Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:18 AM UTC

PDB ID	:	1NTZ / pdb_00001ntz
Title	:	Crystal Structure of Mitochondrial Cytochrome bc1 Complex Bound with Ubiquinone
Authors	:	Gao, X.; Wen, X.; Esser, L.; Quinn, B.; Yu, L.; Yu, C.-A.; Xia, D.
Deposited on	:	2003-01-30
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

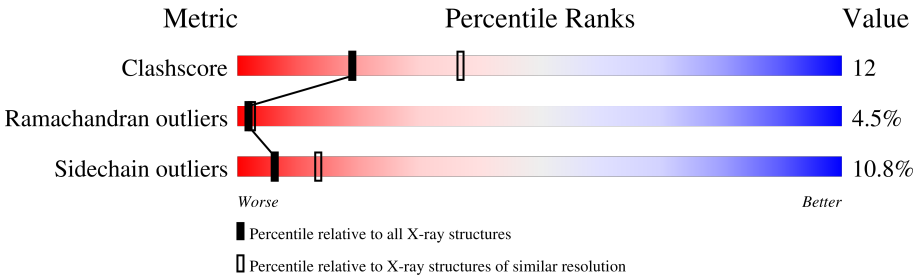
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	71% 23% 5%
2	B	439	68% 23% • • •
3	C	379	69% 22% 8% •
4	D	241	54% 34% 10% •
5	E	196	72% 24% •
6	F	110	69% 16% 7% • 5%
7	G	81	63% 17% 9% • 7%
8	H	78	40% 38% 10% • 10%

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Mol	Chain	Length	Quality of chain
9	I	57	19% 37% 32% 12%
10	J	62	52% 34% 13%
11	K	56	68% 23% 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	UQ2	C	383	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 16896 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
6	F	105	Total	C	N	O	S	0	0	0
			911	576	165	168	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	75	Total	C	N	O	S	0	0	0
			628	410	118	99	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			575	347	102	121	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	61	Total	C	N	O	0	0	0
			483	316	82	85			

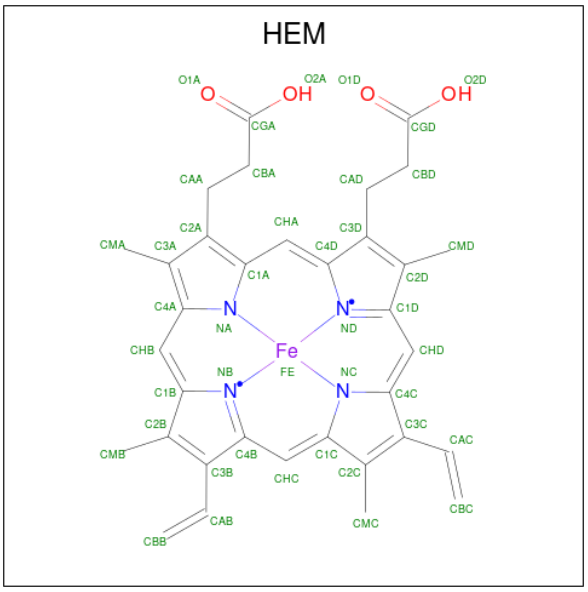
- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase complex 6.4 kDa protein.

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

There is a discrepancy between the modelled and reference sequences:

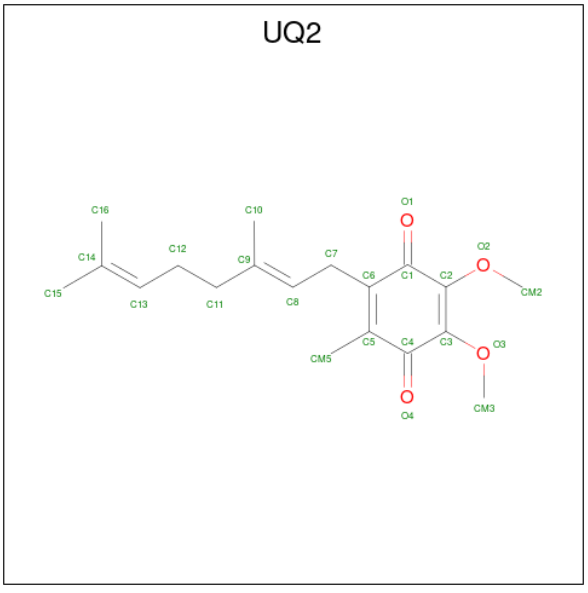
Chain	Residue	Modelled	Actual	Comment	Reference
K	22	GLN	SER	SEE REMARK 999	UNP P07552

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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 UBIQUINONE-2 (CCD ID: UQ2) (formula: $C_{19}H_{26}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			23	19	4		

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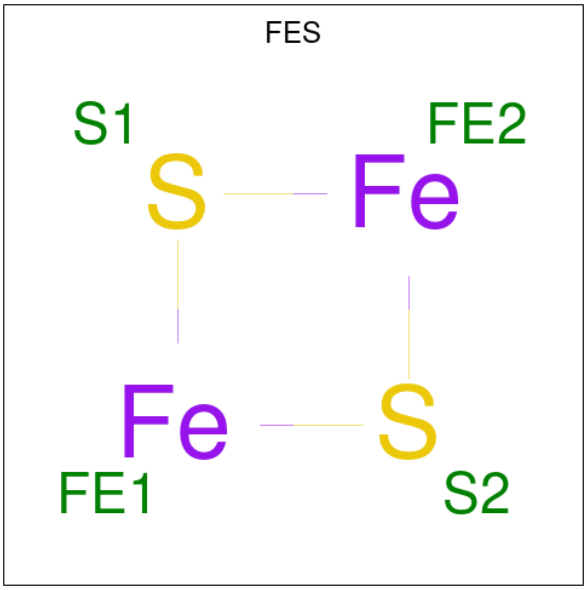
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C O 23 19 4	0	0

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	29	Total O 29 29	0	0
15	B	39	Total O 39 39	0	0
15	C	78	Total O 78 78	0	0
15	D	30	Total O 30 30	0	0
15	E	3	Total O 3 3	0	0
15	F	14	Total O 14 14	0	0
15	G	4	Total O 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total O 1 1	0	0
15	I	4	Total O 4 4	0	0
15	J	2	Total O 2 2	0	0
15	K	3	Total O 3 3	0	0

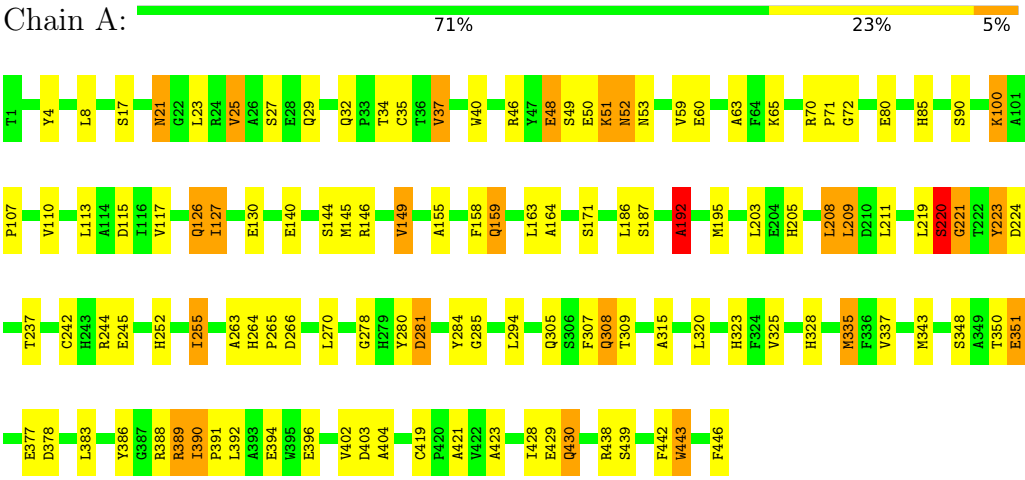
3 Residue-property plots (i)

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.

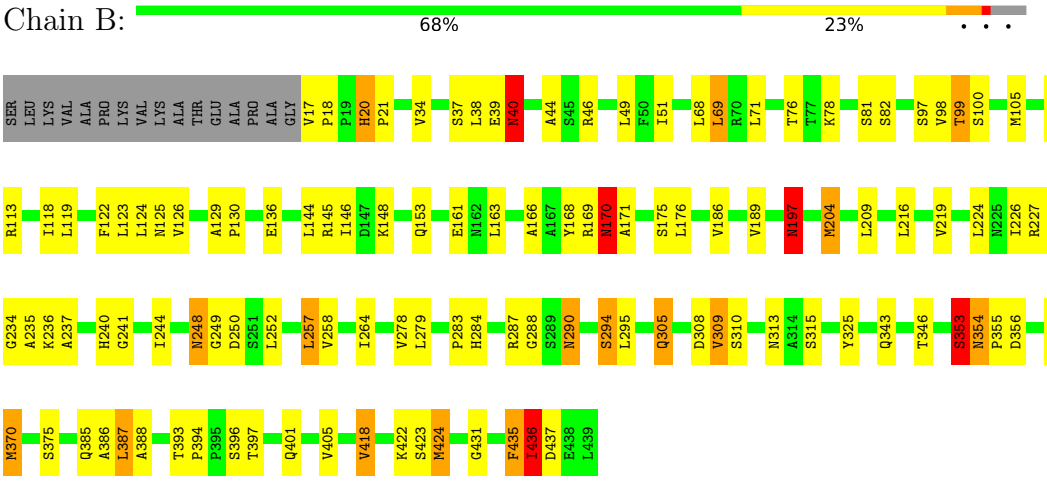
• Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Chain A:



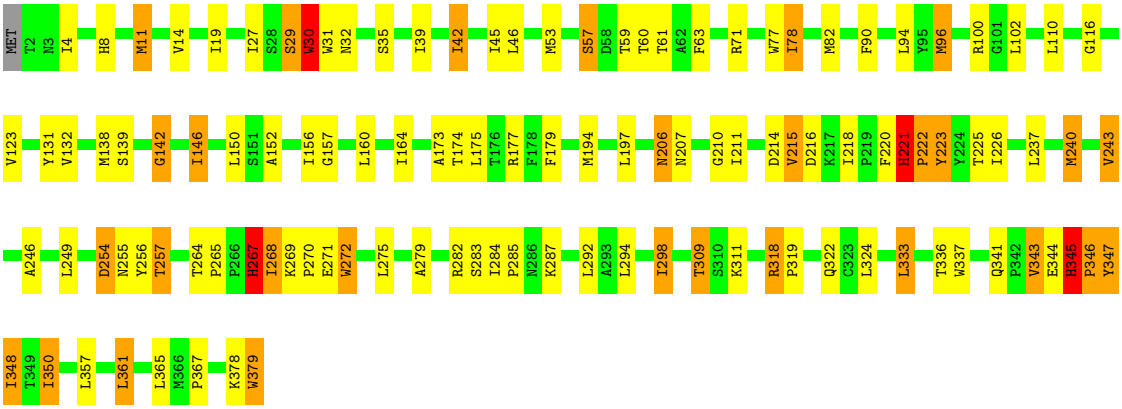
• Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

Chain B:



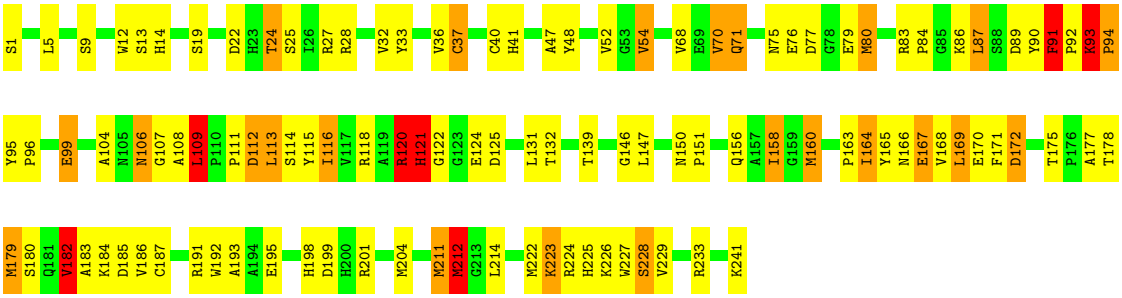
• Molecule 3: Cytochrome b

Chain C:



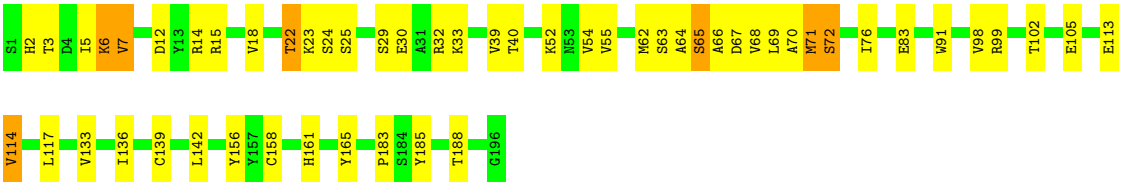
• Molecule 4: cytochrome c1

Chain D:



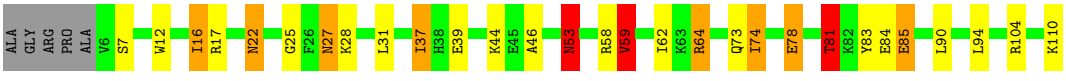
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, mitochondrial

