Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:00 AM EDT

PDB ID	:	1L0L
Title	:	structure of bovine mitochondrial cytochrome bc1 complex with a bound fungicide famoxadone
Authors	:	Gao, X.; Wen, X.; Yu, C.A.; Esser, L.; Tsao, S.; Quinn, B.; Zhang, L.; Yu, L.; Xia, D.
Deposited on	:	2002-02-11
Resolution	:	2.35 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:

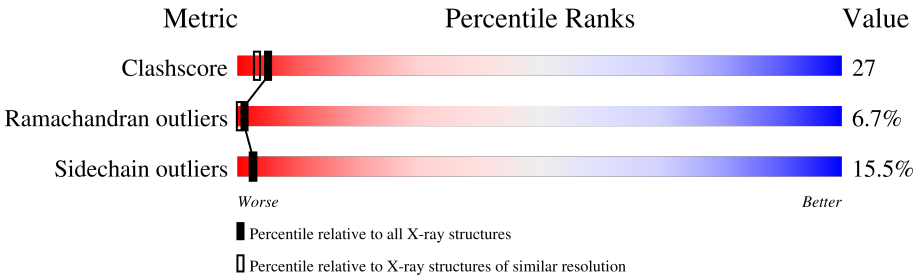
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.35 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	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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	63% 30% 7%
2	B	439	62% 28% 6% • •
3	C	379	64% 29% 6% ••
4	D	241	42% 35% 15% 7%
5	E	196	37% 37% 20% 6%
6	F	110	66% 26% 5% ••
7	G	81	62% 20% 14% • •
8	H	78	33% 41% 19% 6%

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Mol	Chain	Length	Quality of chain
9	I	78	15% 24% 27% 6% 27%
10	J	62	44% 39% 15%
11	K	56	57% 23% 12% 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
14	FES	E	197	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 16795 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.

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.

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	377	2995	2009	470	498	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	240	1909	1219	328	347	15	0	0	0

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

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
6	F	109	Total	C	N	O	S	0	0	0
			938	592	172	172	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	79	Total	C	N	O	S	0	0	0
			662	431	123	107	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	78	Total	C	N	O	S	0	0	0
			639	384	111	139	5			

- Molecule 9 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE 8 KDA PROTEIN.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	60	Total	C	N	O	0	0	0
			495	324	86	85			

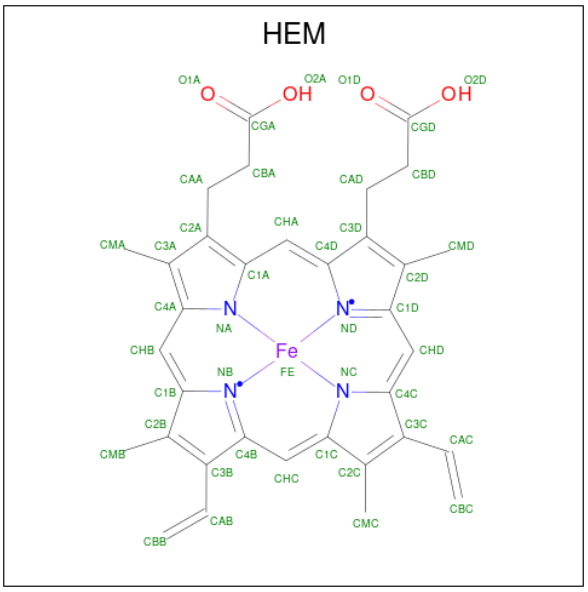
- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase complex 6.4 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	53	Total	C	N	O	S	0	0	0
			441	295	79	66	1			

There is a discrepancy between the modelled and reference sequences:

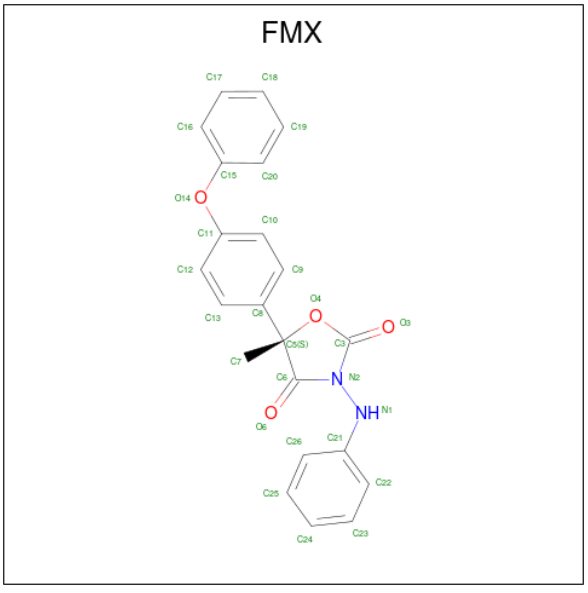
Chain	Residue	Modelled	Actual	Comment	Reference
K	22	GLN	SER	CONFLICT	UNP P07552

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



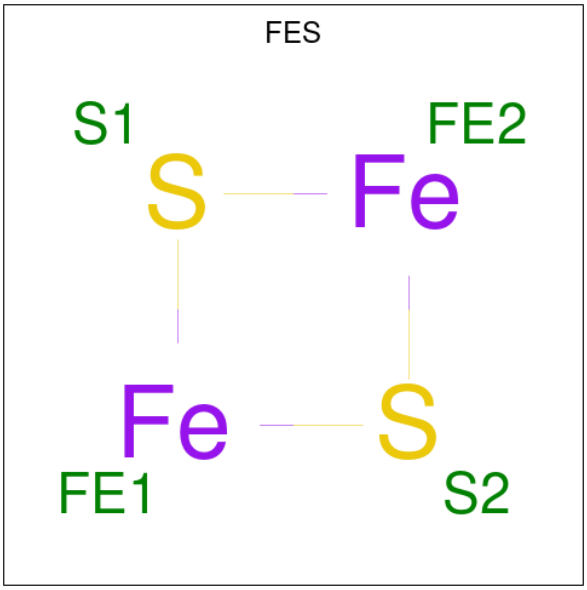
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is FAMOXADONE (three-letter code: FMX) (formula: $C_{22}H_{18}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			28	22	2	4		

- 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

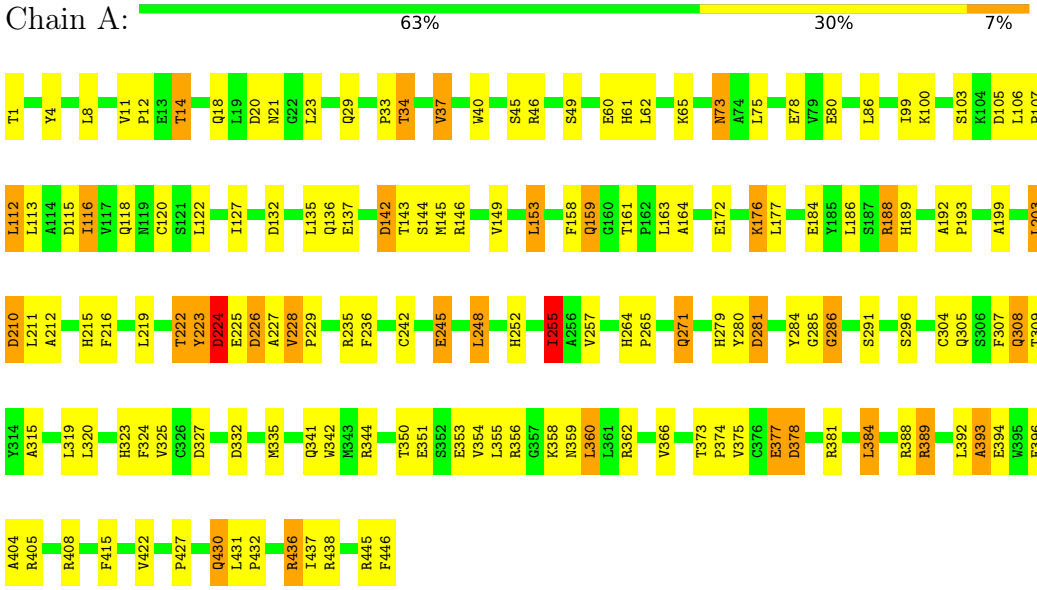
3 Residue-property plots (i)

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.

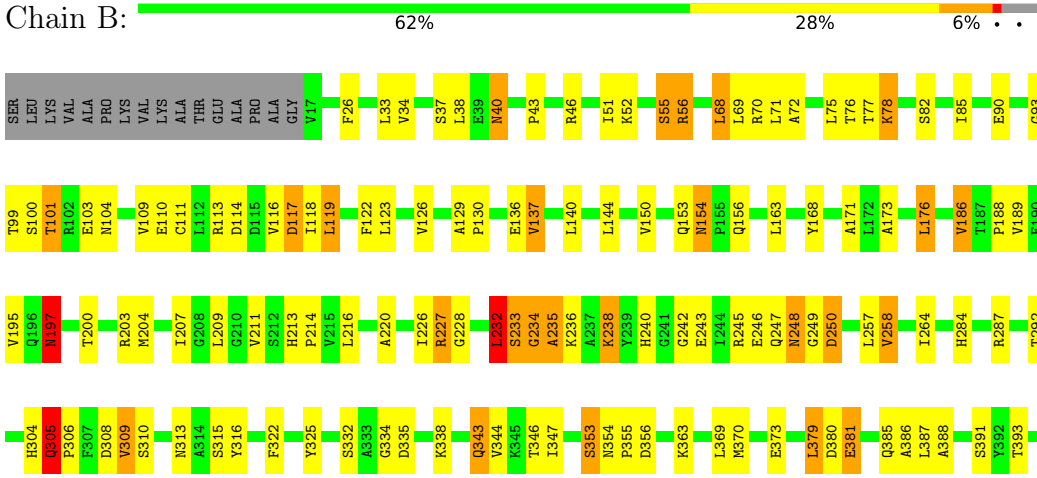
• Molecule 1: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I

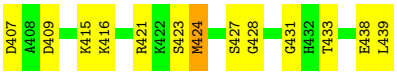
Chain A:



• Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2

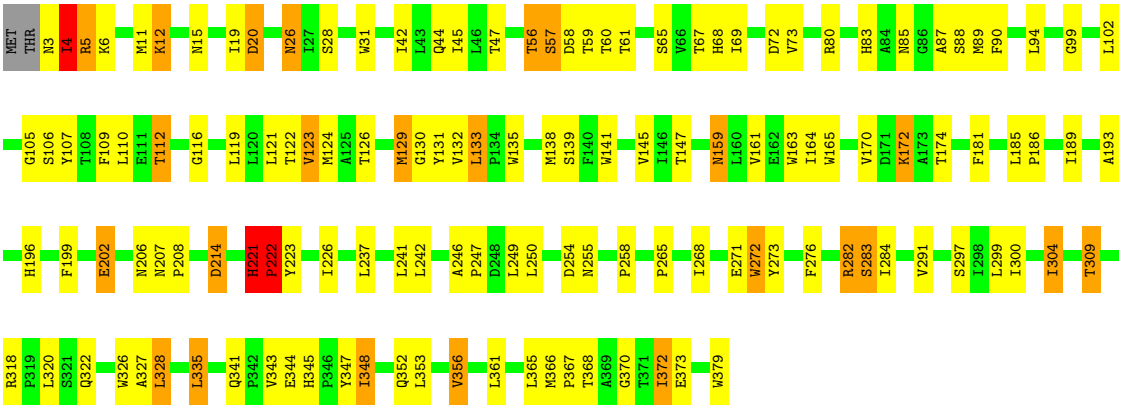
Chain B:





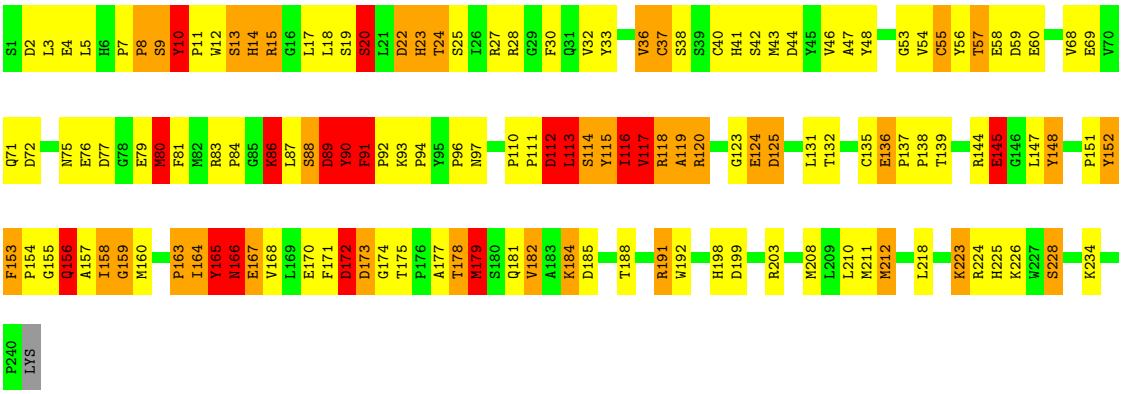
• Molecule 3: Cytochrome B

Chain C:



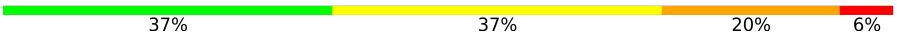
• Molecule 4: Cytochrome c1, heme protein

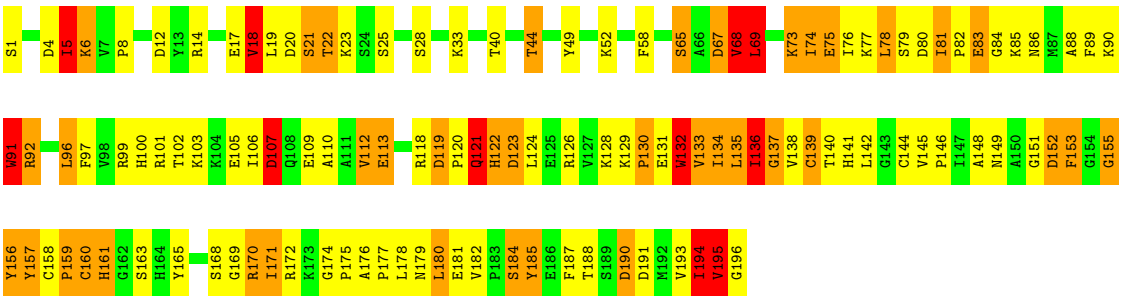
Chain D:



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

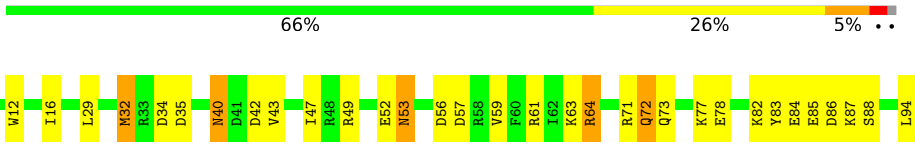
Chain E:





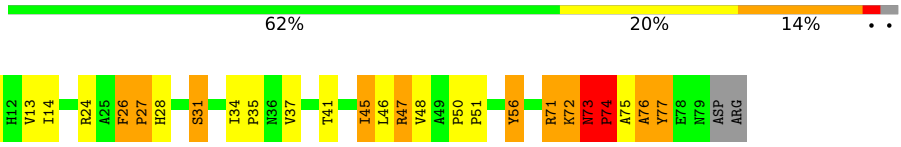
• Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F:



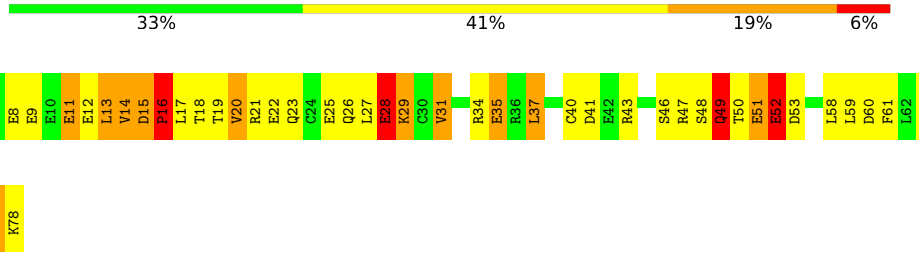
• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain G:



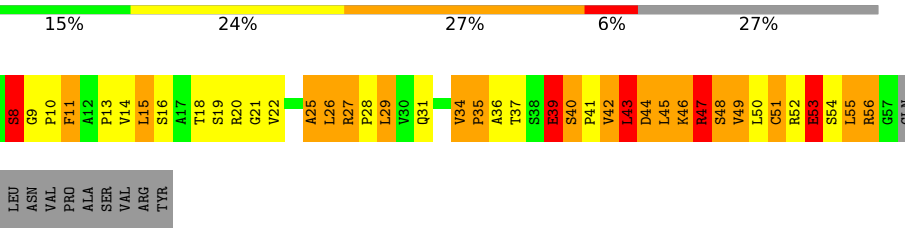
• Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H:



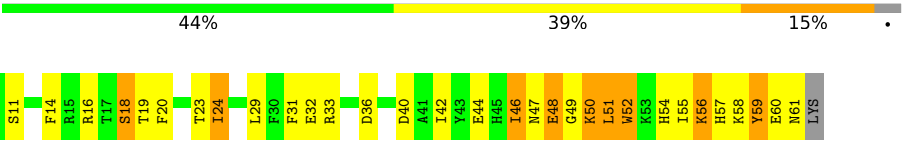
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE 8 KDA PROTEIN

