Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 12:04 PM EDT

PDB ID	:	1NTK
Title	:	Crystal Structure of Mitochondrial Cytochrome bc1 in Complex with Antimycin A1
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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

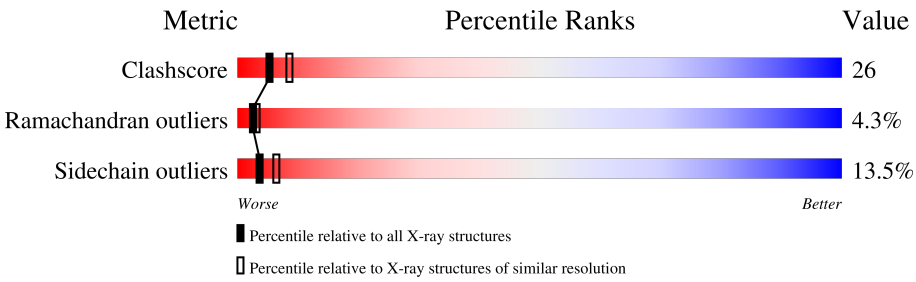
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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	61% 33% 7%
2	B	439	57% 32% 6% •
3	C	379	55% 35% 7% •
4	D	241	42% 44% 11% •
5	E	196	74% 21% • •
6	F	110	50% 37% 8% 5%
7	G	81	58% 28% 11% •
8	H	78	47% 37% 12% • •

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Mol	Chain	Length	Quality of chain
9	I	57	14% 42% 42%
10	J	62	53% 35% 8%
11	K	56	52% 29% 14% 5%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 17118 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	3457	2161	609	667	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	3171	1993	562	609	7	0	0	0

- Molecule 3 is a protein called Cytochrome b.

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

- Molecule 4 is a protein called cytochrome c1.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	105	910	576	165	167	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	79	659	430	122	106	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	76	626	378	109	134	5	0	0	0

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

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

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

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

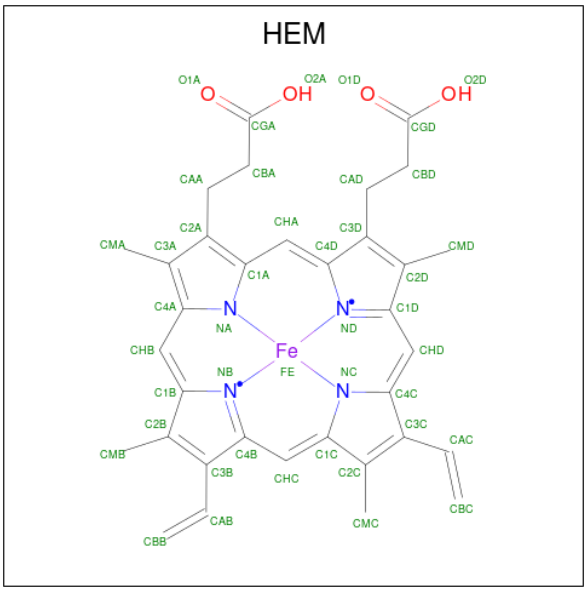
- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase complex 6.4 kDa protein.

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

There is a discrepancy between the modelled and reference sequences:

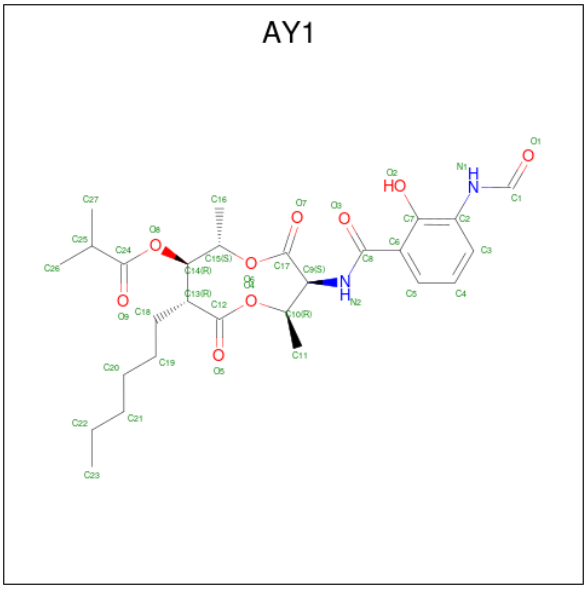
Chain	Residue	Modelled	Actual	Comment	Reference
K	22	GLN	SER	SEE REMARK 999	UNP P07552

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



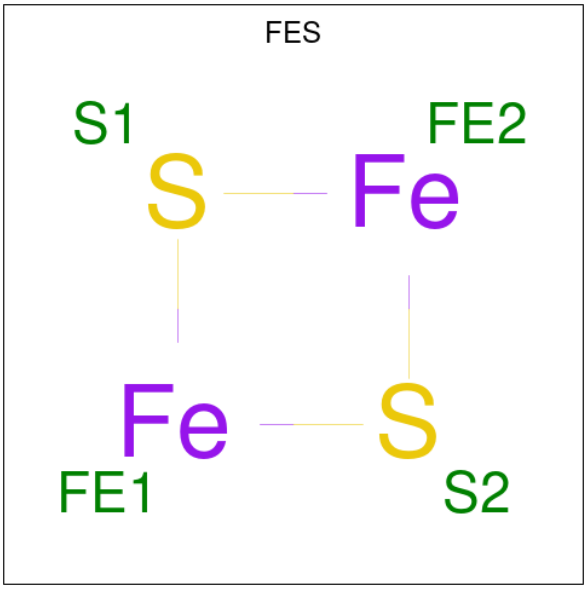
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	D	1	43	34	1	4	4	0	0

- Molecule 13 is [(2R,3S,6S,7R,8R)-3-[(3-formamido-2-oxidanyl-phenyl)carbonylamino]-8-hexyl-2,6-dimethyl-4,9-bis(oxidanylidene)-1,5-dioxonan-7-yl] 2-methylpropanoate (three-letter code: AY1) (formula: $C_{27}H_{38}N_2O_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
13	C	1	38	27	2	9	0	0

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



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O				
15	A	95	95	95			0	0
15	B	83	83	83			0	0
15	C	61	61	61			0	0
15	D	27	27	27			0	0
15	E	3	3	3			0	0
15	F	30	30	30			0	0
15	G	22	22	22			0	0
15	I	6	6	6			0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	J	5	5	5	0	0
			Total	O		
15	K	10	10	10	0	0

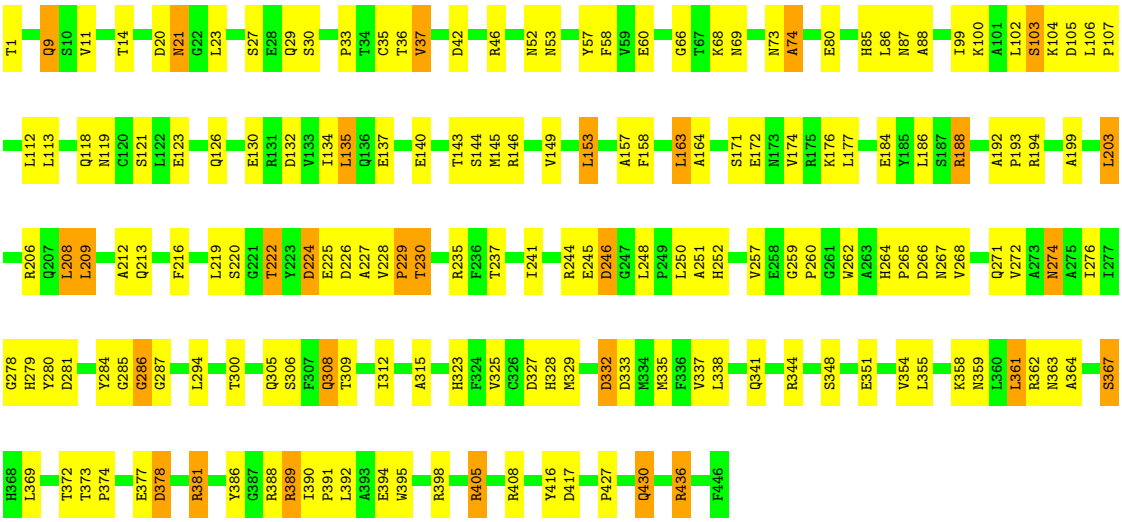
3 Residue-property plots (i)

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.

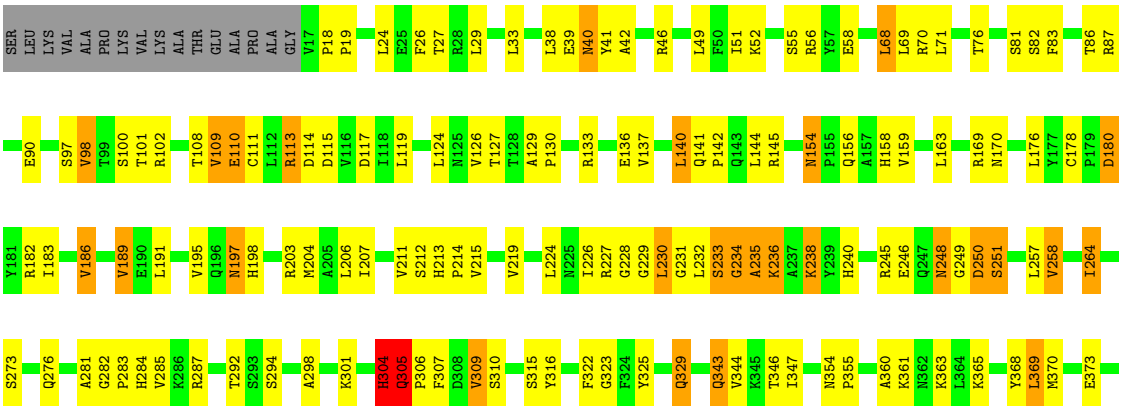
• Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

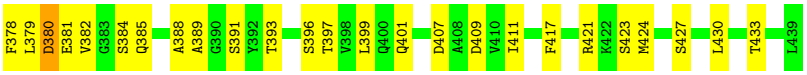
Chain A: 61% 33% 7%



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

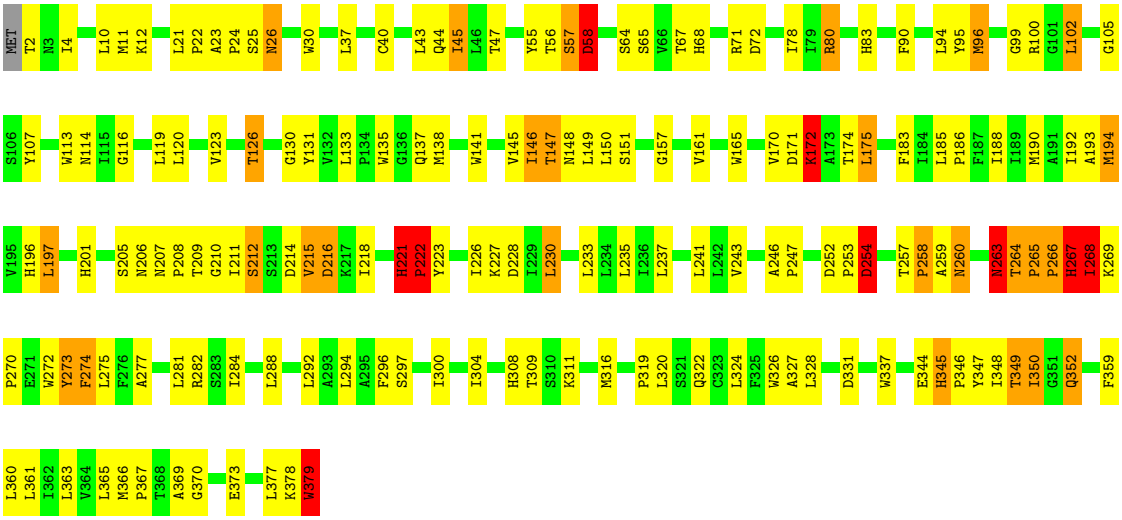
Chain B: 57% 32% 6% •





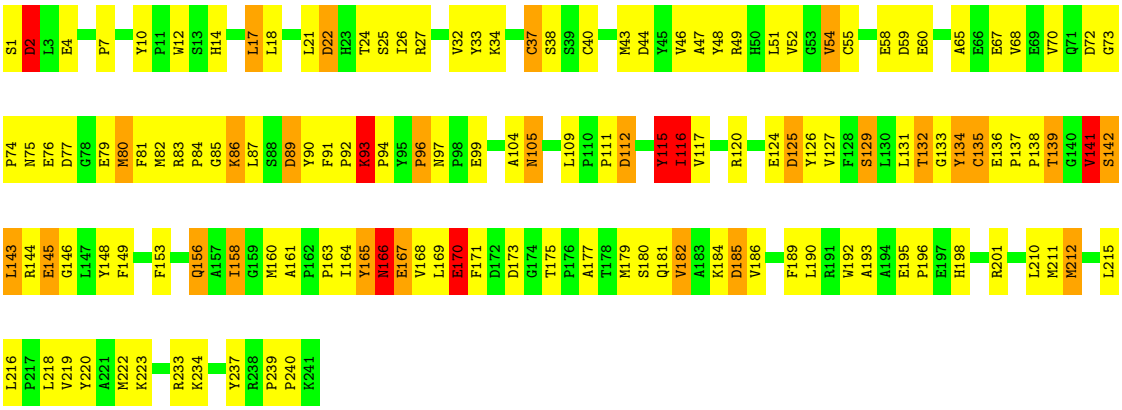
• Molecule 3: Cytochrome b

Chain C:



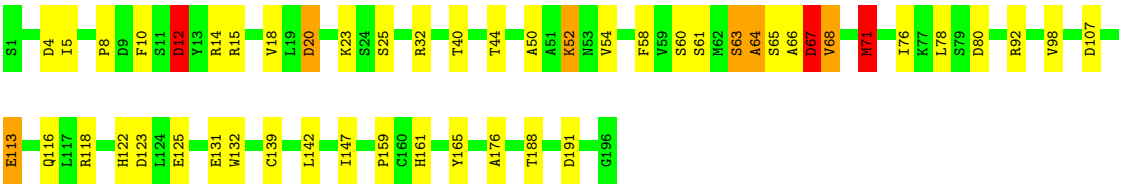
• Molecule 4: cytochrome c1

Chain D:



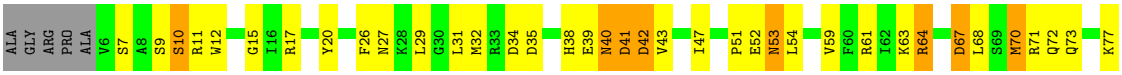
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, MITOCHONDRIAL

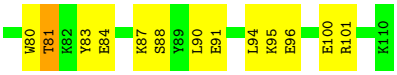
Chain E:



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

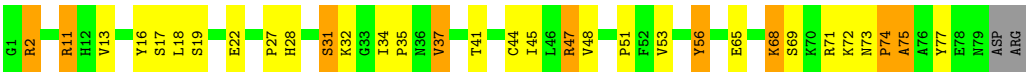
Chain F:





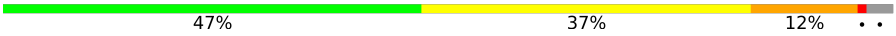
• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