Chain E:



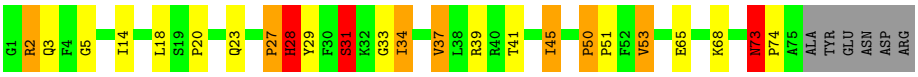
• Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F:



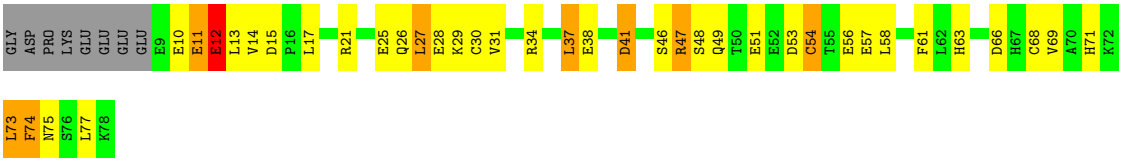
• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain G:



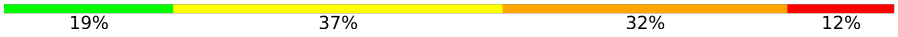
• Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

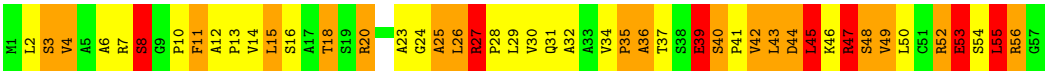
Chain H:



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

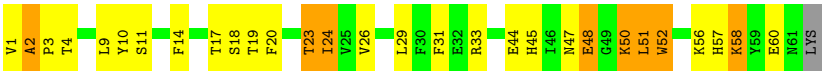
Chain I:





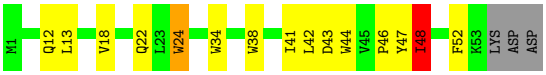
• Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

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	153.83Å 153.83Å 596.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.99 – 2.60	Depositor
% Data completeness (in resolution range)	100.0 (28.99-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.247 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16896	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, UQ2, 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	1.18	6/3531 (0.2%)	1.14	24/4792 (0.5%)
2	B	1.50	22/3232 (0.7%)	1.18	15/4386 (0.3%)
3	C	1.21	14/3100 (0.5%)	1.16	15/4242 (0.4%)
4	D	1.02	7/1977 (0.4%)	1.22	10/2684 (0.4%)
5	E	1.07	6/1553 (0.4%)	1.13	9/2100 (0.4%)
6	F	1.36	5/930 (0.5%)	1.18	7/1246 (0.6%)
7	G	1.29	5/649 (0.8%)	1.16	1/878 (0.1%)
8	H	0.96	2/580 (0.3%)	1.36	7/777 (0.9%)
9	I	1.77	6/411 (1.5%)	1.71	10/558 (1.8%)
10	J	1.08	0/495	1.17	3/672 (0.4%)
11	K	0.99	1/453 (0.2%)	1.07	2/621 (0.3%)
All	All	1.25	74/16911 (0.4%)	1.19	103/22956 (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
1	A	1	0
2	B	1	0
3	C	1	2
4	D	2	0
7	G	1	0
8	H	1	0
9	I	1	0
10	J	1	0
All	All	9	2

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	424	MET	SD-CE	-17.37	1.36	1.79
2	B	105	MET	SD-CE	-13.44	1.46	1.79
3	C	11	MET	SD-CE	11.94	2.09	1.79
3	C	53	MET	SD-CE	-11.77	1.50	1.79
9	I	25	ALA	CA-CB	-9.86	1.36	1.53
1	A	335	MET	SD-CE	-9.19	1.56	1.79
6	F	59	VAL	CA-CB	9.04	1.65	1.54
2	B	370	MET	SD-CE	-8.94	1.57	1.79
2	B	170	ASN	N-CA	-8.87	1.34	1.46
5	E	62	MET	SD-CE	-8.37	1.58	1.79
2	B	118	ILE	CA-CB	8.36	1.65	1.54
5	E	63	SER	CA-C	8.15	1.57	1.52
9	I	42	VAL	CA-CB	8.00	1.65	1.54
4	D	211	MET	SD-CE	-7.71	1.60	1.79
2	B	436	ILE	N-CA	7.49	1.55	1.46
4	D	212	MET	SD-CE	-7.39	1.61	1.79
7	G	3	GLN	C-O	-7.10	1.15	1.24
2	B	204	MET	SD-CE	-6.90	1.62	1.79
3	C	218	ILE	CA-CB	-6.85	1.47	1.55
3	C	19	ILE	CA-CB	-6.76	1.48	1.55
3	C	42	ILE	CA-CB	6.61	1.62	1.54
7	G	73	ASN	CA-C	6.55	1.61	1.52
8	H	69	VAL	CA-CB	6.55	1.61	1.54
9	I	45	LEU	CA-C	6.42	1.61	1.52
5	E	55	VAL	CA-CB	6.30	1.61	1.54
5	E	22	THR	CA-CB	6.27	1.63	1.53
9	I	45	LEU	N-CA	6.24	1.54	1.46
3	C	240	MET	SD-CE	-6.17	1.64	1.79
2	B	226	ILE	CA-C	-6.17	1.45	1.52
2	B	248	ASN	CB-CG	-6.12	1.36	1.52
1	A	106	LEU	CA-C	6.10	1.59	1.52
2	B	431	GLY	C-O	-5.95	1.15	1.23
9	I	12	ALA	CA-CB	-5.86	1.46	1.53
2	B	148	LYS	CA-C	5.84	1.60	1.52
7	G	53	VAL	CA-CB	5.81	1.61	1.54
3	C	257	THR	CA-CB	5.81	1.61	1.52
1	A	281	ASP	CB-CG	-5.79	1.37	1.52
1	A	127	ILE	CA-CB	5.68	1.62	1.54
3	C	194	MET	SD-CE	5.68	1.93	1.79
8	H	31	VAL	CA-CB	5.67	1.61	1.54
2	B	237	ALA	CA-CB	-5.60	1.45	1.53
5	E	133	VAL	CA-CB	5.59	1.60	1.54
1	A	423	ALA	CA-CB	-5.53	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	69	LEU	C-O	-5.53	1.17	1.24
4	D	182	VAL	CA-CB	5.53	1.62	1.54
2	B	197	ASN	CB-CG	-5.52	1.38	1.52
2	B	146	ILE	CA-C	5.49	1.59	1.52
1	A	402	VAL	C-O	-5.48	1.18	1.24
2	B	309	VAL	CA-C	-5.40	1.46	1.52
3	C	156	ILE	CA-CB	5.40	1.61	1.54
4	D	91	PHE	CA-C	5.38	1.59	1.52
4	D	109	LEU	CA-C	-5.34	1.47	1.52
4	D	160	MET	SD-CE	-5.32	1.66	1.79
2	B	168	TYR	CA-C	-5.31	1.46	1.52
6	F	16	ILE	CA-CB	5.29	1.60	1.54
2	B	125	ASN	CA-C	5.26	1.59	1.52
3	C	336	THR	CA-CB	5.25	1.61	1.53
3	C	348	ILE	CA-CB	5.24	1.60	1.54
3	C	221	HIS	C-O	-5.23	1.17	1.24
7	G	28	HIS	CA-C	5.21	1.59	1.52
7	G	34	ILE	CA-CB	5.21	1.60	1.54
4	D	116	ILE	CA-CB	5.20	1.59	1.54
11	K	48	ILE	CA-CB	5.20	1.61	1.54
9	I	54	SER	CA-C	5.09	1.58	1.52
6	F	37	ILE	C-O	5.08	1.29	1.24
5	E	39	VAL	CA-CB	5.08	1.60	1.54
3	C	243	VAL	CA-CB	5.08	1.61	1.54
6	F	46	ALA	CA-CB	-5.06	1.45	1.53
6	F	81	THR	CA-CB	5.06	1.60	1.53
2	B	257	LEU	CA-C	-5.04	1.46	1.52
3	C	379	TRP	CB-CG	-5.04	1.34	1.50
2	B	313	ASN	N-CA	-5.02	1.40	1.46
2	B	405	VAL	CA-C	5.02	1.58	1.52
2	B	170	ASN	CA-C	-5.01	1.46	1.52

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	234	GLY	N-CA-C	14.04	127.78	111.63
8	H	53	ASP	N-CA-C	12.77	127.23	112.93
2	B	235	ALA	N-CA-C	-11.12	99.27	113.72
5	E	66	ALA	N-CA-C	-10.34	102.01	112.97
9	I	44	ASP	N-CA-C	-9.97	95.76	110.52
5	E	68	VAL	N-CA-C	-9.92	103.45	113.47
3	C	221	HIS	N-CA-C	9.90	131.69	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	LYS	N-CA-C	-9.89	93.24	108.96
4	D	70	VAL	N-CA-C	9.68	120.87	111.67
9	I	26	LEU	N-CA-C	9.04	124.13	109.40
1	A	428	ILE	N-CA-C	8.80	119.74	111.91
6	F	85	GLU	N-CA-C	-8.78	92.09	110.80
10	J	52	TRP	N-CA-C	-8.68	102.12	112.89
1	A	443	TRP	N-CA-C	8.67	123.42	108.76
10	J	51	LEU	N-CA-C	8.41	128.72	110.80
4	D	116	ILE	N-CA-C	8.28	118.84	110.23
3	C	29	SER	N-CA-C	-8.11	98.02	110.10
1	A	285	GLY	N-CA-C	-8.11	101.63	112.82
3	C	223	TYR	N-CA-C	7.88	119.50	111.07
1	A	351	GLU	N-CA-C	7.87	119.49	111.07
4	D	120	ARG	N-CA-C	7.76	123.43	111.56
4	D	122	GLY	N-CA-C	-7.74	94.83	113.18
9	I	36	ALA	N-CA-C	7.73	122.34	110.36
8	H	12	GLU	N-CA-C	7.66	127.11	110.80
3	C	243	VAL	N-CA-C	7.58	120.53	111.05
4	D	169	LEU	N-CA-C	7.47	126.72	110.80
2	B	232	LEU	N-CA-C	7.31	119.70	109.31
5	E	2	HIS	N-CA-C	-7.11	104.58	113.18
3	C	255	ASN	N-CA-C	-7.08	104.63	113.20
9	I	52	ARG	N-CA-C	7.06	120.65	109.50
2	B	435	PHE	N-CA-C	6.98	121.40	113.02
1	A	192	ALA	N-CA-C	6.96	125.20	109.81
1	A	159	GLN	N-CA-C	6.95	125.61	110.80
4	D	139	THR	N-CA-C	6.86	119.95	110.35
3	C	157	GLY	N-CA-C	6.81	121.14	112.83
8	H	27	LEU	N-CA-C	6.76	125.20	110.80
5	E	23	LYS	N-CA-C	6.75	119.98	109.52
5	E	63	SER	N-CA-C	6.72	119.57	108.48
9	I	35	PRO	N-CA-C	-6.68	98.70	112.47
5	E	25	SER	N-CA-C	-6.61	105.51	113.97
1	A	48	GLU	N-CA-C	6.60	120.29	110.52
3	C	146	ILE	N-CA-C	6.58	116.60	110.42
1	A	220	SER	N-CA-C	6.53	124.72	110.80
1	A	266	ASP	N-CA-C	6.47	120.85	113.15
1	A	263	ALA	N-CA-C	6.47	119.15	111.33
6	F	59	VAL	N-CA-CB	6.44	119.30	110.54
1	A	430	GLN	N-CA-C	6.42	120.72	113.02
9	I	7	ARG	N-CA-C	-6.36	104.59	113.37
1	A	348	SER	N-CA-C	6.36	120.35	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	197	ASN	N-CA-C	6.25	120.91	113.28
3	C	271	GLU	N-CA-C	-6.13	101.41	110.48
5	E	114	VAL	N-CA-C	6.07	117.54	110.62
4	D	19	SER	N-CA-C	6.07	118.41	108.52
1	A	37	VAL	CB-CA-C	-6.04	101.52	110.82
1	A	421	ALA	N-CA-C	-5.90	99.62	109.24
1	A	305	GLN	N-CA-C	-5.88	106.65	113.88
1	A	389	ARG	CA-C-N	-5.78	118.67	122.60
1	A	389	ARG	C-N-CA	-5.78	118.67	122.60
8	H	47	ARG	N-CA-C	5.78	116.05	108.07
3	C	333	LEU	N-CA-C	-5.73	104.64	111.69
9	I	23	ALA	N-CA-C	-5.73	97.89	107.80
8	H	54	CYS	N-CA-C	5.67	120.02	113.38
11	K	42	LEU	N-CA-C	5.67	117.54	111.36
8	H	66	ASP	N-CA-C	5.64	118.19	111.71
11	K	47	TYR	N-CA-C	-5.61	103.30	110.53
2	B	418	VAL	N-CA-C	5.58	116.31	110.62
1	A	63	ALA	N-CA-C	5.56	118.06	111.33
3	C	110	LEU	N-CA-C	5.55	117.79	111.02
2	B	78	LYS	N-CA-C	-5.51	102.12	110.28
9	I	24	GLY	N-CA-C	5.51	126.24	113.18
2	B	278	VAL	N-CA-C	-5.50	105.36	110.53
2	B	40	ASN	N-CA-C	-5.49	100.35	109.46
6	F	39	GLU	N-CA-C	5.49	118.33	108.17
4	D	52	VAL	N-CA-C	5.45	115.89	110.23
6	F	16	ILE	N-CA-C	-5.43	105.43	110.53
4	D	87	LEU	N-CA-C	-5.42	99.27	110.80
3	C	292	LEU	N-CA-C	-5.40	105.47	111.36
3	C	206	ASN	N-CA-C	-5.36	102.06	110.36
1	A	390	ILE	N-CA-C	5.36	112.43	107.56
6	F	25	GLY	N-CA-C	5.35	123.14	114.90
6	F	53	ASN	N-CA-C	5.35	116.80	111.07
9	I	27	ARG	N-CA-C	-5.35	97.99	109.81
3	C	142	GLY	N-CA-C	-5.33	106.04	112.49
3	C	30	TRP	N-CA-C	-5.32	99.48	110.80
4	D	24	THR	N-CA-C	-5.31	105.53	112.23
1	A	389	ARG	N-CA-C	-5.31	99.87	108.52
10	J	26	VAL	N-CA-C	-5.28	105.39	110.72
2	B	78	LYS	CA-C-N	-5.26	113.83	122.20
2	B	78	LYS	C-N-CA	-5.26	113.83	122.20
2	B	309	VAL	CB-CA-C	-5.23	101.77	111.18
3	C	272	TRP	N-CA-C	5.21	118.42	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	437	ASP	CB-CA-C	-5.21	102.09	110.74
6	F	104	ARG	N-CA-C	-5.17	105.54	111.07
1	A	328	HIS	N-CA-C	5.17	117.59	111.33
5	E	70	ALA	N-CA-C	5.17	118.88	112.47
1	A	278	GLY	N-CA-C	5.17	120.36	111.47
2	B	226	ILE	CB-CA-C	-5.13	102.83	110.33
5	E	185	TYR	N-CA-C	5.13	116.87	109.07
8	H	56	GLU	N-CA-C	5.12	116.55	110.97
2	B	394	PRO	O-C-N	5.07	123.64	121.31
9	I	11	PHE	N-CA-C	5.07	117.99	110.48
1	A	443	TRP	CB-CA-C	5.04	118.82	109.70
7	G	50	PRO	N-CA-C	5.01	116.82	110.70