Chain I:



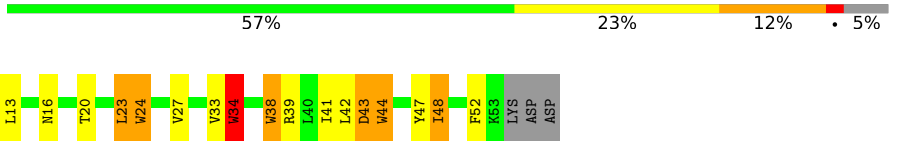
• Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:



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

Chain K:



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	154.09Å 154.09Å 591.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.35	Depositor
% Data completeness (in resolution range)	96.0 (40.00-2.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.259 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16795	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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: FES, FMX, HEM

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	0.86	1/3531 (0.0%)	0.89	13/4792 (0.3%)
2	B	1.11	8/3232 (0.2%)	1.01	19/4386 (0.4%)
3	C	0.84	0/3092	0.88	10/4232 (0.2%)
4	D	0.72	1/1968 (0.1%)	0.96	15/2673 (0.6%)
5	E	0.75	1/1553 (0.1%)	1.04	12/2100 (0.6%)
6	F	1.01	0/958	0.97	7/1284 (0.5%)
7	G	0.91	1/684 (0.1%)	0.86	1/926 (0.1%)
8	H	0.60	0/645	1.01	7/864 (0.8%)
9	I	0.99	2/411 (0.5%)	1.42	8/558 (1.4%)
10	J	0.76	0/508	0.94	1/686 (0.1%)
11	K	0.79	1/457 (0.2%)	0.77	1/625 (0.2%)
All	All	0.89	15/17039 (0.1%)	0.96	94/23126 (0.4%)

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
3	C	0	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	438	GLU	CD-OE2	7.77	1.34	1.25
1	A	304	CYS	CB-SG	-7.46	1.69	1.82
2	B	424	MET	SD-CE	-7.18	1.37	1.77
2	B	195	VAL	CB-CG1	7.08	1.67	1.52
5	E	91	TRP	CB-CG	5.82	1.60	1.50
2	B	90	GLU	CD-OE2	5.74	1.31	1.25
7	G	4	PHE	CB-CG	-5.69	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	55	SER	CB-OG	-5.53	1.35	1.42
9	I	43	LEU	N-CA	-5.46	1.35	1.46
9	I	25	ALA	CA-CB	-5.43	1.41	1.52
2	B	247	GLN	CB-CG	-5.40	1.38	1.52
4	D	90	TYR	CD1-CE1	-5.26	1.31	1.39
11	K	34	TRP	CB-CG	-5.21	1.40	1.50
2	B	381	GLU	CD-OE2	-5.15	1.20	1.25
2	B	137	VAL	CB-CG2	-5.11	1.42	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	42	VAL	O-C-N	10.88	140.12	122.70
3	C	221	HIS	C-N-CD	-10.49	97.52	120.60
9	I	42	VAL	CA-C-N	-9.26	96.84	117.20
2	B	304	HIS	O-C-N	9.08	137.23	122.70
3	C	222	PRO	N-CD-CG	-8.92	89.82	103.20
6	F	42	ASP	CB-CG-OD2	8.17	125.66	118.30
4	D	159	GLY	N-CA-C	8.14	133.46	113.10
2	B	117	ASP	CB-CG-OD2	8.00	125.50	118.30
3	C	4	ILE	O-C-N	7.95	135.42	122.70
3	C	4	ILE	CA-C-N	-7.54	100.61	117.20
5	E	69	LEU	N-CA-C	7.42	131.03	111.00
1	A	327	ASP	CB-CG-OD2	7.38	124.94	118.30
8	H	15	ASP	N-CA-C	7.26	130.60	111.00
3	C	221	HIS	N-CA-C	6.88	129.59	111.00
6	F	57	ASP	CB-CG-OD2	6.85	124.46	118.30
1	A	378	ASP	CB-CG-OD2	6.77	124.39	118.30
2	B	233	SER	N-CA-C	-6.71	92.88	111.00
4	D	10	TYR	N-CA-C	6.68	129.03	111.00
3	C	5	ARG	NE-CZ-NH2	6.58	123.59	120.30
7	G	77	TYR	N-CA-C	-6.50	93.44	111.00
2	B	304	HIS	CA-C-N	-6.50	102.90	117.20
1	A	255	ILE	CG1-CB-CG2	-6.35	97.42	111.40
2	B	250	ASP	N-CA-C	-6.34	93.88	111.00
2	B	304	HIS	C-N-CA	6.22	137.25	121.70
9	I	44	ASP	CB-CG-OD2	6.19	123.87	118.30
2	B	309	VAL	CB-CA-C	-6.17	99.67	111.40
2	B	114	ASP	CB-CG-OD2	6.13	123.82	118.30
5	E	12	ASP	CB-CG-OD2	6.08	123.78	118.30
5	E	152	ASP	CB-CG-OD2	6.03	123.73	118.30
6	F	34	ASP	CB-CG-OD2	5.98	123.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	190	ASP	CB-CG-OD2	5.92	123.63	118.30
2	B	56	ARG	NE-CZ-NH1	-5.92	117.34	120.30
5	E	174	GLY	N-CA-C	5.92	127.89	113.10
1	A	105	ASP	CB-CG-OD2	5.89	123.60	118.30
4	D	112	ASP	CB-CG-OD2	5.86	123.57	118.30
4	D	9	SER	N-CA-C	5.85	126.80	111.00
1	A	210	ASP	CB-CG-OD2	5.82	123.54	118.30
3	C	58	ASP	CB-CG-OD2	5.79	123.51	118.30
3	C	20	ASP	CB-CG-OD2	5.74	123.47	118.30
2	B	193	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	224	ASP	CB-CG-OD2	5.70	123.43	118.30
4	D	185	ASP	CB-CG-OD2	5.67	123.41	118.30
6	F	4	PRO	N-CA-C	5.65	126.78	112.10
2	B	305	GLN	CA-CB-CG	-5.62	101.02	113.40
1	A	159	GLN	N-CA-C	5.59	126.10	111.00
4	D	44	ASP	CB-CG-OD2	5.59	123.33	118.30
5	E	123	ASP	CB-CG-OD2	5.59	123.33	118.30
9	I	46	LYS	N-CA-C	5.59	126.08	111.00
1	A	226	ASP	CB-CG-OD2	5.54	123.29	118.30
5	E	96	LEU	CA-CB-CG	5.53	128.02	115.30
10	J	36	ASP	CB-CG-OD2	5.53	123.27	118.30
3	C	222	PRO	N-CA-C	-5.51	97.77	112.10
5	E	4	ASP	CB-CG-OD2	5.51	123.26	118.30
4	D	166	ASN	N-CA-C	-5.51	96.12	111.00
4	D	118	ARG	N-CA-C	5.50	125.85	111.00
4	D	22	ASP	CB-CG-OD2	5.47	123.22	118.30
8	H	14	VAL	N-CA-C	5.46	125.73	111.00
9	I	36	ALA	N-CA-C	5.42	125.63	111.00
8	H	60	ASP	CB-CG-OD2	5.41	123.17	118.30
4	D	89	ASP	CB-CG-OD2	5.41	123.17	118.30
2	B	409	ASP	CB-CG-OD2	5.39	123.15	118.30
6	F	56	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	304	CYS	N-CA-CB	-5.38	100.92	110.60
8	H	15	ASP	CB-CG-OD2	5.38	123.14	118.30
3	C	214	ASP	CB-CG-OD2	5.36	123.13	118.30
2	B	78	LYS	N-CA-C	-5.36	96.53	111.00
8	H	27	LEU	N-CA-C	5.36	125.46	111.00
2	B	356	ASP	CB-CG-OD2	5.32	123.09	118.30
8	H	66	ASP	CB-CG-OD2	5.32	123.09	118.30
4	D	125	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	20	ASP	CB-CG-OD2	5.28	123.06	118.30
4	D	172	ASP	CB-CG-OD2	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	79	SER	N-CA-C	-5.28	96.75	111.00
1	A	281	ASP	CB-CG-OD2	5.28	123.05	118.30
2	B	197	ASN	CB-CA-C	5.27	120.93	110.40
5	E	107	ASP	CB-CG-OD2	5.27	123.04	118.30
4	D	199	ASP	CB-CG-OD2	5.26	123.04	118.30
2	B	335	ASP	CB-CG-OD2	5.26	123.03	118.30
11	K	43	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	115	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	142	ASP	CB-CG-OD2	5.21	122.99	118.30
6	F	86	ASP	CB-CG-OD2	5.17	122.95	118.30
2	B	305	GLN	N-CA-C	5.15	124.90	111.00
9	I	35	PRO	N-CA-C	-5.14	98.73	112.10
5	E	68	VAL	N-CA-C	-5.11	97.21	111.00
8	H	2	ASP	CB-CG-OD2	5.11	122.89	118.30
2	B	407	ASP	CB-CG-OD2	5.10	122.89	118.30
2	B	380	ASP	CB-CG-OD2	5.08	122.87	118.30
9	I	42	VAL	CB-CA-C	5.05	120.99	111.40
4	D	59	ASP	CB-CG-OD2	5.03	122.82	118.30
9	I	26	LEU	N-CA-C	5.02	124.55	111.00
5	E	191	ASP	CB-CG-OD2	5.01	122.81	118.30
6	F	85	GLU	N-CA-C	-5.00	97.49	111.00
4	D	165	TYR	N-CA-CB	5.00	119.60	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	221	HIS	Peptide,Mainchain

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	149	0
2	B	3172	0	3152	121	0
3	C	2995	0	3058	121	0
4	D	1909	0	1857	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1519	0	1503	172	0
6	F	938	0	932	26	0
7	G	662	0	662	32	0
8	H	639	0	604	50	0
9	I	406	0	437	98	0
10	J	495	0	493	70	0
11	K	441	0	450	26	0
12	C	86	0	60	23	0
12	D	43	0	30	6	0
13	C	28	0	18	0	0
14	E	4	0	0	2	0
All	All	16795	0	16612	902	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 27.

