3	1.92	0.51
4:D:158:ILE:CG1	4:D:160:MET:H	2.23	0.51
2:B:368:TYR:O	2:B:369:LEU:C	2.48	0.51
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:CYS:SG	12:D:242:HEM:HAC	2.51	0.51
5:E:161:HIS:CE1	14:E:200:FES:S2	3.03	0.51
1:A:46:ARG:HD2	1:A:163:LEU:HD13	1.91	0.51
1:A:75:LEU:HD21	1:A:116:ILE:HG12	1.92	0.51
12:C:382:HEM:HBA1	12:C:382:HEM:CHA	2.37	0.51
3:C:5:ARG:NE	3:C:15:ASN:OD1	2.42	0.51
1:A:38:GLY:HA2	1:A:113:LEU:HD21	1.92	0.51
1:A:49:SER:O	1:A:51:LYS:N	2.44	0.51
1:A:252:HIS:HE1	9:I:42:VAL:O	1.91	0.51
2:B:227:ARG:HD3	2:B:228:GLY:N	2.26	0.51
2:B:312:PHE:N	2:B:323:GLY:O	2.36	0.51
3:C:135:TRP:HH2	3:C:170:VAL:HG12	1.75	0.51
4:D:33:TYR:OH	4:D:41:HIS:O	2.21	0.51
7:G:28:HIS:HB3	7:G:31:SER:CB	2.35	0.51
1:A:64:PHE:CE1	1:A:86:LEU:HG	2.46	0.51
6:F:75:LEU:O	6:F:80:TRP:NE1	2.41	0.51
2:B:232:LEU:HD22	2:B:232:LEU:H	1.76	0.50
3:C:220:PHE:HE2	13:C:383:QNO:C6	2.24	0.50
4:D:208:MET:O	4:D:212:MET:HB2	2.11	0.50
1:A:74:ALA:HA	1:A:77:LYS:HB2	1.94	0.50
1:A:168:GLU:OE2	1:A:168:GLU:N	2.43	0.50
3:C:77:TRP:O	3:C:78:ILE:C	2.48	0.50
2:B:354:ASN:HB3	2:B:355:PRO:CD	2.41	0.50
2:B:84:LYS:O	2:B:88:GLY:N	2.39	0.50
10:J:47:ASN:O	10:J:48:GLU:HB2	2.12	0.50
2:B:116:VAL:HG23	2:B:117:ASP:N	2.26	0.50
2:B:258:VAL:HG22	2:B:322:PHE:C	2.31	0.50
2:B:397:THR:HA	2:B:400:GLN:HB3	1.92	0.50
10:J:44:GLU:HG3	10:J:52:TRP:CZ2	2.46	0.50
1:A:61:HIS:CE1	1:A:137:GLU:OE2	2.65	0.50
1:A:220:SER:HA	1:A:223:TYR:CB	2.41	0.50
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.12	0.50
1:A:86:LEU:HB3	2:B:285:VAL:HG13	1.93	0.50
1:A:173:ASN:O	1:A:177:LEU:HB2	2.11	0.50
5:E:7:VAL:HG13	7:G:16:TYR:HD2	1.77	0.50
6:F:35:ASP:OD2	6:F:61:ARG:NH1	2.45	0.50
1:A:3:THR:HG23	1:A:6:GLN:OE1	2.11	0.49
4:D:236:ALA:HB3	7:G:14:ILE:HB	1.94	0.49
7:G:37:VAL:O	7:G:41:THR:OG1	2.30	0.49
1:A:260:PRO:HG3	1:A:414:TYR:CZ	2.47	0.49
3:C:74:ASN:HD21	5:E:64:ALA:HB3	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:223:LYS:HG3	4:D:224:ARG:N	2.28	0.49
5:E:158:CYS:SG	5:E:160:CYS:HB2	2.52	0.49
9:I:49:VAL:HG12	9:I:50:LEU:H	1.76	0.49
2:B:59:ASN:O	2:B:61:ASN:N	2.45	0.49
2:B:236:LYS:HA	2:B:318:ASP:OD1	2.12	0.49
5:E:7:VAL:HG13	7:G:16:TYR:CD2	2.46	0.49
3:C:51:LEU:HD13	3:C:79:ILE:CG2	2.42	0.49
3:C:139:SER:O	3:C:143:ALA:N	2.33	0.49
4:D:195:GLU:OE1	4:D:201:ARG:NH1	2.44	0.49
5:E:5:ILE:HA	5:E:6:LYS:HD3	1.94	0.49
1:A:123:GLU:O	1:A:127:ILE:HG22	2.13	0.49
1:A:305:GLN:O	1:A:306:SER:HB3	2.13	0.49
2:B:325:TYR:HB3	9:I:28:PRO:HD3	1.95	0.49
10:J:29:LEU:HD13	11:K:34:TRP:CD1	2.47	0.49
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.47	0.49
6:F:64:ARG:HB3	6:F:64:ARG:NH1	2.22	0.49
1:A:146:ARG:NH2	1:A:308:GLN:HE22	2.11	0.49
3:C:104:TYR:CD2	3:C:208:PRO:HA	2.48	0.49
10:J:44:GLU:HG3	10:J:52:TRP:HZ2	1.77	0.49
6:F:64:ARG:HH11	6:F:64:ARG:CB	2.23	0.49
4:D:74:PRO:HG3	4:D:80:MET:SD	2.53	0.48
4:D:91:PHE:N	4:D:92:PRO:HD3	2.28	0.48
11:K:38:TRP:HE1	11:K:39:ARG:HH21	1.61	0.48
1:A:156:THR:O	1:A:159:GLN:HG3	2.13	0.48
2:B:146:ILE:HD13	2:B:146:ILE:N	2.28	0.48
1:A:158:PHE:O	1:A:161:THR:HG23	2.13	0.48
1:A:158:PHE:HB3	1:A:161:THR:OG1	2.14	0.48
1:A:436:ARG:NH2	3:C:20:ASP:OD2	2.44	0.48
2:B:35:ILE:CD1	2:B:220:ALA:HB2	2.43	0.48
2:B:116:VAL:CG2	2:B:117:ASP:N	2.75	0.48
3:C:107:TYR:HB2	3:C:305:PRO:HG3	1.95	0.48
3:C:184:ILE:HG12	3:C:184:ILE:O	2.14	0.48
3:C:69:ILE:O	3:C:73:VAL:HB	2.14	0.48
4:D:126:TYR:C	4:D:126:TYR:CD2	2.86	0.48
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.49	0.48
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.95	0.48
3:C:207:ASN:HB2	3:C:208:PRO:CD	2.44	0.48
4:D:12:TRP:NE1	4:D:125:ASP:OD2	2.46	0.48
5:E:44:THR:HB	10:J:24:ILE:CD1	2.43	0.48
1:A:124:ASP:HA	1:A:127:ILE:HG22	1.94	0.48
3:C:24:PRO:C	3:C:26:ASN:N	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:GLU:OE1	10:J:57:HIS:HB3	2.14	0.48
3:C:324:LEU:N	3:C:324:LEU:HD23	2.29	0.48
4:D:68:VAL:HG12	4:D:69:GLU:H	1.77	0.48
5:E:72:SER:CB	5:E:91:TRP:CD1	2.93	0.48
1:A:360:LEU:HD23	1:A:360:LEU:HA	1.64	0.48
5:E:73:LYS:HG2	5:E:196:GLY:HA3	1.95	0.48
6:F:27:ASN:CA	6:F:81:THR:HG23	2.39	0.48
1:A:390:ILE:HB	1:A:395:TRP:CZ2	2.49	0.48
2:B:113:ARG:C	2:B:115:ASP:H	2.17	0.48
3:C:344:GLU:O	3:C:348:ILE:HG13	2.13	0.48
9:I:9:GLY:HA2	9:I:26:LEU:N	2.29	0.48
9:I:24:GLY:O	9:I:25:ALA:HB2	2.13	0.48
3:C:34:GLY:HA2	3:C:97:HIS:CE1	2.48	0.48
3:C:334:THR:OG1	7:G:55:PHE:HD2	1.97	0.47
1:A:37:VAL:HG21	1:A:106:LEU:HD11	1.95	0.47
1:A:149:VAL:HG21	1:A:252:HIS:CB	2.41	0.47
2:B:72:ALA:HB1	2:B:75:LEU:HG	1.94	0.47
3:C:359:PHE:O	3:C:363:LEU:HB2	2.13	0.47
1:A:90:SER:HB3	1:A:95:THR:HG23	1.96	0.47
3:C:140:PHE:CE1	3:C:170:VAL:HB	2.50	0.47
4:D:86:LYS:HD3	5:E:71:MET:HG3	1.96	0.47
1:A:22:GLY:HA3	1:A:193:PRO:HG3	1.97	0.47
2:B:243:GLU:OE2	2:B:435:PHE:O	2.33	0.47
4:D:70:VAL:O	4:D:71:GLN:HB3	2.15	0.47
1:A:35:CYS:HA	1:A:372:THR:HG21	1.95	0.47
3:C:240:MET:HA	3:C:240:MET:CE	2.45	0.47
9:I:41:PRO:HB3	9:I:44:ASP:HB2	1.97	0.47
1:A:49:SER:O	1:A:50:GLU:C	2.53	0.47
2:B:35:ILE:CD1	2:B:220:ALA:CB	2.86	0.47
3:C:253:PRO:HB3	4:D:118:ARG:O	2.15	0.47
5:E:94:LYS:HD2	5:E:138:VAL:HG21	1.96	0.47
1:A:309:THR:HA	1:A:322:ALA:HA	1.97	0.47
1:A:341:GLN:NE2	1:A:344:ARG:HH21	2.12	0.47
1:A:372:THR:OG1	2:B:373:GLU:OE1	2.21	0.47
2:B:158:HIS:CD2	2:B:158:HIS:H	2.31	0.47
2:B:368:TYR:O	2:B:371:SER:N	2.47	0.47
3:C:318:ARG:HB2	3:C:373:GLU:OE1	2.14	0.47
4:D:135:CYS:SG	4:D:136:GLU:N	2.88	0.47
1:A:346:CYS:SG	1:A:412:SER:HA	2.55	0.47
2:B:350:GLY:HA2	2:B:411:ILE:HD13	1.97	0.47
3:C:377:LEU:HD23	3:C:377:LEU:HA	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:171:PHE:CE1	4:D:177:ALA:HB2	2.38	0.47
3:C:48:GLY:HA2	3:C:83:HIS:CE1	2.50	0.47
6:F:21:TYR:CG	6:F:83:TYR:HD2	2.33	0.47
3:C:20:ASP:O	3:C:21:LEU:C	2.53	0.47
4:D:66:GLU:HA	4:D:84:PRO:O	2.15	0.47
1:A:8:LEU:HD22	1:A:392:LEU:HB3	1.97	0.46
1:A:284:TYR:OH	9:I:20:ARG:NE	2.43	0.46
3:C:131:TYR:HE1	15:C:1029:HOH:O	1.98	0.46
4:D:235:LEU:N	4:D:235:LEU:HD23	2.30	0.46
1:A:325:VAL:O	1:A:326:CYS:HB3	2.15	0.46
2:B:153:GLN:NE2	9:I:46:LYS:HD2	2.28	0.46
4:D:5:LEU:HG	4:D:6:HIS:N	2.29	0.46
4:D:131:LEU:HD11	12:D:242:HEM:HMB2	1.97	0.46
4:D:220:TYR:CE2	7:G:26:PHE:HE2	2.34	0.46
9:I:49:VAL:C	9:I:51:CYS:H	2.19	0.46
1:A:432:PRO:HB2	1:A:437:ILE:HG13	1.97	0.46
2:B:141:GLN:HB2	2:B:142:PRO:HD3	1.98	0.46
5:E:90:LYS:HE3	5:E:93:GLY:HA2	1.96	0.46
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.96	0.46
6:F:54:LEU:O	6:F:55:TYR:C	2.54	0.46
1:A:230:THR:HG22	1:A:231:LEU:H	1.81	0.46
2:B:332:SER:O	2:B:333:ALA:C	2.53	0.46
3:C:244:LEU:HD23	3:C:244:LEU:HA	1.71	0.46
3:C:337:TRP:CZ3	3:C:350:ILE:HD11	2.50	0.46
4:D:70:VAL:O	4:D:71:GLN:CB	2.63	0.46
6:F:43:VAL:HG22	6:F:94:LEU:HD11	1.96	0.46
10:J:13:LEU:HD23	10:J:19:THR:HB	1.97	0.46
10:J:19:THR:O	10:J:23:THR:HG22	2.16	0.46
1:A:279:HIS:HB2	9:I:20:ARG:NH2	2.31	0.46
3:C:21:LEU:HA	3:C:22:PRO:HD3	1.72	0.46
10:J:44:GLU:CG	10:J:52:TRP:CZ2	2.99	0.46
2:B:275:LEU:O	2:B:278:VAL:N	2.48	0.46
3:C:92:ILE:HD13	3:C:92:ILE:HA	1.84	0.46
4:D:138:PRO:HG3	8:H:58:LEU:HD22	1.97	0.46
5:E:54:VAL:O	5:E:58:PHE:HD1	1.99	0.46
3:C:8:HIS:CD2	3:C:11:MET:H	2.32	0.46
3:C:318:ARG:HA	3:C:319:PRO:HD3	1.81	0.46
3:C:337:TRP:HZ3	3:C:350:ILE:HD11	1.80	0.46
4:D:112:ASP:OD2	4:D:115:TYR:HE2	1.98	0.46
4:D:115:TYR:HD1	4:D:119:ALA:HB2	1.81	0.46
10:J:9:LEU:HD23	10:J:9:LEU:HA	1.72	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:48:ILE:O	11:K:48:ILE:HG22	2.16	0.46
1:A:85:HIS:HB2	1:A:100:LYS:HB3	1.98	0.46
1:A:308:GLN:HE21	1:A:323:HIS:HD2	1.63	0.46
1:A:351:GLU:HA	1:A:404:ALA:HB2	1.98	0.46
5:E:52:LYS:HD2	11:K:34:TRP:CE2	2.51	0.46
2:B:143:GLN:HE21	2:B:143:GLN:HB2	1.53	0.46
3:C:33:PHE:O	3:C:37:LEU:HD12	2.16	0.46
2:B:75:LEU:HD23	2:B:75:LEU:N	2.31	0.45
2:B:152:LEU:O	2:B:158:HIS:NE2	2.47	0.45
13:C:383:QNO:H242	13:C:383:QNO:H271	1.49	0.45
4:D:14:HIS:NE2	4:D:191:ARG:HD3	2.30	0.45
4:D:234:LYS:HD3	5:E:8:PRO:HB3	1.98	0.45
6:F:51:PRO:HB2	6:F:53:ASN:HD21	1.80	0.45
2:B:156:GLN:HE22	9:I:29:LEU:HB2	1.81	0.45
4:D:223:LYS:HD2	4:D:227:TRP:CD1	2.51	0.45
6:F:52:GLU:OE2	7:G:11:ARG:HD3	2.17	0.45
8:H:15:ASP:HA	8:H:16:PRO:HD3	1.85	0.45
3:C:36:LEU:HD23	3:C:36:LEU:HA	1.69	0.45
3:C:281:LEU:HB2	3:C:294:LEU:HB2	1.98	0.45
4:D:56:TYR:HD1	4:D:60:GLU:OE2	1.99	0.45
3:C:185:LEU:HD23	3:C:185:LEU:HA	1.83	0.45
2:B:343:GLN:HA	2:B:343:GLN:OE1	2.17	0.45
3:C:237:LEU:HD13	4:D:212:MET:HG2	1.99	0.45
10:J:29:LEU:HA	11:K:34:TRP:CD1	2.51	0.45
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.77	0.45
2:B:216:LEU:HD23	2:B:216:LEU:HA	1.78	0.45
3:C:132:VAL:HA	3:C:139:SER:HB3	1.99	0.45
4:D:5:LEU:CD1	8:H:63:HIS:HB2	2.46	0.45
4:D:27:ARG:HE	4:D:27:ARG:HB3	1.60	0.45
2:B:162:ASN:HD22	2:B:162:ASN:HA	1.57	0.45
2:B:209:LEU:HD11	2:B:378:PHE:HE2	1.81	0.45
5:E:176:ALA:HA	5:E:177:PRO:HD3	1.76	0.45
1:A:29:GLN:HG3	1:A:30:SER:N	2.32	0.45
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.54	0.45
1:A:240:GLN:HA	1:A:422:VAL:O	2.15	0.45
2:B:369:LEU:HA	2:B:369:LEU:HD23	1.70	0.45
2:B:439:LEU:HD23	2:B:439:LEU:HA	1.61	0.45
3:C:220:PHE:CE2	13:C:383:QNO:C61	2.97	0.45
3:C:286:ASN:HB3	3:C:289:GLY:HA3	1.99	0.45
4:D:211:MET:CE	10:J:31:PHE:CE2	2.88	0.45
4:D:224:ARG:HD3	4:D:224:ARG:HA	1.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:22:VAL:HG12	9:I:23:ALA:H	1.81	0.45
3:C:90:PHE:CE1	3:C:123:VAL:HG21	2.52	0.45
3:C:100:ARG:HD2	3:C:100:ARG:C	2.37	0.45
3:C:150:LEU:HB2	3:C:161:VAL:HG23	1.99	0.45
3:C:152:ALA:HB1	3:C:291:VAL:HG11	1.99	0.45
3:C:206:ASN:ND2	3:C:207:ASN:H	2.15	0.45
5:E:73:LYS:HA	5:E:195:VAL:O	2.17	0.45
9:I:26:LEU:C	9:I:27:ARG:HG3	2.37	0.45
1:A:291:SER:HB3	1:A:356:ARG:CZ	2.47	0.45
2:B:264:ILE:HD11	9:I:2:LEU:HA	1.99	0.45
2:B:345:LYS:HA	2:B:418:VAL:HG21	1.99	0.45
3:C:135:TRP:CH2	3:C:170:VAL:HG12	2.51	0.45
6:F:78:GLU:H	6:F:78:GLU:HG3	1.40	0.45
1:A:211:LEU:O	1:A:214:LYS:N	2.50	0.44