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	443	TRP	CA
2	B	305	GLN	CA
3	C	221	HIS	CA
4	D	145	GLU	CA
4	D	169	LEU	CA
7	G	2	ARG	CA
8	H	12	GLU	CA
9	I	42	VAL	CA
10	J	51	LEU	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	221	HIS	Mainchain
3	C	345	HIS	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	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3172	0	3152	72	0
3	C	3003	0	3065	81	0
4	D	1918	0	1870	69	0
5	E	1519	0	1504	21	0
6	F	911	0	904	15	0
7	G	628	0	636	15	0
8	H	575	0	550	14	0
9	I	406	0	437	61	0
10	J	483	0	465	23	0
11	K	437	0	439	7	0
12	C	86	0	60	5	0
12	D	43	0	30	3	0
13	C	46	0	52	18	0
14	E	4	0	0	0	0
15	A	29	0	0	3	0
15	B	39	0	0	2	0
15	C	78	0	0	7	0
15	D	30	0	0	1	0
15	E	3	0	0	0	0
15	F	14	0	0	3	0
15	G	4	0	0	0	0
15	H	1	0	0	0	0
15	I	4	0	0	1	0
15	J	2	0	0	0	0
15	K	3	0	0	0	0
All	All	16896	0	16520	391	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 12.