All (902) 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)
4:D:40:CYS:SG	12:D:242:HEM:HAC	1.76	1.26
10:J:49:GLY:C	10:J:54:HIS:HE1	1.40	1.23
10:J:51:LEU:O	10:J:55:ILE:HG13	1.43	1.18
3:C:129:MET:CE	3:C:181:PHE:HB2	1.75	1.17
9:I:47:ARG:HG2	9:I:48:SER:H	1.09	1.16
10:J:18:SER:HA	11:K:24:TRP:CZ3	1.81	1.16
3:C:222:PRO:CD	3:C:223:TYR:H	1.52	1.15
5:E:101:ARG:NH2	5:E:106:ILE:HA	1.62	1.14
3:C:222:PRO:HD2	3:C:223:TYR:N	1.51	1.13
5:E:21:SER:O	5:E:23:LYS:N	1.83	1.11
4:D:20:SER:HB2	10:J:47:ASN:OD1	1.48	1.11
5:E:112:VAL:HG13	5:E:113:GLU:H	1.05	1.10
10:J:60:GLU:O	10:J:61:ASN:CG	1.90	1.10
6:F:3:ARG:HB3	6:F:4:PRO:HD3	1.30	1.08
10:J:18:SER:HA	11:K:24:TRP:HZ3	0.93	1.07
3:C:129:MET:HE1	3:C:181:PHE:HB2	1.35	1.07
5:E:18:VAL:CG2	5:E:19:LEU:H	1.67	1.06
1:A:325:VAL:HG21	9:I:43:LEU:HD12	1.38	1.05
10:J:49:GLY:C	10:J:54:HIS:CE1	2.30	1.03
2:B:154:ASN:N	2:B:154:ASN:HD22	1.54	1.02
7:G:77:TYR:OH	8:H:52:GLU:OE1	1.77	1.02
1:A:144:SER:HA	9:I:42:VAL:HB	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:159:PRO:C	5:E:161:HIS:H	1.61	1.00
1:A:309:THR:O	9:I:52:ARG:NH1	1.94	1.00
3:C:5:ARG:HH11	3:C:15:ASN:HD21	1.09	1.00
9:I:20:ARG:HG3	9:I:51:CYS:SG	2.02	1.00
1:A:341:GLN:HE22	1:A:344:ARG:NH2	1.58	0.99
2:B:385:GLN:HE22	2:B:393:THR:H	1.06	0.96
6:F:64:ARG:HH11	6:F:64:ARG:HG2	1.28	0.96
3:C:5:ARG:NH1	3:C:15:ASN:HD21	1.62	0.96
9:I:41:PRO:O	9:I:42:VAL:HG23	1.66	0.95
9:I:47:ARG:HG2	9:I:48:SER:N	1.73	0.95
2:B:154:ASN:HD22	2:B:154:ASN:H	1.13	0.95
6:F:64:ARG:HH11	6:F:64:ARG:CG	1.80	0.94
4:D:116:ILE:HD11	4:D:191:ARG:HA	1.47	0.94
6:F:3:ARG:HB3	6:F:4:PRO:CD	1.97	0.94
4:D:42:SER:O	4:D:113:LEU:HB3	1.68	0.93
5:E:101:ARG:HH22	5:E:106:ILE:HA	1.25	0.93
3:C:271:GLU:O	3:C:272:TRP:HB2	1.66	0.92
4:D:37:CYS:SG	12:D:242:HEM:HAB	2.10	0.92
1:A:146:ARG:H	9:I:42:VAL:CG1	1.80	0.92
4:D:10:TYR:HD2	4:D:125:ASP:OD1	1.52	0.91
10:J:55:ILE:O	10:J:57:HIS:N	2.03	0.91
4:D:114:SER:O	4:D:114:SER:OG	1.75	0.91
3:C:69:ILE:HA	3:C:73:VAL:HG22	1.52	0.91
4:D:114:SER:O	4:D:118:ARG:HD2	1.70	0.91
6:F:83:TYR:O	6:F:84:GLU:HG2	1.70	0.91
3:C:221:HIS:O	3:C:222:PRO:HG3	1.69	0.91
4:D:115:TYR:OH	4:D:120:ARG:NH1	2.04	0.91
2:B:240:HIS:O	2:B:421:ARG:NH1	2.03	0.91
5:E:136:ILE:HG23	5:E:137:GLY:N	1.83	0.91
9:I:2:LEU:O	9:I:3:SER:HB3	1.69	0.90
3:C:5:ARG:HH11	3:C:15:ASN:ND2	1.68	0.90
1:A:284:TYR:HE1	9:I:20:ARG:HG2	1.36	0.90
5:E:18:VAL:HG23	5:E:19:LEU:H	1.37	0.90
9:I:4:VAL:HG12	9:I:10:PRO:HG2	1.49	0.90
3:C:69:ILE:HA	3:C:73:VAL:CG2	2.00	0.89
5:E:74:ILE:O	5:E:76:ILE:HG13	1.72	0.89
5:E:134:ILE:O	5:E:134:ILE:CG2	2.20	0.89
2:B:76:THR:HG22	2:B:82:SER:H	1.37	0.89
4:D:147:LEU:O	4:D:148:TYR:CD2	2.26	0.88
1:A:311:ASN:C	1:A:311:ASN:HD22	1.77	0.88
5:E:5:ILE:CG2	5:E:6:LYS:H	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.54	0.88
2:B:305:GLN:HB3	2:B:306:PRO:HD3	1.56	0.87
5:E:136:ILE:HG23	5:E:137:GLY:H	1.38	0.86
10:J:50:LYS:N	10:J:54:HIS:HE1	1.73	0.86
9:I:34:VAL:HB	9:I:35:PRO:HD3	1.58	0.86
5:E:135:LEU:HA	5:E:182:VAL:HG11	1.57	0.86
1:A:80:GLU:OE2	2:B:292:THR:HG22	1.75	0.86
5:E:112:VAL:HG13	5:E:113:GLU:N	1.89	0.86
4:D:211:MET:CE	10:J:31:PHE:HE2	1.88	0.85
10:J:29:LEU:HD13	11:K:34:TRP:HB2	1.57	0.85
5:E:179:ASN:O	5:E:180:LEU:HB2	1.76	0.85
4:D:138:PRO:HG3	8:H:58:LEU:HD22	1.59	0.84
4:D:113:LEU:HG	4:D:118:ARG:HH12	1.43	0.84
5:E:18:VAL:HG22	5:E:19:LEU:H	1.39	0.84
1:A:252:HIS:HD2	1:A:323:HIS:HE1	1.25	0.84
5:E:18:VAL:CG2	5:E:19:LEU:N	2.33	0.84
4:D:27:ARG:NH1	10:J:58:LYS:NZ	2.26	0.83
3:C:361:LEU:HA	3:C:365:LEU:HB2	1.61	0.83
9:I:6:ALA:C	9:I:8:SER:H	1.82	0.83
9:I:47:ARG:CG	9:I:48:SER:H	1.90	0.83
10:J:18:SER:CA	11:K:24:TRP:HZ3	1.86	0.83
5:E:97:PHE:CE2	5:E:137:GLY:HA3	2.14	0.83
5:E:5:ILE:CG2	5:E:6:LYS:N	2.42	0.83
5:E:135:LEU:HA	5:E:182:VAL:CG1	2.09	0.82
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.60	0.82
8:H:25:GLU:HG3	8:H:61:PHE:HZ	1.43	0.82
9:I:51:CYS:SG	9:I:52:ARG:N	2.52	0.82
1:A:228:VAL:H	1:A:229:PRO:HD3	1.45	0.82
2:B:385:GLN:HE22	2:B:393:THR:N	1.77	0.82
4:D:10:TYR:CD2	4:D:125:ASP:OD1	2.32	0.82
3:C:226:ILE:HG22	4:D:223:LYS:HB2	1.62	0.82
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.43	0.82
3:C:186:PRO:HG2	12:C:610:HEM:HHC	1.63	0.81
1:A:252:HIS:CD2	1:A:323:HIS:HE1	1.98	0.81
3:C:129:MET:HE2	3:C:181:PHE:HB2	1.62	0.81
3:C:4:ILE:HG12	3:C:6:LYS:HG3	1.63	0.81
1:A:146:ARG:H	9:I:42:VAL:HG11	1.43	0.81
4:D:79:GLU:O	4:D:80:MET:HB2	1.81	0.80
2:B:153:GLN:HE22	9:I:46:LYS:HG3	1.47	0.80
4:D:40:CYS:HG	12:D:242:HEM:HAC	1.44	0.79
4:D:152:TYR:O	4:D:153:PHE:O	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.11	0.79
1:A:341:GLN:HE22	1:A:344:ARG:HH22	1.25	0.79
3:C:207:ASN:HB2	3:C:208:PRO:HD2	1.65	0.79
9:I:10:PRO:O	9:I:25:ALA:HB1	1.82	0.79
2:B:154:ASN:N	2:B:154:ASN:ND2	2.25	0.79
4:D:165:TYR:HD2	4:D:165:TYR:O	1.66	0.79
3:C:222:PRO:HD2	3:C:223:TYR:H	0.67	0.79
1:A:29:GLN:HG3	1:A:203:LEU:O	1.83	0.79
8:H:5:GLU:HA	8:H:8:GLU:HB3	1.64	0.79
9:I:43:LEU:HA	9:I:46:LYS:HD2	1.65	0.79
5:E:5:ILE:HG22	5:E:6:LYS:H	1.47	0.78
5:E:159:PRO:C	5:E:161:HIS:N	2.35	0.78
2:B:71:LEU:HD23	9:I:15:LEU:HG	1.66	0.78
2:B:325:TYR:CD2	9:I:28:PRO:HD2	2.18	0.78
5:E:100:HIS:HD1	5:E:132:TRP:HZ3	1.29	0.78
10:J:60:GLU:O	10:J:61:ASN:OD1	2.00	0.78
3:C:129:MET:CE	3:C:181:PHE:CB	2.60	0.78
5:E:159:PRO:O	5:E:161:HIS:N	2.12	0.78
9:I:10:PRO:O	9:I:25:ALA:CB	2.31	0.78
3:C:186:PRO:HG3	12:C:610:HEM:HMC2	1.67	0.77
1:A:284:TYR:CE1	9:I:20:ARG:HG2	2.18	0.77
3:C:206:ASN:ND2	3:C:207:ASN:H	1.82	0.77
5:E:91:TRP:O	5:E:92:ARG:HB2	1.83	0.77
4:D:71:GLN:HE21	4:D:80:MET:HG3	1.49	0.77
4:D:178:THR:OG1	8:H:16:PRO:HG2	1.84	0.77
5:E:184:SER:HB2	5:E:196:GLY:HA2	1.67	0.77
5:E:18:VAL:HG22	5:E:19:LEU:N	1.97	0.76
2:B:111:CYS:HB3	2:B:119:LEU:HD13	1.68	0.76
4:D:20:SER:HB2	10:J:47:ASN:CG	2.05	0.76
3:C:138:MET:HB2	3:C:255:ASN:HD21	1.49	0.76
5:E:156:TYR:CB	5:E:165:TYR:HB2	2.15	0.76
3:C:31:TRP:NE1	12:C:609:HEM:O1D	2.19	0.75
4:D:43:MET:HA	4:D:113:LEU:HB3	1.68	0.75
8:H:1:GLY:O	8:H:2:ASP:HB2	1.87	0.74
5:E:5:ILE:HG23	5:E:6:LYS:N	2.02	0.74
4:D:147:LEU:O	4:D:148:TYR:CG	2.40	0.74
5:E:120:PRO:O	5:E:121:GLN:HB2	1.86	0.74
8:H:50:THR:O	8:H:51:GLU:HB2	1.85	0.74
4:D:43:MET:HA	4:D:113:LEU:CB	2.17	0.74
10:J:50:LYS:HD3	10:J:52:TRP:HB2	1.67	0.74
2:B:76:THR:HG23	2:B:136:GLU:OE1	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:LEU:HA	3:C:124:MET:HE2	1.70	0.74
5:E:112:VAL:CG1	5:E:113:GLU:H	1.87	0.74
5:E:194:ILE:O	5:E:195:VAL:HG22	1.87	0.73
2:B:101:THR:HG22	2:B:103:GLU:H	1.52	0.73
6:F:64:ARG:HG2	6:F:64:ARG:NH1	2.02	0.73
1:A:144:SER:CA	9:I:42:VAL:HB	2.18	0.73
4:D:72:ASP:OD2	4:D:83:ARG:HD3	1.88	0.73
5:E:170:ARG:HH21	5:E:170:ARG:HG2	1.53	0.73
1:A:146:ARG:NH2	1:A:308:GLN:OE1	2.21	0.73
2:B:95:LYS:HG2	2:B:110:GLU:HG2	1.71	0.73
4:D:211:MET:HE1	10:J:31:PHE:HE2	1.54	0.72
3:C:5:ARG:NH1	3:C:15:ASN:ND2	2.33	0.72
5:E:101:ARG:HH22	5:E:106:ILE:CA	2.00	0.72
5:E:134:ILE:O	5:E:134:ILE:HG22	1.89	0.72
1:A:341:GLN:NE2	1:A:344:ARG:NH2	2.37	0.72
4:D:27:ARG:NH1	10:J:58:LYS:HZ3	1.84	0.72
7:G:71:ARG:O	7:G:74:PRO:HD2	1.89	0.72
10:J:50:LYS:N	10:J:54:HIS:CE1	2.57	0.72
3:C:73:VAL:HG12	5:E:65:SER:HB3	1.70	0.72
3:C:226:ILE:CG2	4:D:223:LYS:HB2	2.20	0.72
4:D:46:VAL:O	4:D:90:TYR:HB2	1.89	0.72
5:E:124:LEU:HG	5:E:130:PRO:HB3	1.72	0.71
10:J:51:LEU:O	10:J:55:ILE:CG1	2.33	0.71
4:D:28:ARG:NH1	8:H:78:LYS:HE2	2.06	0.71
4:D:54:VAL:HG11	4:D:192:TRP:NE1	2.05	0.71
4:D:211:MET:HE3	10:J:31:PHE:HE2	1.55	0.71
4:D:157:ALA:O	4:D:158:ILE:HB	1.90	0.71
4:D:211:MET:HE1	10:J:31:PHE:CE2	2.26	0.71
5:E:91:TRP:O	5:E:92:ARG:CB	2.39	0.71
7:G:77:TYR:CZ	8:H:52:GLU:OE1	2.43	0.71
1:A:378:ASP:OD2	1:A:389:ARG:NH1	2.24	0.71
5:E:138:VAL:HG23	5:E:139:CYS:H	1.54	0.71
4:D:116:ILE:C	4:D:118:ARG:H	1.94	0.71
5:E:91:TRP:HE1	5:E:195:VAL:HG23	1.55	0.71
4:D:91:PHE:HE2	4:D:93:LYS:HD2	1.55	0.71
5:E:78:LEU:HD21	5:E:187:PHE:CE1	2.26	0.71
1:A:146:ARG:H	9:I:42:VAL:HG12	1.53	0.70
1:A:227:ALA:O	1:A:228:VAL:HG22	1.91	0.70
3:C:129:MET:HE1	3:C:181:PHE:CB	2.16	0.70
7:G:56:TYR:C	7:G:56:TYR:HD1	1.95	0.70
3:C:221:HIS:O	3:C:222:PRO:CG	2.30	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:GLY:O	4:D:157:ALA:N	2.25	0.70
1:A:222:THR:HG23	1:A:223:TYR:H	1.56	0.70
4:D:114:SER:O	4:D:118:ARG:CD	2.39	0.70
10:J:59:TYR:O	10:J:59:TYR:CD1	2.44	0.69
9:I:44:ASP:O	9:I:46:LYS:HB2	1.92	0.69
3:C:138:MET:HB2	3:C:255:ASN:ND2	2.07	0.69
9:I:6:ALA:C	9:I:8:SER:N	2.44	0.69
1:A:392:LEU:O	1:A:393:ALA:CB	2.41	0.69
4:D:10:TYR:CD1	4:D:12:TRP:HD1	2.10	0.69
1:A:255:ILE:HG12	1:A:422:VAL:HG22	1.74	0.69
1:A:408:ARG:NH1	11:K:16:ASN:ND2	2.40	0.68
4:D:28:ARG:HB3	4:D:171:PHE:HE2	1.58	0.68
3:C:44:GLN:HG3	12:C:610:HEM:HBC2	1.75	0.68
5:E:135:LEU:HD21	5:E:169:GLY:HA3	1.75	0.68
3:C:47:THR:HG22	5:E:58:PHE:HZ	1.59	0.68
5:E:102:THR:OG1	5:E:105:GLU:HB2	1.94	0.68
2:B:176:LEU:HG	9:I:13:PRO:HG2	1.73	0.68
5:E:82:PRO:O	5:E:100:HIS:HD2	1.76	0.68
1:A:252:HIS:HD2	1:A:323:HIS:CE1	2.11	0.68
3:C:309:THR:HG21	3:C:367:PRO:O	1.93	0.68
9:I:44:ASP:O	9:I:46:LYS:N	2.26	0.68
10:J:14:PHE:HD1	10:J:20:PHE:HD1	1.41	0.68
10:J:49:GLY:O	10:J:54:HIS:CE1	2.45	0.68
2:B:68:LEU:HD12	2:B:186:VAL:HG22	1.76	0.67
2:B:51:ILE:O	2:B:104:ASN:HB2	1.95	0.67
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.27	0.67
1:A:351:GLU:H	11:K:12:GLN:NE2	1.92	0.67
2:B:305:GLN:O	2:B:306:PRO:C	2.29	0.67
10:J:60:GLU:C	10:J:61:ASN:CG	2.51	0.67
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.76	0.67
3:C:343:VAL:HG13	3:C:343:VAL:O	1.93	0.67
2:B:111:CYS:CB	2:B:119:LEU:HD13	2.24	0.67
10:J:14:PHE:HD1	10:J:20:PHE:CD1	2.13	0.67
1:A:392:LEU:O	1:A:393:ALA:HB2	1.94	0.67
5:E:76:ILE:HB	5:E:193:VAL:HG13	1.75	0.67
5:E:134:ILE:O	5:E:134:ILE:HG23	1.94	0.67
1:A:142:ASP:OD1	5:E:1:SER:HB3	1.95	0.67
2:B:156:GLN:HB3	9:I:27:ARG:HG2	1.76	0.67
3:C:271:GLU:O	3:C:272:TRP:CB	2.41	0.67
4:D:163:PRO:O	4:D:164:ILE:HG12	1.95	0.67
8:H:77:LEU:O	8:H:78:LYS:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:NZ	2:B:287:ARG:O	2.29	0.66
5:E:14:ARG:HE	5:E:18:VAL:CG2	2.09	0.66
9:I:21:GLY:O	9:I:47:ARG:NH2	2.27	0.66
2:B:100:SER:O	9:I:13:PRO:HD2	1.96	0.66
4:D:30:PHE:CE1	4:D:90:TYR:OH	2.48	0.66
5:E:88:ALA:HB2	5:E:97:PHE:HB3	1.77	0.66
5:E:194:ILE:HD12	5:E:195:VAL:H	1.61	0.66
2:B:46:ARG:NH1	2:B:110:GLU:OE2	2.29	0.66
2:B:70:ARG:HG3	2:B:98:VAL:HG22	1.76	0.66
1:A:378:ASP:OD1	9:I:56:ARG:CZ	2.44	0.66
5:E:40:THR:O	5:E:44:THR:HG22	1.95	0.66
5:E:136:ILE:CG2	5:E:137:GLY:N	2.56	0.66
9:I:39:GLU:O	9:I:40:SER:HB3	1.96	0.65
1:A:408:ARG:HH12	11:K:16:ASN:ND2	1.94	0.65
4:D:47:ALA:HA	4:D:90:TYR:HB2	1.77	0.65
9:I:8:SER:OG	9:I:26:LEU:HD13	1.95	0.65
10:J:49:GLY:O	10:J:54:HIS:HE1	1.78	0.64
1:A:61:HIS:CE1	1:A:137:GLU:OE2	2.50	0.64
6:F:64:ARG:HH11	6:F:64:ARG:CB	2.10	0.64
5:E:182:VAL:O	5:E:182:VAL:HG22	1.98	0.64
1:A:118:GLN:HG2	1:A:219:LEU:HD21	1.80	0.64
5:E:141:HIS:CE1	5:E:161:HIS:CE1	2.86	0.64
9:I:11:PHE:HA	9:I:25:ALA:CB	2.27	0.64
9:I:55:LEU:O	9:I:56:ARG:HB2	1.98	0.64
2:B:353:SER:OG	2:B:355:PRO:HD2	1.98	0.64
7:G:73:ASN:O	7:G:74:PRO:C	2.35	0.63
3:C:56:THR:HG23	3:C:65:SER:HB3	1.80	0.63
4:D:12:TRP:O	4:D:13:SER:CB	2.45	0.63
8:H:73:LEU:O	8:H:75:ASN:N	2.31	0.63
4:D:20:SER:CB	10:J:47:ASN:OD1	2.38	0.63
5:E:101:ARG:HB2	5:E:131:GLU:C	2.18	0.63
5:E:182:VAL:O	5:E:182:VAL:CG2	2.46	0.63
4:D:166:ASN:HD22	4:D:166:ASN:H	1.45	0.63
9:I:46:LYS:HG2	9:I:47:ARG:N	2.13	0.63
1:A:61:HIS:HE1	1:A:137:GLU:OE2	1.80	0.63
4:D:208:MET:O	4:D:212:MET:HB2	1.98	0.63
4:D:10:TYR:OH	4:D:124:GLU:OE2	2.14	0.63
7:G:56:TYR:C	7:G:56:TYR:CD1	2.70	0.63
1:A:110:VAL:HG11	1:A:211:LEU:HB3	1.80	0.63
5:E:84:GLY:HA2	5:E:100:HIS:HB2	1.81	0.62
9:I:39:GLU:O	9:I:40:SER:CB	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:VAL:O	2:B:130:PRO:HG3	1.99	0.62
4:D:157:ALA:O	4:D:158:ILE:CB	2.47	0.62
2:B:209:LEU:HG	2:B:379:LEU:HD23	1.81	0.62
12:C:609:HEM:CMB	12:C:609:HEM:HBB2	2.30	0.62
4:D:10:TYR:CD1	4:D:12:TRP:CD1	2.88	0.62
1:A:255:ILE:HD12	1:A:335:MET:CE	2.29	0.62
4:D:165:TYR:O	4:D:167:GLU:N	2.32	0.62
4:D:172:ASP:O	4:D:174:GLY:N	2.33	0.62
3:C:226:ILE:HG21	4:D:223:LYS:HA	1.81	0.62
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.40	0.62
4:D:135:CYS:SG	4:D:151:PRO:HG3	2.39	0.62
3:C:147:THR:HG21	3:C:165:TRP:NE1	2.15	0.62
1:A:14:THR:HG21	1:A:389:ARG:HG3	1.81	0.61
3:C:126:THR:HG21	12:C:610:HEM:CMC	2.30	0.61
5:E:131:GLU:HG3	5:E:131:GLU:O	2.00	0.61
9:I:4:VAL:HG12	9:I:10:PRO:CG	2.26	0.61
3:C:129:MET:HE2	3:C:181:PHE:CB	2.26	0.61
11:K:42:LEU:O	11:K:44:TRP:N	2.33	0.61
1:A:252:HIS:CD2	1:A:323:HIS:CE1	2.86	0.61
2:B:233:SER:O	2:B:235:ALA:N	2.32	0.61
4:D:48:TYR:CE1	4:D:90:TYR:HA	2.35	0.61
4:D:211:MET:CE	10:J:31:PHE:CE2	2.77	0.61
5:E:52:LYS:HE2	10:J:32:GLU:OE1	2.00	0.61
4:D:178:THR:HG23	4:D:181:GLN:HB2	1.81	0.61
2:B:315:SER:O	9:I:4:VAL:HG13	2.01	0.61
3:C:112:THR:HG22	3:C:199:PHE:HB3	1.83	0.61
1:A:285:GLY:O	1:A:286:GLY:O	2.19	0.61
4:D:57:THR:HG22	4:D:60:GLU:H	1.66	0.61
9:I:41:PRO:O	9:I:42:VAL:CG2	2.45	0.61
10:J:60:GLU:HB3	10:J:61:ASN:ND2	2.16	0.61
1:A:311:ASN:C	1:A:311:ASN:ND2	2.51	0.61
4:D:10:TYR:O	4:D:12:TRP:CD1	2.53	0.61
5:E:121:GLN:HG3	5:E:122:HIS:H	1.66	0.61
1:A:291:SER:HB3	1:A:356:ARG:CZ	2.30	0.60
1:A:354:VAL:O	1:A:358:LYS:HG3	2.02	0.60
4:D:138:PRO:CG	8:H:58:LEU:HD22	2.29	0.60
4:D:184:LYS:HD3	8:H:78:LYS:NZ	2.16	0.60
8:H:21:ARG:O	8:H:25:GLU:HB2	2.02	0.60
3:C:56:THR:HG23	3:C:65:SER:CB	2.32	0.60
3:C:186:PRO:HG2	12:C:610:HEM:CHC	2.31	0.60