2:B:58:GLU:OE2	2:B:63:LEU:HA	2.17	0.44
3:C:115:ILE:O	3:C:119:LEU:N	2.47	0.44
9:I:5:ALA:C	9:I:7:ARG:H	2.19	0.44
1:A:86:LEU:HD13	1:A:99:ILE:HG12	1.99	0.44
2:B:58:GLU:CD	2:B:64:GLY:H	2.21	0.44
2:B:242:GLY:O	2:B:423:SER:HA	2.17	0.44
2:B:299:VAL:HG11	2:B:336:VAL:HG13	2.00	0.44
3:C:298:ILE:C	3:C:300:ILE:H	2.20	0.44
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.82	0.44
6:F:83:TYR:O	6:F:84:GLU:C	2.55	0.44
9:I:41:PRO:O	9:I:42:VAL:CG2	2.56	0.44
11:K:39:ARG:H	11:K:39:ARG:HG3	1.44	0.44
1:A:102:LEU:HD12	1:A:102:LEU:HA	1.67	0.44
3:C:104:TYR:CE2	3:C:208:PRO:HA	2.52	0.44
4:D:10:TYR:HB2	4:D:125:ASP:OD2	2.16	0.44
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.52	0.44
1:A:236:PHE:CG	1:A:258:GLU:HB2	2.53	0.44
1:A:292:SER:HA	1:A:293:PRO:HD3	1.81	0.44
1:A:329:MET:SD	7:G:5:GLY:HA3	2.57	0.44
2:B:83:PHE:CE2	2:B:87:ARG:HG3	2.53	0.44
2:B:120:MET:HE2	2:B:120:MET:HB2	1.79	0.44
3:C:324:LEU:HD13	3:C:365:LEU:HB3	1.99	0.44
4:D:21:LEU:HD13	4:D:192:TRP:HB2	2.00	0.44
5:E:19:LEU:HA	5:E:19:LEU:HD23	1.81	0.44
5:E:189:SER:OG	5:E:192:MET:HB2	2.18	0.44
6:F:77:LYS:HA	6:F:80:TRP:NE1	2.32	0.44
1:A:173:ASN:HB3	1:A:177:LEU:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ALA:CB	1:A:427:PRO:HD2	2.45	0.44
4:D:92:PRO:C	4:D:93:LYS:HG2	2.38	0.44
9:I:56:ARG:HB3	9:I:57:GLY:H	1.46	0.44
1:A:36:THR:O	1:A:199:ALA:HA	2.17	0.44
2:B:217:LYS:O	2:B:221:GLU:HG3	2.18	0.44
3:C:10:LEU:HA	3:C:10:LEU:HD23	1.77	0.44
3:C:110:LEU:HD23	3:C:110:LEU:HA	1.66	0.44
4:D:23:HIS:NE2	10:J:50:LYS:HG2	2.33	0.44
5:E:160:CYS:HB3	14:E:200:FES:S2	2.58	0.44
6:F:40:ASN:O	6:F:44:LYS:HB2	2.18	0.44
1:A:388:ARG:HH22	1:A:394:GLU:CD	2.16	0.44
2:B:143:GLN:O	2:B:143:GLN:HG3	2.17	0.44
3:C:90:PHE:O	3:C:90:PHE:CD1	2.66	0.44
4:D:161:ALA:O	4:D:163:PRO:HD3	2.18	0.44
2:B:40:ASN:C	2:B:42:ALA:H	2.20	0.44
3:C:33:PHE:O	3:C:37:LEU:HG	2.18	0.44
3:C:191:ALA:O	3:C:194:MET:HB2	2.18	0.44
4:D:203:ARG:O	4:D:206:LEU:HB3	2.18	0.44
5:E:65:SER:HB3	5:E:66:ALA:H	1.28	0.44
6:F:31:LEU:HD23	6:F:31:LEU:HA	1.73	0.44
2:B:176:LEU:HD23	9:I:13:PRO:HD3	1.99	0.44
4:D:164:ILE:HB	4:D:179:MET:SD	2.57	0.44
6:F:96:GLU:O	6:F:100:GLU:HG3	2.18	0.44
4:D:230:LEU:HD23	4:D:230:LEU:HA	1.78	0.43
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.49	0.43
2:B:73:SER:HB3	2:B:98:VAL:HG11	1.99	0.43
2:B:77:THR:HG23	2:B:85:ILE:HD11	1.98	0.43
4:D:10:TYR:HA	4:D:11:PRO:HD3	1.70	0.43
1:A:284:TYR:CE1	9:I:20:ARG:HG2	2.51	0.43
3:C:27:ILE:HA	3:C:208:PRO:HD3	1.99	0.43
10:J:20:PHE:O	10:J:24:ILE:HG23	2.17	0.43
1:A:48:GLU:HB2	1:A:52:ASN:HB3	2.00	0.43
1:A:412:SER:O	10:J:15:ARG:NH2	2.51	0.43
2:B:275:LEU:O	2:B:276:GLN:C	2.55	0.43
3:C:186:PRO:HA	3:C:189:ILE:HD12	1.99	0.43
3:C:276:PHE:HB3	3:C:336:THR:HG23	2.00	0.43
4:D:47:ALA:HA	4:D:90:TYR:HA	2.01	0.43
2:B:160:ILE:HD12	9:I:11:PHE:CE1	2.53	0.43
2:B:258:VAL:HG22	2:B:322:PHE:O	2.18	0.43
1:A:140:GLU:OE2	9:I:37:THR:N	2.50	0.43
2:B:258:VAL:HG13	2:B:259:ALA:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:ILE:HG21	3:C:196:HIS:HB2	2.01	0.43
3:C:122:THR:HG22	3:C:189:ILE:HG12	2.00	0.43
1:A:425:PHE:CD2	1:A:426:GLY:N	2.87	0.43
2:B:170:ASN:HB2	2:B:238:LYS:H	1.83	0.43
3:C:3:ASN:CG	3:C:4:ILE:N	2.71	0.43
9:I:34:VAL:CB	9:I:35:PRO:HD3	2.30	0.43
11:K:45:VAL:HG11	11:K:48:ILE:HD12	2.00	0.43
3:C:3:ASN:ND2	3:C:6:LYS:HG3	2.30	0.43
5:E:64:ALA:O	5:E:65:SER:HB2	2.17	0.43
6:F:89:TYR:C	6:F:89:TYR:CD2	2.91	0.43
2:B:310:SER:HB3	9:I:28:PRO:HG3	2.01	0.43
3:C:335:LEU:HG	3:C:354:ALA:HB1	2.00	0.43
1:A:180:ALA:O	1:A:184:GLU:HB2	2.19	0.43
1:A:403:ASP:OD1	1:A:406:VAL:HG23	2.19	0.43
2:B:176:LEU:CD2	9:I:13:PRO:CD	2.97	0.43
3:C:37:LEU:HD13	12:C:382:HEM:C4B	2.54	0.43
3:C:141:TRP:O	3:C:145:VAL:HG23	2.18	0.43
4:D:5:LEU:HD13	8:H:63:HIS:HB2	2.01	0.43
4:D:95:TYR:HA	4:D:96:PRO:HD3	1.90	0.43
4:D:134:TYR:CD1	4:D:162:PRO:HB3	2.54	0.43
4:D:137:PRO:HA	4:D:138:PRO:HD3	1.89	0.43
4:D:171:PHE:O	4:D:172:ASP:C	2.58	0.43
7:G:18:LEU:HB3	7:G:23:GLN:NE2	2.34	0.43
1:A:255:ILE:CG2	1:A:342:TRP:HH2	2.32	0.42
2:B:243:GLU:HB2	2:B:424:MET:O	2.19	0.42
5:E:157:TYR:HE1	5:E:162:GLY:HA2	1.82	0.42
2:B:322:PHE:CG	2:B:323:GLY:N	2.86	0.42
3:C:288:LEU:O	3:C:292:LEU:HB2	2.19	0.42
3:C:329:VAL:HG12	7:G:52:PHE:HZ	1.84	0.42
9:I:11:PHE:HZ	9:I:27:ARG:NE	2.17	0.42
1:A:429:GLU:HG2	7:G:5:GLY:H	1.85	0.42
2:B:176:LEU:HG	9:I:13:PRO:CG	2.38	0.42
3:C:335:LEU:HD23	3:C:335:LEU:HA	1.80	0.42
4:D:96:PRO:HB2	4:D:97:ASN:H	1.70	0.42
4:D:110:PRO:HA	12:D:242:HEM:C4D	2.54	0.42
9:I:18:THR:H	9:I:18:THR:HG22	1.51	0.42
9:I:42:VAL:HG22	9:I:43:LEU:HD23	2.01	0.42
2:B:156:GLN:HG3	2:B:325:TYR:OH	2.19	0.42
2:B:165:ALA:HA	2:B:173:ALA:HB1	2.00	0.42
3:C:48:GLY:CA	3:C:83:HIS:CE1	3.03	0.42
3:C:121:LEU:HA	3:C:124:MET:HE2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:VAL:HG13	3:C:143:ALA:HB2	2.01	0.42
4:D:22:ASP:O	4:D:26:ILE:HG13	2.19	0.42
2:B:385:GLN:NE2	2:B:393:THR:H	2.13	0.42
3:C:119:LEU:HD22	12:C:382:HEM:HBB2	2.02	0.42
3:C:322:GLN:O	3:C:326:TRP:CD1	2.72	0.42
5:E:71:MET:HB3	5:E:72:SER:H	1.61	0.42
6:F:82:LYS:HB2	6:F:85:GLU:HB3	2.02	0.42
1:A:34:THR:CG2	2:B:373:GLU:OE1	2.67	0.42
2:B:83:PHE:CZ	2:B:87:ARG:HG3	2.55	0.42
3:C:75:TYR:HD2	3:C:78:ILE:HD11	1.85	0.42
3:C:94:LEU:O	3:C:98:VAL:HG23	2.19	0.42
3:C:149:LEU:HD22	3:C:291:VAL:HG23	2.01	0.42
3:C:291:VAL:CG1	3:C:292:LEU:N	2.82	0.42
5:E:136:ILE:C	5:E:138:VAL:H	2.23	0.42
6:F:29:LEU:O	6:F:31:LEU:N	2.53	0.42
2:B:68:LEU:HD23	2:B:186:VAL:CG2	2.49	0.42
2:B:87:ARG:HA	2:B:87:ARG:HD3	1.76	0.42
2:B:113:ARG:C	2:B:115:ASP:N	2.72	0.42
2:B:332:SER:O	2:B:336:VAL:HG23	2.19	0.42
4:D:49:ARG:HA	4:D:52:VAL:HG23	2.02	0.42
4:D:232:SER:OG	7:G:23:GLN:OE1	2.33	0.42
6:F:64:ARG:NH1	6:F:64:ARG:CB	2.83	0.42
1:A:57:TYR:CE2	1:A:134:ILE:HG23	2.50	0.42
1:A:79:VAL:HG11	1:A:86:LEU:HB2	2.01	0.42
1:A:115:ASP:OD1	1:A:119:ASN:HB2	2.20	0.42
2:B:132:PHE:CD2	2:B:191:LEU:HD13	2.55	0.42
3:C:66:VAL:HA	3:C:69:ILE:HD12	2.02	0.42
3:C:75:TYR:CE2	5:E:57:GLN:HG2	2.54	0.42
3:C:246:ALA:HB1	3:C:249:LEU:HD12	2.02	0.42
4:D:128:PHE:CE2	4:D:132:THR:HG21	2.54	0.42
4:D:234:LYS:C	4:D:235:LEU:HD23	2.40	0.42
6:F:61:ARG:HH12	6:F:89:TYR:HE1	1.66	0.42
1:A:305:GLN:HG3	9:I:46:LYS:O	2.19	0.42
2:B:42:ALA:HA	2:B:43:PRO:HD3	1.88	0.42
2:B:204:MET:CE	2:B:224:LEU:HD22	2.50	0.42
5:E:60:SER:C	5:E:62:MET:H	2.24	0.42
3:C:94:LEU:HG	3:C:120:LEU:HD13	2.02	0.41
4:D:79:GLU:O	4:D:80:MET:CB	2.66	0.41
2:B:161:GLU:OE1	2:B:175:SER:OG	2.24	0.41
2:B:290:ASN:O	2:B:293:SER:HB3	2.20	0.41
3:C:119:LEU:HD11	3:C:193:ALA:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:156:ILE:O	3:C:157:GLY:C	2.58	0.41
4:D:218:LEU:HD22	5:E:39:VAL:HG13	2.02	0.41
3:C:171:ASP:HB3	3:C:172:LYS:H	1.61	0.41
4:D:83:ARG:NH2	4:D:89:ASP:OD2	2.54	0.41
1:A:360:LEU:CD2	2:B:93:GLY:HA2	2.50	0.41
2:B:42:ALA:O	2:B:113:ARG:NE	2.50	0.41
3:C:31:TRP:CD1	3:C:100:ARG:NH1	2.89	0.41
3:C:92:ILE:HD12	3:C:92:ILE:HG23	1.82	0.41
5:E:50:ALA:O	5:E:54:VAL:CG2	2.68	0.41
6:F:16:ILE:HD13	6:F:16:ILE:HA	1.95	0.41
10:J:22:LEU:CA	11:K:27:VAL:HG22	2.47	0.41
1:A:77:LYS:O	1:A:81:SER:HB2	2.21	0.41
1:A:272:VAL:O	1:A:276:ILE:HG13	2.21	0.41
2:B:308:ASP:OD2	9:I:31:GLN:HB2	2.21	0.41
2:B:385:GLN:HE22	2:B:393:THR:N	2.13	0.41
3:C:83:HIS:CD2	12:C:381:HEM:ND	2.89	0.41
4:D:116:ILE:HD13	4:D:116:ILE:HA	1.87	0.41
1:A:75:LEU:HD21	1:A:116:ILE:CG1	2.51	0.41
1:A:428:ILE:H	1:A:428:ILE:HG12	1.61	0.41
3:C:213:SER:C	3:C:215:VAL:N	2.73	0.41
4:D:137:PRO:HG3	4:D:149:PHE:HB2	2.02	0.41
9:I:44:ASP:O	9:I:45:LEU:C	2.59	0.41
1:A:363:ASN:O	1:A:367:SER:HB2	2.20	0.41
2:B:25:GLU:O	2:B:36:ALA:HA	2.20	0.41
2:B:55:SER:O	2:B:58:GLU:HG3	2.20	0.41
2:B:327:ILE:HG21	2:B:327:ILE:HD13	1.71	0.41
3:C:75:TYR:CD2	3:C:78:ILE:HD11	2.55	0.41
3:C:240:MET:HB3	4:D:208:MET:HG3	2.01	0.41
3:C:311:LYS:HE3	3:C:311:LYS:HB3	1.85	0.41
4:D:152:TYR:OH	8:H:66:ASP:OD2	2.35	0.41
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.80	0.41
5:E:160:CYS:HB3	5:E:161:HIS:ND1	2.36	0.41
7:G:73:ASN:HB3	7:G:74:PRO:CD	2.36	0.41
1:A:113:LEU:HA	1:A:113:LEU:HD12	1.63	0.41
2:B:154:ASN:O	2:B:155:PRO:C	2.59	0.41
3:C:8:HIS:HB3	3:C:11:MET:HB2	2.03	0.41
4:D:29:GLY:HA3	4:D:185:ASP:O	2.20	0.41
9:I:5:ALA:O	9:I:8:SER:N	2.49	0.41
9:I:30:VAL:C	9:I:32:ALA:H	2.24	0.41
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.96	0.41
1:A:419:CYS:HA	1:A:420:PRO:HD3	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:GLU:O	2:B:39:GLU:HG3	2.21	0.41
2:B:178:CYS:SG	2:B:182:ARG:HB2	2.61	0.41
2:B:209:LEU:HD11	2:B:378:PHE:CE2	2.56	0.41
2:B:354:ASN:HB3	2:B:355:PRO:HD2	2.02	0.41
2:B:375:SER:O	2:B:376:GLU:C	2.60	0.41
3:C:122:THR:HG22	3:C:189:ILE:CG1	2.50	0.41
4:D:232:SER:HB3	5:E:13:TYR:CD1	2.55	0.41
9:I:42:VAL:O	9:I:43:LEU:CB	2.69	0.41
2:B:176:LEU:HA	2:B:176:LEU:HD12	1.43	0.41
4:D:164:ILE:HG23	4:D:182:VAL:HG13	2.03	0.41
6:F:101:ARG:HA	6:F:104:ARG:CZ	2.51	0.41
1:A:207:GLN:O	1:A:211:LEU:HG	2.21	0.40
2:B:253:VAL:CG2	2:B:330:ALA:HA	2.50	0.40
3:C:107:TYR:CD1	3:C:107:TYR:N	2.89	0.40
3:C:234:LEU:CD2	4:D:216:LEU:HD21	2.51	0.40
4:D:164:ILE:HG23	4:D:182:VAL:CG1	2.51	0.40
1:A:133:VAL:HG12	1:A:134:ILE:N	2.36	0.40
2:B:256:ALA:O	2:B:424:MET:HA	2.22	0.40
2:B:366:ALA:O	2:B:370:MET:HB2	2.20	0.40
2:B:368:TYR:O	2:B:371:SER:HB3	2.22	0.40
5:E:81:ILE:HA	5:E:82:PRO:HD2	1.91	0.40
1:A:18:GLN:HE21	1:A:18:GLN:HB2	1.74	0.40
2:B:213:HIS:N	2:B:214:PRO:CD	2.84	0.40
4:D:156:GLN:HE21	4:D:156:GLN:HB2	1.43	0.40
1:A:146:ARG:NH1	1:A:308:GLN:NE2	2.68	0.40
1:A:363:ASN:O	1:A:367:SER:CB	2.69	0.40
5:E:134:ILE:O	5:E:183:PRO:HD2	2.21	0.40
9:I:39:GLU:HB3	9:I:40:SER:H	1.58	0.40
3:C:51:LEU:HD12	3:C:51:LEU:HA	1.99	0.40
3:C:236:ILE:HD13	3:C:236:ILE:HA	1.76	0.40
13:C:383:QNO:H3	15:C:1010:HOH:O	2.13	0.40
5:E:45:VAL:O	5:E:48:ALA:HB3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ARG:NH1	2:B:437:ASP:OD2[10_665]	1.98	0.22