All (391) 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	2.09	1.41
4:D:37:CYS:SG	12:D:242:HEM:HAB	1.90	1.12
10:J:18:SER:HA	11:K:24:TRP:HZ3	1.19	1.03
1:A:325:VAL:HG21	9:I:43:LEU:HD12	1.44	0.98
3:C:221:HIS:CG	3:C:221:HIS:O	2.13	0.98
10:J:18:SER:HA	11:K:24:TRP:CZ3	2.00	0.96
7:G:73:ASN:HB3	7:G:74:PRO:HD3	1.43	0.96
2:B:76:THR:HG22	2:B:82:SER:H	1.28	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:GLN:HE22	2:B:393:THR:H	1.03	0.93
3:C:221:HIS:O	3:C:221:HIS:CD2	2.26	0.87
3:C:146:ILE:HD11	13:C:383:UQ2:C4	2.06	0.85
13:C:384:UQ2:H5M1	13:C:384:UQ2:H8	1.60	0.81
13:C:384:UQ2:H5M2	15:C:1010:HOH:O	1.81	0.81
2:B:169:ARG:HD3	2:B:240:HIS:HB2	1.62	0.80
4:D:37:CYS:SG	12:D:242:HEM:CAB	2.70	0.79
1:A:51:LYS:O	1:A:52:ASN:HB2	1.80	0.78
9:I:34:VAL:HB	9:I:35:PRO:HD3	1.65	0.78
2:B:325:TYR:CD2	9:I:28:PRO:HD2	2.19	0.77
1:A:446:PHE:OXT	10:J:17:THR:HB	1.85	0.77
2:B:99:THR:HB	9:I:14:VAL:HG22	1.66	0.77
3:C:45:ILE:HA	12:C:381:HEM:HAB	1.66	0.76
7:G:27:PRO:O	7:G:29:TYR:N	2.20	0.75
2:B:161:GLU:OE1	2:B:175:SER:OG	2.05	0.74
10:J:44:GLU:HG2	10:J:52:TRP:HZ2	1.52	0.74
9:I:47:ARG:HG2	9:I:48:SER:H	1.53	0.73
3:C:131:TYR:HA	12:C:381:HEM:HAD2	1.71	0.73
2:B:100:SER:O	9:I:13:PRO:HD2	1.87	0.73
4:D:164:ILE:HG22	4:D:179:MET:HG2	1.70	0.73
6:F:31:LEU:O	6:F:81:THR:HG21	1.89	0.73
3:C:211:ILE:HG21	6:F:62:ILE:HD12	1.71	0.72
1:A:48:GLU:OE2	15:A:471:HOH:O	2.06	0.72
4:D:195:GLU:OE1	4:D:201:ARG:NH1	2.23	0.71
3:C:322:GLN:NE2	15:C:1048:HOH:O	2.23	0.70
1:A:146:ARG:H	9:I:42:VAL:HG12	1.56	0.70
4:D:120:ARG:O	4:D:121:HIS:HB2	1.91	0.70
9:I:47:ARG:CG	9:I:48:SER:H	2.05	0.70
9:I:6:ALA:C	9:I:8:SER:H	1.99	0.69
2:B:325:TYR:HB3	9:I:28:PRO:CD	2.22	0.69
2:B:385:GLN:HE22	2:B:393:THR:N	1.85	0.69
1:A:34:THR:HG21	2:B:370:MET:HG3	1.75	0.69
9:I:4:VAL:HG12	9:I:10:PRO:HG2	1.76	0.68
2:B:283:PRO:HG3	9:I:31:GLN:HG3	1.74	0.68
4:D:27:ARG:NH1	10:J:57:HIS:NE2	2.41	0.68
4:D:79:GLU:O	4:D:80:MET:HB2	1.94	0.68
6:F:58:ARG:NE	15:F:1902:HOH:O	2.27	0.68
2:B:435:PHE:O	2:B:436:ILE:HB	1.94	0.67
3:C:214:ASP:OD2	7:G:2:ARG:NH2	2.21	0.67
1:A:145:MET:O	1:A:149:VAL:HG23	1.94	0.67
6:F:58:ARG:NH2	15:F:1902:HOH:O	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:THR:O	15:C:1066:HOH:O	2.14	0.66
7:G:73:ASN:HB3	7:G:74:PRO:CD	2.23	0.65
2:B:310:SER:HB3	9:I:28:PRO:HG3	1.76	0.65
2:B:354:ASN:H	2:B:355:PRO:HD2	1.61	0.65
1:A:252:HIS:HD2	1:A:323:HIS:HE1	1.42	0.65
1:A:244:ARG:NH2	15:A:461:HOH:O	2.05	0.65
15:B:462:HOH:O	9:I:4:VAL:HG21	1.95	0.65
2:B:40:ASN:O	2:B:40:ASN:ND2	2.28	0.64
10:J:50:LYS:O	10:J:52:TRP:N	2.27	0.64
4:D:40:CYS:SG	12:D:242:HEM:HAC	2.37	0.64
1:A:252:HIS:CD2	1:A:323:HIS:HE1	2.17	0.63
3:C:309:THR:HG21	3:C:367:PRO:O	1.99	0.63
3:C:322:GLN:OE1	15:C:1076:HOH:O	2.15	0.63
9:I:42:VAL:HG22	9:I:43:LEU:HD23	1.79	0.63
4:D:90:TYR:C	4:D:92:PRO:HD3	2.24	0.63
7:G:73:ASN:CB	7:G:74:PRO:HD3	2.23	0.62
2:B:76:THR:HG23	2:B:136:GLU:OE1	1.99	0.62
2:B:315:SER:O	9:I:4:VAL:HG13	2.00	0.62
1:A:244:ARG:NE	15:A:461:HOH:O	2.23	0.62
1:A:51:LYS:O	1:A:52:ASN:CB	2.47	0.61
1:A:144:SER:HA	9:I:42:VAL:HB	1.80	0.61
4:D:165:TYR:O	4:D:165:TYR:CD2	2.54	0.61
7:G:41:THR:O	7:G:45:ILE:HG12	1.99	0.61
5:E:18:VAL:HG12	5:E:18:VAL:O	1.99	0.61
3:C:222:PRO:HD2	3:C:223:TYR:H	1.65	0.61
1:A:65:LYS:NZ	2:B:287:ARG:O	2.33	0.61
2:B:385:GLN:NE2	2:B:393:THR:H	1.87	0.61
1:A:284:TYR:HE1	9:I:20:ARG:HG2	1.66	0.61
4:D:224:ARG:HD3	15:D:267:HOH:O	2.00	0.61
1:A:237:THR:OG1	5:E:14:ARG:NH2	2.34	0.60
9:I:47:ARG:HG2	9:I:48:SER:N	2.16	0.60
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.82	0.60
13:C:384:UQ2:H5M1	13:C:384:UQ2:C8	2.31	0.60
4:D:75:ASN:O	4:D:77:ASP:N	2.35	0.60
10:J:33:ARG:HD3	11:K:48:ILE:HA	1.83	0.60
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.83	0.59
6:F:27:ASN:HA	6:F:81:THR:HG23	1.83	0.59
6:F:28:LYS:HB3	6:F:74:ILE:HG12	1.83	0.59
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.21	0.59
4:D:165:TYR:O	4:D:165:TYR:HD2	1.86	0.59
3:C:206:ASN:ND2	3:C:207:ASN:H	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:GLY:C	12:C:382:HEM:HBC2	2.26	0.59
3:C:138:MET:HE1	3:C:268:ILE:HA	1.84	0.59
1:A:351:GLU:H	11:K:12:GLN:NE2	2.00	0.59
2:B:290:ASN:HD22	2:B:290:ASN:N	2.00	0.59
3:C:345:HIS:O	3:C:347:TYR:N	2.36	0.59
2:B:325:TYR:HB3	9:I:28:PRO:HD3	1.84	0.59
9:I:44:ASP:O	9:I:46:LYS:HB2	2.03	0.58
2:B:71:LEU:HD23	9:I:15:LEU:HG	1.85	0.58
3:C:30:TRP:HZ3	3:C:96:MET:HG3	1.67	0.58
9:I:2:LEU:O	9:I:3:SER:HB3	2.03	0.58
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.39	0.58
3:C:132:VAL:HA	3:C:139:SER:HB3	1.86	0.58
4:D:83:ARG:NH2	4:D:89:ASP:OD1	2.36	0.58
9:I:46:LYS:HG2	9:I:47:ARG:H	1.68	0.58
3:C:282:ARG:NH2	3:C:341:GLN:O	2.38	0.57
10:J:58:LYS:C	10:J:60:GLU:H	2.13	0.57
4:D:180:SER:HB3	8:H:77:LEU:HD11	1.85	0.57
3:C:257:THR:HG22	4:D:115:TYR:HE1	1.69	0.56
1:A:27:SER:HB3	1:A:208:LEU:HD12	1.86	0.56
9:I:39:GLU:O	9:I:40:SER:HB3	2.05	0.56
10:J:19:THR:O	10:J:23:THR:HG22	2.05	0.56
1:A:388:ARG:NH2	1:A:394:GLU:OE2	2.39	0.56
4:D:93:LYS:H	4:D:94:PRO:HD2	1.71	0.56
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.88	0.56
9:I:11:PHE:HZ	9:I:27:ARG:HH21	1.53	0.56
1:A:140:GLU:OE2	9:I:36:ALA:HB1	2.05	0.56
3:C:142:GLY:HA2	13:C:383:UQ2:CM3	2.35	0.56
3:C:146:ILE:HD11	13:C:383:UQ2:C5	2.36	0.56
4:D:12:TRP:NE1	4:D:125:ASP:OD2	2.32	0.56
9:I:55:LEU:O	9:I:56:ARG:HB2	2.05	0.56
9:I:8:SER:OG	9:I:26:LEU:HD13	2.05	0.55
9:I:10:PRO:O	9:I:25:ALA:CB	2.54	0.55
2:B:39:GLU:OE2	2:B:113:ARG:NH2	2.38	0.55
2:B:76:THR:HG22	2:B:82:SER:N	2.11	0.55
2:B:325:TYR:CG	9:I:28:PRO:HD2	2.41	0.55
9:I:41:PRO:O	9:I:42:VAL:HG23	2.05	0.55
1:A:255:ILE:HD13	1:A:335:MET:HE1	1.87	0.55
9:I:6:ALA:C	9:I:8:SER:N	2.64	0.55
4:D:211:MET:HE1	10:J:31:PHE:HE2	1.71	0.55
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.89	0.55
2:B:129:ALA:N	2:B:130:PRO:HD3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.42	0.55
1:A:46:ARG:HG3	1:A:163:LEU:HD13	1.89	0.55
4:D:178:THR:O	4:D:182:VAL:HG12	2.07	0.55
10:J:44:GLU:HG2	10:J:52:TRP:CZ2	2.38	0.55
9:I:44:ASP:O	9:I:45:LEU:C	2.50	0.54
2:B:145:ARG:NH2	15:B:475:HOH:O	2.35	0.54
3:C:240:MET:HE2	3:C:240:MET:HA	1.89	0.54
4:D:167:GLU:HG3	4:D:177:ALA:HB3	1.88	0.54
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.90	0.54
9:I:46:LYS:HG2	9:I:47:ARG:N	2.22	0.54
10:J:2:ALA:HB3	10:J:3:PRO:HD3	1.90	0.54
3:C:357:LEU:O	3:C:361:LEU:HB2	2.08	0.53
8:H:38:GLU:HA	8:H:41:ASP:HB2	1.90	0.53
2:B:153:GLN:NE2	9:I:46:LYS:HG3	2.23	0.53
4:D:211:MET:HE1	10:J:31:PHE:CE2	2.42	0.53
5:E:6:LYS:H	5:E:6:LYS:HD3	1.71	0.53
1:A:309:THR:O	9:I:52:ARG:NH1	2.40	0.53
4:D:83:ARG:HG2	4:D:84:PRO:HD2	1.91	0.53
1:A:378:ASP:OD2	1:A:389:ARG:NH1	2.39	0.53
3:C:226:ILE:HG23	4:D:223:LYS:HB2	1.90	0.53
3:C:272:TRP:HA	3:C:275:LEU:HG	1.90	0.53
7:G:28:HIS:HB3	7:G:31:SER:HB2	1.91	0.53
3:C:146:ILE:HD13	3:C:146:ILE:N	2.19	0.53
4:D:158:ILE:HG13	4:D:160:MET:H	1.72	0.53
3:C:146:ILE:HD11	13:C:383:UQ2:C3	2.38	0.52
9:I:34:VAL:HB	9:I:35:PRO:CD	2.36	0.52
4:D:54:VAL:HG21	4:D:192:TRP:CZ2	2.45	0.52
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.91	0.52
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.91	0.52
4:D:48:TYR:OH	4:D:93:LYS:NZ	2.36	0.52
6:F:64:ARG:HH11	6:F:64:ARG:HB3	1.73	0.52
4:D:109:LEU:O	4:D:111:PRO:HD3	2.10	0.51
6:F:83:TYR:CE1	6:F:84:GLU:HG3	2.46	0.51
4:D:165:TYR:O	4:D:167:GLU:N	2.43	0.51
4:D:124:GLU:HB3	4:D:187:CYS:HB3	1.92	0.51
2:B:250:ASP:C	2:B:252:LEU:H	2.19	0.51
6:F:12:TRP:O	6:F:16:ILE:HG12	2.10	0.51
2:B:39:GLU:CD	2:B:113:ARG:HH22	2.19	0.50
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.92	0.50
3:C:63:PHE:HB2	15:C:1042:HOH:O	2.10	0.50
3:C:223:TYR:HB3	4:D:227:TRP:CZ2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:14:PHE:HD1	10:J:20:PHE:CD1	2.28	0.50
2:B:68:LEU:HD13	2:B:144:LEU:HD11	1.93	0.50
3:C:270:PRO:HG3	13:C:383:UQ2:C4	2.41	0.50
6:F:58:ARG:CZ	15:F:1902:HOH:O	2.55	0.50
8:H:25:GLU:HG3	8:H:61:PHE:HZ	1.77	0.50
4:D:222:MET:HG2	5:E:40:THR:HG22	1.93	0.49
4:D:112:ASP:OD1	4:D:112:ASP:N	2.36	0.49
3:C:279:ALA:O	3:C:283:SER:OG	2.30	0.49
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.94	0.49
1:A:255:ILE:HD13	1:A:335:MET:CE	2.42	0.49
1:A:429:GLU:OE2	7:G:5:GLY:N	2.35	0.49
2:B:170:ASN:HB3	2:B:171:ALA:H	1.41	0.49
6:F:53:ASN:N	6:F:53:ASN:HD22	2.11	0.49
4:D:92:PRO:C	4:D:93:LYS:HG2	2.36	0.49
2:B:308:ASP:HB2	9:I:32:ALA:HB2	1.95	0.48
3:C:29:SER:HA	3:C:32:ASN:HD22	1.78	0.48
4:D:28:ARG:O	4:D:32:VAL:HG23	2.13	0.48
4:D:86:LYS:HE2	5:E:71:MET:HE2	1.95	0.48
6:F:78:GLU:H	6:F:78:GLU:HG3	1.42	0.48
1:A:85:HIS:ND1	2:B:370:MET:HE1	2.28	0.48
1:A:100:LYS:HD3	2:B:370:MET:HE3	1.96	0.48
4:D:91:PHE:N	4:D:92:PRO:HD3	2.28	0.48
1:A:187:SER:O	1:A:223:TYR:OH	2.28	0.48
4:D:70:VAL:O	4:D:71:GLN:HB3	2.14	0.48
1:A:145:MET:H	9:I:42:VAL:HA	1.78	0.48
1:A:146:ARG:HH12	1:A:308:GLN:NE2	2.11	0.48
3:C:173:ALA:O	3:C:177:ARG:HB2	2.13	0.48
5:E:139:CYS:SG	5:E:165:TYR:OH	2.67	0.48
1:A:219:LEU:O	1:A:221:GLY:N	2.46	0.47
10:J:20:PHE:O	10:J:24:ILE:HG23	2.15	0.47
4:D:147:LEU:HA	4:D:158:ILE:O	2.15	0.47
9:I:52:ARG:O	9:I:53:GLU:HB2	2.14	0.47
3:C:78:ILE:H	3:C:78:ILE:HG13	1.47	0.47
2:B:46:ARG:HD2	2:B:375:SER:HB3	1.95	0.47
2:B:388:ALA:HB3	9:I:2:LEU:HD13	1.96	0.47
3:C:267:HIS:HE1	3:C:269:LYS:HE2	1.79	0.47
4:D:28:ARG:HD2	4:D:185:ASP:OD2	2.15	0.47
1:A:48:GLU:HG3	1:A:53:ASN:HA	1.96	0.47
1:A:155:ALA:O	5:E:7:VAL:HG21	2.15	0.47
1:A:158:PHE:O	1:A:164:ALA:HB2	2.14	0.47
1:A:308:GLN:HE21	1:A:323:HIS:HD2	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:ALA:HA	2:B:112:LEU:HA	1.97	0.47
3:C:254:ASP:C	3:C:256:TYR:H	2.22	0.47
5:E:29:SER:O	5:E:33:LYS:HG2	2.15	0.47
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.97	0.47
9:I:15:LEU:HA	9:I:15:LEU:HD22	1.49	0.47
10:J:9:LEU:HB3	10:J:14:PHE:HE2	1.79	0.47
3:C:142:GLY:HA2	13:C:383:UQ2:H3M2	1.97	0.47
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.45	0.47
5:E:136:ILE:HD11	5:E:183:PRO:HB3	1.97	0.47
9:I:11:PHE:HZ	9:I:27:ARG:NH2	2.12	0.47
2:B:354:ASN:H	2:B:355:PRO:CD	2.27	0.46
3:C:152:ALA:HB2	3:C:287:LYS:HG2	1.96	0.46
3:C:220:PHE:HE2	13:C:384:UQ2:C2	2.28	0.46
3:C:270:PRO:HB3	13:C:383:UQ2:C2	2.45	0.46
4:D:47:ALA:HA	4:D:90:TYR:HA	1.97	0.46
3:C:57:SER:O	3:C:57:SER:OG	2.32	0.46
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.96	0.46
3:C:378:LYS:HE2	6:F:17:ARG:HD3	1.98	0.46
4:D:99:GLU:H	4:D:99:GLU:HG2	1.23	0.46
2:B:49:LEU:HD11	2:B:204:MET:HE3	1.96	0.46
5:E:65:SER:C	5:E:67:ASP:H	2.23	0.46
8:H:73:LEU:O	8:H:75:ASN:N	2.48	0.46
9:I:20:ARG:NH1	15:I:58:HOH:O	2.44	0.46
2:B:204:MET:HE1	2:B:224:LEU:HD22	1.98	0.46
4:D:22:ASP:HB3	4:D:25:SER:HB3	1.96	0.46
1:A:25:VAL:HG23	1:A:208:LEU:HD13	1.97	0.46
3:C:361:LEU:HA	3:C:365:LEU:HB2	1.98	0.46
1:A:34:THR:HG22	1:A:35:CYS:N	2.31	0.46
2:B:435:PHE:O	2:B:436:ILE:CB	2.63	0.46
4:D:170:GLU:C	4:D:172:ASP:H	2.24	0.46
3:C:71:ARG:NH1	4:D:193:ALA:O	2.49	0.45
10:J:14:PHE:CD1	10:J:20:PHE:HD1	2.34	0.45
1:A:255:ILE:HG21	1:A:335:MET:HE1	1.98	0.45
3:C:284:ILE:HA	3:C:285:PRO:HD3	1.82	0.45
3:C:345:HIS:O	3:C:346:PRO:C	2.59	0.45
8:H:25:GLU:OE1	8:H:34:ARG:NH1	2.49	0.45
8:H:17:LEU:HG	8:H:21:ARG:HD2	1.99	0.45
8:H:37:LEU:HD11	8:H:58:LEU:HA	1.98	0.45
3:C:142:GLY:HA2	13:C:383:UQ2:H3M1	1.97	0.45
9:I:46:LYS:CG	9:I:47:ARG:H	2.23	0.45
4:D:184:LYS:HB2	8:H:74:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:25:GLU:O	8:H:30:CYS:HB2	2.17	0.45
1:A:442:PHE:CD2	1:A:442:PHE:C	2.94	0.45
13:C:383:UQ2:H121	13:C:383:UQ2:H101	1.72	0.45
4:D:225:HIS:O	4:D:228:SER:HB2	2.16	0.45
3:C:222:PRO:CD	3:C:223:TYR:H	2.29	0.45
3:C:267:HIS:HB2	15:C:1068:HOH:O	2.16	0.45
4:D:33:TYR:HA	4:D:37:CYS:SG	2.57	0.45
1:A:307:PHE:C	1:A:307:PHE:CD2	2.94	0.45
3:C:8:HIS:CD2	3:C:11:MET:HG3	2.51	0.45
3:C:90:PHE:O	3:C:94:LEU:HB2	2.17	0.45
4:D:93:LYS:O	4:D:94:PRO:C	2.60	0.45
9:I:49:VAL:O	9:I:50:LEU:HB2	2.17	0.45
9:I:47:ARG:CG	9:I:48:SER:N	2.75	0.45
1:A:29:GLN:HG2	2:B:18:PRO:HG3	1.99	0.44
2:B:325:TYR:HB3	9:I:28:PRO:HD2	1.97	0.44
4:D:5:LEU:HD11	8:H:63:HIS:HB2	1.99	0.44
9:I:44:ASP:O	9:I:46:LYS:N	2.50	0.44
1:A:386:TYR:C	1:A:388:ARG:H	2.26	0.44
5:E:6:LYS:H	5:E:6:LYS:CD	2.29	0.44
5:E:15:ARG:HH11	5:E:32:ARG:HG2	1.83	0.44
2:B:34:VAL:HG11	2:B:386:ALA:HB1	2.00	0.44
2:B:393:THR:HG21	2:B:401:GLN:HE22	1.82	0.44
4:D:120:ARG:HD3	4:D:120:ARG:HA	1.60	0.44
6:F:22:ASN:HA	6:F:27:ASN:HD21	1.81	0.44
7:G:18:LEU:HB3	7:G:23:GLN:NE2	2.32	0.44
2:B:283:PRO:HG3	9:I:31:GLN:CG	2.46	0.44
3:C:318:ARG:HA	3:C:319:PRO:HD3	1.73	0.44
9:I:18:THR:OG1	9:I:53:GLU:OE2	2.24	0.44
2:B:288:GLY:O	2:B:290:ASN:ND2	2.51	0.44
5:E:114:VAL:HA	5:E:117:LEU:HD12	2.00	0.44
2:B:385:GLN:HG2	9:I:2:LEU:HD12	2.00	0.44
3:C:82:MET:HG2	3:C:240:MET:HE1	1.99	0.44
2:B:126:VAL:O	2:B:130:PRO:HG3	2.18	0.44
4:D:28:ARG:HB3	4:D:171:PHE:CE2	2.53	0.44
4:D:79:GLU:HB2	4:D:80:MET:H	1.62	0.44
9:I:39:GLU:O	9:I:40:SER:CB	2.65	0.44
3:C:237:LEU:HD13	4:D:212:MET:HG2	1.99	0.43
3:C:311:LYS:NZ	15:C:1007:HOH:O	2.48	0.43
4:D:223:LYS:HD2	4:D:227:TRP:CD1	2.53	0.43
8:H:11:GLU:O	8:H:12:GLU:HB2	2.18	0.43
3:C:8:HIS:HD2	3:C:11:MET:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:CYS:SG	1:A:438:ARG:NH1	2.92	0.43
2:B:124:LEU:HD11	2:B:219:VAL:HG13	2.01	0.43
3:C:197:LEU:HD12	3:C:197:LEU:HA	1.86	0.43
3:C:346:PRO:HG3	7:G:65:GLU:HB3	1.99	0.43
4:D:14:HIS:NE2	4:D:124:GLU:OE1	2.45	0.43
4:D:183:ALA:HA	4:D:186:VAL:HG12	2.00	0.43
5:E:64:ALA:O	5:E:65:SER:OG	2.28	0.43
3:C:27:ILE:HD12	13:C:384:UQ2:H2M1	2.00	0.43
10:J:29:LEU:HA	11:K:34:TRP:CD1	2.54	0.43
1:A:126:GLN:O	1:A:130:GLU:HG2	2.19	0.43
10:J:14:PHE:CD1	10:J:20:PHE:CD1	3.06	0.43
1:A:219:LEU:HB3	1:A:220:SER:H	1.65	0.43
4:D:131:LEU:HD13	4:D:164:ILE:HD11	2.01	0.43
2:B:76:THR:HB	2:B:81:SER:HA	2.00	0.43
5:E:99:ARG:NH2	5:E:105:GLU:OE2	2.51	0.43
10:J:29:LEU:HD13	11:K:34:TRP:HB2	2.00	0.43
1:A:209:LEU:HA	1:A:209:LEU:HD23	1.81	0.43
1:A:373:THR:HB	1:A:374:PRO:HD3	2.01	0.43
3:C:31:TRP:HB3	13:C:384:UQ2:H2M1	2.01	0.43
5:E:72:SER:HB3	5:E:91:TRP:CD1	2.54	0.43
1:A:104:LYS:O	1:A:107:PRO:HD2	2.19	0.42
7:G:34:ILE:HA	7:G:37:VAL:HG13	2.01	0.42
3:C:35:SER:HB3	13:C:384:UQ2:H71	2.00	0.42
1:A:17:SER:HB3	1:A:205:HIS:NE2	2.34	0.42
1:A:294:LEU:HG	1:A:307:PHE:CE1	2.55	0.42
2:B:197:ASN:C	2:B:197:ASN:HD22	2.26	0.42
3:C:215:VAL:HG21	6:F:59:VAL:HB	2.00	0.42
1:A:80:GLU:HG2	2:B:284:HIS:HB2	2.00	0.42
3:C:150:LEU:HB3	3:C:160:LEU:HD22	2.02	0.42
7:G:29:TYR:O	7:G:33:GLY:HA3	2.20	0.42
2:B:20:HIS:CD2	2:B:20:HIS:H	2.37	0.42
1:A:252:HIS:HE1	9:I:43:LEU:HB2	1.85	0.42
3:C:265:PRO:HD2	3:C:268:ILE:HD11	2.02	0.42
1:A:220:SER:HA	1:A:223:TYR:HB3	2.01	0.42
1:A:343:MET:HE2	1:A:343:MET:HA	2.01	0.42
4:D:28:ARG:HD3	4:D:171:PHE:CD2	2.55	0.42
4:D:41:HIS:ND1	4:D:113:LEU:HD13	2.34	0.42
2:B:353:SER:HB3	2:B:356:ASP:H	1.85	0.42
1:A:70:ARG:NH1	1:A:115:ASP:OD2	2.52	0.42
1:A:270:LEU:HD22	1:A:320:LEU:HD21	2.02	0.41
3:C:298:ILE:HD13	3:C:298:ILE:HA	1.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:345:HIS:ND1	3:C:346:PRO:HD3	2.34	0.41
3:C:179:PHE:HE2	12:C:381:HEM:HMA1	1.85	0.41
9:I:46:LYS:CG	9:I:47:ARG:N	2.77	0.41
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.90	0.41
2:B:122:PHE:O	2:B:126:VAL:HG23	2.19	0.41
2:B:308:ASP:OD2	9:I:31:GLN:HB2	2.19	0.41
3:C:100:ARG:NH2	12:C:382:HEM:HBD1	2.36	0.41
3:C:216:ASP:OD2	4:D:233:ARG:NH2	2.45	0.41
3:C:267:HIS:HB3	3:C:268:ILE:H	1.34	0.41
4:D:106:ASN:O	4:D:108:ALA:N	2.52	0.41
2:B:418:VAL:O	2:B:422:LYS:NZ	2.54	0.41
3:C:343:VAL:HG12	3:C:348:ILE:HG12	2.03	0.41
2:B:294:SER:CB	2:B:343:GLN:HE21	2.33	0.41
2:B:361:LYS:O	2:B:365:LYS:HG3	2.20	0.41
3:C:337:TRP:CZ3	3:C:350:ILE:HD11	2.55	0.41
8:H:54:CYS:HA	8:H:57:GLU:OE1	2.21	0.41
1:A:294:LEU:HD13	1:A:337:VAL:HG12	2.02	0.41
1:A:378:ASP:OD2	9:I:56:ARG:NH2	2.53	0.41
1:A:390:ILE:HA	1:A:391:PRO:HD3	1.91	0.41
2:B:216:LEU:HD23	2:B:216:LEU:HA	1.90	0.41
2:B:241:GLY:HA2	2:B:423:SER:OG	2.20	0.41
4:D:116:ILE:HD13	4:D:116:ILE:HA	1.92	0.41
2:B:294:SER:HB3	2:B:343:GLN:HE21	1.85	0.41
8:H:77:LEU:HD23	8:H:77:LEU:HA	1.81	0.41
9:I:2:LEU:H	9:I:2:LEU:HG	1.71	0.41
1:A:59:VAL:HG11	1:A:186:LEU:HD21	2.03	0.41
1:A:280:TYR:CG	1:A:281:ASP:N	2.89	0.41
3:C:254:ASP:C	3:C:256:TYR:N	2.77	0.41
1:A:21:ASN:HB3	1:A:192:ALA:HB1	2.03	0.41
2:B:387:LEU:HD12	2:B:387:LEU:HA	1.87	0.41
3:C:270:PRO:HG3	13:C:383:UQ2:C3	2.51	0.41
3:C:344:GLU:O	3:C:348:ILE:HG13	2.20	0.41
4:D:113:LEU:HD12	4:D:113:LEU:HA	1.84	0.41
4:D:150:ASN:HA	4:D:151:PRO:HD3	1.93	0.41
5:E:72:SER:HB3	5:E:91:TRP:HD1	1.86	0.41
9:I:47:ARG:CD	9:I:48:SER:H	2.33	0.41
10:J:47:ASN:O	10:J:48:GLU:HB2	2.21	0.41
10:J:58:LYS:C	10:J:60:GLU:N	2.77	0.41
1:A:110:VAL:HG11	1:A:211:LEU:HB3	2.03	0.41
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.74	0.41
3:C:324:LEU:HD23	3:C:324:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:13:LEU:HD23	11:K:13:LEU:HA	1.94	0.40
8:H:47:ARG:HB3	8:H:48:SER:H	1.76	0.40
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.56	0.40
2:B:37:SER:HB3	2:B:216:LEU:HD12	2.04	0.40
13:C:383:UQ2:H5M1	13:C:383:UQ2:H72	1.79	0.40
4:D:198:HIS:ND1	4:D:199:ASP:OD1	2.48	0.40
1:A:4:TYR:OH	1:A:396:GLU:OE1	2.36	0.40
1:A:8:LEU:HD22	1:A:392:LEU:HB3	2.04	0.40
1:A:242:CYS:O	7:G:14:ILE:HA	2.21	0.40
3:C:77:TRP:CH2	4:D:204:MET:HE2	2.56	0.40
3:C:206:ASN:HD21	3:C:210:GLY:HA2	1.85	0.40
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.86	0.40
2:B:290:ASN:OD1	9:I:31:GLN:NE2	2.54	0.40
4:D:170:GLU:O	4:D:172:ASP:N	2.45	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%)	409 (92%)	21 (5%)	14 (3%)	3 5
2	B	421/439 (96%)	393 (93%)	20 (5%)	8 (2%)	6 13
3	C	376/379 (99%)	349 (93%)	18 (5%)	9 (2%)	4 9
4	D	239/241 (99%)	183 (77%)	36 (15%)	20 (8%)	0 0
5	E	194/196 (99%)	175 (90%)	15 (8%)	4 (2%)	5 11
6	F	103/110 (94%)	98 (95%)	3 (3%)	2 (2%)	6 13
7	G	73/81 (90%)	65 (89%)	3 (4%)	5 (7%)	1 1
8	H	68/78 (87%)	49 (72%)	10 (15%)	9 (13%)	0 0
9	I	55/57 (96%)	26 (47%)	16 (29%)	13 (24%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	59/62 (95%)	45 (76%)	9 (15%)	5 (8%)	0	0
11	K	51/56 (91%)	42 (82%)	4 (8%)	5 (10%)	0	0
All	All	2083/2145 (97%)	1834 (88%)	155 (7%)	94 (4%)	2	2