5:E:107:ASP:HA	5:E:110:ALA:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:140:THR:HG21	5:E:178:LEU:HB2	1.84	0.60
5:E:141:HIS:CE1	5:E:161:HIS:HE1	2.18	0.60
9:I:34:VAL:HB	9:I:35:PRO:CD	2.31	0.60
3:C:165:TRP:O	3:C:174:THR:HG22	2.01	0.60
4:D:113:LEU:HG	4:D:118:ARG:NH1	2.17	0.60
4:D:147:LEU:HD22	4:D:159:GLY:H	1.66	0.60
2:B:248:ASN:C	2:B:248:ASN:HD22	2.02	0.60
11:K:47:TYR:O	11:K:48:ILE:HB	2.02	0.60
4:D:28:ARG:HB3	4:D:171:PHE:CE2	2.36	0.59
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.13	0.59
8:H:66:ASP:HA	8:H:69:VAL:HB	1.84	0.59
3:C:26:ASN:HD22	3:C:26:ASN:H	1.50	0.59
4:D:165:TYR:O	4:D:165:TYR:CD2	2.53	0.59
5:E:184:SER:O	5:E:185:TYR:HB2	2.02	0.59
10:J:46:ILE:HG13	10:J:46:ILE:O	2.02	0.59
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.37	0.59
4:D:9:SER:O	4:D:11:PRO:HD3	2.02	0.59
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.31	0.59
5:E:107:ASP:OD1	5:E:107:ASP:N	2.29	0.59
10:J:14:PHE:CD1	10:J:20:PHE:HD1	2.20	0.59
4:D:113:LEU:CG	4:D:118:ARG:HH12	2.16	0.59
1:A:73:ASN:C	1:A:73:ASN:HD22	2.06	0.58
5:E:135:LEU:HD13	5:E:156:TYR:CE1	2.38	0.58
3:C:237:LEU:HD13	4:D:212:MET:HG2	1.84	0.58
5:E:84:GLY:O	5:E:99:ARG:NE	2.36	0.58
9:I:41:PRO:HB3	9:I:44:ASP:CG	2.23	0.58
1:A:172:GLU:O	1:A:176:LYS:HG3	2.04	0.58
1:A:405:ARG:HA	1:A:408:ARG:HH21	1.68	0.58
5:E:184:SER:O	5:E:185:TYR:CB	2.51	0.58
1:A:308:GLN:HG3	9:I:52:ARG:CZ	2.33	0.58
2:B:344:VAL:O	2:B:347:ILE:HG12	2.02	0.58
8:H:52:GLU:OE2	8:H:53:ASP:O	2.21	0.58
5:E:18:VAL:HG23	5:E:19:LEU:N	2.07	0.58
5:E:128:LYS:HB2	5:E:185:TYR:CD2	2.39	0.58
2:B:76:THR:HG22	2:B:82:SER:N	2.15	0.58
2:B:343:GLN:O	2:B:346:THR:HG22	2.03	0.57
2:B:129:ALA:N	2:B:130:PRO:HD3	2.19	0.57
4:D:23:HIS:HE1	4:D:54:VAL:HG12	1.69	0.57
5:E:97:PHE:CZ	5:E:137:GLY:HA3	2.38	0.57
2:B:248:ASN:ND2	2:B:250:ASP:H	2.02	0.57
3:C:341:GLN:HG3	3:C:347:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:64:ARG:HH11	6:F:64:ARG:HB3	1.68	0.57
1:A:184:GLU:O	1:A:188:ARG:HB2	2.05	0.57
1:A:252:HIS:HE1	9:I:43:LEU:HB2	1.70	0.57
3:C:326:TRP:CE2	7:G:48:VAL:HG22	2.40	0.57
5:E:78:LEU:O	5:E:100:HIS:CE1	2.58	0.57
8:H:25:GLU:HG3	8:H:61:PHE:CZ	2.33	0.57
10:J:55:ILE:C	10:J:57:HIS:N	2.58	0.57
1:A:405:ARG:CA	1:A:408:ARG:HH21	2.18	0.57
3:C:368:THR:O	3:C:372:ILE:HG12	2.03	0.57
4:D:115:TYR:HA	4:D:118:ARG:HD3	1.86	0.57
3:C:85:ASN:O	3:C:89:MET:HG2	2.05	0.56
2:B:118:ILE:HG13	2:B:122:PHE:CE1	2.40	0.56
8:H:47:ARG:O	8:H:49:GLN:N	2.30	0.56
9:I:26:LEU:C	9:I:27:ARG:HG3	2.24	0.56
4:D:3:LEU:O	4:D:4:GLU:HB3	2.05	0.56
5:E:122:HIS:O	5:E:126:ARG:N	2.36	0.56
1:A:360:LEU:HD22	2:B:93:GLY:HA2	1.87	0.56
5:E:91:TRP:HB2	5:E:96:LEU:HD11	1.86	0.56
6:F:64:ARG:NH1	6:F:64:ARG:HB3	2.21	0.56
10:J:59:TYR:O	10:J:59:TYR:CG	2.55	0.56
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.40	0.56
2:B:385:GLN:NE2	2:B:393:THR:H	1.90	0.56
7:G:41:THR:O	7:G:45:ILE:HG12	2.06	0.56
1:A:252:HIS:CE1	9:I:43:LEU:HB2	2.41	0.56
5:E:82:PRO:O	5:E:100:HIS:CD2	2.57	0.56
5:E:101:ARG:O	5:E:131:GLU:HB2	2.05	0.56
10:J:57:HIS:O	10:J:58:LYS:HG3	2.06	0.56
3:C:326:TRP:NE1	7:G:48:VAL:HG22	2.21	0.56
1:A:145:MET:HB2	9:I:42:VAL:O	2.06	0.56
9:I:44:ASP:O	9:I:45:LEU:C	2.44	0.56
10:J:42:ILE:O	10:J:46:ILE:HG22	2.06	0.56
3:C:116:GLY:HA3	12:C:609:HEM:C3C	2.41	0.56
5:E:86:ASN:HD22	5:E:148:ALA:HB2	1.71	0.55
1:A:146:ARG:N	9:I:42:VAL:HG12	2.22	0.55
1:A:436:ARG:NH1	3:C:20:ASP:OD1	2.39	0.55
3:C:15:ASN:ND2	3:C:19:ILE:HB	2.22	0.55
3:C:73:VAL:CG1	5:E:65:SER:HB3	2.36	0.55
5:E:100:HIS:O	5:E:101:ARG:HG2	2.06	0.55
5:E:163:SER:HB3	14:E:197:FES:S2	2.47	0.55
1:A:14:THR:HG21	1:A:389:ARG:HE	1.71	0.55
4:D:22:ASP:O	4:D:25:SER:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:90:TYR:C	4:D:92:PRO:HD3	2.27	0.55
4:D:136:GLU:H	4:D:136:GLU:CD	2.09	0.55
10:J:48:GLU:HA	10:J:50:LYS:HE3	1.89	0.55
4:D:167:GLU:HG3	4:D:177:ALA:O	2.06	0.55
5:E:170:ARG:HG2	5:E:170:ARG:NH2	2.14	0.55
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.72	0.55
12:C:609:HEM:HBB2	12:C:609:HEM:HMB1	1.88	0.55
4:D:115:TYR:HD2	4:D:116:ILE:H	1.55	0.55
3:C:202:GLU:OE1	3:C:202:GLU:HA	2.07	0.54
4:D:47:ALA:HA	4:D:90:TYR:H	1.72	0.54
5:E:69:LEU:HB2	5:E:92:ARG:HE	1.71	0.54
9:I:46:LYS:CG	9:I:47:ARG:N	2.68	0.54
2:B:246:GLU:O	2:B:427:SER:HA	2.07	0.54
3:C:163:TRP:HE3	3:C:164:ILE:HG13	1.72	0.54
3:C:268:ILE:O	3:C:268:ILE:HG13	2.06	0.54
4:D:115:TYR:O	4:D:116:ILE:HG12	2.07	0.54
4:D:116:ILE:HD11	4:D:191:ARG:CA	2.30	0.54
5:E:82:PRO:HB2	5:E:85:LYS:HG3	1.88	0.54
5:E:109:GLU:HB3	5:E:123:ASP:CB	2.37	0.54
9:I:31:GLN:O	9:I:35:PRO:HD2	2.08	0.54
9:I:41:PRO:HB3	9:I:44:ASP:OD2	2.06	0.54
6:F:35:ASP:OD1	6:F:61:ARG:NH1	2.41	0.54
1:A:158:PHE:O	1:A:164:ALA:HB2	2.08	0.54
1:A:255:ILE:HD12	1:A:335:MET:HE2	1.88	0.54
3:C:56:THR:OG1	3:C:61:THR:OG1	2.26	0.54
3:C:130:GLY:HA2	3:C:133:LEU:HD22	1.90	0.54
5:E:112:VAL:O	5:E:113:GLU:HB2	2.07	0.54
10:J:60:GLU:O	10:J:61:ASN:ND2	2.41	0.54
4:D:160:MET:HB2	12:D:242:HEM:C1D	2.41	0.54
2:B:68:LEU:HD13	2:B:191:LEU:HD11	1.88	0.54
4:D:27:ARG:NH1	10:J:58:LYS:HZ1	2.04	0.54
4:D:171:PHE:CE1	4:D:177:ALA:HB2	2.43	0.54
6:F:40:ASN:HD22	6:F:40:ASN:C	2.11	0.54
1:A:351:GLU:H	11:K:12:GLN:HE22	1.56	0.54
5:E:136:ILE:HD13	5:E:137:GLY:H	1.73	0.54
3:C:272:TRP:CE3	3:C:273:TYR:HB3	2.42	0.54
4:D:178:THR:CG2	4:D:181:GLN:HB2	2.38	0.54
5:E:132:TRP:HB3	5:E:185:TYR:OH	2.08	0.54
10:J:18:SER:CA	11:K:24:TRP:CZ3	2.73	0.54
2:B:248:ASN:HD22	2:B:249:GLY:N	2.06	0.53
3:C:206:ASN:ND2	3:C:207:ASN:N	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:207:ASN:HB2	3:C:208:PRO:CD	2.37	0.53
3:C:309:THR:HG22	3:C:370:GLY:HA3	1.89	0.53
4:D:43:MET:HA	4:D:113:LEU:HB2	1.88	0.53
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.89	0.53
9:I:11:PHE:HA	9:I:25:ALA:HB2	1.90	0.53
9:I:44:ASP:O	9:I:46:LYS:CB	2.56	0.53
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.24	0.53
4:D:116:ILE:C	4:D:118:ARG:N	2.61	0.53
4:D:43:MET:HG3	4:D:113:LEU:HB2	1.89	0.53
5:E:96:LEU:HD23	5:E:136:ILE:HG12	1.91	0.53
8:H:16:PRO:O	8:H:20:VAL:HG23	2.08	0.53
1:A:192:ALA:HB3	1:A:193:PRO:HD3	1.91	0.53
2:B:154:ASN:H	2:B:154:ASN:ND2	1.92	0.53
10:J:29:LEU:HA	11:K:34:TRP:CD1	2.44	0.53
9:I:43:LEU:HD23	9:I:43:LEU:N	2.22	0.53
2:B:72:ALA:HB1	2:B:75:LEU:HG	1.89	0.53
5:E:101:ARG:CB	5:E:131:GLU:HA	2.39	0.53
5:E:101:ARG:NH1	5:E:105:GLU:OE1	2.42	0.53
10:J:33:ARG:HG2	11:K:47:TYR:CE2	2.43	0.53
1:A:366:VAL:HG11	2:B:43:PRO:HB2	1.90	0.53
12:C:609:HEM:HBD2	12:C:609:HEM:HHA	1.90	0.53
2:B:264:ILE:HG12	2:B:316:TYR:C	2.30	0.53
5:E:122:HIS:N	5:E:170:ARG:HH12	2.06	0.53
1:A:143:THR:HG21	9:I:39:GLU:CG	2.38	0.53
2:B:207:ILE:N	2:B:207:ILE:HD12	2.24	0.53
2:B:388:ALA:HB3	9:I:2:LEU:HD13	1.91	0.53
4:D:113:LEU:O	4:D:115:TYR:N	2.41	0.53
1:A:86:LEU:HD13	1:A:99:ILE:CD1	2.39	0.52
1:A:144:SER:HA	9:I:42:VAL:CB	2.28	0.52
4:D:131:LEU:HD11	12:D:242:HEM:HMB3	1.91	0.52
4:D:14:HIS:HA	4:D:19:SER:HB3	1.91	0.52
5:E:187:PHE:HA	5:E:193:VAL:HG23	1.91	0.52
2:B:242:GLY:O	2:B:423:SER:HA	2.08	0.52
4:D:71:GLN:HE21	4:D:80:MET:CG	2.21	0.52
5:E:138:VAL:HG23	5:E:139:CYS:N	2.24	0.52
1:A:281:ASP:HB2	9:I:20:ARG:NE	2.24	0.52
5:E:82:PRO:O	5:E:84:GLY:N	2.42	0.52
3:C:99:GLY:HA2	3:C:102:LEU:HD12	1.92	0.52
9:I:49:VAL:C	9:I:51:CYS:H	2.13	0.52
1:A:279:HIS:HD2	1:A:284:TYR:OH	1.93	0.52
4:D:166:ASN:O	4:D:168:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:55:ILE:O	10:J:56:LYS:C	2.47	0.52
3:C:226:ILE:CG2	4:D:223:LYS:CB	2.87	0.52
4:D:88:SER:O	4:D:89:ASP:CG	2.48	0.52
2:B:245:ARG:NH2	2:B:433:THR:O	2.43	0.52
3:C:282:ARG:O	3:C:283:SER:C	2.47	0.52
4:D:24:THR:O	4:D:27:ARG:HB2	2.11	0.52
5:E:78:LEU:HD21	5:E:187:PHE:HE1	1.70	0.52
8:H:31:VAL:O	8:H:35:GLU:HB3	2.10	0.52
1:A:33:PRO:HD2	1:A:34:THR:HG22	1.91	0.51
1:A:245:GLU:OE1	7:G:11:ARG:HD3	2.10	0.51
5:E:136:ILE:HB	5:E:181:GLU:O	2.10	0.51
7:G:71:ARG:O	7:G:72:LYS:C	2.49	0.51
10:J:19:THR:O	10:J:23:THR:HG22	2.11	0.51
2:B:76:THR:CG2	2:B:136:GLU:OE1	2.55	0.51
2:B:176:LEU:HG	9:I:13:PRO:CG	2.40	0.51
1:A:212:ALA:O	1:A:216:PHE:HB2	2.11	0.51
2:B:298:ALA:CB	2:B:343:GLN:HG2	2.40	0.51
5:E:20:ASP:OD2	5:E:22:THR:HG22	2.11	0.51
1:A:143:THR:HG21	9:I:39:GLU:HG2	1.92	0.51
5:E:135:LEU:HD13	5:E:156:TYR:HE1	1.75	0.51
8:H:6:GLU:HA	8:H:9:GLU:HB3	1.93	0.51
3:C:102:LEU:CD2	3:C:304:ILE:HD12	2.41	0.51
3:C:328:LEU:HD23	3:C:361:LEU:HD11	1.92	0.51
3:C:344:GLU:O	3:C:348:ILE:HG23	2.10	0.51
3:C:68:HIS:CD2	3:C:72:ASP:HB2	2.45	0.51
3:C:186:PRO:CG	12:C:610:HEM:HHC	2.36	0.51
4:D:75:ASN:O	4:D:77:ASP:N	2.44	0.51
6:F:59:VAL:HG11	7:G:10:VAL:HG13	1.92	0.51
5:E:121:GLN:NE2	5:E:121:GLN:HA	2.26	0.51
1:A:100:LYS:HE2	1:A:373:THR:OG1	2.10	0.51
1:A:62:LEU:HD13	1:A:122:LEU:HD23	1.93	0.51
2:B:99:THR:OG1	9:I:14:VAL:HG22	2.11	0.51
3:C:105:GLY:HA2	3:C:107:TYR:CE1	2.46	0.51
4:D:188:THR:O	4:D:191:ARG:HB3	2.11	0.51
10:J:20:PHE:O	10:J:24:ILE:HG23	2.11	0.51
1:A:320:LEU:CD1	1:A:415:PHE:CZ	2.94	0.50
2:B:68:LEU:HG	2:B:144:LEU:HD11	1.93	0.50
4:D:38:SER:O	4:D:94:PRO:HG3	2.12	0.50
6:F:49:ARG:NH2	6:F:100:GLU:OE2	2.37	0.50
4:D:53:GLY:O	10:J:51:LEU:HG	2.11	0.50
5:E:91:TRP:NE1	5:E:195:VAL:HG23	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:24:ARG:HB2	7:G:27:PRO:HD3	1.93	0.50
1:A:146:ARG:NH2	1:A:308:GLN:CD	2.64	0.50
3:C:226:ILE:HG21	4:D:223:LYS:CA	2.41	0.50
4:D:79:GLU:O	4:D:80:MET:CB	2.57	0.50
3:C:272:TRP:HE3	3:C:273:TYR:HB3	1.77	0.50
4:D:28:ARG:HH11	8:H:78:LYS:HE2	1.76	0.50
9:I:22:VAL:HA	9:I:47:ARG:NH2	2.26	0.50
10:J:40:ASP:O	10:J:44:GLU:HG3	2.10	0.50
2:B:111:CYS:SG	2:B:119:LEU:HD13	2.51	0.50
4:D:20:SER:N	10:J:47:ASN:OD1	2.42	0.50
4:D:37:CYS:SG	12:D:242:HEM:CBB	2.99	0.50
7:G:73:ASN:O	7:G:74:PRO:O	2.30	0.50
9:I:2:LEU:O	9:I:3:SER:CB	2.47	0.50
1:A:222:THR:O	1:A:223:TYR:HB3	2.11	0.50
5:E:107:ASP:HA	5:E:110:ALA:CB	2.41	0.50
3:C:116:GLY:O	12:C:609:HEM:HMC3	2.12	0.50
3:C:129:MET:HE1	3:C:181:PHE:CD2	2.47	0.50
3:C:163:TRP:CE3	3:C:164:ILE:HG13	2.46	0.50
4:D:166:ASN:O	4:D:168:VAL:N	2.44	0.50
5:E:100:HIS:ND1	5:E:132:TRP:HZ3	2.04	0.50
5:E:151:GLY:HA3	5:E:157:TYR:HB2	1.93	0.50
8:H:50:THR:O	8:H:51:GLU:CB	2.58	0.50
1:A:255:ILE:HD12	1:A:335:MET:HE1	1.92	0.49
5:E:132:TRP:O	5:E:185:TYR:HE1	1.94	0.49
8:H:69:VAL:O	8:H:73:LEU:HB2	2.12	0.49
3:C:131:TYR:HA	12:C:610:HEM:HAD2	1.94	0.49
8:H:51:GLU:HG3	8:H:52:GLU:N	2.27	0.49
1:A:245:GLU:OE1	7:G:11:ARG:CD	2.60	0.49
5:E:156:TYR:HB3	5:E:165:TYR:HB2	1.93	0.49
1:A:373:THR:HB	1:A:374:PRO:HD3	1.94	0.49
5:E:165:TYR:HD2	5:E:169:GLY:O	1.95	0.49
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.47	0.49
1:A:228:VAL:N	1:A:229:PRO:HD3	2.19	0.49
3:C:159:ASN:OD1	3:C:159:ASN:N	2.44	0.49
3:C:222:PRO:CD	3:C:223:TYR:N	2.25	0.49
4:D:68:VAL:HG22	4:D:69:GLU:H	1.78	0.49
10:J:60:GLU:HB3	10:J:61:ASN:HD22	1.76	0.49
2:B:308:ASP:OD2	9:I:31:GLN:OE1	2.30	0.49
5:E:193:VAL:HG22	5:E:194:ILE:N	2.27	0.49
2:B:37:SER:HB3	2:B:216:LEU:HD12	1.94	0.49
3:C:126:THR:HG21	12:C:610:HEM:HMC2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:33:TYR:CD1	4:D:37:CYS:HB2	2.47	0.49
5:E:82:PRO:HG2	5:E:85:LYS:NZ	2.28	0.49
1:A:188:ARG:HD2	1:A:189:HIS:NE2	2.27	0.49
1:A:245:GLU:OE1	1:A:245:GLU:CA	2.60	0.49
4:D:27:ARG:HH11	10:J:58:LYS:NZ	2.10	0.49
1:A:222:THR:O	1:A:223:TYR:CB	2.60	0.49
2:B:101:THR:HG22	2:B:104:ASN:H	1.78	0.49
2:B:150:VAL:CG1	9:I:47:ARG:HD2	2.43	0.49
2:B:264:ILE:HG12	2:B:316:TYR:O	2.13	0.49
4:D:124:GLU:OE1	4:D:191:ARG:HD2	2.12	0.48
5:E:14:ARG:HE	5:E:18:VAL:HG21	1.78	0.48
5:E:78:LEU:O	5:E:132:TRP:CH2	2.66	0.48
2:B:137:VAL:HG21	2:B:188:PRO:HG3	1.95	0.48
5:E:142:LEU:HB2	14:E:197:FES:S1	2.53	0.48
1:A:80:GLU:HB3	2:B:292:THR:HG21	1.94	0.48
4:D:88:SER:O	4:D:89:ASP:CB	2.60	0.48
4:D:225:HIS:O	4:D:228:SER:HB2	2.14	0.48
1:A:332:ASP:OD2	3:C:6:LYS:NZ	2.32	0.48
4:D:32:VAL:O	4:D:36:VAL:HG23	2.14	0.48
1:A:252:HIS:NE2	9:I:43:LEU:HG	2.28	0.48
9:I:52:ARG:O	9:I:53:GLU:HB2	2.13	0.48
4:D:30:PHE:HD2	4:D:56:TYR:HH	1.57	0.48
5:E:163:SER:HB2	5:E:175:PRO:HD2	1.94	0.48
9:I:46:LYS:CG	9:I:47:ARG:H	2.25	0.48
5:E:68:VAL:O	5:E:68:VAL:CG1	2.61	0.48
5:E:101:ARG:HB2	5:E:131:GLU:CA	2.44	0.48
1:A:40:TRP:HB3	1:A:384:LEU:CD2	2.44	0.48
1:A:307:PHE:C	1:A:307:PHE:CD2	2.87	0.48
2:B:33:LEU:CD2	2:B:220:ALA:HB1	2.43	0.48
3:C:122:THR:CG2	3:C:189:ILE:HG12	2.43	0.48
4:D:155:GLY:C	4:D:157:ALA:H	2.13	0.48
5:E:138:VAL:O	5:E:139:CYS:CB	2.61	0.48
7:G:26:PHE:N	7:G:27:PRO:CD	2.77	0.48
11:K:42:LEU:C	11:K:44:TRP:H	2.17	0.48
4:D:145:GLU:O	4:D:147:LEU:N	2.43	0.48
4:D:223:LYS:HG3	4:D:224:ARG:N	2.26	0.48
2:B:313:ASN:HD22	2:B:322:PHE:HD1	1.61	0.48
4:D:184:LYS:HD3	8:H:78:LYS:HZ3	1.79	0.48
3:C:31:TRP:O	12:C:609:HEM:O2A	2.32	0.47
5:E:138:VAL:O	5:E:139:CYS:HB3	2.14	0.47
6:F:53:ASN:HD22	6:F:53:ASN:H	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:75:ALA:O	7:G:76:ALA:O	2.32	0.47
5:E:81:ILE:HB	5:E:100:HIS:NE2	2.30	0.47
5:E:128:LYS:HB2	5:E:185:TYR:CE2	2.49	0.47
11:K:48:ILE:O	11:K:48:ILE:HG22	2.15	0.47
1:A:145:MET:N	9:I:42:VAL:HB	2.29	0.47
1:A:396:GLU:HA	1:A:396:GLU:OE1	2.13	0.47
2:B:334:GLY:O	2:B:338:LYS:HG3	2.14	0.47
3:C:185:LEU:O	3:C:189:ILE:HG13	2.14	0.47
3:C:272:TRP:HE3	3:C:273:TYR:CB	2.27	0.47
4:D:12:TRP:O	4:D:13:SER:HB3	2.14	0.47
5:E:18:VAL:O	5:E:19:LEU:CB	2.61	0.47
5:E:77:LYS:HG2	5:E:80:ASP:HB2	1.97	0.47
9:I:11:PHE:HA	9:I:25:ALA:HB3	1.95	0.47
10:J:57:HIS:C	10:J:58:LYS:HG3	2.35	0.47
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.50	0.47
1:A:153:LEU:HD13	1:A:319:LEU:HD13	1.97	0.47