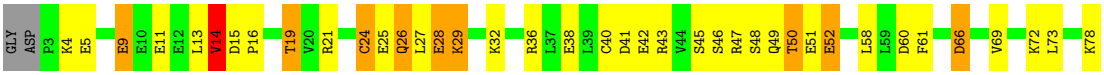
Chain G:



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

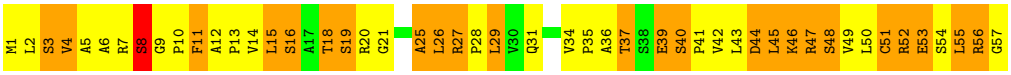
Chain H:





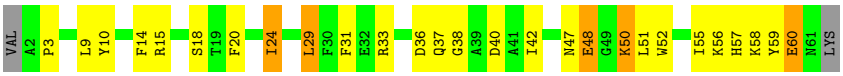
• Molecule 9: Ubiquinol-cytochrome C reductase 8 kDa protein

Chain I:



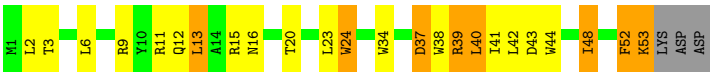
• Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

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	153.78Å 153.78Å 592.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.5 (40.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.233 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17118	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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: AY1, FES, 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	0.84	2/3530 (0.1%)	0.85	11/4792 (0.2%)
2	B	1.11	1/3231 (0.0%)	0.94	11/4386 (0.3%)
3	C	0.78	3/3100 (0.1%)	0.82	9/4242 (0.2%)
4	D	0.60	0/1977	0.87	11/2684 (0.4%)
5	E	0.53	0/1553	0.78	8/2100 (0.4%)
6	F	0.96	0/929	0.91	5/1246 (0.4%)
7	G	0.77	0/681	0.79	0/922
8	H	0.56	0/632	0.83	3/847 (0.4%)
9	I	1.07	1/411 (0.2%)	1.18	1/558 (0.2%)
10	J	0.56	0/508	0.76	2/686 (0.3%)
11	K	0.66	0/457	0.77	2/625 (0.3%)
All	All	0.83	7/17009 (0.0%)	0.86	63/23088 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	1	0
3	C	2	2
7	G	2	0
9	I	1	0
All	All	6	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	25	ALA	CA-CB	-6.95	1.37	1.52
3	C	26	ASN	CB-CG	-6.36	1.36	1.51
3	C	194	MET	SD-CE	5.82	2.10	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	159	VAL	CB-CG2	-5.71	1.40	1.52
3	C	379	TRP	CB-CG	-5.44	1.40	1.50
1	A	436	ARG	CB-CG	-5.32	1.38	1.52
1	A	37	VAL	CB-CG2	-5.05	1.42	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	42	ASP	CB-CG-OD2	7.55	125.10	118.30
3	C	345	HIS	N-CA-C	6.71	129.12	111.00
1	A	333	ASP	CB-CG-OD2	6.66	124.30	118.30
3	C	252	ASP	CB-CG-OD2	6.55	124.19	118.30
5	E	67	ASP	CB-CG-OD2	6.40	124.06	118.30
3	C	254	ASP	CB-CG-OD2	6.37	124.03	118.30
2	B	115	ASP	CB-CG-OD2	6.33	123.99	118.30
6	F	34	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	246	ASP	CB-CG-OD2	6.11	123.80	118.30
9	I	44	ASP	CB-CG-OD2	6.11	123.80	118.30
2	B	309	VAL	CB-CA-C	-6.08	99.84	111.40
11	K	43	ASP	CB-CG-OD2	6.08	123.77	118.30
2	B	409	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	327	ASP	CB-CG-OD2	6.03	123.73	118.30
2	B	117	ASP	CB-CG-OD2	6.03	123.73	118.30
2	B	250	ASP	N-CA-C	-6.00	94.81	111.00
1	A	266	ASP	CB-CG-OD2	5.97	123.67	118.30
4	D	115	TYR	CB-CA-C	-5.94	98.51	110.40
1	A	417	ASP	CB-CG-OD2	5.93	123.64	118.30
3	C	58	ASP	CB-CG-OD2	5.93	123.64	118.30
3	C	216	ASP	CB-CG-OD2	5.74	123.46	118.30
2	B	304	HIS	CB-CA-C	5.73	121.86	110.40
10	J	40	ASP	CB-CG-OD2	5.73	123.45	118.30
2	B	369	LEU	CA-CB-CG	-5.71	102.17	115.30
8	H	60	ASP	CB-CG-OD2	5.68	123.41	118.30
2	B	180	ASP	CB-CG-OD2	5.64	123.38	118.30
4	D	93	LYS	N-CA-C	5.63	126.21	111.00
8	H	15	ASP	CB-CG-OD2	5.61	123.35	118.30
4	D	44	ASP	CB-CG-OD2	5.59	123.33	118.30
2	B	170	ASN	N-CA-C	5.59	126.09	111.00
11	K	37	ASP	CB-CG-OD2	5.57	123.31	118.30
5	E	4	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	224	ASP	CB-CG-OD2	5.54	123.28	118.30
4	D	185	ASP	CB-CG-OD2	5.52	123.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	112	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	380	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	20	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	378	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	332	ASP	CB-CG-OD2	5.39	123.15	118.30
4	D	125	ASP	CB-CG-OD2	5.36	123.13	118.30
8	H	66	ASP	CB-CG-OD2	5.27	123.04	118.30
5	E	107	ASP	CB-CG-OD2	5.26	123.04	118.30
3	C	72	ASP	CB-CG-OD2	5.25	123.02	118.30
4	D	89	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	105	ASP	CB-CG-OD2	5.22	123.00	118.30
4	D	116	ILE	N-CA-C	5.18	125.00	111.00
6	F	67	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	226	ASP	CB-CG-OD2	5.18	122.96	118.30
3	C	267	HIS	N-CA-C	-5.17	97.04	111.00
6	F	90	LEU	CA-CB-CG	5.17	127.19	115.30
6	F	41	ASP	CB-CG-OD2	5.17	122.95	118.30
5	E	191	ASP	CB-CG-OD2	5.16	122.95	118.30
10	J	36	ASP	CB-CG-OD2	5.16	122.94	118.30
5	E	20	ASP	CB-CG-OD2	5.13	122.92	118.30
3	C	214	ASP	CB-CG-OD2	5.13	122.92	118.30
3	C	331	ASP	CB-CG-OD2	5.11	122.89	118.30
2	B	114	ASP	CB-CG-OD2	5.10	122.89	118.30
4	D	59	ASP	CB-CG-OD2	5.08	122.87	118.30
4	D	22	ASP	CB-CG-OD2	5.07	122.86	118.30
5	E	123	ASP	CB-CG-OD2	5.04	122.84	118.30
5	E	80	ASP	CB-CG-OD2	5.04	122.83	118.30
5	E	12	ASP	CB-CG-OD2	5.04	122.83	118.30
4	D	72	ASP	CB-CG-OD2	5.03	122.82	118.30

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	304	HIS	CA
3	C	58	ASP	CA
3	C	221	HIS	CA
7	G	11	ARG	CA
7	G	73	ASN	CA
9	I	42	VAL	CA

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	3457	0	3356	229	0
2	B	3171	0	3152	199	0
3	C	3003	0	3065	153	0
4	D	1918	0	1870	113	0
5	E	1519	0	1504	34	0
6	F	910	0	904	43	0
7	G	659	0	658	27	0
8	H	626	0	595	25	0
9	I	406	0	435	260	0
10	J	495	0	493	27	0
11	K	441	0	450	18	0
12	C	86	0	60	16	0
12	D	43	0	30	6	0
13	C	38	0	37	12	0
14	E	4	0	0	1	0
15	A	95	0	0	10	0
15	B	83	0	0	21	0
15	C	61	0	0	7	0
15	D	27	0	0	2	0
15	E	3	0	0	2	0
15	F	30	0	0	4	0
15	G	22	0	0	3	0
15	I	6	0	0	3	0
15	J	5	0	0	0	0
15	K	10	0	0	2	0
All	All	17118	0	16609	883	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 26.