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	220	SER
1	A	227	ALA
2	B	305	GLN
3	C	222	PRO
3	C	254	ASP
3	C	267	HIS
3	C	345	HIS
3	C	346	PRO
3	C	347	TYR
4	D	71	GLN
4	D	76	GLU
4	D	80	MET
4	D	96	PRO
4	D	121	HIS
4	D	169	LEU
4	D	172	ASP
5	E	65	SER
5	E	69	LEU
7	G	2	ARG
7	G	27	PRO
7	G	28	HIS
7	G	73	ASN
8	H	12	GLU
8	H	27	LEU
8	H	73	LEU
8	H	74	PHE
9	I	29	LEU
9	I	37	THR
9	I	39	GLU
9	I	40	SER
9	I	45	LEU
9	I	53	GLU
9	I	55	LEU

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Mol	Chain	Res	Type
9	I	56	ARG
10	J	48	GLU
10	J	51	LEU
11	K	52	PHE
1	A	50	GLU
1	A	52	ASN
1	A	72	GLY
2	B	21	PRO
3	C	30	TRP
4	D	107	GLY
8	H	11	GLU
8	H	26	GLN
8	H	28	GLU
8	H	49	GLN
9	I	8	SER
9	I	47	ARG
10	J	58	LYS
11	K	48	ILE
1	A	21	ASN
1	A	223	TYR
1	A	315	ALA
2	B	228	GLY
4	D	36	VAL
4	D	87	LEU
4	D	93	LYS
4	D	94	PRO
4	D	167	GLU
5	E	71	MET
5	E	72	SER
6	F	7	SER
6	F	85	GLU
9	I	3	SER
9	I	48	SER
10	J	2	ALA
10	J	56	LYS
11	K	38	TRP
1	A	192	ALA
1	A	224	ASP
2	B	236	LYS
2	B	353	SER
4	D	104	ALA
4	D	146	GLY

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Mol	Chain	Res	Type
4	D	166	ASN
7	G	31	SER
8	H	46	SER
9	I	4	VAL
1	A	49	SER
2	B	354	ASN
4	D	54	VAL
4	D	106	ASN
11	K	43	ASP
3	C	268	ILE
11	K	46	PRO
1	A	71	PRO
2	B	249	GLY
4	D	91	PHE
4	D	163	PRO
2	B	436	ILE
1	A	221	GLY
3	C	221	HIS

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%)	342 (92%)	28 (8%)	12 27
2	B	332/343 (97%)	297 (90%)	35 (10%)	6 14
3	C	326/327 (100%)	297 (91%)	29 (9%)	9 20
4	D	206/206 (100%)	175 (85%)	31 (15%)	3 5
5	E	168/168 (100%)	155 (92%)	13 (8%)	12 27
6	F	96/98 (98%)	82 (85%)	14 (15%)	3 6
7	G	66/71 (93%)	60 (91%)	6 (9%)	9 19
8	H	67/74 (90%)	57 (85%)	10 (15%)	3 5
9	I	44/44 (100%)	31 (70%)	13 (30%)	0 0
10	J	46/52 (88%)	39 (85%)	7 (15%)	3 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	42/46 (91%)	37 (88%)	5 (12%)	5 10
All	All	1763/1799 (98%)	1572 (89%)	191 (11%)	6 13