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/446 (100%)	376 (85%)	53 (12%)	15 (3%)	3	24
2	B	421/439 (96%)	373 (89%)	39 (9%)	9 (2%)	7	37
3	C	376/379 (99%)	302 (80%)	56 (15%)	18 (5%)	2	17
4	D	239/241 (99%)	181 (76%)	38 (16%)	20 (8%)	1	5
5	E	194/196 (99%)	160 (82%)	29 (15%)	5 (3%)	5	31
6	F	103/110 (94%)	84 (82%)	17 (16%)	2 (2%)	8	39
7	G	73/81 (90%)	62 (85%)	5 (7%)	6 (8%)	1	5
8	H	68/78 (87%)	50 (74%)	12 (18%)	6 (9%)	1	4
9	I	55/57 (96%)	25 (46%)	16 (29%)	14 (26%)	0	0
10	J	59/62 (95%)	44 (75%)	11 (19%)	4 (7%)	1	9
11	K	51/56 (91%)	38 (74%)	11 (22%)	2 (4%)	3	22
All	All	2083/2145 (97%)	1695 (81%)	287 (14%)	101 (5%)	2	17

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
2	B	266	SER
2	B	305	GLN
2	B	353	SER
2	B	436	ILE
3	C	3	ASN
3	C	221	HIS
3	C	345	HIS
4	D	71	GLN
4	D	76	GLU
4	D	80	MET
4	D	93	LYS
4	D	96	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	121	HIS
4	D	169	LEU
4	D	172	ASP
5	E	65	SER
5	E	69	LEU
5	E	72	SER
7	G	2	ARG
7	G	28	HIS
7	G	73	ASN
8	H	12	GLU
8	H	27	LEU
8	H	28	GLU
8	H	73	LEU
8	H	74	PHE
9	I	3	SER
9	I	4	VAL
9	I	29	LEU
9	I	39	GLU
9	I	40	SER
9	I	45	LEU
9	I	53	GLU
9	I	56	ARG
10	J	51	LEU
11	K	52	PHE
1	A	72	GLY
1	A	220	SER
1	A	223	TYR
1	A	224	ASP
2	B	60	SER
2	B	354	ASN
3	C	4	ILE
3	C	158	THR
4	D	54	VAL
6	F	30	GLY
8	H	26	GLN
1	A	21	ASN
1	A	71	PRO
1	A	315	ALA
2	B	228	GLY
3	C	157	GLY
3	C	263	ASN
3	C	347	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	355	SER
3	C	378	LYS
4	D	171	PHE
5	E	64	ALA
7	G	3	GLN
7	G	31	SER
9	I	37	THR
9	I	51	CYS
10	J	2	ALA
10	J	18	SER
10	J	48	GLU
1	A	159	GLN
1	A	306	SER
2	B	41	TYR
3	C	73	VAL
3	C	258	PRO
3	C	264	THR
3	C	299	LEU
4	D	38	SER
4	D	94	PRO
4	D	146	GLY
4	D	198	HIS
5	E	113	GLU
6	F	7	SER
7	G	27	PRO
9	I	43	LEU
9	I	48	SER
1	A	107	PRO
1	A	192	ALA
3	C	110	LEU
3	C	159	ASN
4	D	166	ASN
1	A	77	LYS
1	A	183	THR
4	D	154	PRO
4	D	163	PRO
4	D	168	VAL
9	I	34	VAL
11	K	48	ILE
2	B	431	GLY
3	C	268	ILE
3	C	170	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	107	GLY
4	D	123	GLY
1	A	428	ILE
9	I	24	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	370/370 (100%)	322 (87%)	48 (13%)	4 19
2	B	332/343 (97%)	285 (86%)	47 (14%)	3 15
3	C	326/327 (100%)	272 (83%)	54 (17%)	2 10
4	D	206/206 (100%)	172 (84%)	34 (16%)	2 10
5	E	168/168 (100%)	155 (92%)	13 (8%)	13 44
6	F	96/98 (98%)	76 (79%)	20 (21%)	1 6
7	G	66/71 (93%)	57 (86%)	9 (14%)	3 17
8	H	67/74 (90%)	56 (84%)	11 (16%)	2 11
9	I	44/44 (100%)	31 (70%)	13 (30%)	0 1
10	J	46/52 (88%)	36 (78%)	10 (22%)	1 5
11	K	42/46 (91%)	32 (76%)	10 (24%)	0 3
All	All	1763/1799 (98%)	1494 (85%)	269 (15%)	2 13