All (883) 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)
1:A:284:TYR:HE1	9:I:20:ARG:CG	1.09	1.65
1:A:284:TYR:CE1	9:I:20:ARG:HG3	1.24	1.61
1:A:279:HIS:CE1	9:I:52:ARG:HB2	1.56	1.40
2:B:283:PRO:HG3	9:I:31:GLN:CG	1.52	1.39
3:C:194:MET:SD	3:C:194:MET:CE	2.10	1.38
1:A:252:HIS:CE1	9:I:42:VAL:O	1.74	1.37
1:A:252:HIS:HE1	9:I:42:VAL:O	0.95	1.26
2:B:264:ILE:HG22	9:I:7:ARG:NH1	1.51	1.26
1:A:279:HIS:ND1	9:I:52:ARG:HB2	1.52	1.24
1:A:284:TYR:CE1	9:I:20:ARG:CG	1.94	1.23
1:A:279:HIS:CE1	9:I:52:ARG:CB	2.26	1.19
1:A:306:SER:HB3	9:I:47:ARG:O	1.44	1.17
9:I:41:PRO:O	9:I:42:VAL:HG23	1.47	1.13
1:A:305:GLN:HG3	9:I:46:LYS:O	1.48	1.12
1:A:325:VAL:HG11	9:I:43:LEU:HB3	1.15	1.12
2:B:283:PRO:CG	9:I:31:GLN:HG3	1.82	1.09
2:B:283:PRO:HG3	9:I:31:GLN:HG3	1.23	1.09
2:B:385:GLN:HA	9:I:2:LEU:HD12	1.13	1.09
15:A:497:HOH:O	9:I:55:LEU:HD23	1.50	1.09
2:B:381:GLU:OE1	9:I:1:MET:HA	1.50	1.07
4:D:161:ALA:O	4:D:163:PRO:HD3	1.55	1.07
3:C:190:MET:HG3	13:C:383:AY1:H261	1.31	1.07
15:A:497:HOH:O	9:I:55:LEU:CD2	1.99	1.06
2:B:388:ALA:CB	9:I:2:LEU:HD13	1.85	1.05
9:I:18:THR:OG1	9:I:53:GLU:OE2	1.72	1.04
2:B:388:ALA:HB3	9:I:2:LEU:CD1	1.87	1.04
1:A:325:VAL:HG21	9:I:43:LEU:CG	1.88	1.04
2:B:384:SER:OG	9:I:3:SER:HA	1.56	1.03
15:A:448:HOH:O	9:I:15:LEU:HD22	1.58	1.02
1:A:306:SER:CB	9:I:47:ARG:O	2.07	1.02
2:B:287:ARG:HG2	9:I:34:VAL:HG13	1.41	1.02
1:A:284:TYR:CE1	9:I:20:ARG:HG2	1.93	1.01
9:I:11:PHE:HA	9:I:25:ALA:HB2	1.43	1.01
1:A:140:GLU:CD	9:I:36:ALA:HB1	1.81	1.01
1:A:143:THR:HG21	9:I:39:GLU:HG2	1.42	1.00
1:A:146:ARG:HB2	9:I:42:VAL:HG11	1.44	0.99
1:A:140:GLU:OE1	9:I:36:ALA:HB1	1.61	0.99
1:A:284:TYR:CZ	9:I:20:ARG:HG3	1.97	0.98
2:B:283:PRO:CG	9:I:31:GLN:CG	2.40	0.98
2:B:70:ARG:NE	9:I:13:PRO:HB2	1.78	0.97
2:B:70:ARG:NH2	9:I:13:PRO:HG2	1.79	0.97
1:A:280:TYR:N	9:I:20:ARG:HH21	1.62	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:VAL:CG2	9:I:43:LEU:HG	1.94	0.97
2:B:68:LEU:HG	2:B:144:LEU:HD11	1.47	0.97
9:I:20:ARG:NH1	15:I:58:HOH:O	1.92	0.97
6:F:64:ARG:NH1	15:F:1906:HOH:O	1.99	0.96
2:B:384:SER:CB	9:I:3:SER:CA	2.43	0.96
1:A:279:HIS:CG	9:I:52:ARG:HB2	2.01	0.96
2:B:249:GLY:HA2	15:B:506:HOH:O	1.64	0.95
2:B:384:SER:CB	9:I:3:SER:N	2.30	0.95
1:A:281:ASP:HB2	9:I:20:ARG:NE	1.80	0.95
4:D:12:TRP:CH2	4:D:125:ASP:HB3	2.03	0.94
2:B:385:GLN:CA	9:I:2:LEU:HD12	1.98	0.94
2:B:264:ILE:HG22	9:I:7:ARG:HH11	1.16	0.94
1:A:325:VAL:HG21	9:I:43:LEU:HG	0.97	0.94
2:B:384:SER:HB2	9:I:3:SER:N	1.82	0.94
2:B:388:ALA:HB3	9:I:2:LEU:HD13	0.95	0.94
4:D:83:ARG:HG3	4:D:84:PRO:HD2	1.50	0.93
2:B:76:THR:HG22	2:B:82:SER:H	1.34	0.93
2:B:385:GLN:HA	9:I:2:LEU:CD1	1.99	0.93
2:B:264:ILE:CG2	9:I:7:ARG:HH11	1.82	0.92
8:H:51:GLU:HG2	8:H:52:GLU:H	1.30	0.92
9:I:46:LYS:HG2	9:I:47:ARG:H	1.32	0.92
13:C:383:AY1:H5	15:C:412:HOH:O	1.70	0.92
2:B:68:LEU:HD12	2:B:186:VAL:HG22	1.51	0.91
1:A:279:HIS:ND1	9:I:52:ARG:CB	2.30	0.91
2:B:101:THR:HB	15:B:521:HOH:O	1.72	0.90
2:B:384:SER:CB	9:I:3:SER:HA	2.01	0.90
9:I:46:LYS:CG	9:I:47:ARG:H	1.84	0.90
1:A:146:ARG:H	9:I:42:VAL:CG1	1.84	0.90
1:A:364:ALA:HB1	9:I:54:SER:HA	1.53	0.90
9:I:4:VAL:HG12	9:I:10:PRO:HG2	1.55	0.89
2:B:385:GLN:HE22	2:B:393:THR:H	1.19	0.88
1:A:146:ARG:CB	9:I:42:VAL:HG11	2.02	0.88
1:A:325:VAL:CG1	9:I:43:LEU:HB3	2.03	0.88
1:A:281:ASP:OD1	9:I:47:ARG:HG2	1.73	0.88
2:B:154:ASN:N	2:B:154:ASN:HD22	1.71	0.87
2:B:70:ARG:CZ	9:I:13:PRO:HG2	2.05	0.87
2:B:156:GLN:HB3	9:I:27:ARG:HG2	1.57	0.87
2:B:384:SER:OG	9:I:3:SER:CA	2.22	0.87
1:A:281:ASP:OD1	9:I:47:ARG:CG	2.23	0.86
9:I:34:VAL:HB	9:I:35:PRO:HD3	1.57	0.86
2:B:100:SER:O	9:I:12:ALA:HA	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLN:HE22	1:A:344:ARG:HH22	1.24	0.86
2:B:305:GLN:HB2	2:B:306:PRO:CD	2.06	0.85
9:I:8:SER:OG	9:I:26:LEU:HD13	1.75	0.85
4:D:37:CYS:SG	12:D:242:HEM:HAB	2.17	0.85
3:C:26:ASN:ND2	3:C:207:ASN:HD22	1.75	0.85
4:D:138:PRO:HG3	8:H:58:LEU:HD22	1.58	0.84
4:D:12:TRP:HH2	4:D:125:ASP:HB3	1.39	0.84
4:D:131:LEU:HD11	12:D:242:HEM:HMB3	1.59	0.84
3:C:26:ASN:HD22	3:C:207:ASN:ND2	1.74	0.84
4:D:14:HIS:NE2	4:D:124:GLU:OE1	2.10	0.84
2:B:154:ASN:HD22	2:B:154:ASN:H	1.22	0.84
2:B:283:PRO:HG3	9:I:31:GLN:CD	1.96	0.84
2:B:283:PRO:HG3	9:I:31:GLN:NE2	1.93	0.83
1:A:140:GLU:OE1	9:I:36:ALA:CB	2.26	0.83
1:A:284:TYR:CD1	9:I:19:SER:O	2.32	0.83
15:A:448:HOH:O	9:I:21:GLY:CA	2.25	0.83
2:B:283:PRO:HG3	9:I:31:GLN:HG2	1.61	0.83
9:I:47:ARG:HG2	9:I:48:SER:N	1.92	0.83
4:D:10:TYR:O	4:D:12:TRP:CE3	2.33	0.82
1:A:281:ASP:OD2	9:I:47:ARG:HG3	1.80	0.82
1:A:351:GLU:H	11:K:12:GLN:NE2	1.78	0.82
4:D:165:TYR:HD2	4:D:165:TYR:O	1.63	0.82
9:I:46:LYS:HG2	9:I:47:ARG:N	1.93	0.82
1:A:281:ASP:OD1	9:I:47:ARG:CB	2.28	0.81
2:B:70:ARG:HE	9:I:13:PRO:HB2	1.43	0.81
2:B:380:ASP:OD1	9:I:3:SER:OG	1.97	0.81
9:I:11:PHE:HA	9:I:25:ALA:CB	2.10	0.81
9:I:47:ARG:HG2	9:I:48:SER:H	1.43	0.81
1:A:364:ALA:HB1	9:I:54:SER:CA	2.10	0.81
9:I:6:ALA:C	9:I:8:SER:H	1.84	0.81
3:C:45:ILE:HA	12:C:381:HEM:HAB	1.61	0.81
1:A:281:ASP:HB3	9:I:20:ARG:HG2	1.64	0.80
4:D:37:CYS:SG	12:D:242:HEM:CAB	2.70	0.80
1:A:325:VAL:HG11	9:I:43:LEU:CB	2.07	0.79
2:B:401:GLN:HB3	15:B:470:HOH:O	1.81	0.79
2:B:368:TYR:CE1	9:I:1:MET:HG3	2.18	0.79
3:C:24:PRO:C	3:C:26:ASN:H	1.85	0.79
2:B:233:SER:O	2:B:235:ALA:N	2.15	0.79
1:A:29:GLN:HG3	1:A:203:LEU:O	1.83	0.79
1:A:252:HIS:CE1	9:I:43:LEU:HB2	2.18	0.79
9:I:2:LEU:O	9:I:3:SER:HB3	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:HIS:CD2	3:C:222:PRO:HD3	2.19	0.78
1:A:280:TYR:N	9:I:20:ARG:NH2	2.31	0.78
9:I:49:VAL:HG12	9:I:50:LEU:H	1.48	0.78
1:A:271:GLN:NE2	9:I:55:LEU:HD22	1.99	0.78
1:A:140:GLU:OE1	9:I:37:THR:N	2.17	0.78
2:B:283:PRO:CG	9:I:31:GLN:HE21	1.97	0.78
5:E:5:ILE:HA	15:E:1702:HOH:O	1.84	0.77
2:B:305:GLN:HB2	2:B:306:PRO:HD2	1.66	0.77
9:I:5:ALA:HB3	15:I:62:HOH:O	1.83	0.77
1:A:378:ASP:OD2	1:A:389:ARG:NH1	2.18	0.76
3:C:131:TYR:HA	12:C:381:HEM:HAD2	1.67	0.76
7:G:73:ASN:O	7:G:75:ALA:HB3	1.84	0.76
1:A:280:TYR:H	9:I:20:ARG:NH2	1.84	0.76
6:F:64:ARG:HH11	6:F:64:ARG:HG2	1.50	0.76
2:B:385:GLN:HE22	2:B:393:THR:N	1.82	0.76
4:D:54:VAL:HG21	4:D:192:TRP:CZ2	2.21	0.76
4:D:75:ASN:O	4:D:77:ASP:N	2.18	0.76
1:A:146:ARG:HB2	9:I:42:VAL:CG1	2.14	0.75
2:B:86:THR:O	2:B:90:GLU:HG2	1.87	0.75
2:B:251:SER:O	15:B:507:HOH:O	2.04	0.75
2:B:287:ARG:HG2	9:I:34:VAL:CG1	2.15	0.75
1:A:279:HIS:HB2	9:I:20:ARG:NH2	2.01	0.75
3:C:26:ASN:ND2	3:C:207:ASN:ND2	2.31	0.75
10:J:29:LEU:HD13	11:K:34:TRP:HD1	1.51	0.75
2:B:156:GLN:CB	9:I:27:ARG:HG2	2.16	0.74
2:B:39:GLU:OE1	2:B:113:ARG:NH2	2.19	0.74
4:D:40:CYS:SG	12:D:242:HEM:HAC	2.28	0.74
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.22	0.74
1:A:143:THR:CG2	9:I:39:GLU:HG2	2.16	0.74
2:B:240:HIS:O	2:B:421:ARG:NH1	2.21	0.74
1:A:146:ARG:H	9:I:42:VAL:HG12	1.51	0.74
3:C:319:PRO:HG3	7:G:47:ARG:HH12	1.53	0.74
2:B:381:GLU:OE1	9:I:1:MET:CA	2.32	0.73
4:D:7:PRO:HB2	4:D:125:ASP:OD1	1.88	0.73
2:B:329:GLN:HE21	2:B:329:GLN:N	1.86	0.73
6:F:40:ASN:ND2	6:F:43:VAL:H	1.86	0.73
9:I:41:PRO:O	9:I:42:VAL:CG2	2.33	0.73
1:A:281:ASP:CB	9:I:20:ARG:HG2	2.18	0.73
2:B:282:GLY:N	15:B:512:HOH:O	2.22	0.73
1:A:281:ASP:OD1	9:I:47:ARG:C	2.27	0.73
15:A:448:HOH:O	9:I:21:GLY:HA2	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASP:HB2	9:I:20:ARG:CD	2.19	0.73
10:J:18:SER:HA	11:K:24:TRP:CZ3	2.23	0.72
1:A:279:HIS:NE2	9:I:52:ARG:HB2	2.02	0.72
6:F:43:VAL:O	6:F:47:ILE:HG12	1.90	0.72
1:A:308:GLN:NE2	15:I:58:HOH:O	2.18	0.71
1:A:284:TYR:CE1	9:I:19:SER:O	2.43	0.71
2:B:129:ALA:N	2:B:130:PRO:HD3	2.06	0.71
1:A:271:GLN:HE21	9:I:55:LEU:HD13	1.56	0.71
3:C:190:MET:CG	13:C:383:AY1:H261	2.17	0.71
7:G:18:LEU:HD21	7:G:22:GLU:HB3	1.72	0.71
9:I:20:ARG:HD2	9:I:51:CYS:SG	2.31	0.70
1:A:279:HIS:CE1	9:I:52:ARG:C	2.65	0.70
2:B:283:PRO:HG3	9:I:31:GLN:HE21	1.54	0.70
4:D:34:LYS:NZ	4:D:67:GLU:OE1	2.25	0.70
2:B:68:LEU:HD12	2:B:186:VAL:CG2	2.19	0.70
2:B:249:GLY:N	15:B:505:HOH:O	2.22	0.70
2:B:189:VAL:HG12	15:B:496:HOH:O	1.91	0.70
2:B:158:HIS:HB2	15:B:494:HOH:O	1.92	0.70
1:A:279:HIS:CD2	9:I:52:ARG:HB2	2.27	0.70
3:C:26:ASN:HD22	3:C:207:ASN:HD22	1.35	0.70
8:H:51:GLU:CG	8:H:52:GLU:H	2.05	0.69
1:A:281:ASP:CG	9:I:47:ARG:HB2	2.12	0.69
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.75	0.69
3:C:215:VAL:HG11	6:F:59:VAL:HG13	1.73	0.69
6:F:64:ARG:HH11	6:F:64:ARG:CG	2.05	0.69
1:A:118:GLN:HG2	1:A:219:LEU:HD21	1.73	0.69
4:D:166:ASN:HD22	4:D:166:ASN:H	1.38	0.69
2:B:384:SER:OG	9:I:3:SER:CB	2.41	0.69
2:B:40:ASN:O	2:B:41:TYR:HB2	1.92	0.69
7:G:68:LYS:O	7:G:72:LYS:HB3	1.93	0.69
4:D:165:TYR:O	4:D:167:GLU:N	2.25	0.69
9:I:55:LEU:O	9:I:56:ARG:HB2	1.92	0.69
1:A:271:GLN:NE2	9:I:55:LEU:HD13	2.08	0.69
1:A:146:ARG:N	9:I:42:VAL:HG12	2.08	0.68
1:A:271:GLN:NE2	9:I:55:LEU:CD2	2.56	0.68
1:A:286:GLY:N	15:A:452:HOH:O	2.24	0.68
2:B:384:SER:HB3	9:I:3:SER:N	2.07	0.68
9:I:44:ASP:O	9:I:46:LYS:N	2.27	0.68
4:D:86:LYS:NZ	4:D:89:ASP:HB2	2.09	0.68
4:D:161:ALA:O	4:D:163:PRO:CD	2.39	0.68
2:B:70:ARG:NH2	9:I:13:PRO:CG	2.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:181:GLN:HE22	8:H:78:LYS:HB2	1.58	0.67
2:B:264:ILE:CG2	9:I:7:ARG:NH1	2.40	0.67
1:A:364:ALA:CB	9:I:54:SER:HA	2.21	0.67
6:F:68:LEU:HD23	6:F:71:ARG:HH12	1.59	0.67
2:B:283:PRO:CG	9:I:31:GLN:NE2	2.57	0.67
3:C:226:ILE:HD11	4:D:222:MET:HB3	1.76	0.67
9:I:42:VAL:HG13	9:I:43:LEU:HD23	1.74	0.67
1:A:281:ASP:OD2	9:I:47:ARG:CG	2.43	0.66
4:D:141:VAL:HG13	4:D:142:SER:N	2.10	0.66
2:B:329:GLN:HE21	2:B:329:GLN:H	1.43	0.66
2:B:368:TYR:CD1	9:I:1:MET:HG3	2.30	0.66
1:A:250:LEU:HD12	9:I:44:ASP:C	2.16	0.66
2:B:126:VAL:O	2:B:130:PRO:HG3	1.95	0.66
6:F:40:ASN:HD22	6:F:40:ASN:C	1.99	0.66
2:B:70:ARG:HG3	2:B:98:VAL:HG22	1.78	0.66
1:A:146:ARG:N	9:I:42:VAL:CG1	2.58	0.66
9:I:47:ARG:CG	9:I:48:SER:H	2.09	0.66
2:B:283:PRO:HG2	9:I:31:GLN:HG3	1.76	0.65
3:C:273:TYR:HE2	15:C:396:HOH:O	1.78	0.65
6:F:53:ASN:N	6:F:53:ASN:HD22	1.94	0.65
2:B:76:THR:HG22	2:B:82:SER:N	2.10	0.65
1:A:341:GLN:NE2	1:A:344:ARG:HH22	1.93	0.65
1:A:284:TYR:OH	9:I:20:ARG:NE	2.30	0.65
2:B:283:PRO:N	9:I:31:GLN:HE21	1.94	0.65
3:C:263:ASN:O	3:C:264:THR:HB	1.96	0.65
2:B:283:PRO:N	9:I:31:GLN:NE2	2.45	0.65
3:C:273:TYR:HD2	3:C:274:PHE:CE2	2.14	0.65
3:C:215:VAL:CG1	6:F:59:VAL:HG13	2.27	0.64
2:B:46:ARG:NH1	2:B:110:GLU:OE2	2.30	0.64
1:A:27:SER:HB3	1:A:208:LEU:HD12	1.79	0.64
2:B:76:THR:HB	2:B:81:SER:HA	1.80	0.64
1:A:287:GLY:N	15:A:498:HOH:O	2.30	0.64
3:C:227:LYS:HE3	15:D:1061:HOH:O	1.97	0.64
2:B:154:ASN:N	2:B:154:ASN:ND2	2.40	0.64
1:A:146:ARG:H	9:I:42:VAL:HG11	1.62	0.64
1:A:271:GLN:HE22	9:I:55:LEU:CD2	2.10	0.64
6:F:83:TYR:O	6:F:84:GLU:HG2	1.98	0.64
1:A:158:PHE:O	1:A:164:ALA:HB2	1.97	0.64
3:C:193:ALA:O	3:C:196:HIS:HB3	1.98	0.64
3:C:207:ASN:HB2	3:C:208:PRO:CD	2.28	0.64
3:C:230:LEU:HD11	4:D:220:TYR:HD1	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:LEU:O	9:I:3:SER:CB	2.44	0.63
4:D:211:MET:HE3	10:J:31:PHE:HE2	1.63	0.63
1:A:279:HIS:HB2	9:I:20:ARG:HH22	1.63	0.63
1:A:408:ARG:NH1	11:K:16:ASN:ND2	2.46	0.63
1:A:271:GLN:NE2	9:I:55:LEU:CD1	2.62	0.63
4:D:90:TYR:C	4:D:92:PRO:HD3	2.19	0.63
2:B:156:GLN:HG2	9:I:27:ARG:HB2	1.79	0.63
4:D:86:LYS:H	4:D:86:LYS:HD2	1.63	0.63
2:B:264:ILE:HG22	9:I:7:ARG:HH12	1.55	0.63
4:D:182:VAL:O	4:D:186:VAL:HG23	1.99	0.63
1:A:363:ASN:O	1:A:367:SER:HB2	1.99	0.63
2:B:258:VAL:HG12	2:B:423:SER:HB2	1.81	0.63
6:F:96:GLU:O	6:F:100:GLU:HG2	1.99	0.63
2:B:298:ALA:CB	2:B:343:GLN:HG2	2.29	0.62
3:C:309:THR:HG21	3:C:367:PRO:O	1.99	0.62
1:A:280:TYR:O	9:I:20:ARG:NH2	2.32	0.62
1:A:80:GLU:HB3	2:B:292:THR:HG21	1.81	0.62
2:B:111:CYS:SG	2:B:119:LEU:HD13	2.39	0.62
1:A:281:ASP:OD2	9:I:47:ARG:HB2	2.00	0.62
3:C:273:TYR:HD2	3:C:274:PHE:HE2	1.47	0.62
1:A:184:GLU:O	1:A:188:ARG:HB2	2.00	0.62
1:A:281:ASP:CG	9:I:47:ARG:CG	2.68	0.62
7:G:37:VAL:O	7:G:41:THR:OG1	2.15	0.62
9:I:56:ARG:HG2	9:I:57:GLY:H	1.63	0.62
1:A:354:VAL:O	1:A:358:LYS:HG3	2.00	0.62
7:G:18:LEU:CD2	7:G:22:GLU:HB3	2.30	0.61
7:G:56:TYR:C	7:G:56:TYR:CD1	2.73	0.61
8:H:66:ASP:HA	8:H:69:VAL:HB	1.82	0.61
2:B:176:LEU:HD23	9:I:11:PHE:HB3	1.80	0.61
3:C:258:PRO:HD2	4:D:115:TYR:OH	2.00	0.61
1:A:143:THR:HG21	9:I:39:GLU:CG	2.24	0.61
9:I:46:LYS:CG	9:I:47:ARG:N	2.56	0.61
3:C:141:TRP:O	3:C:145:VAL:HG13	2.01	0.61
9:I:34:VAL:HB	9:I:35:PRO:CD	2.28	0.61
4:D:234:LYS:HD3	5:E:8:PRO:HB2	1.83	0.61
7:G:65:GLU:O	7:G:69:SER:HB2	2.00	0.61
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.83	0.61
4:D:120:ARG:HG2	4:D:120:ARG:HH11	1.66	0.61
4:D:32:VAL:HG11	4:D:186:VAL:HG22	1.82	0.61
5:E:40:THR:O	5:E:44:THR:HG22	2.00	0.60
1:A:228:VAL:O	1:A:230:THR:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.36	0.60
5:E:68:VAL:O	5:E:68:VAL:CG1	2.49	0.60
1:A:250:LEU:CD1	9:I:44:ASP:C	2.69	0.60
2:B:384:SER:OG	9:I:3:SER:HB2	2.01	0.60
2:B:281:ALA:N	15:B:512:HOH:O	2.34	0.60
2:B:305:GLN:CB	2:B:306:PRO:CD	2.76	0.60
3:C:105:GLY:HA2	3:C:107:TYR:CE1	2.37	0.60
11:K:3:THR:HA	11:K:6:LEU:HG	1.83	0.60
2:B:198:HIS:NE2	15:B:479:HOH:O	2.32	0.60
4:D:12:TRP:CZ2	4:D:125:ASP:HB3	2.37	0.60
7:G:69:SER:O	7:G:73:ASN:HB2	2.02	0.60
10:J:47:ASN:O	10:J:48:GLU:HB2	2.02	0.60
9:I:10:PRO:O	9:I:25:ALA:HB1	2.02	0.59
3:C:268:ILE:O	3:C:268:ILE:HG13	2.01	0.59
1:A:294:LEU:HD13	1:A:337:VAL:HG12	1.84	0.59
1:A:359:ASN:ND2	1:A:362:ARG:HH11	2.01	0.59
4:D:219:VAL:HG12	4:D:219:VAL:O	2.02	0.59
4:D:27:ARG:HH22	10:J:58:LYS:HE2	1.67	0.59
1:A:252:HIS:NE2	9:I:42:VAL:CG1	2.65	0.59
4:D:171:PHE:HB3	4:D:175:THR:HB	1.84	0.59
3:C:211:ILE:O	3:C:212:SER:CB	2.50	0.59
4:D:165:TYR:OH	8:H:14:VAL:O	2.21	0.59
3:C:259:ALA:O	3:C:260:ASN:HB2	2.01	0.59
4:D:158:ILE:HG13	4:D:160:MET:H	1.68	0.59
5:E:12:ASP:HB2	15:E:1703:HOH:O	2.03	0.59
1:A:213:GLN:HG3	15:A:493:HOH:O	2.03	0.59
2:B:211:VAL:HG12	2:B:212:SER:N	2.18	0.59
3:C:361:LEU:HA	3:C:365:LEU:HB2	1.84	0.59
3:C:267:HIS:CG	3:C:268:ILE:H	2.20	0.58
4:D:22:ASP:HB3	4:D:25:SER:HB3	1.83	0.58
1:A:252:HIS:NE2	9:I:42:VAL:HG12	2.18	0.58
4:D:22:ASP:O	4:D:26:ILE:HG13	2.03	0.58
4:D:165:TYR:O	4:D:165:TYR:CD2	2.51	0.58
3:C:267:HIS:CG	3:C:268:ILE:N	2.71	0.58
1:A:279:HIS:HD2	1:A:284:TYR:OH	1.85	0.58
1:A:308:GLN:HG3	9:I:52:ARG:CZ	2.34	0.58
3:C:221:HIS:CD2	3:C:222:PRO:CD	2.87	0.58
1:A:308:GLN:HG3	9:I:52:ARG:NH2	2.17	0.58
2:B:287:ARG:HA	9:I:34:VAL:HG11	1.86	0.58
3:C:56:THR:O	3:C:57:SER:HB2	2.04	0.58
10:J:29:LEU:HG	11:K:48:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASP:CG	9:I:47:ARG:CB	2.73	0.57
3:C:30:TRP:HZ3	3:C:96:MET:HG3	1.69	0.57
5:E:20:ASP:HB3	5:E:23:LYS:HB2	1.86	0.57
10:J:29:LEU:HD13	11:K:34:TRP:CD1	2.35	0.57
4:D:169:LEU:HD23	4:D:171:PHE:CD1	2.39	0.57
1:A:281:ASP:CB	9:I:20:ARG:CD	2.83	0.57
1:A:308:GLN:O	1:A:308:GLN:HG2	2.05	0.57
3:C:319:PRO:HG3	7:G:47:ARG:NH1	2.18	0.57
1:A:279:HIS:CE1	9:I:52:ARG:HB3	2.30	0.57
1:A:341:GLN:HE22	1:A:344:ARG:NH2	1.96	0.57
1:A:250:LEU:HD12	9:I:44:ASP:CA	2.35	0.57
4:D:169:LEU:HD23	4:D:171:PHE:HD1	1.70	0.57
5:E:147:ILE:HD12	5:E:159:PRO:HD3	1.85	0.57
1:A:87:ASN:OD1	1:A:88:ALA:N	2.37	0.57
3:C:337:TRP:CZ3	3:C:350:ILE:HD11	2.40	0.57
4:D:1:SER:O	4:D:2:ASP:HB2	2.04	0.57
1:A:9:GLN:HE21	1:A:9:GLN:HA	1.70	0.57
1:A:280:TYR:CA	9:I:20:ARG:HH21	2.18	0.57
2:B:227:ARG:NH2	2:B:230:LEU:O	2.38	0.57
8:H:69:VAL:O	8:H:73:LEU:HB2	2.05	0.57
9:I:15:LEU:HD13	9:I:16:SER:H	1.70	0.56
1:A:102:LEU:HD23	1:A:104:LYS:HE2	1.87	0.56
2:B:384:SER:HB3	9:I:3:SER:H	1.69	0.56
9:I:47:ARG:CG	9:I:48:SER:N	2.66	0.56
1:A:140:GLU:OE1	9:I:36:ALA:CA	2.52	0.56
1:A:244:ARG:NH2	1:A:246:ASP:OD2	2.32	0.56
1:A:359:ASN:HD22	1:A:362:ARG:HH11	1.53	0.56
1:A:388:ARG:NH2	1:A:394:GLU:OE2	2.38	0.56
3:C:186:PRO:HG3	12:C:381:HEM:HMC2	1.86	0.56
4:D:142:SER:O	4:D:143:LEU:HG	2.05	0.56
10:J:50:LYS:HB2	10:J:52:TRP:H	1.70	0.56
4:D:240:PRO:O	15:D:1424:HOH:O	2.18	0.56
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.88	0.56
3:C:207:ASN:HB2	3:C:208:PRO:HD2	1.87	0.56
3:C:273:TYR:CD2	3:C:274:PHE:HE2	2.23	0.56
9:I:6:ALA:C	9:I:8:SER:N	2.55	0.56
3:C:68:HIS:NE2	5:E:67:ASP:OD1	2.36	0.56
4:D:79:GLU:O	4:D:80:MET:HB2	2.05	0.56
4:D:86:LYS:HD3	4:D:89:ASP:H	1.71	0.56
1:A:332:ASP:H	1:A:430:GLN:NE2	2.04	0.56
2:B:70:ARG:NE	9:I:13:PRO:CB	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:LEU:O	3:C:123:VAL:HG12	2.05	0.56
9:I:9:GLY:H	9:I:26:LEU:HB2	1.70	0.56
2:B:245:ARG:NH2	2:B:433:THR:O	2.36	0.56
5:E:44:THR:HG23	10:J:24:ILE:HD13	1.88	0.56
9:I:49:VAL:HG12	9:I:50:LEU:N	2.19	0.56
5:E:18:VAL:HG12	5:E:18:VAL:O	2.03	0.55
6:F:91:GLU:HG2	15:F:1075:HOH:O	2.06	0.55
1:A:279:HIS:NE2	9:I:52:ARG:O	2.39	0.55
3:C:94:LEU:HD21	3:C:123:VAL:HG11	1.89	0.55
3:C:235:LEU:O	3:C:235:LEU:HG	2.06	0.55
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.88	0.55
1:A:271:GLN:CD	9:I:55:LEU:HD22	2.26	0.55
2:B:248:ASN:C	2:B:248:ASN:HD22	2.09	0.55
1:A:36:THR:O	1:A:199:ALA:HA	2.07	0.55
9:I:41:PRO:HB3	9:I:44:ASP:OD2	2.06	0.55
3:C:137:GLN:HB2	3:C:254:ASP:O	2.07	0.55
3:C:322:GLN:HE21	7:G:47:ARG:HG3	1.71	0.55
5:E:14:ARG:HE	5:E:18:VAL:HG12	1.71	0.55
1:A:285:GLY:N	9:I:16:SER:O	2.36	0.55
2:B:325:TYR:CD2	9:I:28:PRO:CD	2.90	0.55
3:C:228:ASP:OD2	13:C:383:AY1:O2	2.25	0.55
3:C:273:TYR:CD2	3:C:274:PHE:CE2	2.94	0.55
5:E:68:VAL:O	5:E:68:VAL:HG12	2.08	0.55
10:J:55:ILE:O	10:J:57:HIS:N	2.40	0.55
1:A:279:HIS:CE1	9:I:52:ARG:CA	2.90	0.54
1:A:305:GLN:HG3	9:I:46:LYS:C	2.24	0.54
5:E:122:HIS:O	5:E:125:GLU:HG2	2.06	0.54
1:A:364:ALA:HB1	9:I:54:SER:C	2.28	0.54
2:B:109:VAL:HG22	2:B:119:LEU:HD23	1.88	0.54
3:C:197:LEU:HD21	13:C:383:AY1:H9	1.89	0.54
1:A:46:ARG:HH12	1:A:315:ALA:HB3	1.71	0.54
3:C:206:ASN:HD21	3:C:210:GLY:HA2	1.72	0.54
1:A:143:THR:CB	9:I:39:GLU:HG2	2.37	0.54
2:B:90:GLU:HB2	15:B:484:HOH:O	2.07	0.54
2:B:98:VAL:O	9:I:14:VAL:HA	2.07	0.54
4:D:86:LYS:HZ3	4:D:89:ASP:HB2	1.71	0.54
2:B:248:ASN:ND2	2:B:250:ASP:H	2.05	0.54
10:J:50:LYS:HD3	10:J:52:TRP:HB2	1.89	0.54
1:A:267:ASN:HB3	9:I:57:GLY:C	2.28	0.54
3:C:131:TYR:CA	12:C:381:HEM:HAD2	2.36	0.54
3:C:133:LEU:HA	3:C:175:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:105:ASN:H	4:D:105:ASN:ND2	2.04	0.54
9:I:49:VAL:C	9:I:51:CYS:H	2.09	0.54
2:B:385:GLN:NE2	2:B:393:THR:H	1.99	0.54
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.73	0.54
1:A:395:TRP:HE1	9:I:56:ARG:HH21	1.55	0.54
3:C:40:CYS:HB3	3:C:90:PHE:CD2	2.43	0.54
3:C:116:GLY:HA3	12:C:382:HEM:C4C	2.43	0.54
5:E:118:ARG:NH1	5:E:176:ALA:O	2.41	0.54
9:I:10:PRO:O	9:I:25:ALA:CB	2.56	0.54
9:I:52:ARG:O	9:I:53:GLU:HB2	2.08	0.53
1:A:416:TYR:HB3	10:J:15:ARG:HH22	1.74	0.53
15:C:444:HOH:O	6:F:39:GLU:HG3	2.07	0.53
3:C:288:LEU:O	3:C:292:LEU:HB2	2.08	0.53
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.09	0.53
15:B:458:HOH:O	9:I:15:LEU:HD12	2.08	0.53
2:B:248:ASN:HD22	2:B:249:GLY:N	2.07	0.53
7:G:48:VAL:O	7:G:51:PRO:HD2	2.08	0.53
1:A:21:ASN:HB3	1:A:192:ALA:CB	2.38	0.53
1:A:284:TYR:CZ	9:I:20:ARG:NE	2.76	0.53
3:C:24:PRO:C	3:C:26:ASN:N	2.55	0.53
4:D:33:TYR:HA	4:D:37:CYS:SG	2.49	0.53
5:E:139:CYS:HG	5:E:165:TYR:HH	1.57	0.53
1:A:250:LEU:HD12	9:I:43:LEU:O	2.10	0.52
10:J:29:LEU:HD21	11:K:42:LEU:HD21	1.91	0.52
2:B:133:ARG:O	2:B:137:VAL:HG13	2.09	0.52
1:A:42:ASP:O	1:A:194:ARG:NH2	2.42	0.52
2:B:384:SER:HB2	9:I:2:LEU:C	2.29	0.52
15:B:492:HOH:O	9:I:13:PRO:HB3	2.08	0.52
3:C:349:THR:HA	3:C:352:GLN:HE21	1.73	0.52
6:F:35:ASP:OD1	6:F:61:ARG:HD2	2.10	0.52
1:A:281:ASP:OD1	9:I:48:SER:N	2.42	0.52
9:I:28:PRO:O	9:I:29:LEU:HB2	2.08	0.52
1:A:281:ASP:CB	9:I:20:ARG:CG	2.87	0.52
6:F:83:TYR:O	6:F:84:GLU:CG	2.57	0.52
2:B:283:PRO:CA	9:I:31:GLN:HE21	2.23	0.52
8:H:28:GLU:HB3	8:H:29:LYS:HE2	1.91	0.52
2:B:141:GLN:HB2	2:B:142:PRO:HD3	1.91	0.52
3:C:359:PHE:O	3:C:363:LEU:HB2	2.10	0.52
4:D:75:ASN:HB3	4:D:79:GLU:OE1	2.10	0.52
5:E:50:ALA:O	5:E:54:VAL:HG12	2.09	0.52