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	25	VAL
1	A	32	GLN
1	A	37	VAL
1	A	90	SER
1	A	100	LYS
1	A	102	LEU
1	A	113	LEU
1	A	117	VAL
1	A	126	GLN
1	A	127	ILE
1	A	149	VAL
1	A	171	SER
1	A	195	MET
1	A	203	LEU
1	A	208	LEU
1	A	209	LEU
1	A	226	ASP
1	A	230	THR
1	A	245	GLU
1	A	255	ILE
1	A	308	GLN
1	A	350	THR
1	A	383	LEU
1	A	403	ASP
1	A	430	GLN
1	A	439	SER
1	A	443	TRP
2	B	17	VAL
2	B	20	HIS
2	B	38	LEU
2	B	40	ASN
2	B	69	LEU
2	B	97	SER
2	B	98	VAL
2	B	99	THR

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Mol	Chain	Res	Type
2	B	109	VAL
2	B	110	GLU
2	B	119	LEU
2	B	123	LEU
2	B	163	LEU
2	B	170	ASN
2	B	176	LEU
2	B	186	VAL
2	B	189	VAL
2	B	197	ASN
2	B	209	LEU
2	B	227	ARG
2	B	232	LEU
2	B	248	ASN
2	B	257	LEU
2	B	258	VAL
2	B	264	ILE
2	B	290	ASN
2	B	294	SER
2	B	305	GLN
2	B	309	VAL
2	B	346	THR
2	B	353	SER
2	B	387	LEU
2	B	396	SER
2	B	397	THR
2	B	424	MET
3	C	4	ILE
3	C	14	VAL
3	C	39	ILE
3	C	42	ILE
3	C	46	LEU
3	C	57	SER
3	C	60	THR
3	C	61	THR
3	C	78	ILE
3	C	96	MET
3	C	102	LEU
3	C	123	VAL
3	C	164	ILE
3	C	174	THR
3	C	175	LEU

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Mol	Chain	Res	Type
3	C	215	VAL
3	C	225	THR
3	C	243	VAL
3	C	264	THR
3	C	267	HIS
3	C	294	LEU
3	C	298	ILE
3	C	309	THR
3	C	318	ARG
3	C	333	LEU
3	C	343	VAL
3	C	350	ILE
3	C	361	LEU
3	C	379	TRP
4	D	1	SER
4	D	9	SER
4	D	13	SER
4	D	24	THR
4	D	37	CYS
4	D	68	VAL
4	D	93	LYS
4	D	95	TYR
4	D	99	GLU
4	D	109	LEU
4	D	112	ASP
4	D	113	LEU
4	D	114	SER
4	D	118	ARG
4	D	120	ARG
4	D	121	HIS
4	D	132	THR
4	D	156	GLN
4	D	158	ILE
4	D	164	ILE
4	D	168	VAL
4	D	175	THR
4	D	179	MET
4	D	182	VAL
4	D	191	ARG
4	D	212	MET
4	D	214	LEU
4	D	223	LYS

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Mol	Chain	Res	Type
4	D	226	LYS
4	D	228	SER
4	D	241	LYS
5	E	3	THR
5	E	5	ILE
5	E	6	LYS
5	E	7	VAL
5	E	12	ASP
5	E	22	THR
5	E	24	SER
5	E	30	GLU
5	E	52	LYS
5	E	54	VAL
5	E	113	GLU
5	E	158	CYS
5	E	188	THR
6	F	22	ASN
6	F	27	ASN
6	F	37	ILE
6	F	44	LYS
6	F	53	ASN
6	F	59	VAL
6	F	64	ARG
6	F	73	GLN
6	F	74	ILE
6	F	78	GLU
6	F	81	THR
6	F	90	LEU
6	F	94	LEU
6	F	110	LYS
7	G	31	SER
7	G	37	VAL
7	G	39	ARG
7	G	45	ILE
7	G	53	VAL
7	G	68	LYS
8	H	10	GLU
8	H	13	LEU
8	H	14	VAL
8	H	15	ASP
8	H	29	LYS
8	H	37	LEU

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Mol	Chain	Res	Type
8	H	41	ASP
8	H	51	GLU
8	H	68	CYS
8	H	71	HIS
9	I	8	SER
9	I	15	LEU
9	I	16	SER
9	I	18	THR
9	I	20	ARG
9	I	27	ARG
9	I	30	VAL
9	I	39	GLU
9	I	43	LEU
9	I	47	ARG
9	I	49	VAL
9	I	53	GLU
9	I	55	LEU
10	J	1	VAL
10	J	4	THR
10	J	11	SER
10	J	23	THR
10	J	24	ILE
10	J	45	HIS
10	J	50	LYS
11	K	18	VAL
11	K	22	GLN
11	K	24	TRP
11	K	41	ILE
11	K	44	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	73	ASN
1	A	119	ASN
1	A	126	GLN
1	A	159	GLN
1	A	165	GLN
1	A	173	ASN
1	A	215	HIS
1	A	252	HIS

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Mol	Chain	Res	Type
1	A	267	ASN
1	A	271	GLN
1	A	274	ASN
1	A	305	GLN
1	A	311	ASN
1	A	323	HIS
1	A	341	GLN
1	A	359	ASN
1	A	368	HIS
1	A	418	GLN
2	B	20	HIS
2	B	22	GLN
2	B	143	GLN
2	B	153	GLN
2	B	162	ASN
2	B	174	ASN
2	B	197	ASN
2	B	240	HIS
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	284	HIS
2	B	342	ASN
2	B	343	GLN
2	B	362	ASN
2	B	385	GLN
2	B	401	GLN
2	B	432	HIS
3	C	8	HIS
3	C	32	ASN
3	C	114	ASN
3	C	206	ASN
3	C	260	ASN
3	C	267	HIS
3	C	352	GLN
4	D	71	GLN
4	D	75	ASN
4	D	105	ASN
4	D	121	HIS
4	D	156	GLN
4	D	200	HIS
5	E	53	ASN

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Mol	Chain	Res	Type
5	E	57	GLN
5	E	161	HIS
6	F	53	ASN
6	F	72	GLN
7	G	23	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	381	3	50,50,50	3.31	26 (52%)	67,82,82	2.48	28 (41%)
12	HEM	D	242	4	50,50,50	3.33	25 (50%)	67,82,82	2.54	30 (44%)
13	UQ2	C	383	-	23,23,23	2.38	6 (26%)	30,31,31	1.78	7 (23%)
12	HEM	C	382	3	50,50,50	3.29	23 (46%)	67,82,82	2.42	27 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	UQ2	C	384	-	23,23,23	2.62	5 (21%)	30,31,31	1.52	5 (16%)

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	381	3	-	8/14/54/54	-
12	HEM	D	242	4	-	6/14/54/54	-
13	UQ2	C	383	-	-	5/15/39/39	0/1/1/1
12	HEM	C	382	3	-	4/14/54/54	-
13	UQ2	C	384	-	-	3/15/39/39	0/1/1/1

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	384	UQ2	C6-C5	10.22	1.53	1.35
13	C	383	UQ2	C6-C5	8.18	1.49	1.35
12	C	382	HEM	C3C-C4C	-7.96	1.32	1.46
12	C	381	HEM	C3C-C4C	-7.69	1.32	1.46
12	D	242	HEM	C4D-C3D	-7.32	1.32	1.45
12	C	382	HEM	C1C-C2C	-6.88	1.31	1.45
12	D	242	HEM	FE-NA	6.72	2.17	1.95
12	D	242	HEM	C1B-C2B	-6.47	1.31	1.44
12	C	381	HEM	FE-NA	6.36	2.16	1.95
12	D	242	HEM	C3C-C4C	-6.21	1.35	1.46
12	C	381	HEM	C1C-C2C	-5.98	1.33	1.45
12	C	381	HEM	C4D-C3D	-5.95	1.34	1.45
12	C	382	HEM	C3B-C4B	-5.91	1.33	1.44
12	C	382	HEM	CHA-C4D	5.87	1.50	1.38
12	D	242	HEM	C1C-C2C	-5.81	1.33	1.45
12	D	242	HEM	CHD-C4C	5.75	1.49	1.38
12	C	381	HEM	CHD-C4C	5.70	1.49	1.38
12	D	242	HEM	C3B-C4B	-5.70	1.33	1.44
12	C	382	HEM	C1B-C2B	-5.61	1.33	1.44
12	D	242	HEM	CHC-C1C	5.56	1.49	1.38
12	C	382	HEM	CHD-C4C	5.51	1.49	1.38
12	D	242	HEM	C1D-C2D	-5.35	1.33	1.44
12	C	382	HEM	CHC-C1C	5.32	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	382	HEM	FE-NA	5.18	2.12	1.95
12	C	381	HEM	CHA-C1A	5.08	1.50	1.39
12	C	381	HEM	C3B-C4B	-5.03	1.35	1.44
12	D	242	HEM	CBC-CAC	4.98	1.54	1.30
12	C	381	HEM	CHA-C4D	4.91	1.48	1.38
12	C	381	HEM	CHC-C4B	4.88	1.50	1.39
12	C	381	HEM	CHC-C1C	4.84	1.47	1.38
12	C	382	HEM	C4D-C3D	-4.78	1.36	1.45
12	C	381	HEM	C1B-C2B	-4.76	1.34	1.44
12	C	382	HEM	CBB-CAB	4.72	1.53	1.30
12	C	381	HEM	CBC-CAC	4.63	1.52	1.30
12	D	242	HEM	CBB-CAB	4.62	1.52	1.30
12	C	381	HEM	CBB-CAB	4.55	1.52	1.30
12	D	242	HEM	CHB-C1B	4.51	1.47	1.38
12	C	382	HEM	CHA-C1A	4.46	1.49	1.39
12	C	382	HEM	CBC-CAC	4.39	1.51	1.30
12	D	242	HEM	CHA-C4D	4.20	1.46	1.38
12	C	382	HEM	CHD-C1D	4.18	1.48	1.39
12	D	242	HEM	CHD-C1D	4.10	1.48	1.39
12	C	381	HEM	CHB-C1B	4.10	1.46	1.38
12	C	382	HEM	C1D-C2D	-4.05	1.36	1.44
13	C	383	UQ2	C3-C2	4.02	1.50	1.36
12	C	381	HEM	CHB-C4A	4.02	1.48	1.39
12	C	381	HEM	C1D-C2D	-3.94	1.36	1.44
12	C	382	HEM	CHB-C4A	3.93	1.48	1.39
12	D	242	HEM	CHC-C4B	3.92	1.48	1.39
12	C	382	HEM	CHB-C1B	3.90	1.46	1.38
13	C	384	UQ2	C3-C2	3.76	1.49	1.36
12	D	242	HEM	CHB-C4A	3.75	1.47	1.39
12	C	381	HEM	CHD-C1D	3.72	1.47	1.39
12	C	382	HEM	O2A-CGA	-3.65	1.18	1.30
12	D	242	HEM	CHA-C1A	3.46	1.47	1.39
12	C	382	HEM	CHC-C4B	3.45	1.47	1.39
13	C	384	UQ2	C8-C9	3.29	1.40	1.33
12	C	381	HEM	C3C-C2C	-3.25	1.30	1.37
12	C	381	HEM	C1A-C2A	3.05	1.50	1.44
13	C	383	UQ2	C13-C14	2.99	1.41	1.32
13	C	383	UQ2	C8-C9	2.97	1.39	1.33
12	D	242	HEM	C2A-C3A	2.96	1.46	1.38
13	C	384	UQ2	C13-C14	2.80	1.40	1.32
12	C	382	HEM	CAB-C3B	2.69	1.54	1.47
12	C	382	HEM	O2D-CGD	-2.55	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	242	HEM	O2D-CGD	-2.54	1.22	1.30
12	D	242	HEM	C4A-C3A	2.43	1.48	1.43
13	C	383	UQ2	C7-C8	2.36	1.54	1.50
12	D	242	HEM	C3D-C2D	-2.36	1.31	1.36
12	D	242	HEM	O2A-CGA	-2.36	1.23	1.30
12	C	382	HEM	C2A-C3A	2.35	1.45	1.38
12	C	381	HEM	C2A-C3A	2.32	1.45	1.38
12	C	381	HEM	C4A-C3A	2.31	1.48	1.43
12	C	382	HEM	C1A-NA	-2.30	1.35	1.39
13	C	383	UQ2	C6-C1	2.28	1.52	1.46
12	C	381	HEM	O2D-CGD	-2.22	1.23	1.30
12	C	382	HEM	C4A-NA	-2.21	1.35	1.39
12	C	381	HEM	O2A-CGA	-2.17	1.23	1.30
13	C	384	UQ2	C7-C8	2.12	1.53	1.50
12	C	381	HEM	CMB-C2B	2.10	1.55	1.50
12	C	381	HEM	C4B-NB	2.09	1.43	1.38
12	C	381	HEM	C1C-NC	2.08	1.43	1.39
12	D	242	HEM	CAC-C3C	2.06	1.52	1.47
12	D	242	HEM	C3C-C2C	-2.06	1.33	1.37
12	D	242	HEM	C1A-NA	-2.04	1.35	1.39