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	23	LEU
1	A	25	VAL
1	A	31	SER
1	A	32	GLN
1	A	34	THR
1	A	45	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	52	ASN
1	A	53	ASN
1	A	58	PHE
1	A	75	LEU
1	A	108	LYS
1	A	113	LEU
1	A	117	VAL
1	A	122	LEU
1	A	125	SER
1	A	127	ILE
1	A	131	ARG
1	A	137	GLU
1	A	143	THR
1	A	149	VAL
1	A	171	SER
1	A	175	ARG
1	A	177	LEU
1	A	184	GLU
1	A	186	LEU
1	A	188	ARG
1	A	191	LYS
1	A	203	LEU
1	A	208	LEU
1	A	223	TYR
1	A	235	ARG
1	A	244	ARG
1	A	245	GLU
1	A	274	ASN
1	A	300	THR
1	A	308	GLN
1	A	323	HIS
1	A	382	SER
1	A	389	ARG
1	A	398	ARG
1	A	403	ASP
1	A	408	ARG
1	A	418	GLN
1	A	428	ILE
1	A	430	GLN
1	A	438	ARG
1	A	443	TRP
2	B	17	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	24	LEU
2	B	38	LEU
2	B	40	ASN
2	B	69	LEU
2	B	75	LEU
2	B	92	VAL
2	B	98	VAL
2	B	99	THR
2	B	108	THR
2	B	110	GLU
2	B	113	ARG
2	B	123	LEU
2	B	127	THR
2	B	142	PRO
2	B	143	GLN
2	B	158	HIS
2	B	163	LEU
2	B	176	LEU
2	B	186	VAL
2	B	189	VAL
2	B	197	ASN
2	B	227	ARG
2	B	232	LEU
2	B	243	GLU
2	B	248	ASN
2	B	257	LEU
2	B	273	SER
2	B	284	HIS
2	B	289	SER
2	B	292	THR
2	B	305	GLN
2	B	346	THR
2	B	358	GLN
2	B	370	MET
2	B	371	SER
2	B	373	GLU
2	B	374	SER
2	B	387	LEU
2	B	391	SER
2	B	397	THR
2	B	401	GLN
2	B	415	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	421	ARG
2	B	424	MET
2	B	435	PHE
2	B	436	ILE
3	C	4	ILE
3	C	21	LEU
3	C	27	ILE
3	C	43	LEU
3	C	45	ILE
3	C	46	LEU
3	C	51	LEU
3	C	53	MET
3	C	58	ASP
3	C	67	THR
3	C	70	CYS
3	C	78	ILE
3	C	80	ARG
3	C	90	PHE
3	C	92	ILE
3	C	96	MET
3	C	114	ASN
3	C	118	ILE
3	C	124	MET
3	C	131	TYR
3	C	135	TRP
3	C	144	THR
3	C	165	TRP
3	C	171	ASP
3	C	175	LEU
3	C	177	ARG
3	C	185	LEU
3	C	197	LEU
3	C	202	GLU
3	C	212	SER
3	C	225	THR
3	C	226	ILE
3	C	241	LEU
3	C	243	VAL
3	C	244	LEU
3	C	249	LEU
3	C	252	ASP
3	C	254	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	263	ASN
3	C	264	THR
3	C	267	HIS
3	C	281	LEU
3	C	309	THR
3	C	311	LYS
3	C	316	MET
3	C	320	LEU
3	C	328	LEU
3	C	333	LEU
3	C	336	THR
3	C	349	THR
3	C	350	ILE
3	C	365	LEU
3	C	366	MET
3	C	379	TRP
4	D	9	SER
4	D	17	LEU
4	D	36	VAL
4	D	37	CYS
4	D	42	SER
4	D	43	MET
4	D	55	CYS
4	D	79	GLU
4	D	80	MET
4	D	88	SER
4	D	93	LYS
4	D	95	TYR
4	D	112	ASP
4	D	113	LEU
4	D	114	SER
4	D	120	ARG
4	D	121	HIS
4	D	132	THR
4	D	135	CYS
4	D	139	THR
4	D	141	VAL
4	D	156	GLN
4	D	158	ILE
4	D	164	ILE
4	D	165	TYR
4	D	175	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	179	MET
4	D	191	ARG
4	D	211	MET
4	D	216	LEU
4	D	223	LYS
4	D	224	ARG
4	D	226	LYS
4	D	241	LYS
5	E	6	LYS
5	E	22	THR
5	E	24	SER
5	E	25	SER
5	E	27	GLU
5	E	28	SER
5	E	44	THR
5	E	54	VAL
5	E	79	SER
5	E	113	GLU
5	E	144	CYS
5	E	160	CYS
5	E	188	THR
6	F	10	SER
6	F	22	ASN
6	F	27	ASN
6	F	33	ARG
6	F	37	ILE
6	F	44	LYS
6	F	47	ILE
6	F	53	ASN
6	F	59	VAL
6	F	64	ARG
6	F	73	GLN
6	F	74	ILE
6	F	77	LYS
6	F	78	GLU
6	F	81	THR
6	F	85	GLU
6	F	86	ASP
6	F	90	LEU
6	F	105	GLU
6	F	110	LYS
7	G	2	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	3	GLN
7	G	31	SER
7	G	34	ILE
7	G	37	VAL
7	G	39	ARG
7	G	41	THR
7	G	45	ILE
7	G	63	THR
8	H	9	GLU
8	H	15	ASP
8	H	18	THR
8	H	19	THR
8	H	37	LEU
8	H	39	LEU
8	H	48	SER
8	H	51	GLU
8	H	65	ARG
8	H	68	CYS
8	H	76	SER
9	I	8	SER
9	I	15	LEU
9	I	16	SER
9	I	18	THR
9	I	20	ARG
9	I	26	LEU
9	I	27	ARG
9	I	30	VAL
9	I	37	THR
9	I	43	LEU
9	I	47	ARG
9	I	51	CYS
9	I	56	ARG
10	J	1	VAL
10	J	4	THR
10	J	5	LEU
10	J	6	THR
10	J	16	ARG
10	J	18	SER
10	J	23	THR
10	J	24	ILE
10	J	36	ASP
10	J	45	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	12	GLN
11	K	13	LEU
11	K	15	ARG
11	K	18	VAL
11	K	23	LEU
11	K	24	TRP
11	K	34	TRP
11	K	41	ILE
11	K	44	TRP
11	K	52	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	53	ASN
1	A	85	HIS
1	A	119	ASN
1	A	126	GLN
1	A	136	GLN
1	A	141	ASN
1	A	173	ASN
1	A	189	HIS
1	A	252	HIS
1	A	271	GLN
1	A	274	ASN
1	A	305	GLN
1	A	308	GLN
1	A	323	HIS
1	A	341	GLN
1	A	359	ASN
1	A	363	ASN
1	A	368	HIS
1	A	418	GLN
2	B	20	HIS
2	B	125	ASN
2	B	143	GLN
2	B	153	GLN
2	B	162	ASN
2	B	170	ASN
2	B	174	ASN
2	B	197	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	248	ASN
2	B	270	ASN
2	B	342	ASN
2	B	343	GLN
2	B	362	ASN
2	B	385	GLN
3	C	3	ASN
3	C	8	HIS
3	C	26	ASN
3	C	68	HIS
3	C	85	ASN
3	C	114	ASN
3	C	206	ASN
3	C	322	GLN
3	C	345	HIS
3	C	352	GLN
4	D	71	GLN
4	D	105	ASN
4	D	156	GLN
4	D	166	ASN
5	E	53	ASN
5	E	57	GLN
6	F	53	ASN
6	F	72	GLN
9	I	31	GLN
11	K	12	GLN
11	K	16	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
14	FES	E	200	5	0,4,4	-	-	-		
12	HEM	C	382	3	41,50,50	2.96	18 (43%)	45,82,82	2.54	14 (31%)
12	HEM	C	381	3	41,50,50	2.88	20 (48%)	45,82,82	2.75	19 (42%)
13	QNO	C	383	-	22,22,22	2.62	3 (13%)	20,28,28	1.35	4 (20%)
12	HEM	D	242	4	41,50,50	3.07	20 (48%)	45,82,82	2.80	24 (53%)