5:E:113:GLU:OE1	5:E:116:GLN:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ARG:N	1:A:408:ARG:HH21	2.08	0.52
2:B:108:THR:HB	15:B:485:HOH:O	2.09	0.52
3:C:206:ASN:ND2	3:C:207:ASN:H	2.07	0.52
9:I:42:VAL:HG13	9:I:43:LEU:CD2	2.40	0.52
9:I:51:CYS:SG	9:I:52:ARG:N	2.82	0.52
1:A:251:ALA:HB2	1:A:427:PRO:HD2	1.92	0.52
1:A:341:GLN:NE2	1:A:344:ARG:NH2	2.55	0.52
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.90	0.51
15:A:448:HOH:O	9:I:21:GLY:N	2.40	0.51
4:D:132:THR:O	8:H:21:ARG:NH2	2.43	0.51
1:A:344:ARG:O	1:A:348:SER:N	2.40	0.51
2:B:283:PRO:CB	9:I:31:GLN:HE21	2.23	0.51
3:C:196:HIS:CE1	12:C:382:HEM:NC	2.77	0.51
9:I:15:LEU:HD13	9:I:16:SER:N	2.25	0.51
1:A:361:LEU:HD11	9:I:56:ARG:O	2.10	0.51
2:B:70:ARG:CZ	9:I:13:PRO:CG	2.84	0.51
2:B:287:ARG:CG	9:I:34:VAL:HG13	2.29	0.51
4:D:125:ASP:OD2	4:D:126:TYR:N	2.43	0.51
1:A:80:GLU:HB3	2:B:292:THR:CG2	2.41	0.51
1:A:281:ASP:HB2	9:I:20:ARG:HE	1.72	0.51
13:C:383:AY1:O7	13:C:383:AY1:O3	2.28	0.51
1:A:373:THR:HB	1:A:374:PRO:HD3	1.93	0.51
2:B:384:SER:HB3	9:I:3:SER:HA	1.90	0.51
3:C:311:LYS:HD3	3:C:379:TRP:HB3	1.92	0.51
6:F:7:SER:HB2	6:F:10:SER:H	1.76	0.51
11:K:48:ILE:O	11:K:48:ILE:HG22	2.10	0.51
1:A:220:SER:C	1:A:222:THR:H	2.14	0.51
1:A:416:TYR:HB3	10:J:15:ARG:NH2	2.25	0.51
3:C:243:VAL:O	3:C:247:PRO:HG3	2.11	0.51
1:A:252:HIS:CD2	1:A:323:HIS:HE1	2.30	0.51
1:A:359:ASN:ND2	1:A:362:ARG:NH1	2.58	0.50
3:C:265:PRO:HD2	3:C:268:ILE:CG2	2.41	0.50
4:D:21:LEU:HD13	4:D:192:TRP:HB2	1.93	0.50
3:C:277:ALA:HB1	3:C:294:LEU:HD11	1.92	0.50
4:D:47:ALA:HB2	4:D:90:TYR:CD2	2.46	0.50
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.46	0.50
2:B:124:LEU:HD11	2:B:219:VAL:HG13	1.94	0.50
4:D:138:PRO:CG	8:H:58:LEU:HD22	2.36	0.50
7:G:2:ARG:HB2	15:G:95:HOH:O	2.11	0.50
2:B:76:THR:HG22	2:B:82:SER:HB2	1.94	0.50
2:B:176:LEU:CD2	9:I:11:PHE:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:344:GLU:O	3:C:348:ILE:HG13	2.12	0.50
1:A:30:SER:HA	2:B:18:PRO:HG2	1.93	0.50
3:C:11:MET:O	3:C:12:LYS:C	2.49	0.50
3:C:65:SER:O	3:C:68:HIS:HB3	2.12	0.50
3:C:100:ARG:HD2	3:C:100:ARG:C	2.32	0.50
13:C:383:AY1:C8	13:C:383:AY1:H113	2.42	0.50
11:K:39:ARG:NH2	15:K:1093:HOH:O	2.37	0.50
2:B:304:HIS:O	2:B:305:GLN:O	2.30	0.50
5:E:142:LEU:HB2	14:E:197:FES:S2	2.52	0.50
1:A:212:ALA:O	1:A:216:PHE:HB2	2.12	0.50
3:C:55:TYR:CG	3:C:56:THR:N	2.80	0.50
3:C:216:ASP:OD2	4:D:233:ARG:NH2	2.42	0.50
6:F:38:HIS:HB3	15:F:1910:HOH:O	2.11	0.50
10:J:18:SER:CA	11:K:24:TRP:CZ3	2.93	0.50
8:H:24:CYS:C	8:H:26:GLN:H	2.14	0.50
1:A:80:GLU:OE2	2:B:292:THR:HG22	2.12	0.50
1:A:9:GLN:HE21	1:A:9:GLN:CA	2.25	0.49
4:D:184:LYS:HD3	4:D:185:ASP:OD1	2.12	0.49
1:A:281:ASP:OD1	9:I:47:ARG:CA	2.60	0.49
2:B:102:ARG:HG2	15:B:465:HOH:O	2.12	0.49
1:A:305:GLN:HG2	9:I:46:LYS:H	1.77	0.49
3:C:94:LEU:HD21	3:C:123:VAL:CG1	2.42	0.49
3:C:145:VAL:HG11	3:C:268:ILE:CD1	2.42	0.49
4:D:141:VAL:CG1	4:D:142:SER:N	2.74	0.49
6:F:40:ASN:H	6:F:43:VAL:HB	1.77	0.49
3:C:326:TRP:NE1	7:G:48:VAL:HG22	2.27	0.49
4:D:43:MET:HA	4:D:112:ASP:OD1	2.12	0.49
1:A:11:VAL:HG21	1:A:392:LEU:HD12	1.94	0.49
1:A:280:TYR:C	9:I:20:ARG:HH21	2.16	0.49
2:B:129:ALA:N	2:B:130:PRO:CD	2.74	0.49
3:C:378:LYS:HE2	6:F:17:ARG:HD3	1.94	0.49
1:A:172:GLU:O	1:A:176:LYS:N	2.45	0.49
3:C:207:ASN:ND2	3:C:209:THR:H	2.10	0.49
4:D:116:ILE:CG2	4:D:127:VAL:HG21	2.43	0.49
1:A:252:HIS:HD2	1:A:323:HIS:HE1	1.61	0.49
13:C:383:AY1:O2	13:C:383:AY1:O3	2.28	0.49
7:G:2:ARG:CB	15:G:95:HOH:O	2.60	0.49
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.43	0.49
1:A:35:CYS:HA	1:A:372:THR:HG21	1.95	0.49
3:C:145:VAL:HG23	3:C:146:ILE:N	2.28	0.49
3:C:211:ILE:O	3:C:212:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ARG:CA	1:A:408:ARG:HH21	2.26	0.48
2:B:68:LEU:HD22	2:B:140:LEU:HD13	1.93	0.48
3:C:150:LEU:HB2	3:C:161:VAL:HG22	1.94	0.48
6:F:9:SER:O	6:F:12:TRP:HB3	2.13	0.48
6:F:70:MET:HG3	6:F:71:ARG:N	2.28	0.48
8:H:42:GLU:O	8:H:46:SER:N	2.46	0.48
1:A:37:VAL:HG21	1:A:106:LEU:HD11	1.94	0.48
3:C:71:ARG:NH2	15:C:425:HOH:O	2.45	0.48
3:C:130:GLY:C	12:C:381:HEM:HAD2	2.33	0.48
4:D:153:PHE:CG	4:D:158:ILE:HG22	2.48	0.48
2:B:206:LEU:C	2:B:207:ILE:HD12	2.34	0.48
2:B:282:GLY:C	9:I:31:GLN:NE2	2.66	0.48
4:D:163:PRO:HG2	12:D:242:HEM:HMC2	1.95	0.48
2:B:384:SER:HB3	9:I:3:SER:CA	2.36	0.48
3:C:253:PRO:O	3:C:254:ASP:HB2	2.13	0.48
4:D:91:PHE:O	4:D:93:LYS:HG2	2.13	0.48
5:E:52:LYS:HE2	11:K:34:TRP:O	2.12	0.48
1:A:361:LEU:HD21	9:I:56:ARG:H	1.77	0.48
2:B:235:ALA:O	2:B:236:LYS:CB	2.61	0.48
3:C:282:ARG:C	3:C:284:ILE:H	2.17	0.48
2:B:49:LEU:HD23	2:B:127:THR:HG21	1.95	0.48
8:H:47:ARG:O	8:H:49:GLN:N	2.47	0.48
1:A:281:ASP:OD1	9:I:47:ARG:HB2	2.07	0.48
2:B:70:ARG:HE	9:I:13:PRO:CB	2.22	0.48
3:C:113:TRP:HA	12:C:382:HEM:HHD	1.96	0.48
3:C:233:LEU:HD23	4:D:216:LEU:HD23	1.96	0.48
8:H:51:GLU:HG2	8:H:52:GLU:HG2	1.96	0.48
2:B:384:SER:HB2	9:I:3:SER:CA	2.30	0.48
3:C:126:THR:OG1	3:C:185:LEU:HB3	2.13	0.48
9:I:42:VAL:O	9:I:43:LEU:HB2	2.14	0.48
1:A:268:VAL:HG22	9:I:57:GLY:HA3	1.95	0.48
1:A:386:TYR:HE1	9:I:56:ARG:HH12	1.62	0.47
3:C:141:TRP:CH2	3:C:260:ASN:O	2.66	0.47
4:D:54:VAL:HG21	4:D:192:TRP:CE2	2.48	0.47
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.46	0.47
2:B:113:ARG:HG3	2:B:113:ARG:HH11	1.79	0.47
2:B:124:LEU:HD11	2:B:219:VAL:CG1	2.43	0.47
3:C:71:ARG:HG2	4:D:196:PRO:HG2	1.96	0.47
3:C:270:PRO:HB2	3:C:274:PHE:HB2	1.96	0.47
12:C:382:HEM:HHA	12:C:382:HEM:HBD1	1.96	0.47
12:C:382:HEM:HMC2	12:C:382:HEM:CBC	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:64:ARG:NH1	6:F:64:ARG:HG2	2.23	0.47
1:A:361:LEU:HD21	9:I:56:ARG:O	2.14	0.47
3:C:300:ILE:HD11	3:C:363:LEU:HD13	1.96	0.47
6:F:40:ASN:ND2	6:F:40:ASN:C	2.67	0.47
8:H:38:GLU:HA	8:H:41:ASP:HB2	1.96	0.47
1:A:361:LEU:HD23	9:I:55:LEU:HB2	1.97	0.47
4:D:48:TYR:HA	4:D:51:LEU:HD12	1.95	0.47
4:D:137:PRO:HG3	4:D:149:PHE:HB2	1.96	0.47
4:D:10:TYR:O	4:D:12:TRP:CZ3	2.67	0.47
9:I:54:SER:O	9:I:55:LEU:HG	2.13	0.47
1:A:278:GLY:O	1:A:309:THR:HG23	2.14	0.47
1:A:284:TYR:CE1	9:I:19:SER:C	2.87	0.47
1:A:335:MET:CE	1:A:338:LEU:HD23	2.45	0.47
3:C:23:ALA:HA	15:C:436:HOH:O	2.15	0.47
3:C:246:ALA:N	3:C:247:PRO:HD3	2.30	0.47
3:C:263:ASN:O	3:C:264:THR:CB	2.61	0.47
4:D:49:ARG:HA	4:D:52:VAL:HG23	1.95	0.47
4:D:171:PHE:CB	4:D:175:THR:HB	2.45	0.47
8:H:69:VAL:HG13	8:H:73:LEU:HD12	1.97	0.47
10:J:14:PHE:HD1	10:J:20:PHE:CD1	2.33	0.47
3:C:71:ARG:NH1	4:D:193:ALA:O	2.47	0.47
5:E:18:VAL:O	5:E:18:VAL:CG1	2.62	0.47
6:F:81:THR:HG22	15:F:1925:HOH:O	2.14	0.47
1:A:73:ASN:O	1:A:74:ALA:C	2.53	0.47
1:A:272:VAL:O	1:A:276:ILE:HG13	2.15	0.47
1:A:281:ASP:OD2	9:I:47:ARG:CB	2.61	0.47
2:B:232:LEU:HG	2:B:234:GLY:N	2.30	0.47
3:C:369:ALA:O	3:C:373:GLU:HG3	2.15	0.47
1:A:86:LEU:HD13	1:A:99:ILE:HG12	1.96	0.46
4:D:46:VAL:O	4:D:90:TYR:HB3	2.14	0.46
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.97	0.46
2:B:156:GLN:HG2	9:I:27:ARG:CG	2.45	0.46
2:B:211:VAL:CG1	2:B:212:SER:N	2.78	0.46
5:E:44:THR:CG2	10:J:24:ILE:HD13	2.45	0.46
7:G:73:ASN:HA	7:G:74:PRO:HD3	1.79	0.46
3:C:237:LEU:HD13	4:D:212:MET:HG2	1.97	0.46
6:F:40:ASN:HD21	6:F:43:VAL:H	1.61	0.46
9:I:15:LEU:HD22	9:I:15:LEU:HA	1.47	0.46
11:K:11:ARG:HH21	11:K:15:ARG:NH2	2.14	0.46
1:A:364:ALA:CA	9:I:54:SER:HA	2.46	0.46
3:C:171:ASP:O	3:C:172:LYS:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:327:ALA:HA	7:G:51:PRO:HB3	1.97	0.46
1:A:126:GLN:HA	1:A:126:GLN:NE2	2.29	0.46
1:A:57:TYR:HE2	1:A:134:ILE:HG23	1.80	0.46
1:A:386:TYR:HE1	9:I:56:ARG:NH1	2.13	0.46
3:C:107:TYR:OH	3:C:308:HIS:ND1	2.29	0.46
4:D:160:MET:HB2	12:D:242:HEM:C3D	2.51	0.46
8:H:32:LYS:O	8:H:36:ARG:HG3	2.15	0.46
1:A:405:ARG:HA	1:A:408:ARG:HH21	1.80	0.46
4:D:156:GLN:HE21	4:D:156:GLN:HB2	1.54	0.46
3:C:324:LEU:HD13	3:C:365:LEU:HB3	1.97	0.46
2:B:169:ARG:HD2	2:B:238:LYS:HB3	1.97	0.46
1:A:68:LYS:HG2	1:A:119:ASN:HB3	1.98	0.46
2:B:407:ASP:O	2:B:411:ILE:HG13	2.15	0.46
3:C:90:PHE:O	3:C:94:LEU:HB2	2.16	0.46
13:C:383:AY1:C17	13:C:383:AY1:C12	2.94	0.46
7:G:28:HIS:HB3	7:G:31:SER:HB2	1.97	0.46
11:K:11:ARG:O	11:K:15:ARG:HG3	2.16	0.46
1:A:281:ASP:HB3	1:A:284:TYR:CD1	2.51	0.45
3:C:311:LYS:HE2	3:C:311:LYS:HB3	1.79	0.45
4:D:91:PHE:N	4:D:92:PRO:HD3	2.31	0.45
4:D:167:GLU:HG3	4:D:177:ALA:HB3	1.99	0.45
1:A:325:VAL:HG21	9:I:43:LEU:CB	2.43	0.45
2:B:369:LEU:HA	2:B:369:LEU:HD23	1.68	0.45
4:D:169:LEU:O	4:D:170:GLU:HB2	2.17	0.45
4:D:215:LEU:HD23	4:D:215:LEU:HA	1.65	0.45
5:E:15:ARG:HD2	5:E:32:ARG:HG2	1.98	0.45
1:A:66:GLY:O	1:A:121:SER:HB2	2.16	0.45
13:C:383:AY1:O3	13:C:383:AY1:C11	2.65	0.45
7:G:56:TYR:C	7:G:56:TYR:HD1	2.16	0.45
8:H:4:LYS:O	8:H:4:LYS:HG3	2.17	0.45
1:A:252:HIS:NE2	9:I:42:VAL:HG13	2.31	0.45
1:A:280:TYR:CG	1:A:281:ASP:N	2.84	0.45
2:B:145:ARG:NH2	15:B:490:HOH:O	2.49	0.45
3:C:47:THR:HG22	5:E:58:PHE:HZ	1.81	0.45
8:H:51:GLU:CG	8:H:52:GLU:N	2.77	0.45
9:I:46:LYS:CD	9:I:47:ARG:H	2.29	0.45
1:A:37:VAL:HG21	1:A:106:LEU:CD1	2.47	0.45
2:B:169:ARG:HG3	2:B:240:HIS:HB2	1.99	0.45
3:C:83:HIS:CD2	12:C:381:HEM:ND	2.84	0.45
3:C:337:TRP:HZ3	3:C:350:ILE:HD11	1.82	0.45
4:D:237:TYR:CZ	4:D:239:PRO:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:LEU:O	2:B:195:VAL:HG23	2.16	0.45
4:D:166:ASN:H	4:D:166:ASN:ND2	2.10	0.45
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.52	0.45
10:J:38:GLY:O	10:J:42:ILE:HG12	2.16	0.45
1:A:281:ASP:CB	9:I:20:ARG:NE	2.67	0.45
2:B:232:LEU:C	2:B:234:GLY:H	2.20	0.45
2:B:389:ALA:HB1	15:B:516:HOH:O	2.17	0.45
2:B:156:GLN:HG2	9:I:27:ARG:CB	2.44	0.45
2:B:248:ASN:ND2	2:B:250:ASP:N	2.64	0.45
2:B:354:ASN:HB3	2:B:355:PRO:HD3	1.99	0.45
9:I:39:GLU:O	9:I:40:SER:CB	2.64	0.45
11:K:52:PHE:O	11:K:53:LYS:C	2.55	0.45
2:B:108:THR:HG21	15:B:472:HOH:O	2.16	0.45
3:C:145:VAL:HG11	3:C:268:ILE:HD11	1.99	0.45
4:D:60:GLU:OE1	10:J:58:LYS:HG2	2.17	0.45
2:B:207:ILE:HD12	2:B:207:ILE:N	2.33	0.44
2:B:307:PHE:C	2:B:307:PHE:CD2	2.90	0.44
3:C:263:ASN:HB3	3:C:264:THR:H	1.54	0.44
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.53	0.44
4:D:135:CYS:SG	4:D:136:GLU:N	2.90	0.44
9:I:45:LEU:HD23	9:I:45:LEU:HA	1.72	0.44
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.59	0.44
2:B:101:THR:CA	15:B:521:HOH:O	2.65	0.44
3:C:185:LEU:HD23	3:C:185:LEU:HA	1.75	0.44
3:C:373:GLU:HB3	6:F:20:TYR:OH	2.18	0.44
4:D:137:PRO:HA	4:D:138:PRO:HD3	1.82	0.44
6:F:53:ASN:HD22	6:F:53:ASN:H	1.62	0.44
5:E:71:MET:HB3	5:E:92:ARG:HA	1.98	0.44
8:H:69:VAL:CG1	8:H:73:LEU:HD12	2.47	0.44
1:A:241:ILE:HG23	1:A:241:ILE:O	2.18	0.44
1:A:405:ARG:HA	1:A:408:ARG:NH2	2.32	0.44
3:C:309:THR:CG2	3:C:370:GLY:HA3	2.48	0.44
8:H:41:ASP:O	8:H:45:SER:OG	2.36	0.44
1:A:192:ALA:HB3	1:A:193:PRO:HD3	2.00	0.44
2:B:176:LEU:HD12	2:B:176:LEU:HA	1.78	0.44
2:B:276:GLN:HE21	2:B:276:GLN:HB3	1.66	0.44
3:C:44:GLN:HA	3:C:44:GLN:NE2	2.32	0.44
4:D:195:GLU:O	4:D:198:HIS:HB2	2.17	0.44
2:B:281:ALA:HA	2:B:310:SER:HB2	2.00	0.44
4:D:34:LYS:O	4:D:38:SER:OG	2.28	0.44
4:D:195:GLU:OE2	4:D:201:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:63:SER:O	5:E:64:ALA:HB2	2.17	0.44
1:A:135:LEU:HD13	1:A:174:VAL:HG11	2.00	0.43
1:A:220:SER:C	1:A:222:THR:N	2.70	0.43
1:A:250:LEU:CD1	9:I:44:ASP:O	2.66	0.43
3:C:116:GLY:C	12:C:382:HEM:HBC2	2.39	0.43
3:C:237:LEU:HD22	4:D:216:LEU:HD11	2.00	0.43
10:J:14:PHE:HD1	10:J:20:PHE:HD1	1.66	0.43
2:B:264:ILE:HG12	2:B:316:TYR:O	2.18	0.43
4:D:129:SER:O	4:D:133:GLY:N	2.51	0.43
5:E:65:SER:O	5:E:67:ASP:N	2.51	0.43
2:B:29:LEU:HD23	2:B:29:LEU:HA	1.76	0.43
5:E:14:ARG:NE	5:E:18:VAL:HG12	2.33	0.43
1:A:364:ALA:HB1	9:I:55:LEU:N	2.34	0.43
2:B:283:PRO:CD	9:I:31:GLN:NE2	2.81	0.43
3:C:26:ASN:ND2	3:C:208:PRO:HD2	2.33	0.43
4:D:83:ARG:CG	4:D:84:PRO:HD2	2.34	0.43
4:D:211:MET:HE3	10:J:31:PHE:CE2	2.47	0.43
8:H:25:GLU:HG3	8:H:61:PHE:CZ	2.54	0.43
2:B:55:SER:HA	2:B:58:GLU:HG3	2.00	0.43
2:B:385:GLN:HG2	9:I:2:LEU:HG	2.01	0.43
3:C:131:TYR:N	12:C:381:HEM:HAD2	2.34	0.43
3:C:148:ASN:O	3:C:150:LEU:N	2.51	0.43
3:C:294:LEU:O	3:C:297:SER:HB3	2.18	0.43
4:D:190:LEU:HD23	4:D:190:LEU:HA	1.87	0.43
6:F:51:PRO:HD2	6:F:54:LEU:HD12	2.01	0.43
8:H:9:GLU:HG3	8:H:13:LEU:HD12	2.00	0.43
1:A:259:GLY:HA3	15:A:496:HOH:O	2.17	0.43
1:A:227:ALA:C	1:A:229:PRO:HD3	2.39	0.43
2:B:370:MET:O	2:B:373:GLU:HB2	2.19	0.43
2:B:385:GLN:HA	9:I:2:LEU:CG	2.47	0.43
4:D:136:GLU:HA	4:D:137:PRO:HD3	1.86	0.43
1:A:21:ASN:HB3	1:A:192:ALA:HB1	2.01	0.43
2:B:197:ASN:C	2:B:197:ASN:HD22	2.21	0.43
3:C:94:LEU:HG	3:C:120:LEU:HD13	2.00	0.43
9:I:49:VAL:CG1	9:I:50:LEU:H	2.26	0.43
1:A:146:ARG:N	9:I:42:VAL:HG11	2.30	0.43
3:C:157:GLY:O	3:C:161:VAL:HG23	2.19	0.43
1:A:144:SER:O	1:A:145:MET:C	2.57	0.43
6:F:40:ASN:HD22	6:F:43:VAL:H	1.62	0.43
1:A:86:LEU:HB3	2:B:285:VAL:HG13	2.00	0.42
1:A:391:PRO:O	1:A:392:LEU:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:LEU:CD2	9:I:15:LEU:HG	2.49	0.42
2:B:213:HIS:N	2:B:214:PRO:CD	2.82	0.42
3:C:265:PRO:HD2	3:C:268:ILE:HG21	2.01	0.42
3:C:146:ILE:O	3:C:147:THR:C	2.57	0.42
1:A:250:LEU:HD11	9:I:44:ASP:C	2.39	0.42
2:B:384:SER:C	9:I:2:LEU:HB2	2.40	0.42
3:C:21:LEU:HA	3:C:22:PRO:HD3	1.86	0.42
3:C:148:ASN:O	3:C:151:SER:N	2.33	0.42
3:C:272:TRP:CE2	3:C:273:TYR:HD1	2.38	0.42
10:J:50:LYS:H	10:J:50:LYS:HG3	1.19	0.42
1:A:188:ARG:NH1	1:A:224:ASP:OD2	2.52	0.42
2:B:97:SER:HB2	15:B:486:HOH:O	2.19	0.42
2:B:227:ARG:HD2	15:B:499:HOH:O	2.18	0.42
2:B:264:ILE:HG23	2:B:315:SER:OG	2.20	0.42
3:C:57:SER:HB3	3:C:58:ASP:H	1.58	0.42
3:C:207:ASN:CB	3:C:208:PRO:CD	2.93	0.42
3:C:326:TRP:CE2	7:G:48:VAL:HG22	2.55	0.42
8:H:16:PRO:HA	8:H:19:THR:CG2	2.50	0.42
10:J:59:TYR:CE2	10:J:60:GLU:HG3	2.55	0.42
1:A:140:GLU:CD	9:I:36:ALA:CB	2.68	0.42
2:B:40:ASN:HB3	2:B:42:ALA:H	1.84	0.42
2:B:245:ARG:HB3	2:B:430:LEU:CD1	2.50	0.42
3:C:57:SER:O	3:C:58:ASP:C	2.58	0.42
5:E:10:PHE:O	5:E:12:ASP:N	2.52	0.42
7:G:18:LEU:HD23	7:G:19:SER:O	2.19	0.42
1:A:33:PRO:O	1:A:103:SER:HB3	2.19	0.42
1:A:60:GLU:HG2	2:B:287:ARG:NH2	2.33	0.42
2:B:40:ASN:O	2:B:41:TYR:CB	2.64	0.42
4:D:81:PHE:HB2	4:D:82:MET:H	1.68	0.42
6:F:27:ASN:HA	6:F:81:THR:OG1	2.19	0.42
6:F:53:ASN:ND2	6:F:54:LEU:H	2.18	0.42
7:G:47:ARG:H	7:G:47:ARG:HG2	1.77	0.42
9:I:34:VAL:CB	9:I:35:PRO:HD3	2.39	0.42
1:A:52:ASN:HA	1:A:177:LEU:HD21	2.02	0.42
1:A:135:LEU:HD12	1:A:135:LEU:HA	1.76	0.42
2:B:233:SER:C	2:B:235:ALA:H	2.15	0.42
3:C:37:LEU:HD13	12:C:382:HEM:C3B	2.54	0.42
4:D:27:ARG:HH22	10:J:58:LYS:CE	2.30	0.42
4:D:86:LYS:H	4:D:86:LYS:CD	2.26	0.42
11:K:13:LEU:HD23	11:K:13:LEU:HA	1.69	0.42
1:A:308:GLN:HE21	1:A:308:GLN:HB3	1.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ARG:CZ	9:I:13:PRO:CB	2.98	0.42
2:B:212:SER:HB2	2:B:215:VAL:HG23	2.01	0.42
3:C:186:PRO:CG	12:C:381:HEM:HMC2	2.49	0.42
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.87	0.42
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.86	0.42
1:A:271:GLN:HE22	9:I:55:LEU:HD21	1.82	0.42
3:C:114:ASN:N	3:C:114:ASN:HD22	2.18	0.42
3:C:221:HIS:CG	3:C:222:PRO:N	2.88	0.42
6:F:67:ASP:O	6:F:70:MET:HG2	2.20	0.42
3:C:90:PHE:O	3:C:90:PHE:HD1	2.03	0.42
3:C:165:TRP:O	3:C:174:THR:OG1	2.34	0.42
1:A:209:LEU:HD23	1:A:209:LEU:HA	1.86	0.41
1:A:328:HIS:CE1	1:A:329:MET:HG2	2.55	0.41
2:B:180:ASP:HA	2:B:183:ILE:HG13	2.02	0.41
3:C:10:LEU:HA	3:C:10:LEU:HD23	1.77	0.41
3:C:95:TYR:HD1	3:C:95:TYR:HA	1.73	0.41
5:E:18:VAL:HG11	7:G:22:GLU:HG3	2.02	0.41
6:F:63:LYS:HE3	6:F:63:LYS:HB3	1.81	0.41
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.97	0.41
2:B:322:PHE:CG	2:B:323:GLY:N	2.88	0.41
3:C:201:HIS:CE1	15:C:432:HOH:O	2.73	0.41
4:D:17:LEU:HD23	4:D:17:LEU:HA	1.81	0.41
1:A:130:GLU:O	1:A:134:ILE:HG13	2.21	0.41
2:B:113:ARG:HG3	2:B:113:ARG:NH1	2.35	0.41
2:B:378:PHE:O	2:B:382:VAL:HG23	2.20	0.41
3:C:145:VAL:CG2	3:C:146:ILE:N	2.84	0.41
3:C:272:TRP:HA	3:C:275:LEU:HG	2.03	0.41
13:C:383:AY1:C8	13:C:383:AY1:C11	2.99	0.41
2:B:224:LEU:HA	2:B:224:LEU:HD23	1.80	0.41
3:C:80:ARG:C	3:C:80:ARG:HD3	2.41	0.41
3:C:135:TRP:CE3	3:C:175:LEU:HG	2.56	0.41
4:D:145:GLU:HB3	4:D:146:GLY:H	1.46	0.41
6:F:64:ARG:HH11	6:F:64:ARG:CB	2.32	0.41
11:K:9:ARG:HB2	15:K:89:HOH:O	2.20	0.41
3:C:135:TRP:HH2	3:C:170:VAL:HG12	1.85	0.41
7:G:2:ARG:NH1	15:G:84:HOH:O	2.28	0.41
1:A:140:GLU:CD	9:I:37:THR:H	2.18	0.41
2:B:46:ARG:HG2	2:B:379:LEU:HD22	2.03	0.41
2:B:344:VAL:HG11	2:B:417:PHE:CD2	2.55	0.41
8:H:40:CYS:HA	8:H:43:ARG:HB3	2.02	0.41
9:I:34:VAL:CB	9:I:35:PRO:CD	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:29:LEU:HD22	11:K:34:TRP:HB2	2.02	0.41
1:A:29:GLN:CG	1:A:203:LEU:O	2.63	0.41
1:A:279:HIS:NE2	9:I:52:ARG:C	2.73	0.41
1:A:281:ASP:CG	9:I:20:ARG:HG2	2.41	0.41
2:B:70:ARG:CZ	9:I:13:PRO:HB2	2.45	0.41
2:B:368:TYR:O	2:B:369:LEU:C	2.59	0.41
13:C:383:AY1:O1	13:C:383:AY1:H3	2.20	0.41
4:D:26:ILE:HG23	4:D:189:PHE:HA	2.02	0.41
4:D:120:ARG:HG2	4:D:120:ARG:NH1	2.34	0.41
4:D:219:VAL:O	4:D:219:VAL:CG1	2.67	0.41
1:A:106:LEU:N	1:A:107:PRO:CD	2.83	0.41
1:A:118:GLN:HE21	1:A:118:GLN:HB2	1.74	0.41
2:B:292:THR:HG23	2:B:363:LYS:NZ	2.35	0.41
3:C:377:LEU:O	3:C:378:LYS:HB2	2.20	0.41
4:D:96:PRO:HB2	4:D:97:ASN:H	1.62	0.41
1:A:106:LEU:HD22	1:A:203:LEU:HB3	2.02	0.41
1:A:157:ALA:O	1:A:237:THR:N	2.53	0.41
2:B:83:PHE:CZ	2:B:87:ARG:HG3	2.56	0.41
2:B:156:GLN:NE2	9:I:29:LEU:HB2	2.36	0.41
2:B:248:ASN:C	2:B:248:ASN:ND2	2.74	0.41
2:B:325:TYR:HD2	9:I:28:PRO:HG2	1.85	0.41
2:B:365:LYS:HG2	2:B:399:LEU:HG	2.03	0.41
3:C:2:THR:HA	15:C:385:HOH:O	2.21	0.41
3:C:188:ILE:O	3:C:192:ILE:HG12	2.21	0.41
3:C:264:THR:HA	3:C:265:PRO:HD3	1.83	0.41
3:C:264:THR:O	3:C:266:PRO:CD	2.69	0.41
4:D:109:LEU:O	4:D:111:PRO:HD3	2.21	0.41
4:D:117:VAL:CG1	4:D:124:GLU:HG3	2.51	0.41
6:F:11:ARG:O	6:F:15:GLY:N	2.52	0.41
6:F:64:ARG:HH11	6:F:64:ARG:HB3	1.85	0.41
7:G:16:TYR:CD1	7:G:16:TYR:N	2.89	0.41
9:I:47:ARG:O	9:I:48:SER:CB	2.69	0.41
1:A:335:MET:HA	1:A:335:MET:HE3	2.03	0.41
2:B:360:ALA:O	2:B:361:LYS:C	2.58	0.41
3:C:44:GLN:HG3	12:C:381:HEM:C1C	2.56	0.41
2:B:26:PHE:CZ	2:B:391:SER:HA	2.56	0.40
2:B:246:GLU:O	2:B:427:SER:HA	2.21	0.40
3:C:99:GLY:HA2	3:C:102:LEU:HD12	2.03	0.40
3:C:322:GLN:NE2	7:G:47:ARG:HG3	2.36	0.40
4:D:139:THR:O	4:D:141:VAL:HB	2.21	0.40
1:A:390:ILE:HA	1:A:391:PRO:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:VAL:O	2:B:141:GLN:HG2	2.22	0.40
4:D:73:GLY:HA2	4:D:74:PRO:HD3	1.92	0.40
4:D:166:ASN:O	4:D:168:VAL:HG23	2.22	0.40
6:F:40:ASN:O	6:F:41:ASP:C	2.58	0.40
6:F:68:LEU:HA	6:F:71:ARG:NH1	2.35	0.40
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.90	0.40
1:A:381:ARG:HG2	1:A:381:ARG:NH1	2.37	0.40
1:A:389:ARG:O	1:A:391:PRO:HD3	2.22	0.40
4:D:93:LYS:HE2	4:D:93:LYS:HB3	1.73	0.40
4:D:133:GLY:O	4:D:134:TYR:C	2.59	0.40
10:J:33:ARG:O	10:J:37:GLN:HG2	2.22	0.40
2:B:197:ASN:HB2	2:B:229:GLY:HA2	2.04	0.40
3:C:25:SER:HA	3:C:218:ILE:HG12	2.04	0.40
3:C:148:ASN:HA	3:C:161:VAL:HG11	2.03	0.40
4:D:65:ALA:O	4:D:85:GLY:HA3	2.20	0.40
6:F:26:PHE:HB2	6:F:31:LEU:HB2	2.02	0.40
1:A:227:ALA:O	1:A:229:PRO:HD3	2.21	0.40
2:B:178:CYS:SG	2:B:182:ARG:HB2	2.62	0.40
2:B:325:TYR:CD2	9:I:28:PRO:HD2	2.56	0.40
5:E:10:PHE:C	5:E:12:ASP:N	2.74	0.40
6:F:53:ASN:N	6:F:53:ASN:ND2	2.64	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%)	396 (89%)	42 (10%)	6 (1%)	11 22
2	B	421/439 (96%)	389 (92%)	24 (6%)	8 (2%)	8 15
3	C	376/379 (99%)	317 (84%)	37 (10%)	22 (6%)	1 1
4	D	239/241 (99%)	172 (72%)	47 (20%)	20 (8%)	1 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	194/196 (99%)	181 (93%)	9 (5%)	4 (2%)	7	13
6	F	103/110 (94%)	95 (92%)	8 (8%)	0	100	100
7	G	77/81 (95%)	65 (84%)	8 (10%)	4 (5%)	2	2
8	H	74/78 (95%)	58 (78%)	11 (15%)	5 (7%)	1	1
9	I	55/57 (96%)	25 (46%)	17 (31%)	13 (24%)	0	0
10	J	58/62 (94%)	46 (79%)	8 (14%)	4 (7%)	1	1
11	K	51/56 (91%)	41 (80%)	7 (14%)	3 (6%)	1	1
All	All	2092/2145 (98%)	1785 (85%)	218 (10%)	89 (4%)	2	3