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	382	HEM	C4C-CHD-C1D	-6.85	111.47	126.02
12	C	381	HEM	C1C-CHC-C4B	-6.09	113.08	126.02
12	C	382	HEM	C1C-CHC-C4B	-5.82	113.65	126.02
12	D	242	HEM	C1C-CHC-C4B	-5.63	114.05	126.02
12	C	381	HEM	C4C-CHD-C1D	-5.49	114.36	126.02
12	D	242	HEM	C4C-CHD-C1D	-5.47	114.39	126.02
12	C	382	HEM	CHB-C4A-NA	5.20	133.28	123.86
12	D	242	HEM	CHB-C1B-NB	4.96	130.50	124.37
12	C	381	HEM	CHB-C4A-NA	4.95	132.84	123.86
12	C	382	HEM	C4A-CHB-C1B	-4.94	114.62	126.25
12	C	382	HEM	C4A-NA-C1A	4.89	113.80	105.82
12	D	242	HEM	CHB-C4A-NA	4.64	132.28	123.86
12	C	382	HEM	CHA-C1A-NA	4.63	132.26	123.86
12	D	242	HEM	CHA-C1A-NA	4.62	132.24	123.86
12	D	242	HEM	CHC-C1C-NC	4.52	129.38	124.45
12	C	381	HEM	C4A-CHB-C1B	-4.52	115.62	126.25
12	D	242	HEM	C4A-CHB-C1B	-4.50	115.67	126.25
12	C	381	HEM	C4A-NA-C1A	4.48	113.12	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	383	UQ2	C7-C6-C1	4.32	123.53	118.52
12	D	242	HEM	C1A-CHA-C4D	-4.29	116.15	126.25
12	C	381	HEM	C4C-C3C-C2C	4.24	110.49	106.81
12	D	242	HEM	C4A-NA-C1A	4.23	112.72	105.82
12	C	381	HEM	CHA-C1A-NA	4.23	131.53	123.86
12	C	381	HEM	CHC-C4B-NB	4.23	128.97	124.42
12	C	382	HEM	C1A-CHA-C4D	-4.18	116.41	126.25
12	D	242	HEM	CHD-C1D-ND	4.05	128.78	124.42
12	C	382	HEM	CHC-C1C-NC	4.03	128.84	124.45
12	D	242	HEM	CHA-C4D-ND	4.03	129.35	124.37
12	C	381	HEM	C1A-CHA-C4D	-4.02	116.78	126.25
12	D	242	HEM	CHC-C4B-NB	3.94	128.66	124.42
13	C	383	UQ2	C7-C6-C5	-3.82	118.34	124.89
12	C	381	HEM	CHB-C1B-NB	3.81	129.08	124.37
12	C	381	HEM	CHD-C4C-NC	3.73	128.51	124.45
12	D	242	HEM	CHD-C4C-NC	3.57	128.34	124.45
12	C	381	HEM	CBC-CAC-C3C	-3.57	109.71	127.53
13	C	383	UQ2	CM5-C5-C6	-3.52	118.66	124.45
12	C	382	HEM	C1B-NB-C4B	-3.51	101.06	105.21
12	C	381	HEM	CBB-CAB-C3B	-3.45	110.29	127.53
12	D	242	HEM	C3B-C2B-C1B	3.41	108.97	106.41
12	D	242	HEM	CBC-CAC-C3C	-3.40	110.56	127.53
13	C	383	UQ2	C10-C9-C11	3.39	121.11	115.23
12	C	381	HEM	C4C-NC-C1C	-3.34	100.38	105.82
12	C	381	HEM	C4B-C3B-C2B	3.29	110.31	107.28
12	C	382	HEM	C3B-C2B-C1B	3.27	108.86	106.41
12	C	382	HEM	C2A-C1A-NA	-3.22	106.58	110.15
12	C	381	HEM	CHA-C4D-ND	3.13	128.23	124.37
13	C	384	UQ2	C7-C6-C1	-3.09	114.92	118.52
12	C	381	HEM	CHD-C1D-ND	3.06	127.72	124.42
12	C	382	HEM	CBC-CAC-C3C	-3.02	112.44	127.53
12	C	381	HEM	C2A-C1A-NA	-2.92	106.91	110.15
12	C	382	HEM	C4C-NC-C1C	-2.85	101.17	105.82
12	D	242	HEM	C4C-C3C-C2C	2.85	109.29	106.81
12	C	381	HEM	CHB-C4A-C3A	-2.84	119.18	127.43
13	C	384	UQ2	CM2-O2-C2	-2.83	106.52	116.47
12	D	242	HEM	CBB-CAB-C3B	-2.82	113.44	127.53
12	D	242	HEM	C3C-C2C-C1C	2.81	109.70	107.05
13	C	384	UQ2	C10-C9-C11	2.81	120.10	115.23
12	C	381	HEM	CHC-C1C-NC	2.80	127.50	124.45
12	C	382	HEM	CHD-C1D-ND	2.79	127.43	124.42
12	D	242	HEM	C4B-C3B-C2B	2.79	109.85	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	242	HEM	CAA-CBA-CGA	-2.75	106.37	113.67
12	C	381	HEM	C4D-ND-C1D	-2.74	101.96	105.21
12	C	382	HEM	CHB-C1B-NB	2.74	127.75	124.37
12	D	242	HEM	C1D-C2D-C3D	2.73	109.85	106.98
12	C	382	HEM	CHB-C4A-C3A	-2.69	119.61	127.43
12	C	382	HEM	CHC-C4B-NB	2.69	127.31	124.42
12	D	242	HEM	CHA-C1A-C2A	-2.65	119.49	125.30
12	D	242	HEM	CHB-C4A-C3A	-2.57	119.97	127.43
12	C	381	HEM	C1B-NB-C4B	-2.56	102.17	105.21
12	D	242	HEM	CHB-C1B-C2B	-2.54	119.73	126.95
12	D	242	HEM	CAD-CBD-CGD	-2.51	107.01	113.67
12	C	382	HEM	CHD-C4C-NC	2.47	127.15	124.45
13	C	384	UQ2	C8-C7-C6	2.46	118.14	112.08
12	C	381	HEM	C3B-C2B-C1B	2.46	108.26	106.41
12	D	242	HEM	CHA-C4D-C3D	-2.46	120.70	125.23
13	C	383	UQ2	C12-C13-C14	-2.42	119.56	127.64
13	C	383	UQ2	C6-C5-C4	2.42	121.08	119.17
12	D	242	HEM	C4D-ND-C1D	-2.41	102.36	105.21
12	C	382	HEM	CHC-C1C-C2C	-2.38	120.53	125.49
12	C	382	HEM	CHA-C4D-ND	2.38	127.31	124.37
12	C	382	HEM	C3C-C2C-C1C	2.35	109.27	107.05
12	C	381	HEM	C1D-C2D-C3D	2.32	109.42	106.98
12	C	381	HEM	CHA-C4D-C3D	-2.27	121.04	125.23
13	C	384	UQ2	C7-C8-C9	-2.26	122.95	126.83
12	C	382	HEM	O2A-CGA-O1A	-2.25	117.54	123.33
12	C	381	HEM	CHB-C1B-C2B	-2.25	120.56	126.95
13	C	383	UQ2	C10-C9-C8	-2.18	118.03	123.63
12	C	381	HEM	CHD-C4C-C3C	-2.17	121.54	125.21
12	C	382	HEM	C4C-C3C-C2C	2.11	108.64	106.81
12	C	382	HEM	O2D-CGD-CBD	2.10	120.64	114.00
12	C	382	HEM	CBB-CAB-C3B	-2.10	117.05	127.53
12	C	382	HEM	C1D-C2D-C3D	2.08	109.17	106.98
12	D	242	HEM	C1B-NB-C4B	-2.07	102.76	105.21
12	D	242	HEM	O2A-CGA-CBA	2.05	120.49	114.00
12	C	382	HEM	CHB-C1B-C2B	-2.04	121.15	126.95
12	C	381	HEM	C3C-C2C-C1C	2.04	108.97	107.05
12	D	242	HEM	CHC-C1C-C2C	-2.04	121.25	125.49

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	381	HEM	C2B-C3B-CAB-CBB
12	C	381	HEM	C2C-C3C-CAC-CBC
12	C	381	HEM	C4C-C3C-CAC-CBC
12	C	382	HEM	C2C-C3C-CAC-CBC
12	D	242	HEM	C2B-C3B-CAB-CBB
12	D	242	HEM	C2C-C3C-CAC-CBC
12	D	242	HEM	C4C-C3C-CAC-CBC
13	C	383	UQ2	C1-C6-C7-C8
13	C	384	UQ2	C1-C6-C7-C8
13	C	384	UQ2	C5-C6-C7-C8
13	C	383	UQ2	C12-C11-C9-C10
13	C	383	UQ2	C9-C11-C12-C13
13	C	383	UQ2	C12-C11-C9-C8
13	C	383	UQ2	C5-C6-C7-C8
12	C	381	HEM	C4B-C3B-CAB-CBB
12	C	382	HEM	C4C-C3C-CAC-CBC
12	D	242	HEM	C4B-C3B-CAB-CBB
13	C	384	UQ2	C9-C11-C12-C13
12	C	381	HEM	C2A-CAA-CBA-CGA
12	C	381	HEM	C3D-CAD-CBD-CGD
12	C	382	HEM	CAA-CBA-CGA-O1A
12	C	382	HEM	CAA-CBA-CGA-O2A
12	D	242	HEM	CAD-CBD-CGD-O2D
12	D	242	HEM	CAD-CBD-CGD-O1D
12	C	381	HEM	CAD-CBD-CGD-O1D
12	C	381	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

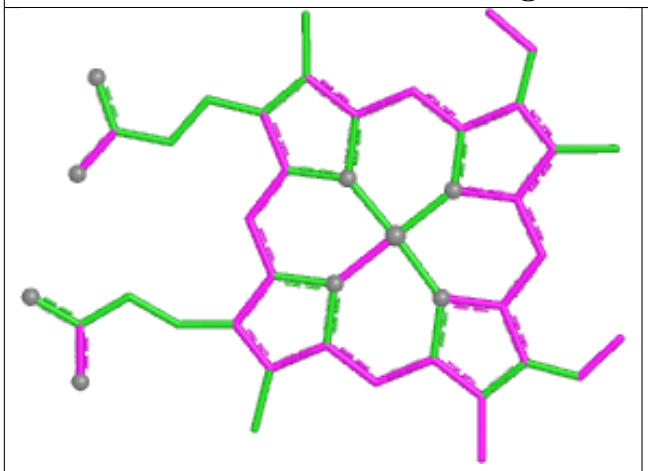
5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	381	HEM	3	0
12	D	242	HEM	3	0
13	C	383	UQ2	11	0
12	C	382	HEM	2	0
13	C	384	UQ2	7	0

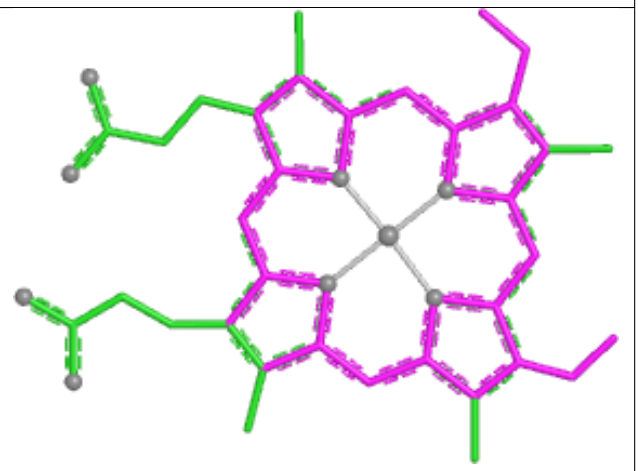
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