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
14	FES	E	200	5	-	-	0/1/1/1
12	HEM	C	382	3	-	9/12/54/54	-
12	HEM	C	381	3	-	7/12/54/54	-
13	QNO	C	383	-	1/1/0/0	7/9/9/9	0/2/2/2
12	HEM	D	242	4	-	4/12/54/54	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	383	QNO	OH-N1	-10.50	1.24	1.38
12	C	382	HEM	C4D-C3D	-7.67	1.31	1.45
12	C	382	HEM	C1B-C2B	-6.89	1.31	1.44
12	C	381	HEM	C4D-C3D	-6.77	1.33	1.45
12	D	242	HEM	C1B-C2B	-6.76	1.31	1.44
12	D	242	HEM	C4D-C3D	-6.54	1.33	1.45
12	C	382	HEM	C1D-C2D	-6.19	1.32	1.44
12	C	381	HEM	C3C-C2C	-6.16	1.31	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	242	HEM	C1D-C2D	-5.88	1.33	1.44
12	D	242	HEM	C3B-C4B	-5.81	1.33	1.44
12	D	242	HEM	C3C-C2C	-5.62	1.32	1.40
12	D	242	HEM	CHA-C4D	5.21	1.48	1.35
12	C	381	HEM	CHB-C1B	5.14	1.48	1.35
12	D	242	HEM	CHB-C1B	5.11	1.48	1.35
12	C	382	HEM	CHA-C4D	5.05	1.47	1.35
12	C	381	HEM	C1D-C2D	-5.04	1.34	1.44
12	C	382	HEM	C3B-C4B	-5.01	1.34	1.44
12	C	381	HEM	CHA-C4D	5.01	1.47	1.35
12	C	381	HEM	C3B-C4B	-4.91	1.35	1.44
12	D	242	HEM	CBB-CAB	4.65	1.53	1.30
12	C	382	HEM	CHB-C1B	4.55	1.46	1.35
12	C	382	HEM	C3C-C2C	-4.47	1.34	1.40
12	C	381	HEM	CBB-CAB	4.34	1.51	1.30
12	C	382	HEM	CBB-CAB	4.28	1.51	1.30
12	C	381	HEM	C1B-C2B	-4.26	1.36	1.44
12	D	242	HEM	C2C-C1C	-4.00	1.33	1.42
13	C	383	QNO	O41-C4	-3.93	1.25	1.36
12	D	242	HEM	CBC-CAC	3.74	1.54	1.29
12	C	382	HEM	C2C-C1C	-3.65	1.34	1.42
12	C	381	HEM	CHC-C4B	3.61	1.51	1.41
12	C	381	HEM	C2C-C1C	-3.55	1.34	1.42
12	C	381	HEM	CBC-CAC	3.49	1.52	1.29
12	C	382	HEM	CHC-C4B	3.48	1.51	1.41
12	C	382	HEM	CBC-CAC	3.42	1.52	1.29
12	D	242	HEM	C2A-C3A	3.33	1.47	1.37
12	C	381	HEM	C2A-C3A	3.30	1.47	1.37
12	C	382	HEM	C4A-CHB	3.20	1.49	1.41
12	D	242	HEM	CHC-C4B	3.08	1.50	1.41
12	C	381	HEM	C4A-CHB	3.08	1.49	1.41
12	C	382	HEM	C1A-CHA	3.01	1.49	1.41
13	C	383	QNO	C6-N1	-2.95	1.33	1.39
12	D	242	HEM	C3B-C2B	-2.94	1.31	1.37
12	D	242	HEM	C4A-CHB	2.90	1.49	1.41
12	D	242	HEM	CHD-C1D	2.89	1.49	1.41
12	C	381	HEM	C1A-CHA	2.84	1.48	1.41
12	D	242	HEM	C1A-CHA	2.77	1.48	1.41
12	D	242	HEM	C3D-C2D	-2.72	1.30	1.36
12	C	382	HEM	CHD-C1D	2.66	1.48	1.41
12	C	381	HEM	C4B-NB	2.61	1.44	1.38
12	C	381	HEM	C3D-C2D	-2.57	1.31	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	242	HEM	C3C-CAC	2.49	1.52	1.47
12	C	381	HEM	CHD-C1D	2.47	1.48	1.41
12	C	382	HEM	C3B-C2B	-2.43	1.32	1.37
12	D	242	HEM	O2A-CGA	-2.43	1.22	1.30
12	C	381	HEM	O2A-CGA	-2.35	1.22	1.30
12	D	242	HEM	O2D-CGD	-2.35	1.22	1.30
12	C	381	HEM	C1B-NB	2.21	1.44	1.40
12	C	382	HEM	O2D-CGD	-2.18	1.23	1.30
12	C	382	HEM	C2A-C3A	2.14	1.44	1.37
12	C	381	HEM	O2D-CGD	-2.10	1.23	1.30
12	C	382	HEM	O2A-CGA	-2.09	1.23	1.30