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ALA
1	A	225	GLU
2	B	234	GLY
2	B	304	HIS
2	B	305	GLN
3	C	57	SER
3	C	58	ASP
3	C	149	LEU
3	C	172	LYS
3	C	212	SER
3	C	222	PRO
3	C	223	TYR
3	C	254	ASP
3	C	258	PRO
3	C	263	ASN
3	C	264	THR
3	C	267	HIS
3	C	268	ILE
4	D	76	GLU
4	D	87	LEU
4	D	93	LYS
4	D	115	TYR
4	D	116	ILE
4	D	134	TYR
4	D	139	THR
4	D	141	VAL
4	D	143	LEU
4	D	148	TYR

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Mol	Chain	Res	Type
4	D	166	ASN
4	D	170	GLU
7	G	11	ARG
8	H	48	SER
8	H	52	GLU
9	I	3	SER
9	I	29	LEU
9	I	37	THR
9	I	39	GLU
9	I	45	LEU
9	I	48	SER
9	I	53	GLU
9	I	55	LEU
9	I	56	ARG
10	J	48	GLU
1	A	229	PRO
3	C	146	ILE
3	C	260	ASN
3	C	266	PRO
3	C	347	TYR
4	D	54	VAL
4	D	80	MET
4	D	96	PRO
4	D	142	SER
5	E	64	ALA
5	E	66	ALA
5	E	71	MET
8	H	28	GLU
9	I	4	VAL
9	I	8	SER
10	J	56	LYS
10	J	60	GLU
11	K	48	ILE
2	B	235	ALA
3	C	147	THR
4	D	2	ASP
4	D	167	GLU
7	G	27	PRO
8	H	14	VAL
10	J	3	PRO
1	A	262	TRP
3	C	257	THR