1:A:224:ASP:HB3	1:A:227:ALA:HB2	1.96	0.47
1:A:388:ARG:NH2	1:A:394:GLU:OE1	2.47	0.47
2:B:232:LEU:HD12	2:B:234:GLY:CA	2.44	0.47
3:C:57:SER:O	3:C:57:SER:OG	2.32	0.47
3:C:119:LEU:O	3:C:123:VAL:HG13	2.15	0.47
6:F:82:LYS:O	6:F:83:TYR:C	2.53	0.47
6:F:83:TYR:O	6:F:84:GLU:CG	2.54	0.47
7:G:77:TYR:CD1	7:G:77:TYR:O	2.68	0.47
9:I:49:VAL:HG12	9:I:50:LEU:H	1.80	0.47
10:J:60:GLU:C	10:J:61:ASN:ND2	2.67	0.47
7:G:56:TYR:HD1	7:G:56:TYR:O	1.97	0.47
9:I:2:LEU:H	9:I:2:LEU:HG	1.57	0.47
9:I:15:LEU:HD22	9:I:15:LEU:HA	1.39	0.47
2:B:95:LYS:NZ	2:B:110:GLU:OE1	2.44	0.47
2:B:248:ASN:C	2:B:248:ASN:ND2	2.67	0.47
3:C:65:SER:O	3:C:68:HIS:HB3	2.15	0.47
12:C:609:HEM:HMB1	12:C:609:HEM:CBB	2.45	0.47
4:D:54:VAL:O	10:J:51:LEU:HD23	2.15	0.47
5:E:96:LEU:HA	5:E:136:ILE:HA	1.97	0.47
8:H:3:PRO:O	8:H:6:GLU:HB2	2.14	0.47
10:J:29:LEU:HD12	11:K:34:TRP:HD1	1.80	0.47
1:A:255:ILE:CG2	1:A:342:TRP:HH2	2.28	0.46
1:A:311:ASN:ND2	1:A:313:CYS:SG	2.88	0.46
4:D:116:ILE:O	4:D:117:VAL:HG22	2.16	0.46
5:E:81:ILE:HG22	5:E:82:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:42:ILE:O	10:J:46:ILE:CG2	2.63	0.46
1:A:37:VAL:HG13	1:A:199:ALA:HB2	1.97	0.46
1:A:332:ASP:H	1:A:430:GLN:NE2	2.13	0.46
3:C:327:ALA:HA	7:G:51:PRO:HB3	1.96	0.46
4:D:4:GLU:OE1	4:D:154:PRO:HA	2.15	0.46
8:H:1:GLY:O	8:H:2:ASP:CB	2.60	0.46
5:E:123:ASP:CG	5:E:168:SER:HB3	2.35	0.46
7:G:28:HIS:HB3	7:G:31:SER:HB2	1.98	0.46
10:J:14:PHE:CD1	10:J:20:PHE:CD1	2.99	0.46
1:A:446:PHE:OXT	10:J:16:ARG:HB3	2.16	0.46
2:B:200:THR:OG1	2:B:227:ARG:NH1	2.48	0.46
2:B:369:LEU:HD11	2:B:399:LEU:HD21	1.97	0.46
4:D:163:PRO:C	4:D:164:ILE:HG12	2.35	0.46
8:H:17:LEU:HG	8:H:21:ARG:HD2	1.98	0.46
1:A:358:LYS:HD2	1:A:399:ILE:O	2.15	0.46
5:E:112:VAL:O	5:E:113:GLU:CB	2.63	0.46
7:G:24:ARG:CB	7:G:27:PRO:HD3	2.45	0.46
10:J:9:LEU:HB3	10:J:14:PHE:HE2	1.81	0.46
1:A:146:ARG:HH22	1:A:308:GLN:NE2	2.14	0.46
2:B:150:VAL:O	2:B:153:GLN:HB2	2.16	0.46
4:D:54:VAL:HG23	4:D:55:CYS:H	1.80	0.46
5:E:132:TRP:HA	5:E:132:TRP:CE3	2.50	0.46
5:E:165:TYR:CD2	5:E:169:GLY:O	2.68	0.46
1:A:245:GLU:OE2	7:G:11:ARG:NH2	2.43	0.46
1:A:341:GLN:NE2	1:A:344:ARG:HH22	2.04	0.46
2:B:308:ASP:OD1	9:I:28:PRO:HB3	2.15	0.46
2:B:325:TYR:HB3	9:I:28:PRO:HD3	1.97	0.46
4:D:178:THR:CB	8:H:16:PRO:HG2	2.45	0.46
11:K:39:ARG:H	11:K:39:ARG:HG3	1.26	0.46
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.98	0.46
4:D:90:TYR:HB3	4:D:91:PHE:H	1.27	0.46
3:C:226:ILE:HD12	3:C:226:ILE:HG23	1.68	0.45
4:D:54:VAL:HG21	4:D:192:TRP:CZ2	2.51	0.45
5:E:126:ARG:HD3	5:E:168:SER:HB2	1.98	0.45
6:F:72:GLN:HE21	6:F:72:GLN:HB2	1.56	0.45
10:J:33:ARG:CG	11:K:47:TYR:CE2	2.99	0.45
2:B:197:ASN:C	2:B:197:ASN:HD22	2.20	0.45
2:B:439:LEU:HD23	2:B:439:LEU:HA	1.73	0.45
3:C:141:TRP:CD1	3:C:265:PRO:HD3	2.51	0.45
3:C:214:ASP:CG	7:G:2:ARG:HH22	2.20	0.45
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:28:PRO:O	9:I:29:LEU:HB2	2.15	0.45
2:B:232:LEU:H	2:B:232:LEU:HG	1.25	0.45
3:C:272:TRP:HE3	3:C:273:TYR:CA	2.29	0.45
5:E:83:GLU:HG3	5:E:102:THR:HG22	1.97	0.45
1:A:158:PHE:HB3	1:A:161:THR:OG1	2.16	0.45
5:E:91:TRP:CD1	5:E:96:LEU:HD11	2.51	0.45
6:F:32:MET:HE3	6:F:61:ARG:CZ	2.46	0.45
8:H:40:CYS:HA	8:H:43:ARG:HG2	1.97	0.45
1:A:284:TYR:CE1	9:I:19:SER:O	2.69	0.45
2:B:213:HIS:N	2:B:214:PRO:CD	2.80	0.45
2:B:235:ALA:O	2:B:236:LYS:HB3	2.16	0.45
4:D:5:LEU:HB2	8:H:59:LEU:HD22	1.98	0.45
5:E:149:ASN:HA	5:E:155:GLY:CA	2.47	0.45
1:A:344:ARG:NH1	1:A:353:GLU:OE2	2.50	0.45
2:B:51:ILE:O	2:B:104:ASN:CB	2.62	0.45
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.98	0.45
5:E:97:PHE:CZ	5:E:137:GLY:CA	3.00	0.45
1:A:378:ASP:OD2	9:I:56:ARG:NH2	2.50	0.45
5:E:88:ALA:HA	5:E:96:LEU:O	2.17	0.45
6:F:40:ASN:ND2	6:F:43:VAL:H	2.15	0.45
3:C:87:ALA:HB2	12:C:610:HEM:HHD	1.99	0.45
3:C:246:ALA:N	3:C:247:PRO:HD3	2.32	0.45
3:C:343:VAL:O	3:C:343:VAL:CG1	2.65	0.45
1:A:311:ASN:ND2	1:A:311:ASN:O	2.49	0.44
3:C:249:LEU:HD23	3:C:250:LEU:HD23	1.98	0.44
5:E:102:THR:O	5:E:106:ILE:HG13	2.17	0.44
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.99	0.44
12:C:609:HEM:CMB	12:C:609:HEM:CBB	2.96	0.44
5:E:185:TYR:CE1	5:E:187:PHE:HE2	2.34	0.44
1:A:14:THR:CB	1:A:389:ARG:HG3	2.48	0.44
1:A:252:HIS:CE1	9:I:42:VAL:O	2.71	0.44
5:E:152:ASP:HB3	5:E:153:PHE:H	1.57	0.44
10:J:55:ILE:C	10:J:57:HIS:H	2.19	0.44
2:B:129:ALA:N	2:B:130:PRO:CD	2.80	0.44
9:I:39:GLU:HB3	9:I:40:SER:H	1.36	0.44
11:K:47:TYR:O	11:K:48:ILE:CB	2.64	0.44
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.99	0.44
2:B:150:VAL:HG13	9:I:47:ARG:HD2	1.99	0.44
2:B:308:ASP:OD2	9:I:31:GLN:HB2	2.17	0.44
3:C:185:LEU:HA	3:C:185:LEU:HD23	1.67	0.44
12:C:609:HEM:HBC2	12:C:609:HEM:CMC	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:TRP:HD1	5:E:96:LEU:HD11	1.83	0.44
8:H:8:GLU:O	8:H:12:GLU:N	2.30	0.44
8:H:11:GLU:C	8:H:13:LEU:N	2.71	0.44
1:A:11:VAL:HG21	1:A:392:LEU:HD12	1.99	0.44
1:A:46:ARG:HD2	1:A:163:LEU:CD1	2.48	0.44
1:A:242:CYS:O	7:G:14:ILE:HA	2.18	0.44
1:A:350:THR:HG21	11:K:9:ARG:HE	1.83	0.44
2:B:232:LEU:HB2	2:B:234:GLY:N	2.33	0.44
2:B:325:TYR:CD2	9:I:28:PRO:CD	2.97	0.44
3:C:322:GLN:NE2	7:G:47:ARG:HG3	2.32	0.44
4:D:10:TYR:CD1	4:D:15:ARG:HG3	2.53	0.44
4:D:27:ARG:HH12	10:J:58:LYS:HZ3	1.61	0.44
4:D:116:ILE:O	4:D:117:VAL:HG13	2.18	0.44
5:E:17:GLU:HB3	5:E:28:SER:CB	2.47	0.44
5:E:73:LYS:HG3	5:E:194:ILE:HB	1.99	0.44
10:J:29:LEU:CD1	11:K:34:TRP:HD1	2.30	0.44
10:J:47:ASN:O	10:J:48:GLU:HB2	2.18	0.44
1:A:112:LEU:O	1:A:116:ILE:HG12	2.17	0.44
3:C:272:TRP:HE3	3:C:273:TYR:N	2.14	0.44
4:D:41:HIS:HE1	4:D:111:PRO:HD2	1.83	0.44
4:D:178:THR:HG21	8:H:16:PRO:HG2	1.99	0.44
5:E:171:ILE:HG13	5:E:172:ARG:N	2.31	0.44
1:A:436:ARG:HH21	1:A:436:ARG:HG3	1.82	0.44
2:B:381:GLU:OE2	2:B:381:GLU:HA	2.17	0.44
5:E:129:LYS:HA	5:E:130:PRO:HD2	1.81	0.44
5:E:132:TRP:CB	5:E:185:TYR:OH	2.65	0.44
1:A:271:GLN:HE21	1:A:271:GLN:HA	1.83	0.43
1:A:375:VAL:HG13	1:A:389:ARG:NH2	2.33	0.43
3:C:352:GLN:O	3:C:356:VAL:HG13	2.18	0.43
4:D:152:TYR:C	4:D:153:PHE:O	2.53	0.43
5:E:101:ARG:HB3	5:E:131:GLU:HA	1.99	0.43
7:G:71:ARG:O	7:G:73:ASN:N	2.51	0.43
2:B:156:GLN:HG2	9:I:27:ARG:CD	2.49	0.43
2:B:213:HIS:HB3	2:B:214:PRO:HD3	2.00	0.43
2:B:370:MET:HB3	2:B:370:MET:HE2	1.76	0.43
4:D:136:GLU:HA	4:D:137:PRO:HD3	1.86	0.43
5:E:149:ASN:HA	5:E:155:GLY:C	2.37	0.43
4:D:171:PHE:HE1	4:D:177:ALA:HB2	1.83	0.43
5:E:135:LEU:CD2	5:E:169:GLY:HA3	2.45	0.43
8:H:49:GLN:O	8:H:50:THR:OG1	2.30	0.43
1:A:86:LEU:HD13	1:A:99:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HB3	1:A:107:PRO:HD3	2.01	0.43
4:D:8:PRO:HG3	8:H:66:ASP:HB3	2.01	0.43
4:D:184:LYS:HG3	8:H:74:PHE:HE2	1.82	0.43
9:I:34:VAL:CB	9:I:35:PRO:HD3	2.38	0.43
1:A:106:LEU:N	1:A:107:PRO:CD	2.82	0.43
3:C:276:PHE:HA	3:C:335:LEU:HB3	2.01	0.43
8:H:37:LEU:HD23	8:H:40:CYS:SG	2.59	0.43
11:K:42:LEU:C	11:K:44:TRP:N	2.72	0.43
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.65	0.43
4:D:10:TYR:O	4:D:12:TRP:N	2.52	0.43
4:D:91:PHE:CE2	4:D:93:LYS:HD2	2.45	0.43
6:F:64:ARG:NH1	6:F:64:ARG:CB	2.78	0.43
1:A:33:PRO:HG2	2:B:369:LEU:HD22	2.01	0.43
2:B:34:VAL:HG11	2:B:386:ALA:HB1	1.99	0.43
4:D:81:PHE:CD2	4:D:81:PHE:N	2.86	0.43
5:E:121:GLN:C	5:E:170:ARG:HH12	2.21	0.43
9:I:20:ARG:NH1	9:I:48:SER:OG	2.51	0.43
9:I:49:VAL:O	9:I:50:LEU:HB2	2.17	0.43
1:A:14:THR:CG2	1:A:389:ARG:HG3	2.48	0.43
1:A:46:ARG:HH12	1:A:315:ALA:HB3	1.83	0.43
8:H:18:THR:O	8:H:22:GLU:HB2	2.17	0.43
11:K:23:LEU:O	11:K:27:VAL:HG23	2.19	0.43
4:D:24:THR:OG1	10:J:54:HIS:CD2	2.72	0.43
3:C:138:MET:HE1	3:C:268:ILE:HB	2.01	0.42
1:A:80:GLU:HG2	2:B:284:HIS:HB2	2.01	0.42
2:B:77:THR:HG23	2:B:85:ILE:HD11	2.01	0.42
3:C:318:ARG:HD2	3:C:373:GLU:OE1	2.18	0.42
4:D:184:LYS:HD3	8:H:78:LYS:HZ2	1.84	0.42
8:H:23:GLN:O	8:H:26:GLN:HB3	2.19	0.42
1:A:248:LEU:O	1:A:427:PRO:HG3	2.18	0.42
1:A:307:PHE:HB2	1:A:324:PHE:HB3	2.00	0.42
2:B:243:GLU:HA	2:B:424:MET:O	2.20	0.42
4:D:7:PRO:HA	4:D:8:PRO:HD3	1.92	0.42
5:E:135:LEU:HA	5:E:182:VAL:CB	2.49	0.42
5:E:142:LEU:HD12	5:E:161:HIS:NE2	2.34	0.42
8:H:2:ASP:HA	8:H:3:PRO:HD3	1.84	0.42
4:D:12:TRP:HB3	4:D:14:HIS:CE1	2.55	0.42
6:F:64:ARG:CG	6:F:64:ARG:NH1	2.53	0.42
2:B:116:VAL:HG23	2:B:117:ASP:OD1	2.19	0.42
3:C:83:HIS:CD2	12:C:610:HEM:ND	2.88	0.42
1:A:120:CYS:SG	1:A:122:LEU:HG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:CD1	1:A:319:LEU:HD13	2.50	0.42
2:B:264:ILE:HD12	2:B:388:ALA:HB1	2.00	0.42
3:C:122:THR:HG21	3:C:189:ILE:HG12	2.02	0.42
4:D:234:LYS:HD3	5:E:8:PRO:HB2	2.01	0.42
5:E:176:ALA:HA	5:E:177:PRO:HD3	1.79	0.42
1:A:11:VAL:HA	1:A:12:PRO:HD3	1.91	0.42
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.95	0.42
2:B:325:TYR:HB3	9:I:28:PRO:CD	2.49	0.42
3:C:322:GLN:HE21	7:G:47:ARG:HG3	1.84	0.42
5:E:112:VAL:HG21	5:E:122:HIS:HA	2.02	0.42
5:E:121:GLN:HG2	5:E:126:ARG:HA	2.00	0.42
5:E:185:TYR:CZ	5:E:187:PHE:CE2	3.08	0.42
9:I:43:LEU:HD22	9:I:46:LYS:CD	2.50	0.42
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.34	0.42
1:A:280:TYR:HB3	1:A:307:PHE:CE1	2.55	0.42
2:B:258:VAL:HG12	2:B:423:SER:HB2	2.01	0.42
4:D:110:PRO:HA	4:D:111:PRO:HD3	1.80	0.42
6:F:12:TRP:O	6:F:16:ILE:HG12	2.20	0.42
2:B:200:THR:O	2:B:204:MET:HG3	2.20	0.42
3:C:12:LYS:HB2	3:C:12:LYS:HE3	1.84	0.42
3:C:106:SER:HB3	12:C:609:HEM:O2D	2.19	0.42
9:I:54:SER:O	9:I:55:LEU:HG	2.20	0.42
11:K:13:LEU:HA	11:K:13:LEU:HD23	1.58	0.42
2:B:26:PHE:CZ	2:B:391:SER:HA	2.54	0.42
3:C:226:ILE:HD13	3:C:226:ILE:HA	1.96	0.42
5:E:97:PHE:HZ	5:E:146:PRO:HD2	1.85	0.42
6:F:43:VAL:O	6:F:47:ILE:HG12	2.20	0.42
6:F:63:LYS:HB3	6:F:63:LYS:HE3	1.74	0.42
11:K:1:MET:C	11:K:3:THR:H	2.23	0.42
3:C:45:ILE:HA	12:C:610:HEM:CBB	2.50	0.41
3:C:45:ILE:HG12	12:C:610:HEM:HBB1	2.01	0.41
4:D:86:LYS:H	4:D:86:LYS:HG2	1.50	0.41
5:E:82:PRO:HG2	5:E:85:LYS:HE2	2.02	0.41
7:G:26:PHE:O	7:G:27:PRO:C	2.59	0.41
4:D:75:ASN:HB3	4:D:79:GLU:OE2	2.20	0.41
4:D:112:ASP:HB3	4:D:118:ARG:CZ	2.50	0.41
5:E:132:TRP:HA	5:E:132:TRP:HE3	1.86	0.41
5:E:179:ASN:O	5:E:180:LEU:CB	2.57	0.41
5:E:185:TYR:CZ	5:E:187:PHE:HE2	2.38	0.41
8:H:25:GLU:HG2	8:H:34:ARG:HH11	1.85	0.41
11:K:33:VAL:CG2	11:K:41:ILE:HD12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:28:GLU:HB3	8:H:29:LYS:HE2	2.02	0.41
10:J:50:LYS:H	10:J:50:LYS:HG3	1.49	0.41
2:B:370:MET:O	2:B:373:GLU:HB2	2.20	0.41
3:C:132:VAL:HA	3:C:139:SER:HB3	2.03	0.41
3:C:141:TRP:O	3:C:145:VAL:HG23	2.19	0.41
8:H:5:GLU:O	8:H:9:GLU:N	2.53	0.41
9:I:9:GLY:H	9:I:26:LEU:HB2	1.86	0.41
10:J:58:LYS:C	10:J:60:GLU:H	2.23	0.41
2:B:117:ASP:OD1	2:B:117:ASP:N	2.52	0.41
2:B:232:LEU:CD1	2:B:234:GLY:HA2	2.51	0.41
5:E:78:LEU:HD22	5:E:193:VAL:CG1	2.49	0.41
10:J:50:LYS:HB2	10:J:52:TRP:H	1.85	0.41
5:E:78:LEU:HA	5:E:81:ILE:HG13	2.02	0.41
1:A:255:ILE:CD1	1:A:335:MET:CE	2.98	0.41
3:C:129:MET:HE1	3:C:181:PHE:HD2	1.84	0.41
5:E:84:GLY:HA3	5:E:99:ARG:HH21	1.86	0.41
1:A:236:PHE:CD2	1:A:236:PHE:C	2.94	0.41
1:A:305:GLN:HA	1:A:305:GLN:HE21	1.86	0.41
1:A:360:LEU:CD2	2:B:93:GLY:HA2	2.51	0.41
3:C:193:ALA:O	3:C:196:HIS:HB3	2.21	0.41
4:D:117:VAL:HG12	4:D:191:ARG:HH22	1.84	0.41
4:D:118:ARG:O	4:D:119:ALA:HB2	2.21	0.41
4:D:157:ALA:O	4:D:158:ILE:HG13	2.21	0.41
4:D:166:ASN:H	4:D:166:ASN:ND2	2.16	0.41
6:F:53:ASN:HD22	6:F:53:ASN:N	2.19	0.41
8:H:15:ASP:O	8:H:16:PRO:C	2.59	0.41
9:I:55:LEU:HB3	9:I:56:ARG:H	1.19	0.41
1:A:305:GLN:HA	1:A:305:GLN:NE2	2.36	0.41
1:A:438:ARG:HH21	5:E:33:LYS:NZ	2.19	0.41
5:E:49:TYR:CD2	5:E:49:TYR:C	2.94	0.41
5:E:157:TYR:O	5:E:159:PRO:HD3	2.21	0.41
1:A:40:TRP:HB3	1:A:384:LEU:HD21	2.03	0.40
1:A:245:GLU:OE1	1:A:245:GLU:C	2.60	0.40
2:B:200:THR:HB	2:B:227:ARG:HG2	2.04	0.40
2:B:292:THR:HG23	2:B:363:LYS:NZ	2.36	0.40
3:C:42:ILE:HD13	3:C:42:ILE:HA	1.96	0.40
4:D:165:TYR:HD1	4:D:179:MET:HG2	1.86	0.40
5:E:121:GLN:C	5:E:170:ARG:NH1	2.75	0.40
10:J:55:ILE:O	10:J:58:LYS:N	2.54	0.40
4:D:156:GLN:HE21	4:D:156:GLN:HB2	1.64	0.40
7:G:2:ARG:H	7:G:2:ARG:HG2	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ASN:ND2	1:A:362:ARG:HH11	2.19	0.40
2:B:40:ASN:HD22	2:B:40:ASN:HA	1.66	0.40
2:B:52:LYS:HD2	2:B:387:LEU:HD22	2.04	0.40
2:B:236:LYS:O	2:B:238:LYS:HD2	2.21	0.40
2:B:354:ASN:HB3	2:B:355:PRO:HD3	2.04	0.40
2:B:385:GLN:HA	9:I:2:LEU:HD12	2.03	0.40
3:C:109:PHE:HB3	3:C:112:THR:HG23	2.04	0.40
3:C:226:ILE:HG21	4:D:223:LYS:CB	2.51	0.40
4:D:171:PHE:HZ	4:D:182:VAL:HG23	1.86	0.40
4:D:178:THR:CG2	8:H:16:PRO:HG2	2.52	0.40
4:D:116:ILE:HD12	4:D:124:GLU:HG2	2.03	0.40
4:D:181:GLN:HG2	8:H:78:LYS:HZ1	1.87	0.40
1:A:422:VAL:HG21	1:A:437:ILE:HD13	2.04	0.40
2:B:68:LEU:HD23	2:B:68:LEU:HA	1.85	0.40
2:B:369:LEU:HD23	2:B:369:LEU:HA	1.98	0.40
2:B:381:GLU:OE2	9:I:3:SER:HB3	2.21	0.40
4:D:5:LEU:HD11	8:H:63:HIS:ND1	2.36	0.40
4:D:28:ARG:O	4:D:32:VAL:HG23	2.20	0.40
6:F:82:LYS:C	6:F:83:TYR:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/446 (100%)	408 (92%)	28 (6%)	8 (2%)	8	6
2	B	421/439 (96%)	397 (94%)	17 (4%)	7 (2%)	9	7
3	C	375/379 (99%)	352 (94%)	16 (4%)	7 (2%)	8	6
4	D	238/241 (99%)	164 (69%)	35 (15%)	39 (16%)	0	0
5	E	194/196 (99%)	123 (63%)	35 (18%)	36 (19%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	F	107/110 (97%)	96 (90%)	8 (8%)	3 (3%)	5 2
7	G	77/81 (95%)	64 (83%)	7 (9%)	6 (8%)	1 0
8	H	76/78 (97%)	57 (75%)	7 (9%)	12 (16%)	0 0
9	I	55/78 (70%)	28 (51%)	11 (20%)	16 (29%)	0 0
10	J	58/62 (94%)	46 (79%)	9 (16%)	3 (5%)	2 0
11	K	51/56 (91%)	43 (84%)	4 (8%)	4 (8%)	1 0
All	All	2096/2166 (97%)	1778 (85%)	177 (8%)	141 (7%)	1 0