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	382	HEM	C4C-CHD-C1D	-10.36	108.88	122.56
12	D	242	HEM	C4B-CHC-C1C	-8.06	111.92	122.56
12	D	242	HEM	C4C-CHD-C1D	-7.62	112.50	122.56
12	C	382	HEM	C4B-CHC-C1C	-7.50	112.66	122.56
12	C	381	HEM	C4B-CHC-C1C	-7.47	112.70	122.56
12	C	381	HEM	C4C-CHD-C1D	-7.16	113.11	122.56
12	D	242	HEM	C4D-ND-C1D	-5.39	99.51	105.07
12	D	242	HEM	C1B-NB-C4B	-5.24	99.66	105.07
12	C	381	HEM	C4B-C3B-C2B	5.03	111.11	107.11
12	C	381	HEM	C4D-ND-C1D	-5.00	99.91	105.07
12	C	381	HEM	CHC-C4B-NB	4.61	129.44	124.43
12	C	381	HEM	CBB-CAB-C3B	-4.61	104.69	127.62
12	D	242	HEM	CHB-C1B-NB	4.26	129.65	124.38
12	C	381	HEM	C2C-C3C-C4C	4.23	109.85	106.90
12	C	382	HEM	C1B-NB-C4B	-4.03	100.91	105.07
12	C	382	HEM	C3B-C2B-C1B	3.91	109.39	106.49
12	C	381	HEM	C1B-NB-C4B	-3.89	101.06	105.07
12	C	381	HEM	CBA-CAA-C2A	-3.81	106.12	112.62
13	C	383	QNO	O41-C4-C5	3.55	120.75	116.31
12	C	382	HEM	CAA-CBA-CGA	-3.48	104.02	113.76
12	D	242	HEM	CHC-C4B-NB	3.29	128.00	124.43
12	C	381	HEM	CHA-C4D-ND	3.26	128.41	124.38
12	D	242	HEM	CHD-C1D-ND	3.21	127.92	124.43
12	C	381	HEM	CHA-C4D-C3D	-3.17	119.38	125.33
12	D	242	HEM	C3B-C2B-C1B	3.07	108.77	106.49
12	D	242	HEM	C2C-C3C-C4C	3.07	109.04	106.90
12	D	242	HEM	CHB-C1B-C2B	-3.00	118.43	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	242	HEM	C4B-C3B-C2B	2.91	109.43	107.11
12	C	382	HEM	CHA-C4D-ND	2.90	127.96	124.38
12	D	242	HEM	CBB-CAB-C3B	-2.89	113.26	127.62
12	C	382	HEM	CHB-C1B-NB	2.88	127.94	124.38
12	C	381	HEM	CHB-C1B-NB	2.73	127.75	124.38
12	D	242	HEM	C4A-C3A-C2A	-2.72	105.11	107.00
12	C	381	HEM	C4A-C3A-C2A	-2.71	105.11	107.00
12	D	242	HEM	CHD-C1D-C2D	-2.54	121.00	124.98
13	C	383	QNO	C3-C2-N1	2.48	121.67	118.94
12	D	242	HEM	CAD-CBD-CGD	-2.48	108.27	113.60
12	C	382	HEM	CHD-C1D-ND	2.44	127.09	124.43
13	C	383	QNO	C51-C5-C6	2.44	120.83	118.17
12	D	242	HEM	C1D-C2D-C3D	2.43	109.51	106.96
12	D	242	HEM	CAD-C3D-C2D	-2.38	123.44	127.88
12	C	382	HEM	CBB-CAB-C3B	-2.38	115.80	127.62
12	D	242	HEM	CHA-C4D-C3D	-2.36	120.90	125.33
12	C	381	HEM	CMB-C2B-C1B	2.34	128.61	125.04
12	C	382	HEM	CAD-CBD-CGD	-2.33	108.59	113.60
12	C	382	HEM	CMC-C2C-C3C	2.30	128.98	124.68
12	C	382	HEM	CHB-C1B-C2B	-2.29	120.39	126.72
12	D	242	HEM	CMA-C3A-C2A	2.27	129.22	124.94
12	D	242	HEM	CAA-CBA-CGA	-2.26	107.43	113.76
12	C	381	HEM	CHD-C1D-ND	2.23	126.86	124.43
12	C	382	HEM	C4D-ND-C1D	-2.23	102.77	105.07
12	D	242	HEM	CHA-C4D-ND	2.23	127.13	124.38
12	C	381	HEM	CHC-C4B-C3B	-2.22	121.17	124.57
13	C	383	QNO	C3-C4-C5	-2.20	117.90	120.52
12	D	242	HEM	O2D-CGD-CBD	2.19	121.08	114.03
12	C	381	HEM	CHB-C1B-C2B	-2.09	120.95	126.72
12	D	242	HEM	O2A-CGA-CBA	2.06	120.64	114.03
12	C	381	HEM	O2D-CGD-CBD	2.05	120.61	114.03
12	C	382	HEM	C4B-C3B-C2B	2.04	108.73	107.11
12	C	381	HEM	CHD-C1D-C2D	-2.02	121.82	124.98
12	D	242	HEM	CAD-C3D-C4D	2.01	128.17	124.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	C	383	QNO	C2