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Mol	Chain	Res	Type
3	C	346	PRO
5	E	68	VAL
8	H	50	THR
9	I	51	CYS
11	K	40	LEU
2	B	236	LYS
3	C	345	HIS
4	D	104	ALA
7	G	75	ALA
9	I	40	SER
11	K	2	LEU
1	A	286	GLY
7	G	74	PRO
2	B	228	GLY
3	C	221	HIS
4	D	94	PRO
2	B	19	PRO
1	A	260	PRO
2	B	231	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	370/370 (100%)	324 (88%)	46 (12%)	4 8
2	B	332/343 (97%)	291 (88%)	41 (12%)	4 9
3	C	326/327 (100%)	286 (88%)	40 (12%)	4 9
4	D	206/206 (100%)	172 (84%)	34 (16%)	2 3
5	E	168/168 (100%)	158 (94%)	10 (6%)	19 39
6	F	96/98 (98%)	81 (84%)	15 (16%)	2 4
7	G	68/71 (96%)	53 (78%)	15 (22%)	1 1
8	H	73/74 (99%)	62 (85%)	11 (15%)	3 4
9	I	44/44 (100%)	33 (75%)	11 (25%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	50/52 (96%)	45 (90%)	5 (10%)	7 14
11	K	43/46 (94%)	31 (72%)	12 (28%)	0 1
All	All	1776/1799 (99%)	1536 (86%)	240 (14%)	4 6