All (141) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	VAL
2	B	232	LEU
2	B	234	GLY
2	B	305	GLN
3	C	172	LYS
3	C	222	PRO
3	C	258	PRO
3	C	272	TRP
4	D	10	TYR
4	D	76	GLU
4	D	80	MET
4	D	86	LYS
4	D	87	LEU
4	D	89	ASP
4	D	90	TYR
4	D	112	ASP
4	D	116	ILE
4	D	117	VAL
4	D	119	ALA
4	D	123	GLY
4	D	148	TYR
4	D	153	PHE
4	D	156	GLN
4	D	158	ILE
4	D	165	TYR
4	D	167	GLU
4	D	170	GLU
4	D	173	ASP
5	E	21	SER

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Mol	Chain	Res	Type
5	E	22	THR
5	E	67	ASP
5	E	69	LEU
5	E	83	GLU
5	E	92	ARG
5	E	113	GLU
5	E	121	GLN
5	E	139	CYS
5	E	156	TYR
5	E	160	CYS
5	E	185	TYR
5	E	188	THR
5	E	195	VAL
6	F	3	ARG
6	F	7	SER
7	G	27	PRO
7	G	73	ASN
7	G	74	PRO
7	G	76	ALA
8	H	2	ASP
8	H	16	PRO
8	H	48	SER
8	H	52	GLU
8	H	73	LEU
8	H	74	PHE
9	I	3	SER
9	I	29	LEU
9	I	37	THR
9	I	39	GLU
9	I	40	SER
9	I	45	LEU
9	I	47	ARG
9	I	53	GLU
9	I	55	LEU
9	I	56	ARG
10	J	56	LYS
11	K	52	PHE
1	A	286	GLY
1	A	393	ALA
3	C	283	SER
4	D	2	ASP
4	D	13	SER