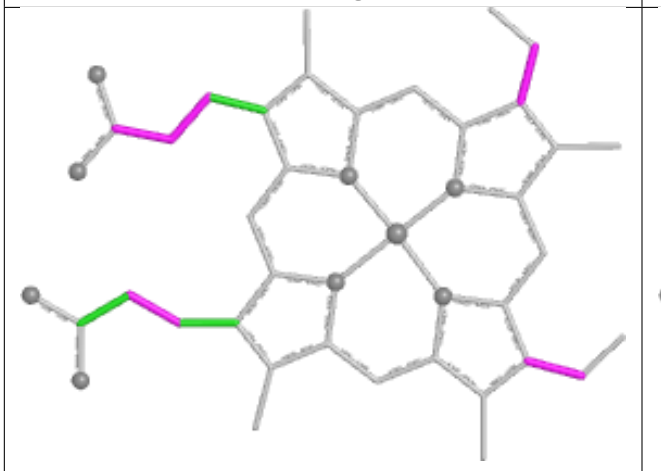
Ligand HEM C 381



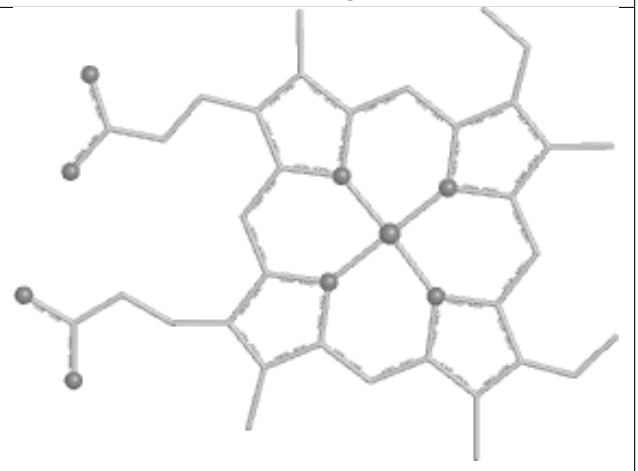
Bond lengths



Bond angles

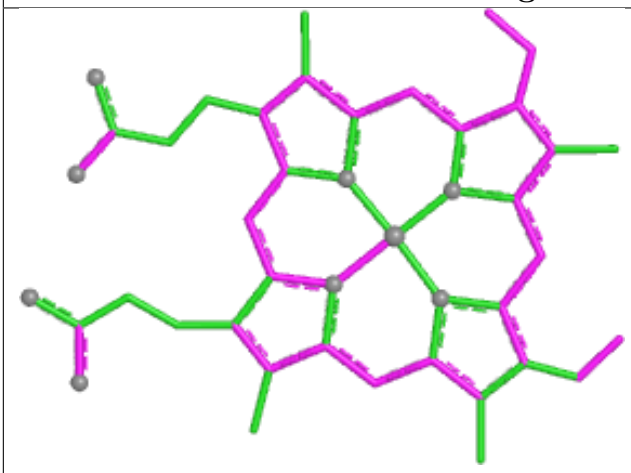


Torsions

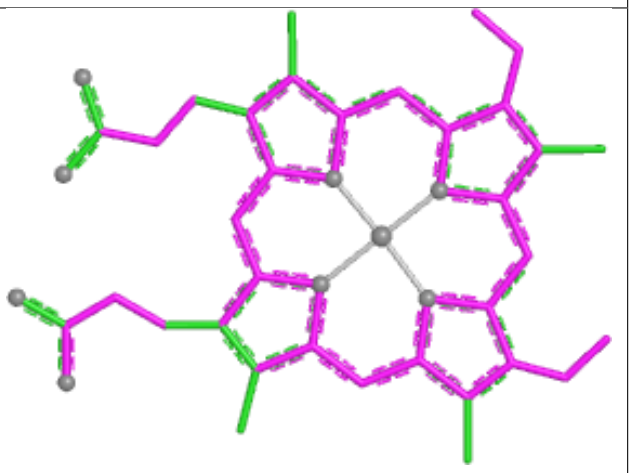


Rings

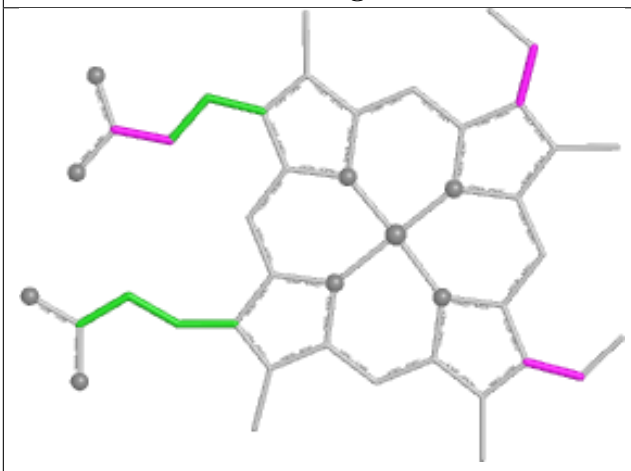
Ligand HEM D 242



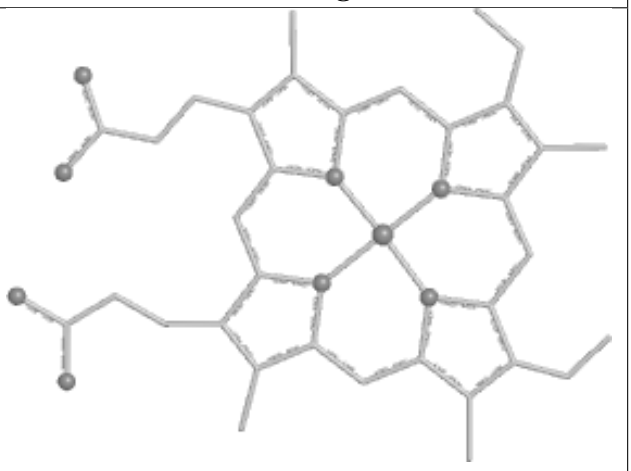
Bond lengths



Bond angles

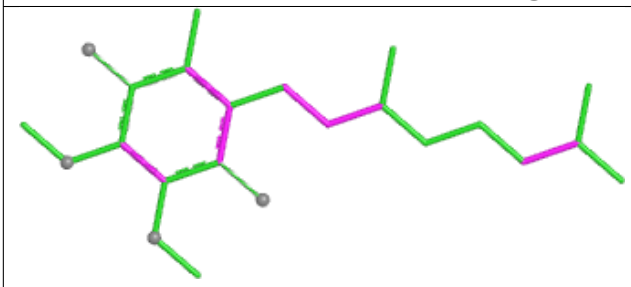


Torsions

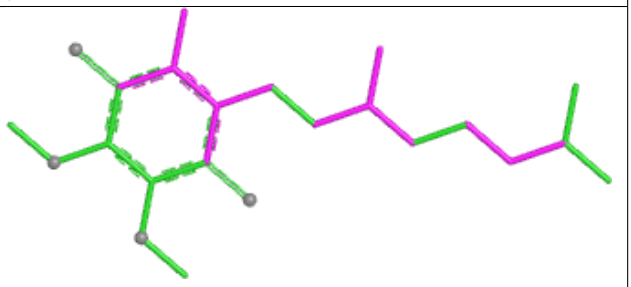


Rings

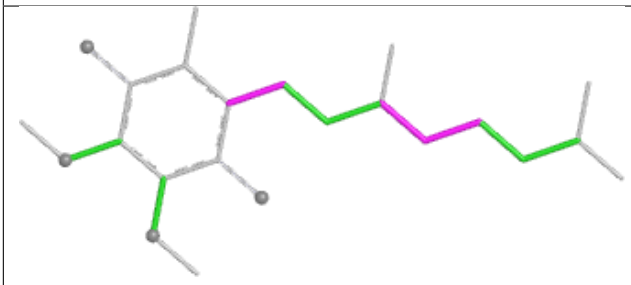
Ligand UQ2 C 383



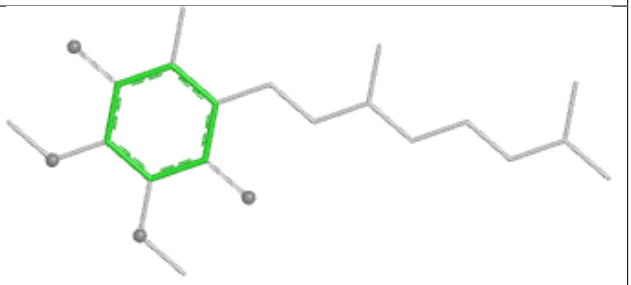
Bond lengths



Bond angles

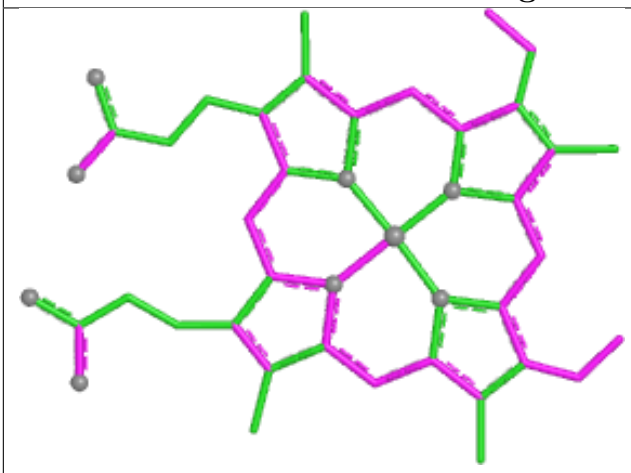


Torsions

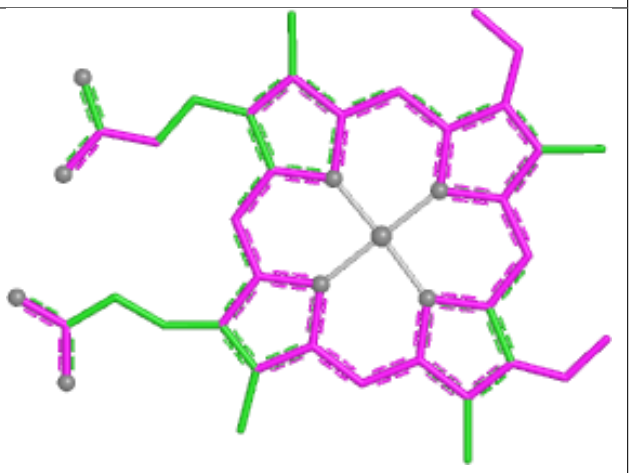


Rings

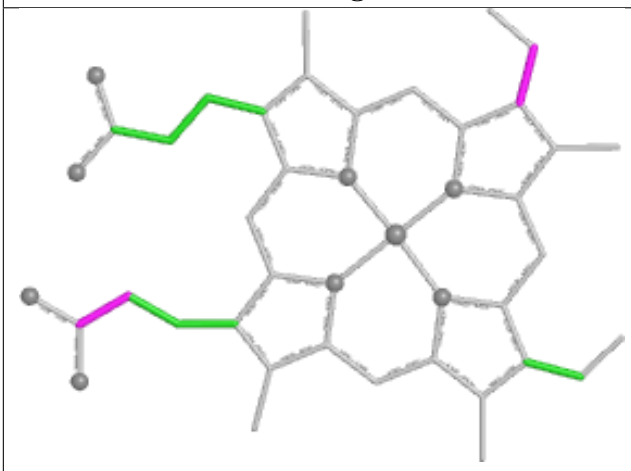
Ligand HEM C 382



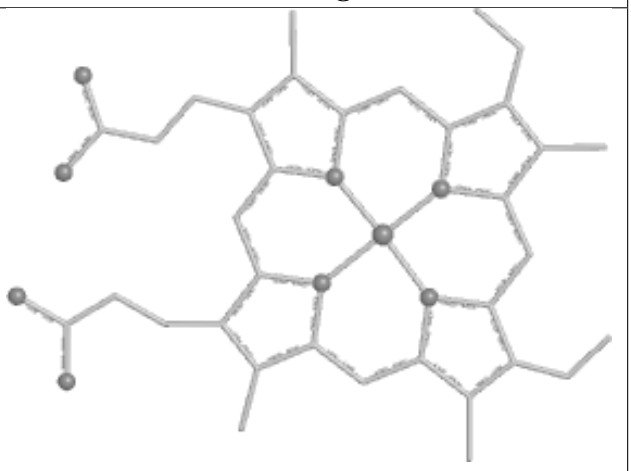
Bond lengths



Bond angles

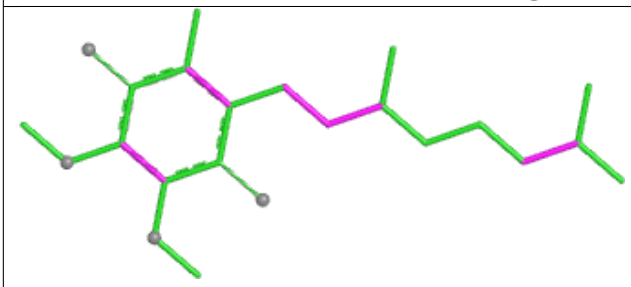


Torsions

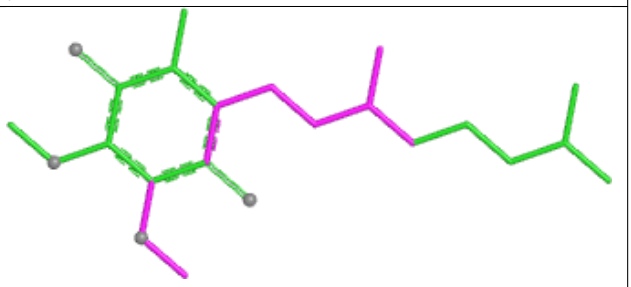


Rings

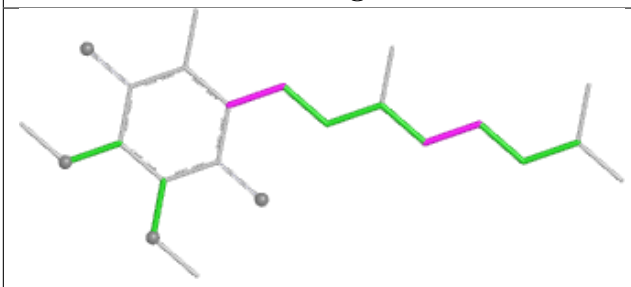
Ligand UQ2 C 384



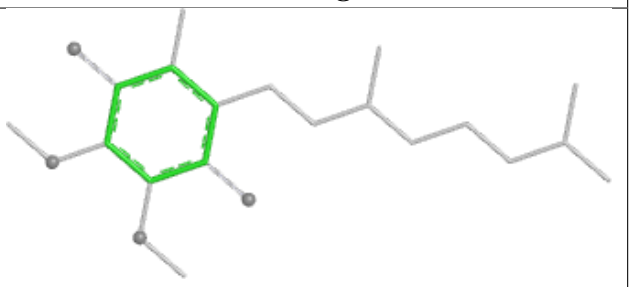
Bond lengths



Bond angles



Torsions



Rings

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.