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	9	GLN
1	A	14	THR
1	A	21	ASN
1	A	23	LEU
1	A	53	ASN
1	A	58	PHE
1	A	69	ASN
1	A	103	SER
1	A	112	LEU
1	A	113	LEU
1	A	123	GLU
1	A	132	ASP
1	A	135	LEU
1	A	137	GLU
1	A	149	VAL
1	A	153	LEU
1	A	163	LEU
1	A	171	SER
1	A	186	LEU
1	A	188	ARG
1	A	203	LEU
1	A	206	ARG
1	A	208	LEU
1	A	209	LEU
1	A	222	THR
1	A	230	THR
1	A	235	ARG
1	A	245	GLU
1	A	248	LEU
1	A	257	VAL
1	A	274	ASN
1	A	300	THR
1	A	308	GLN

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Mol	Chain	Res	Type
1	A	312	ILE
1	A	355	LEU
1	A	361	LEU
1	A	367	SER
1	A	369	LEU
1	A	377	GLU
1	A	381	ARG
1	A	389	ARG
1	A	398	ARG
1	A	405	ARG
1	A	430	GLN
1	A	436	ARG
2	B	24	LEU
2	B	27	THR
2	B	33	LEU
2	B	38	LEU
2	B	40	ASN
2	B	56	ARG
2	B	68	LEU
2	B	69	LEU
2	B	98	VAL
2	B	109	VAL
2	B	110	GLU
2	B	113	ARG
2	B	140	LEU
2	B	154	ASN
2	B	163	LEU
2	B	186	VAL
2	B	189	VAL
2	B	197	ASN
2	B	226	ILE
2	B	230	LEU
2	B	233	SER
2	B	238	LYS
2	B	248	ASN
2	B	251	SER
2	B	257	LEU
2	B	258	VAL
2	B	264	ILE
2	B	273	SER
2	B	284	HIS
2	B	294	SER

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Mol	Chain	Res	Type
2	B	301	LYS
2	B	304	HIS
2	B	305	GLN
2	B	309	VAL
2	B	329	GLN
2	B	343	GLN
2	B	346	THR
2	B	347	ILE
2	B	396	SER
2	B	397	THR
2	B	424	MET
3	C	4	ILE
3	C	43	LEU
3	C	45	ILE
3	C	58	ASP
3	C	64	SER
3	C	67	THR
3	C	78	ILE
3	C	80	ARG
3	C	96	MET
3	C	102	LEU
3	C	126	THR
3	C	138	MET
3	C	172	LYS
3	C	175	LEU
3	C	183	PHE
3	C	197	LEU
3	C	205	SER
3	C	215	VAL
3	C	222	PRO
3	C	230	LEU
3	C	241	LEU
3	C	263	ASN
3	C	265	PRO
3	C	267	HIS
3	C	268	ILE
3	C	269	LYS
3	C	273	TYR
3	C	274	PHE
3	C	281	LEU
3	C	296	PHE
3	C	304	ILE

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Mol	Chain	Res	Type
3	C	316	MET
3	C	320	LEU
3	C	328	LEU
3	C	349	THR
3	C	350	ILE
3	C	352	GLN
3	C	360	LEU
3	C	366	MET
3	C	379	TRP
4	D	2	ASP
4	D	4	GLU
4	D	17	LEU
4	D	18	LEU
4	D	24	THR
4	D	37	CYS
4	D	55	CYS
4	D	58	GLU
4	D	68	VAL
4	D	70	VAL
4	D	86	LYS
4	D	93	LYS
4	D	99	GLU
4	D	105	ASN
4	D	129	SER
4	D	132	THR
4	D	135	CYS
4	D	141	VAL
4	D	144	ARG
4	D	145	GLU
4	D	156	GLN
4	D	158	ILE
4	D	164	ILE
4	D	165	TYR
4	D	166	ASN
4	D	170	GLU
4	D	173	ASP
4	D	179	MET
4	D	180	SER
4	D	182	VAL
4	D	210	LEU
4	D	212	MET
4	D	218	LEU

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Mol	Chain	Res	Type
4	D	223	LYS
5	E	12	ASP
5	E	25	SER
5	E	52	LYS
5	E	60	SER
5	E	61	SER
5	E	63	SER
5	E	67	ASP
5	E	71	MET
5	E	113	GLU
5	E	188	THR
6	F	10	SER
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	70	MET
6	F	72	GLN
6	F	73	GLN
6	F	81	THR
6	F	87	LYS
6	F	88	SER
6	F	94	LEU
6	F	95	LYS
7	G	2	ARG
7	G	11	ARG
7	G	13	VAL
7	G	17	SER
7	G	31	SER
7	G	32	LYS
7	G	37	VAL
7	G	44	CYS
7	G	45	ILE
7	G	47	ARG
7	G	53	VAL
7	G	56	TYR
7	G	68	LYS
7	G	71	ARG
7	G	77	TYR
8	H	5	GLU

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Mol	Chain	Res	Type
8	H	9	GLU
8	H	11	GLU
8	H	14	VAL
8	H	19	THR
8	H	24	CYS
8	H	26	GLN
8	H	27	LEU
8	H	29	LYS
8	H	50	THR
8	H	72	LYS
9	I	8	SER
9	I	11	PHE
9	I	15	LEU
9	I	16	SER
9	I	18	THR
9	I	19	SER
9	I	26	LEU
9	I	27	ARG
9	I	46	LYS
9	I	47	ARG
9	I	52	ARG
10	J	9	LEU
10	J	24	ILE
10	J	29	LEU
10	J	50	LYS
10	J	51	LEU
11	K	13	LEU
11	K	20	THR
11	K	23	LEU
11	K	24	TRP
11	K	37	ASP
11	K	38	TRP
11	K	39	ARG
11	K	40	LEU
11	K	41	ILE
11	K	44	TRP
11	K	52	PHE
11	K	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	15	GLN
1	A	21	ASN
1	A	32	GLN
1	A	73	ASN
1	A	85	HIS
1	A	119	ASN
1	A	126	GLN
1	A	173	ASN
1	A	189	HIS
1	A	252	HIS
1	A	271	GLN
1	A	274	ASN
1	A	279	HIS
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	104	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	290	ASN
2	B	329	GLN
2	B	342	ASN
2	B	362	ASN
2	B	385	GLN
3	C	44	GLN
3	C	114	ASN
3	C	206	ASN
3	C	207	ASN
3	C	221	HIS
3	C	322	GLN
3	C	341	GLN
3	C	352	GLN