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Mol	Chain	Res	Type
4	D	14	HIS
4	D	20	SER
4	D	96	PRO
4	D	114	SER
4	D	152	TYR
4	D	172	ASP
5	E	5	ILE
5	E	18	VAL
5	E	73	LYS
5	E	74	ILE
5	E	153	PHE
5	E	155	GLY
5	E	159	PRO
7	G	71	ARG
8	H	13	LEU
8	H	49	GLN
8	H	51	GLU
9	I	2	LEU
11	K	43	ASP
11	K	48	ILE
1	A	45	SER
2	B	171	ALA
2	B	228	GLY
2	B	235	ALA
4	D	23	HIS
4	D	91	PHE
4	D	113	LEU
4	D	166	ASN
4	D	198	HIS
5	E	103	LYS
5	E	157	TYR
5	E	161	HIS
5	E	184	SER
6	F	4	PRO
9	I	48	SER
9	I	51	CYS
10	J	48	GLU
11	K	38	TRP
1	A	159	GLN
1	A	225	GLU
1	A	226	ASP
4	D	8	PRO

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Mol	Chain	Res	Type
4	D	145	GLU
4	D	179	MET
5	E	75	GLU
5	E	130	PRO
5	E	133	VAL
5	E	136	ILE
8	H	28	GLU
8	H	46	SER
9	I	8	SER
1	A	223	TYR
4	D	17	LEU
4	D	163	PRO
5	E	6	LYS
5	E	112	VAL
5	E	132	TRP
5	E	135	LEU
5	E	194	ILE
8	H	77	LEU
2	B	431	GLY
5	E	180	LEU
10	J	52	TRP
5	E	137	GLY
3	C	345	HIS
4	D	84	PRO
9	I	4	VAL
9	I	34	VAL
3	C	170	VAL
7	G	26	PHE

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%)	317 (86%)	53 (14%)	3 3
2	B	332/343 (97%)	293 (88%)	39 (12%)	5 5
3	C	325/327 (99%)	280 (86%)	45 (14%)	3 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	205/206 (100%)	161 (78%)	44 (22%)	1 0
5	E	168/168 (100%)	140 (83%)	28 (17%)	2 1
6	F	98/98 (100%)	83 (85%)	15 (15%)	2 2
7	G	69/71 (97%)	58 (84%)	11 (16%)	2 2
8	H	74/74 (100%)	59 (80%)	15 (20%)	1 1
9	I	44/60 (73%)	33 (75%)	11 (25%)	0 0
10	J	50/52 (96%)	42 (84%)	8 (16%)	2 2
11	K	43/46 (94%)	36 (84%)	7 (16%)	2 1
All	All	1778/1815 (98%)	1502 (84%)	276 (16%)	2 2

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	14	THR
1	A	18	GLN
1	A	21	ASN
1	A	23	LEU
1	A	34	THR
1	A	37	VAL
1	A	49	SER
1	A	73	ASN
1	A	75	LEU
1	A	78	GLU
1	A	103	SER
1	A	108	LYS
1	A	112	LEU
1	A	113	LEU
1	A	116	ILE
1	A	127	ILE
1	A	132	ASP
1	A	135	LEU
1	A	136	GLN
1	A	149	VAL
1	A	153	LEU
1	A	176	LYS
1	A	177	LEU
1	A	186	LEU
1	A	188	ARG

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Mol	Chain	Res	Type
1	A	203	LEU
1	A	204	GLU
1	A	208	LEU
1	A	210	ASP
1	A	222	THR
1	A	224	ASP
1	A	235	ARG
1	A	245	GLU
1	A	248	LEU
1	A	255	ILE
1	A	257	VAL
1	A	271	GLN
1	A	296	SER
1	A	308	GLN
1	A	311	ASN
1	A	312	ILE
1	A	355	LEU
1	A	360	LEU
1	A	377	GLU
1	A	381	ARG
1	A	384	LEU
1	A	389	ARG
1	A	397	SER
1	A	398	ARG
1	A	430	GLN
1	A	436	ARG
1	A	445	ARG
2	B	38	LEU
2	B	40	ASN
2	B	55	SER
2	B	56	ARG
2	B	68	LEU
2	B	69	LEU
2	B	78	LYS
2	B	98	VAL
2	B	101	THR
2	B	109	VAL
2	B	113	ARG
2	B	119	LEU
2	B	123	LEU
2	B	140	LEU
2	B	154	ASN

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Mol	Chain	Res	Type
2	B	163	LEU
2	B	176	LEU
2	B	186	VAL
2	B	189	VAL
2	B	197	ASN
2	B	211	VAL
2	B	226	ILE
2	B	227	ARG
2	B	232	LEU
2	B	238	LYS
2	B	248	ASN
2	B	257	LEU
2	B	258	VAL
2	B	301	LYS
2	B	305	GLN
2	B	309	VAL
2	B	310	SER
2	B	332	SER
2	B	343	GLN
2	B	353	SER
2	B	379	LEU
2	B	397	THR
2	B	415	LYS
2	B	416	LYS
3	C	3	ASN
3	C	4	ILE
3	C	11	MET
3	C	12	LYS
3	C	26	ASN
3	C	28	SER
3	C	56	THR
3	C	57	SER
3	C	59	THR
3	C	60	THR
3	C	67	THR
3	C	80	ARG
3	C	88	SER
3	C	90	PHE
3	C	94	LEU
3	C	110	LEU
3	C	112	THR
3	C	123	VAL

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Mol	Chain	Res	Type
3	C	129	MET
3	C	133	LEU
3	C	135	TRP
3	C	159	ASN
3	C	161	VAL
3	C	172	LYS
3	C	202	GLU
3	C	241	LEU
3	C	242	LEU
3	C	254	ASP
3	C	282	ARG
3	C	284	ILE
3	C	291	VAL
3	C	297	SER
3	C	299	LEU
3	C	300	ILE
3	C	304	ILE
3	C	309	THR
3	C	320	LEU
3	C	328	LEU
3	C	335	LEU
3	C	348	ILE
3	C	353	LEU
3	C	356	VAL
3	C	366	MET
3	C	372	ILE
3	C	379	TRP
4	D	10	TYR
4	D	15	ARG
4	D	18	LEU
4	D	20	SER
4	D	24	THR
4	D	36	VAL
4	D	37	CYS
4	D	55	CYS
4	D	57	THR
4	D	58	GLU
4	D	80	MET
4	D	86	LYS
4	D	88	SER
4	D	90	TYR
4	D	91	PHE

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Mol	Chain	Res	Type
4	D	97	ASN
4	D	113	LEU
4	D	115	TYR
4	D	116	ILE
4	D	117	VAL
4	D	120	ARG
4	D	124	GLU
4	D	132	THR
4	D	136	GLU
4	D	139	THR
4	D	144	ARG
4	D	145	GLU
4	D	156	GLN
4	D	164	ILE
4	D	165	TYR
4	D	173	ASP
4	D	175	THR
4	D	178	THR
4	D	179	MET
4	D	182	VAL
4	D	184	LYS
4	D	191	ARG
4	D	203	ARG
4	D	210	LEU
4	D	212	MET
4	D	218	LEU
4	D	223	LYS
4	D	226	LYS
4	D	228	SER
5	E	5	ILE
5	E	18	VAL
5	E	25	SER
5	E	44	THR
5	E	65	SER
5	E	67	ASP
5	E	68	VAL
5	E	75	GLU
5	E	78	LEU
5	E	81	ILE
5	E	89	PHE
5	E	90	LYS
5	E	91	TRP

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Mol	Chain	Res	Type
5	E	107	ASP
5	E	118	ARG
5	E	119	ASP
5	E	121	GLN
5	E	122	HIS
5	E	132	TRP
5	E	133	VAL
5	E	134	ILE
5	E	136	ILE
5	E	160	CYS
5	E	170	ARG
5	E	171	ILE
5	E	190	ASP
5	E	194	ILE
5	E	195	VAL
6	F	3	ARG
6	F	29	LEU
6	F	32	MET
6	F	40	ASN
6	F	52	GLU
6	F	53	ASN
6	F	64	ARG
6	F	71	ARG
6	F	72	GLN
6	F	73	GLN
6	F	77	LYS
6	F	78	GLU
6	F	87	LYS
6	F	88	SER
6	F	94	LEU
7	G	2	ARG
7	G	13	VAL
7	G	31	SER
7	G	37	VAL
7	G	45	ILE
7	G	46	LEU
7	G	47	ARG
7	G	56	TYR
7	G	72	LYS
7	G	73	ASN
7	G	74	PRO
8	H	2	ASP

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Mol	Chain	Res	Type
8	H	5	GLU
8	H	11	GLU
8	H	14	VAL
8	H	16	PRO
8	H	19	THR
8	H	20	VAL
8	H	28	GLU
8	H	29	LYS
8	H	31	VAL
8	H	35	GLU
8	H	37	LEU
8	H	41	ASP
8	H	49	GLN
8	H	52	GLU
9	I	8	SER
9	I	11	PHE
9	I	15	LEU
9	I	16	SER
9	I	18	THR
9	I	27	ARG
9	I	39	GLU
9	I	43	LEU
9	I	47	ARG
9	I	49	VAL
9	I	53	GLU
10	J	5	LEU
10	J	11	SER
10	J	18	SER
10	J	24	ILE
10	J	46	ILE
10	J	50	LYS
10	J	51	LEU
10	J	59	TYR
11	K	1	MET
11	K	20	THR
11	K	23	LEU
11	K	24	TRP
11	K	34	TRP
11	K	38	TRP
11	K	44	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	61	HIS
1	A	73	ASN
1	A	85	HIS
1	A	118	GLN
1	A	126	GLN
1	A	173	ASN
1	A	252	HIS
1	A	271	GLN
1	A	274	ASN
1	A	279	HIS
1	A	305	GLN
1	A	308	GLN
1	A	311	ASN
1	A	323	HIS
1	A	341	GLN
1	A	359	ASN
1	A	418	GLN
1	A	430	GLN
2	B	20	HIS
2	B	40	ASN
2	B	153	GLN
2	B	154	ASN
2	B	162	ASN
2	B	174	ASN
2	B	197	ASN
2	B	248	ASN
2	B	276	GLN
2	B	313	ASN
2	B	342	ASN
2	B	343	GLN
2	B	354	ASN
2	B	358	GLN
2	B	362	ASN
2	B	385	GLN
3	C	15	ASN
3	C	26	ASN
3	C	44	GLN
3	C	68	HIS
3	C	74	ASN
3	C	114	ASN
3	C	206	ASN
3	C	286	ASN

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Mol	Chain	Res	Type
3	C	322	GLN
3	C	345	HIS
3	C	352	GLN
4	D	23	HIS
4	D	71	GLN
4	D	156	GLN
4	D	166	ASN
4	D	181	GLN
5	E	57	GLN
5	E	121	GLN
5	E	161	HIS
5	E	179	ASN
6	F	40	ASN
6	F	53	ASN
6	F	72	GLN
6	F	73	GLN
8	H	23	GLN
9	I	31	GLN
10	J	61	ASN
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	$\#\|Z\| > 2$
12	HEM	C	610	3	41,50,50	2.90	18 (43%)	45,82,82	2.80	20 (44%)
13	FMX	C	611	-	29,31,31	0.81	1 (3%)	34,44,44	1.19	3 (8%)
12	HEM	C	609	3	41,50,50	3.12	22 (53%)	45,82,82	2.67	19 (42%)
14	FES	E	197	5	0,4,4	-	-	-		
12	HEM	D	242	4	41,50,50	1.89	5 (12%)	45,82,82	1.89	10 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HEM	C	610	3	-	5/12/54/54	-
13	FMX	C	611	-	-	2/14/33/33	0/4/4/4
12	HEM	C	609	3	-	9/12/54/54	-
14	FES	E	197	5	-	-	0/1/1/1
12	HEM	D	242	4	-	4/12/54/54	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	242	HEM	C3D-C2D	7.26	1.52	1.36
12	C	610	HEM	C3C-C2C	-6.98	1.30	1.40
12	C	609	HEM	C3B-C4B	-6.97	1.30	1.44
12	C	609	HEM	CHA-C4D	6.68	1.52	1.35
12	C	609	HEM	C1D-C2D	-6.53	1.31	1.44
12	C	610	HEM	C4D-C3D	-6.40	1.34	1.45
12	C	609	HEM	CHB-C1B	5.62	1.49	1.35
12	C	610	HEM	C3B-C4B	-5.33	1.34	1.44
12	C	609	HEM	C1B-C2B	-5.18	1.34	1.44
12	C	610	HEM	CHB-C1B	5.17	1.48	1.35
12	C	609	HEM	C3C-C2C	-5.13	1.33	1.40
12	C	610	HEM	CHA-C4D	5.11	1.48	1.35
12	C	610	HEM	C1B-C2B	-4.88	1.35	1.44
12	C	609	HEM	CBB-CAB	4.85	1.54	1.30
12	D	242	HEM	C3C-C2C	-4.35	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	609	HEM	C4D-C3D	-4.31	1.37	1.45
12	C	610	HEM	CBB-CAB	4.26	1.51	1.30
12	C	609	HEM	C4A-CHB	4.05	1.52	1.41
12	C	609	HEM	C2C-C1C	-3.84	1.33	1.42
12	D	242	HEM	C3C-CAC	3.67	1.55	1.47
12	C	610	HEM	C1D-C2D	-3.63	1.37	1.44
12	C	610	HEM	C2C-C1C	-3.59	1.34	1.42
12	C	610	HEM	CBC-CAC	3.43	1.52	1.29
12	C	609	HEM	CBC-CAC	3.42	1.52	1.29
12	C	609	HEM	O2D-CGD	-3.26	1.19	1.30
12	C	610	HEM	C4A-CHB	3.22	1.49	1.41
12	C	610	HEM	CHD-C1D	3.19	1.50	1.41
12	C	609	HEM	C4B-NB	3.14	1.45	1.38
12	C	610	HEM	C3D-C2D	-3.11	1.30	1.36
12	D	242	HEM	FE-NB	3.08	2.12	1.96
12	C	610	HEM	CHC-C4B	3.03	1.49	1.41
12	C	610	HEM	C1A-CHA	2.99	1.49	1.41
12	C	609	HEM	C1A-CHA	2.97	1.49	1.41
12	C	609	HEM	C2A-C3A	2.90	1.46	1.37
12	C	610	HEM	C2A-C3A	2.85	1.46	1.37
12	C	609	HEM	C4D-ND	2.77	1.45	1.40
12	C	609	HEM	CHC-C4B	2.74	1.49	1.41
12	C	609	HEM	CHD-C1D	2.70	1.48	1.41
13	C	611	FMX	C7-C5	-2.66	1.46	1.53
12	C	609	HEM	O2A-CGA	-2.60	1.22	1.30
12	D	242	HEM	CAB-C3B	2.51	1.54	1.47
12	C	610	HEM	C4B-NB	2.36	1.43	1.38
12	C	609	HEM	CAB-C3B	2.32	1.53	1.47
12	C	609	HEM	C3C-CAC	2.32	1.52	1.47
12	C	610	HEM	O2A-CGA	-2.20	1.23	1.30
12	C	609	HEM	C3B-C2B	-2.12	1.33	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	610	HEM	C4C-CHD-C1D	-8.21	111.72	122.56
12	C	609	HEM	C4C-CHD-C1D	-7.57	112.57	122.56
12	C	609	HEM	C4B-CHC-C1C	-7.17	113.09	122.56
12	C	610	HEM	C4B-CHC-C1C	-7.13	113.15	122.56
12	D	242	HEM	C4D-ND-C1D	6.02	111.30	105.07
12	C	610	HEM	C2C-C3C-C4C	5.16	110.50	106.90
12	C	610	HEM	CHC-C4B-NB	5.02	129.89	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	610	HEM	CBD-CAD-C3D	-4.88	99.08	112.63
12	C	609	HEM	C1B-NB-C4B	-4.75	100.17	105.07
12	C	609	HEM	CHD-C1D-ND	4.37	129.18	124.43
13	C	611	FMX	C21-N1-N2	4.22	124.35	116.23
12	C	609	HEM	C3B-C2B-C1B	4.20	109.60	106.49
12	D	242	HEM	CAA-CBA-CGA	-4.18	102.05	113.76
12	C	610	HEM	C4D-ND-C1D	-4.13	100.81	105.07
12	C	609	HEM	CAD-C3D-C2D	-4.07	120.30	127.88
12	D	242	HEM	CBA-CAA-C2A	3.96	119.37	112.62
12	C	609	HEM	CAD-C3D-C4D	3.81	131.31	124.66
12	C	609	HEM	CHC-C4B-NB	3.68	128.42	124.43
12	C	610	HEM	CHB-C1B-NB	3.63	128.86	124.38
12	C	609	HEM	C1D-C2D-C3D	3.59	110.73	106.96
12	C	610	HEM	CHA-C4D-ND	3.57	128.79	124.38
12	C	610	HEM	C3B-C2B-C1B	3.48	109.07	106.49
12	C	610	HEM	CBB-CAB-C3B	-3.46	110.38	127.62
12	C	610	HEM	C4B-C3B-C2B	3.19	109.65	107.11
12	D	242	HEM	CAD-CBD-CGD	-3.05	107.03	113.60
12	C	609	HEM	CBA-CAA-C2A	2.99	117.73	112.62
12	C	609	HEM	CHC-C4B-C3B	-2.89	120.15	124.57
12	D	242	HEM	C4B-CHC-C1C	2.88	126.36	122.56
13	C	611	FMX	C13-C8-C5	-2.87	115.97	120.62
12	C	609	HEM	C2C-C3C-C4C	2.79	108.85	106.90
12	C	609	HEM	CHD-C1D-C2D	-2.73	120.72	124.98
12	C	610	HEM	CHA-C4D-C3D	-2.63	120.39	125.33
12	D	242	HEM	C4C-CHD-C1D	2.57	125.95	122.56
12	C	610	HEM	CHD-C1D-ND	2.48	127.13	124.43
12	C	610	HEM	C1D-C2D-C3D	2.42	109.50	106.96
12	C	609	HEM	CBB-CAB-C3B	-2.40	115.69	127.62
13	C	611	FMX	C9-C8-C5	2.32	124.39	120.62
12	C	610	HEM	CMD-C2D-C1D	2.26	128.47	125.04
12	C	610	HEM	CAD-CBD-CGD	2.25	118.45	113.60
12	C	609	HEM	C3D-C4D-ND	-2.24	107.67	110.17
12	C	610	HEM	C4A-C3A-C2A	-2.23	105.44	107.00
12	C	609	HEM	O2D-CGD-O1D	-2.18	117.86	123.30
12	C	609	HEM	CHA-C4D-ND	2.18	127.07	124.38
12	D	242	HEM	O1A-CGA-CBA	-2.17	116.09	123.08
12	D	242	HEM	O2A-CGA-CBA	2.17	120.99	114.03
12	C	610	HEM	CHC-C4B-C3B	-2.09	121.38	124.57
12	C	609	HEM	CHB-C1B-NB	2.08	126.95	124.38
12	C	610	HEM	CAD-C3D-C2D	-2.07	124.02	127.88
12	D	242	HEM	CMA-C3A-C4A	-2.04	125.33	128.46