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	381	HEM	C2B-C3B-CAB-CBB
12	C	381	HEM	C4B-C3B-CAB-CBB
12	C	382	HEM	C1A-C2A-CAA-CBA
12	C	382	HEM	C3A-C2A-CAA-CBA
12	C	382	HEM	C2B-C3B-CAB-CBB
12	C	382	HEM	C4B-C3B-CAB-CBB
13	C	383	QNO	C24-C25-C26-C27
13	C	383	QNO	C2-C21-C22-C23
13	C	383	QNO	C21-C22-C23-C24
13	C	383	QNO	C23-C24-C25-C26
13	C	383	QNO	C22-C23-C24-C25
12	C	381	HEM	C3D-CAD-CBD-CGD
13	C	383	QNO	C26-C27-C28-C29
12	D	242	HEM	C2B-C3B-CAB-CBB
13	C	383	QNO	C25-C26-C27-C28
12	C	381	HEM	CAD-CBD-CGD-O2D
12	D	242	HEM	CAD-CBD-CGD-O1D
12	C	382	HEM	C3D-CAD-CBD-CGD
12	C	381	HEM	C4D-C3D-CAD-CBD
12	D	242	HEM	CAD-CBD-CGD-O2D
12	C	381	HEM	CAD-CBD-CGD-O1D
12	C	381	HEM	C2D-C3D-CAD-CBD
12	C	382	HEM	CAA-CBA-CGA-O1A
12	C	382	HEM	CAA-CBA-CGA-O2A
12	D	242	HEM	C4B-C3B-CAB-CBB
12	C	382	HEM	CAD-CBD-CGD-O2D
12	C	382	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

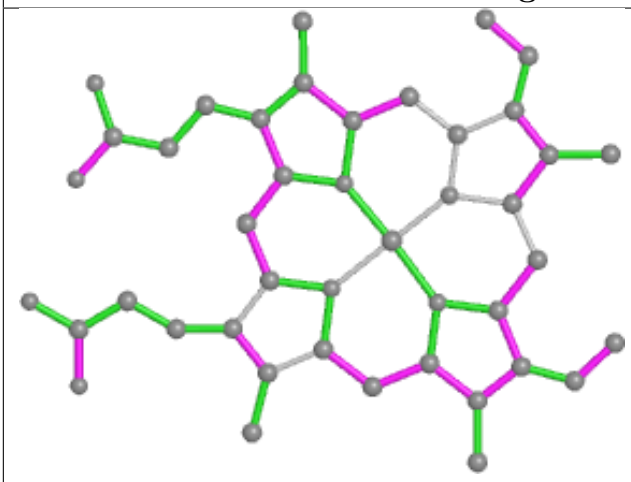
5 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	E	200	FES	2	0
12	C	382	HEM	14	0
12	C	381	HEM	7	0
13	C	383	QNO	6	0
12	D	242	HEM	5	0

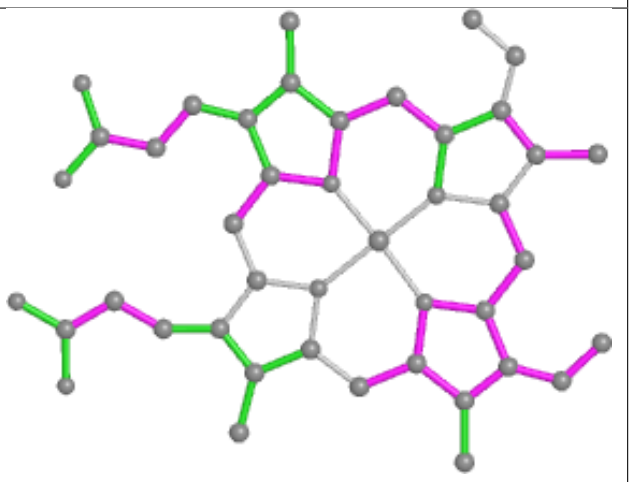
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

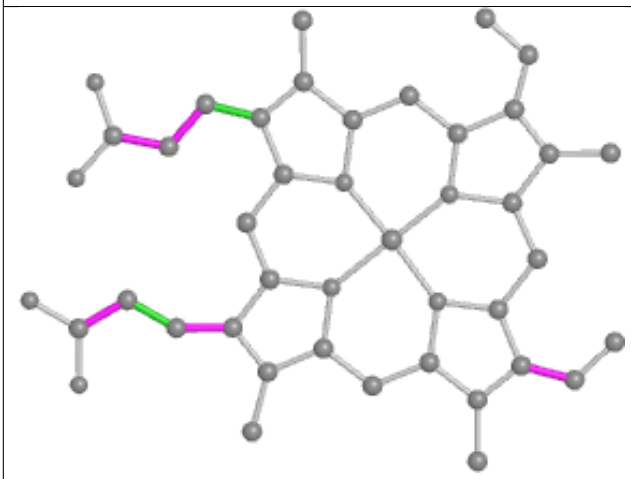
Ligand HEM C 382



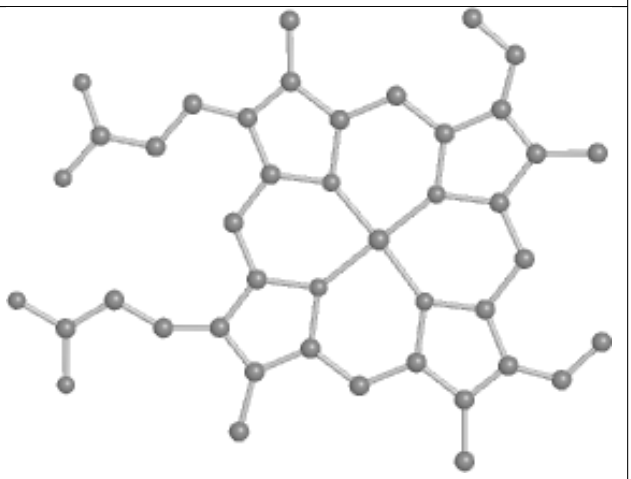
Bond lengths



Bond angles

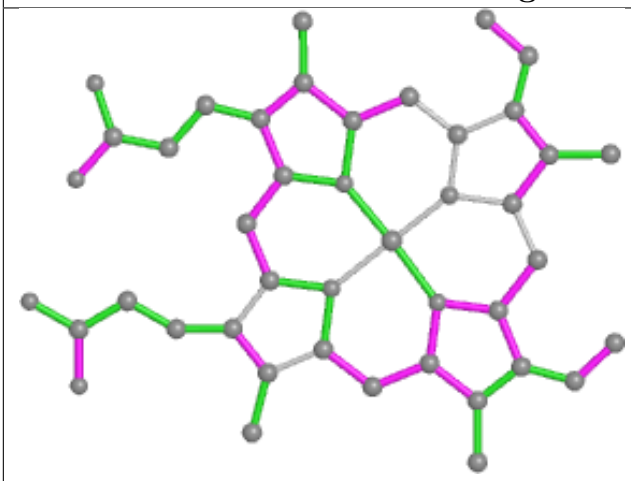


Torsions

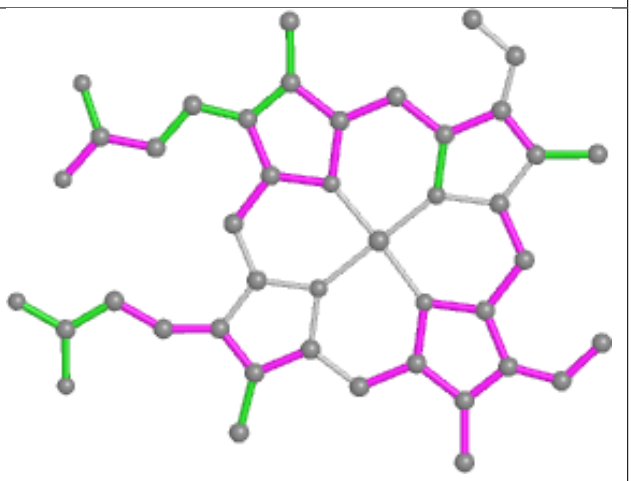


Rings

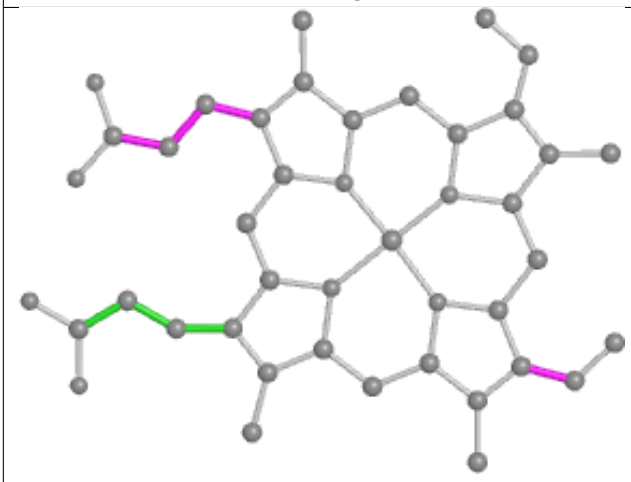
Ligand HEM C 381



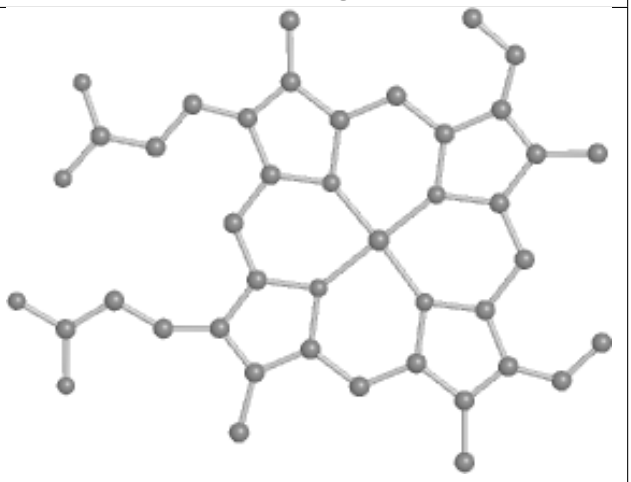
Bond lengths



Bond angles

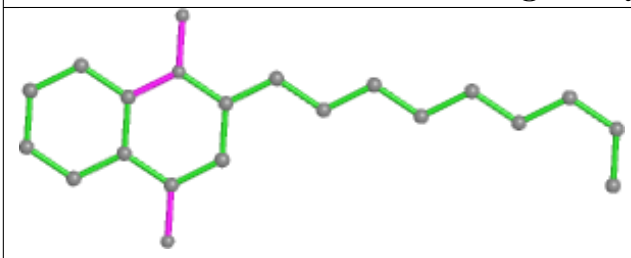


Torsions

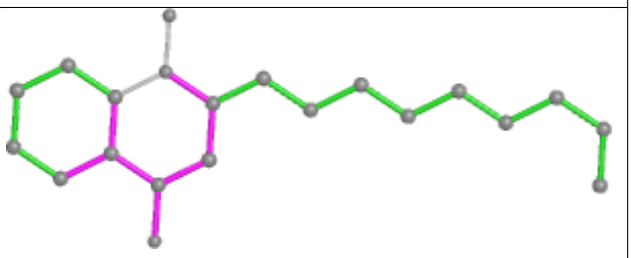


Rings

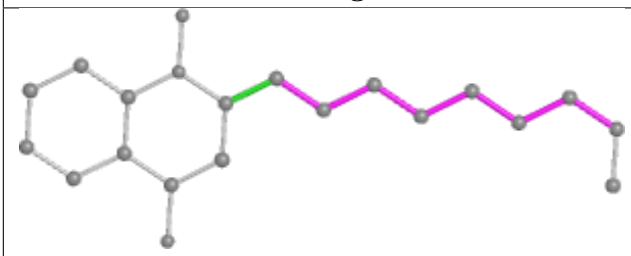
Ligand QNO C 383



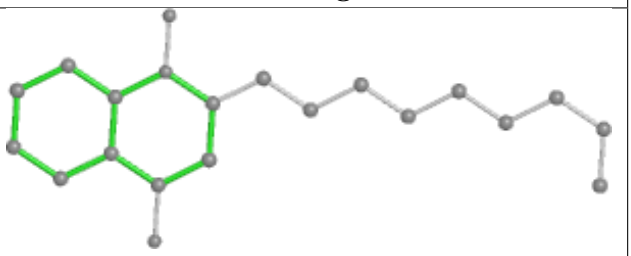
Bond lengths



Bond angles

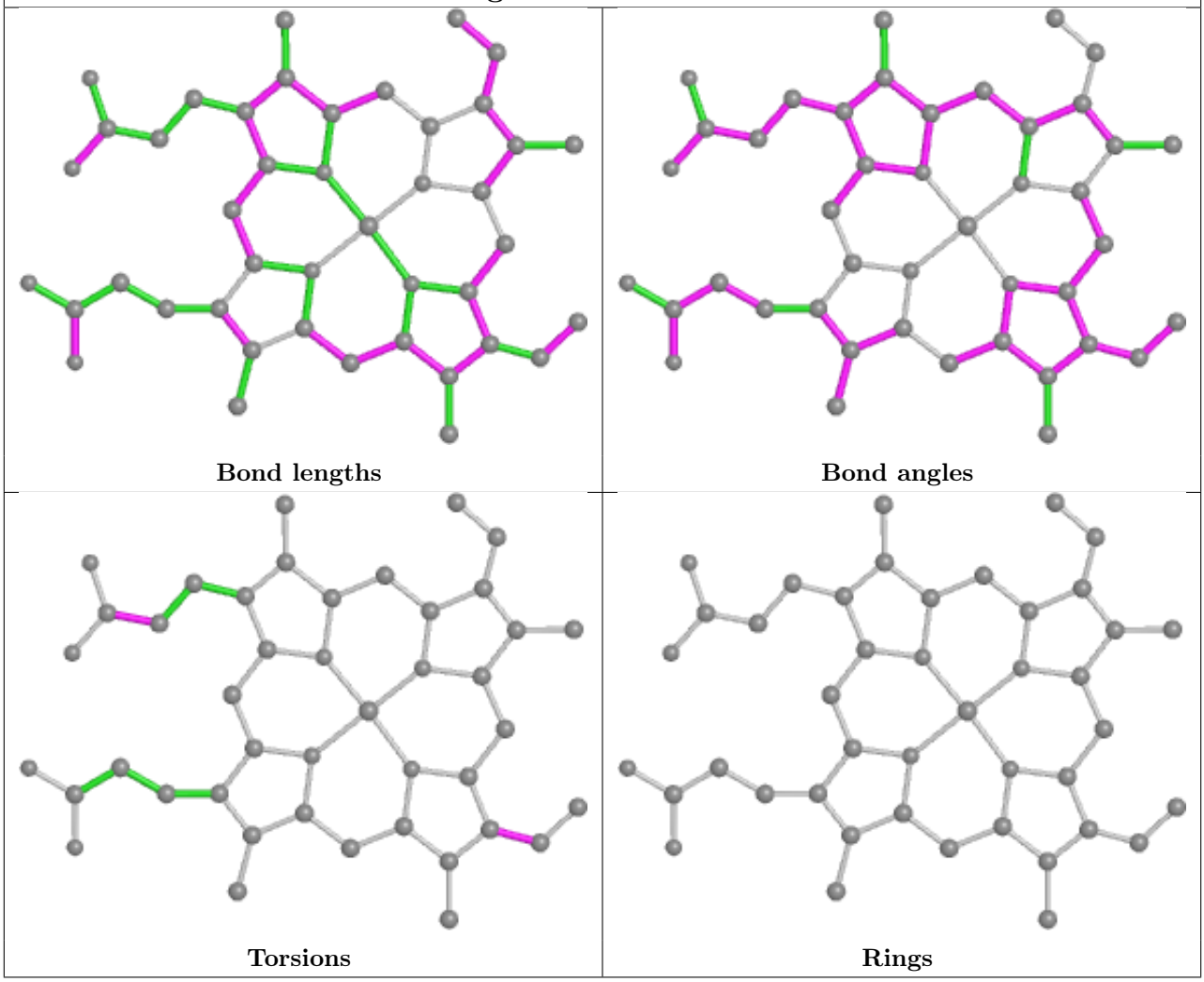


Torsions



Rings

Ligand HEM D 242



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.