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	609	HEM	C4D-ND-C1D	-2.04	102.96	105.07
12	D	242	HEM	O2D-CGD-CBD	2.04	120.58	114.03
12	C	610	HEM	C1B-NB-C4B	-2.03	102.97	105.07

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	609	HEM	C2A-CAA-CBA-CGA
12	C	609	HEM	C2D-C3D-CAD-CBD
12	C	609	HEM	C4D-C3D-CAD-CBD
12	C	610	HEM	C2B-C3B-CAB-CBB
12	C	609	HEM	C3D-CAD-CBD-CGD
12	C	610	HEM	C2A-CAA-CBA-CGA
12	C	610	HEM	C4B-C3B-CAB-CBB
12	C	609	HEM	C3A-C2A-CAA-CBA
12	C	609	HEM	CAA-CBA-CGA-O2A
12	D	242	HEM	CAD-CBD-CGD-O2D
12	C	609	HEM	CAA-CBA-CGA-O1A
12	D	242	HEM	CAD-CBD-CGD-O1D
12	C	610	HEM	CAD-CBD-CGD-O1D
12	C	610	HEM	CAD-CBD-CGD-O2D
12	D	242	HEM	CAA-CBA-CGA-O2A
12	D	242	HEM	CAA-CBA-CGA-O1A
12	C	609	HEM	CAD-CBD-CGD-O2D
13	C	611	FMX	C6-C5-C8-C9
13	C	611	FMX	C6-C5-C8-C13
12	C	609	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

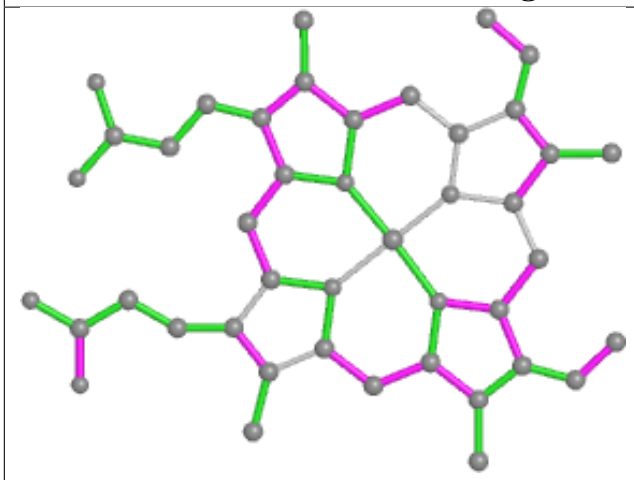
4 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	610	HEM	12	0
12	C	609	HEM	11	0
14	E	197	FES	2	0
12	D	242	HEM	6	0

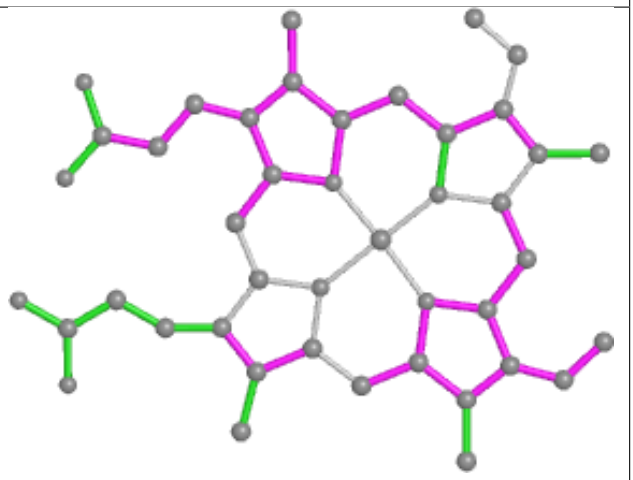
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

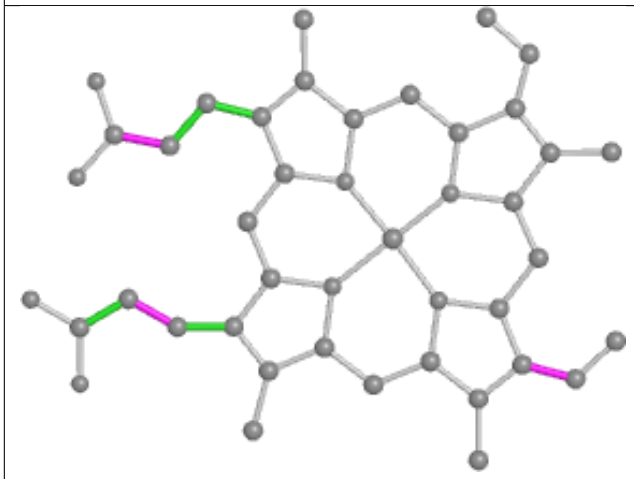
Ligand HEM C 610



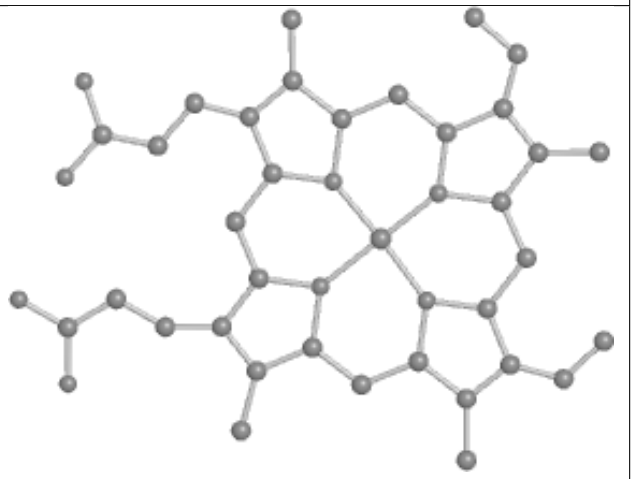
Bond lengths



Bond angles

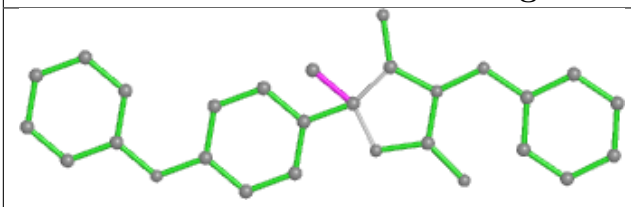


Torsions

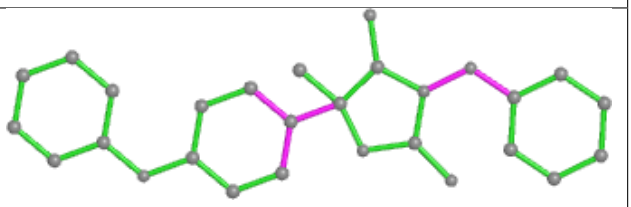


Rings

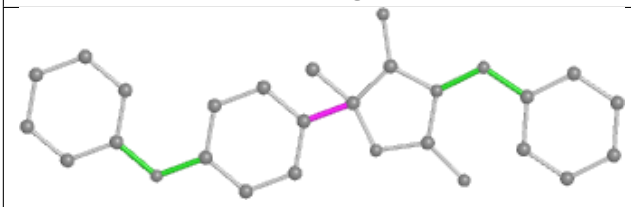
Ligand FMX C 611



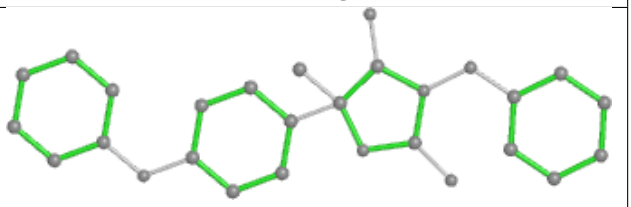
Bond lengths



Bond angles

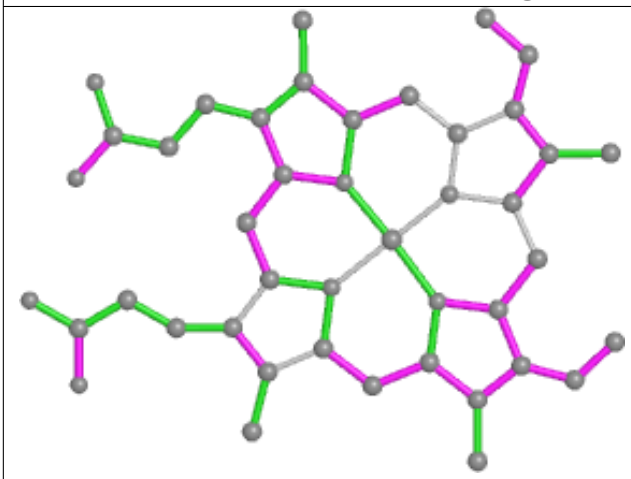


Torsions

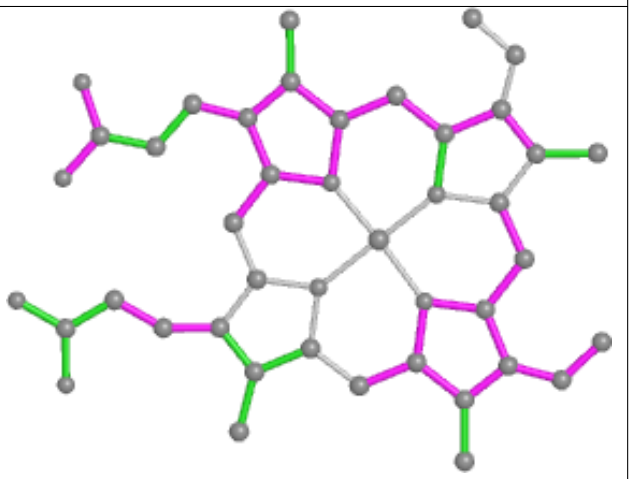


Rings

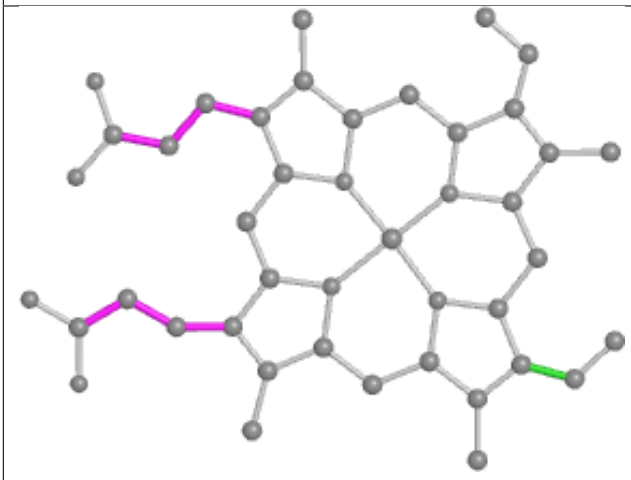
Ligand HEM C 609



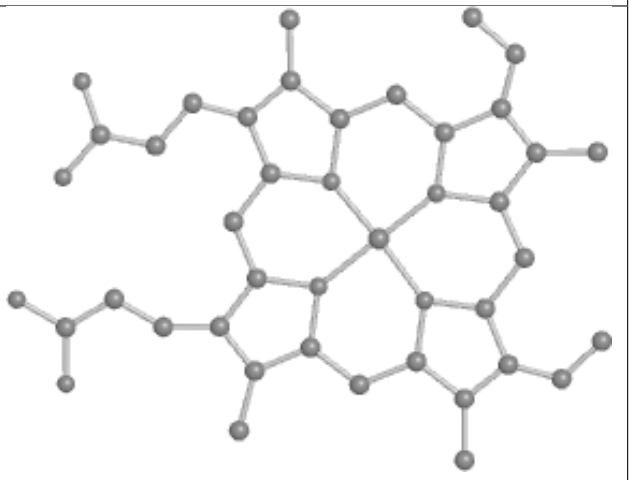
Bond lengths



Bond angles

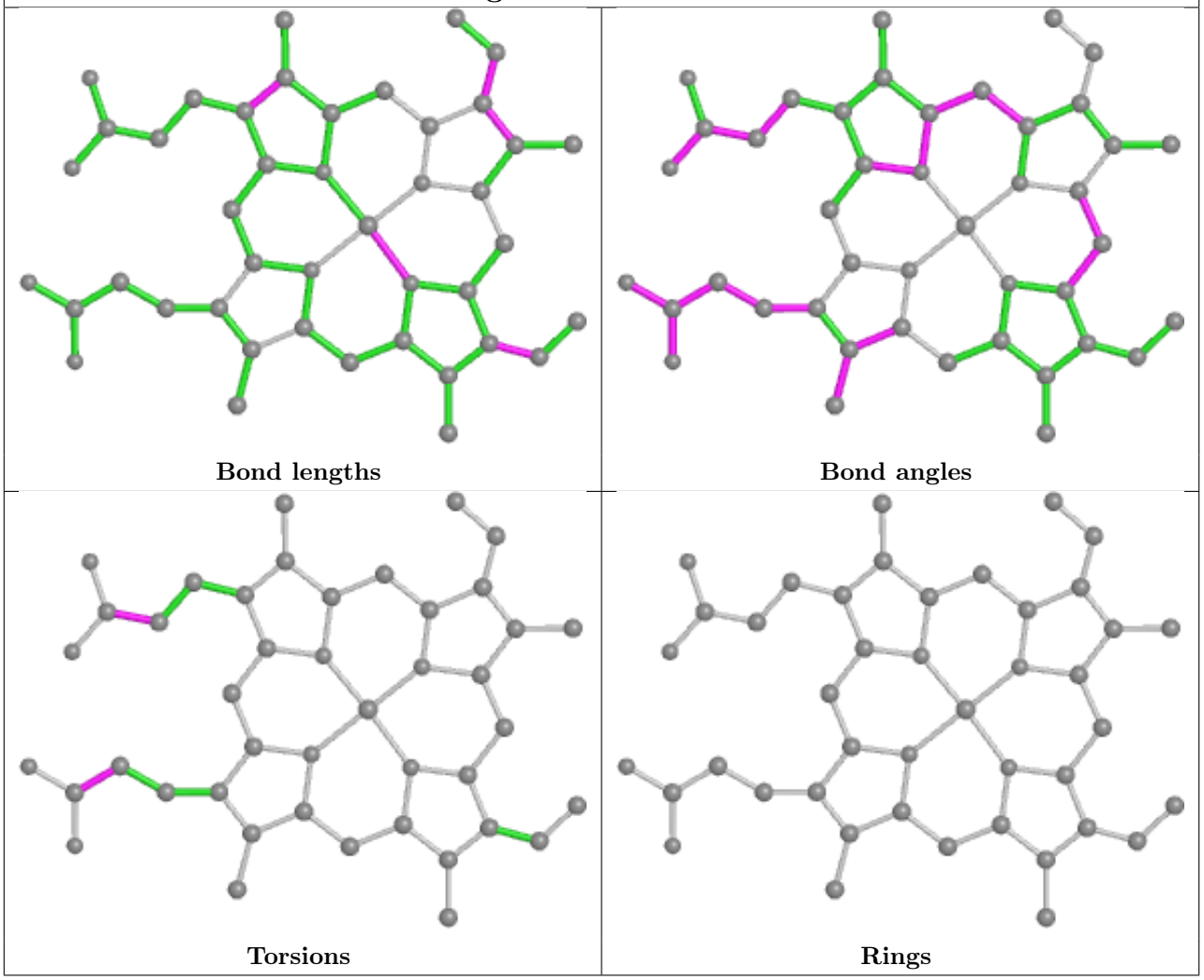


Torsions



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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.