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Mol	Chain	Res	Type
4	D	105	ASN
4	D	156	GLN
4	D	166	ASN
5	E	53	ASN
5	E	57	GLN
6	F	40	ASN
6	F	53	ASN
6	F	72	GLN
8	H	23	GLN
8	H	49	GLN
8	H	63	HIS
9	I	31	GLN
11	K	12	GLN
11	K	16	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FES	E	197	5	0,4,4	-	-	-		
12	HEM	C	382	3	41,50,50	2.94	18 (43%)	45,82,82	2.48	11 (24%)
12	HEM	D	242	4	41,50,50	3.08	20 (48%)	45,82,82	2.70	17 (37%)
13	AY1	C	383	-	39,39,39	2.20	10 (25%)	35,53,53	2.43	11 (31%)
12	HEM	C	381	3	41,50,50	3.00	20 (48%)	45,82,82	2.88	20 (44%)

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	197	5	-	-	0/1/1/1
12	HEM	C	382	3	-	4/12/54/54	-
12	HEM	D	242	4	-	4/12/54/54	-
13	AY1	C	383	-	-	4/38/53/53	0/1/2/2
12	HEM	C	381	3	-	8/12/54/54	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	C4D-C3D	-7.75	1.31	1.45
12	D	242	HEM	C4D-C3D	-7.40	1.32	1.45
13	C	383	AY1	C1-N1	6.56	1.43	1.34
12	C	382	HEM	C4D-C3D	-6.54	1.33	1.45
12	D	242	HEM	C1D-C2D	-6.48	1.32	1.44
12	D	242	HEM	C1B-C2B	-6.33	1.32	1.44
13	C	383	AY1	O2-C7	-6.17	1.22	1.37
12	C	382	HEM	C3C-C2C	-5.97	1.32	1.40
12	C	381	HEM	C3C-C2C	-5.76	1.32	1.40
12	D	242	HEM	C3C-C2C	-5.68	1.32	1.40
12	C	381	HEM	C1D-C2D	-5.67	1.33	1.44
12	C	382	HEM	C1D-C2D	-5.62	1.33	1.44
12	C	382	HEM	C1B-C2B	-5.59	1.33	1.44
12	C	382	HEM	C3B-C4B	-5.56	1.33	1.44
12	C	382	HEM	CHA-C4D	5.51	1.49	1.35
12	C	381	HEM	C3B-C4B	-5.39	1.34	1.44
12	D	242	HEM	C3B-C4B	-5.39	1.34	1.44
12	C	381	HEM	C1B-C2B	-5.18	1.34	1.44
12	D	242	HEM	CHB-C1B	5.07	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	CHA-C4D	5.04	1.47	1.35
12	C	382	HEM	CHB-C1B	4.96	1.47	1.35
12	D	242	HEM	CHA-C4D	4.95	1.47	1.35
12	D	242	HEM	CBB-CAB	4.73	1.53	1.30
13	C	383	AY1	C14-C15	4.52	1.62	1.52
12	C	381	HEM	CHB-C1B	4.52	1.46	1.35
12	C	381	HEM	CBB-CAB	4.50	1.52	1.30
12	C	382	HEM	CBB-CAB	4.45	1.52	1.30
13	C	383	AY1	O8-C24	4.05	1.43	1.34
12	C	381	HEM	C2C-C1C	-4.02	1.33	1.42
12	C	382	HEM	C2C-C1C	-4.00	1.33	1.42
12	D	242	HEM	C2C-C1C	-3.89	1.33	1.42
13	C	383	AY1	O6-C15	3.72	1.52	1.46
12	C	381	HEM	CBC-CAC	3.68	1.53	1.29
12	D	242	HEM	CBC-CAC	3.65	1.53	1.29
12	C	382	HEM	CBC-CAC	3.49	1.52	1.29
12	D	242	HEM	C2A-C3A	3.38	1.47	1.37
13	C	383	AY1	C2-N1	-3.33	1.36	1.41
12	C	381	HEM	C2A-C3A	3.32	1.47	1.37
12	C	382	HEM	C4A-CHB	3.24	1.50	1.41
12	C	381	HEM	C4B-NB	3.24	1.45	1.38
12	C	381	HEM	CHC-C4B	3.19	1.50	1.41
12	C	382	HEM	O2D-CGD	-3.06	1.20	1.30
12	D	242	HEM	C4A-CHB	3.01	1.49	1.41
12	C	382	HEM	O2A-CGA	-2.99	1.20	1.30
13	C	383	AY1	O8-C14	2.97	1.49	1.44
12	C	382	HEM	CHC-C4B	2.89	1.49	1.41
12	C	381	HEM	C1A-CHA	2.88	1.49	1.41
12	D	242	HEM	C1A-CHA	2.86	1.48	1.41
12	D	242	HEM	CHC-C4B	2.82	1.49	1.41
12	C	382	HEM	CHD-C1D	2.79	1.49	1.41
12	D	242	HEM	C3D-C2D	-2.64	1.31	1.36
12	C	382	HEM	C2A-C3A	2.64	1.45	1.37
12	C	381	HEM	C4A-CHB	2.58	1.48	1.41
12	C	381	HEM	CHD-C1D	2.58	1.48	1.41
12	C	381	HEM	C3D-C2D	-2.57	1.31	1.36
12	D	242	HEM	CHD-C1D	2.50	1.48	1.41
12	D	242	HEM	O2D-CGD	-2.49	1.22	1.30
13	C	383	AY1	C10-C9	2.48	1.59	1.53
12	C	381	HEM	C3B-C2B	-2.48	1.32	1.37
12	D	242	HEM	O2A-CGA	-2.47	1.22	1.30
12	D	242	HEM	C3B-C2B	-2.46	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	382	HEM	C1A-CHA	2.40	1.47	1.41
12	C	382	HEM	CAB-C3B	2.31	1.53	1.47
13	C	383	AY1	C6-C7	2.31	1.45	1.41
12	C	381	HEM	O2A-CGA	-2.28	1.23	1.30
13	C	383	AY1	O4-C12	2.19	1.39	1.34
12	D	242	HEM	C3C-CAC	2.18	1.52	1.47
12	C	381	HEM	O2D-CGD	-2.14	1.23	1.30

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	382	HEM	C4C-CHD-C1D	-9.85	109.56	122.56
12	C	381	HEM	C4B-CHC-C1C	-8.27	111.64	122.56
12	C	381	HEM	C4C-CHD-C1D	-7.67	112.43	122.56
12	D	242	HEM	C4C-CHD-C1D	-7.50	112.66	122.56
12	D	242	HEM	C4B-CHC-C1C	-7.30	112.92	122.56
12	C	382	HEM	C4B-CHC-C1C	-7.06	113.24	122.56
13	C	383	AY1	C14-O8-C24	-5.99	107.50	117.78
12	C	381	HEM	C4D-ND-C1D	-5.50	99.40	105.07
13	C	383	AY1	O1-C1-N1	-5.49	118.79	125.80
12	D	242	HEM	C4D-ND-C1D	-5.12	99.79	105.07
12	C	381	HEM	C2C-C3C-C4C	4.97	110.37	106.90
12	C	381	HEM	C1B-NB-C4B	-4.72	100.20	105.07
12	C	381	HEM	C4B-C3B-C2B	4.56	110.74	107.11
13	C	383	AY1	O8-C24-C25	4.55	119.88	111.19
13	C	383	AY1	O8-C14-C15	-4.49	98.54	107.47
12	D	242	HEM	CAD-CBD-CGD	-4.46	104.00	113.60
12	C	381	HEM	CHC-C4B-NB	4.33	129.13	124.43
13	C	383	AY1	C3-C2-N1	4.23	128.96	122.59
12	C	381	HEM	CBB-CAB-C3B	-4.15	106.97	127.62
12	D	242	HEM	CHB-C1B-NB	4.13	129.49	124.38
12	D	242	HEM	C3B-C2B-C1B	4.09	109.52	106.49
12	D	242	HEM	CHD-C1D-ND	3.79	128.55	124.43
12	D	242	HEM	C1B-NB-C4B	-3.77	101.18	105.07
12	C	382	HEM	C3B-C2B-C1B	3.69	109.22	106.49
12	C	382	HEM	C2C-C3C-C4C	3.64	109.44	106.90
12	C	382	HEM	C1B-NB-C4B	-3.56	101.39	105.07
13	C	383	AY1	C9-N2-C8	3.49	127.83	121.52
12	D	242	HEM	CHC-C4B-NB	3.43	128.16	124.43
13	C	383	AY1	O3-C8-C6	-3.40	114.80	121.01
13	C	383	AY1	C6-C8-N2	3.34	122.99	116.80
12	D	242	HEM	C2C-C3C-C4C	3.30	109.20	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	382	HEM	CHA-C4D-ND	3.30	128.45	124.38
12	D	242	HEM	CHA-C4D-ND	3.24	128.39	124.38
12	C	381	HEM	CHB-C1B-NB	3.24	128.38	124.38
13	C	383	AY1	O8-C24-O9	-3.22	117.93	123.94
12	C	381	HEM	CHA-C4D-ND	3.20	128.34	124.38
12	C	381	HEM	CHA-C4D-C3D	-3.00	119.70	125.33
13	C	383	AY1	C5-C6-C8	2.97	126.38	118.43
12	C	381	HEM	CHD-C1D-ND	2.89	127.57	124.43
12	D	242	HEM	CHD-C1D-C2D	-2.82	120.58	124.98
12	C	382	HEM	CBB-CAB-C3B	-2.74	113.98	127.62
12	D	242	HEM	CBB-CAB-C3B	-2.69	114.23	127.62
12	C	382	HEM	CHD-C1D-ND	2.67	127.33	124.43
12	C	382	HEM	CHB-C1B-NB	2.58	127.57	124.38
12	C	382	HEM	CBA-CAA-C2A	-2.56	108.25	112.62
13	C	383	AY1	C3-C2-C7	-2.52	118.15	119.79
12	D	242	HEM	C4B-C3B-C2B	2.51	109.11	107.11
12	D	242	HEM	CHA-C4D-C3D	-2.47	120.68	125.33
12	C	381	HEM	O2D-CGD-CBD	2.44	121.87	114.03
12	D	242	HEM	CHB-C1B-C2B	-2.43	119.99	126.72
12	C	381	HEM	CHD-C1D-C2D	-2.43	121.18	124.98
12	D	242	HEM	C1D-C2D-C3D	2.43	109.51	106.96
12	C	381	HEM	C4A-C3A-C2A	-2.42	105.31	107.00
12	C	381	HEM	C3B-C2B-C1B	2.39	108.26	106.49
12	C	381	HEM	CHB-C1B-C2B	-2.38	120.13	126.72
12	C	382	HEM	CHC-C4B-NB	2.34	126.98	124.43
12	C	381	HEM	CBA-CAA-C2A	-2.29	108.71	112.62
12	C	381	HEM	CAA-CBA-CGA	-2.08	107.92	113.76
12	C	381	HEM	CHC-C4B-C3B	-2.08	121.39	124.57

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	381	HEM	C2B-C3B-CAB-CBB
12	C	381	HEM	C4B-C3B-CAB-CBB
13	C	383	AY1	C9-C10-O4-C12
12	C	381	HEM	C2A-CAA-CBA-CGA
13	C	383	AY1	C19-C20-C21-C22
13	C	383	AY1	C18-C19-C20-C21
12	C	381	HEM	C3D-CAD-CBD-CGD
13	C	383	AY1	C20-C21-C22-C23
12	C	381	HEM	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
12	C	382	HEM	C2B-C3B-CAB-CBB
12	C	381	HEM	C2D-C3D-CAD-CBD
12	D	242	HEM	C1A-C2A-CAA-CBA
12	D	242	HEM	C3A-C2A-CAA-CBA
12	C	381	HEM	CAD-CBD-CGD-O1D
12	D	242	HEM	CAD-CBD-CGD-O1D
12	D	242	HEM	CAD-CBD-CGD-O2D
12	C	381	HEM	CAD-CBD-CGD-O2D
12	C	382	HEM	CAA-CBA-CGA-O2A
12	C	382	HEM	C4B-C3B-CAB-CBB
12	C	382	HEM	CAA-CBA-CGA-O1A

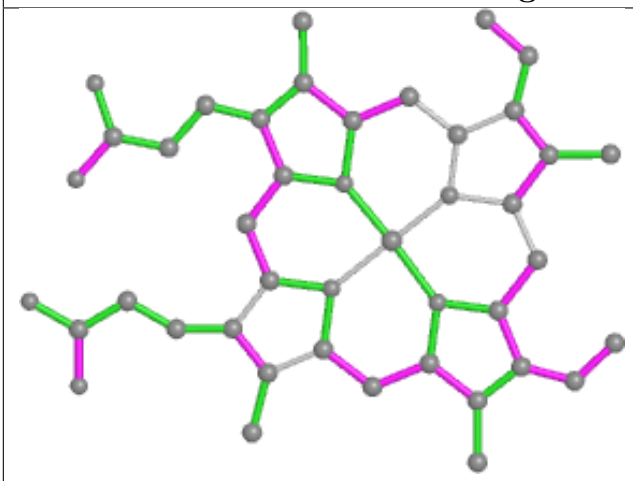
There are no ring outliers.

5 monomers are involved in 35 short contacts:

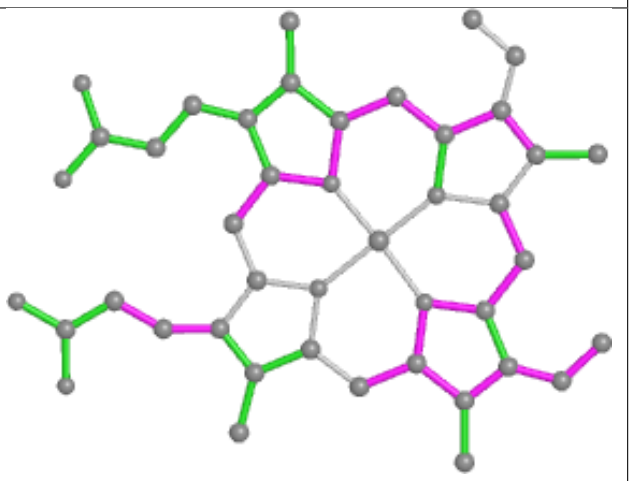
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	E	197	FES	1	0
12	C	382	HEM	7	0
12	D	242	HEM	6	0
13	C	383	AY1	12	0
12	C	381	HEM	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

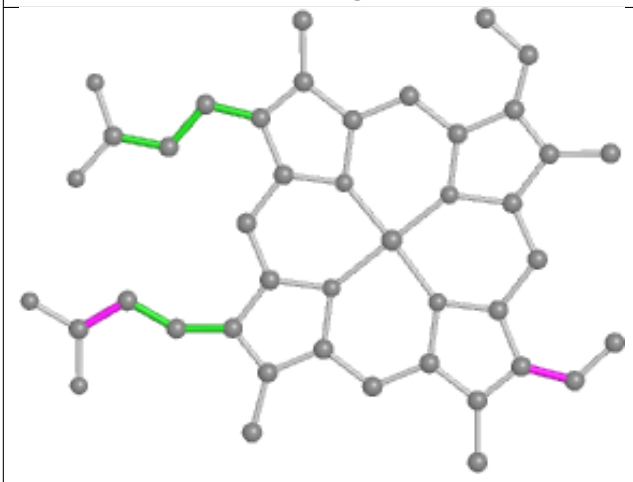
Ligand HEM C 382



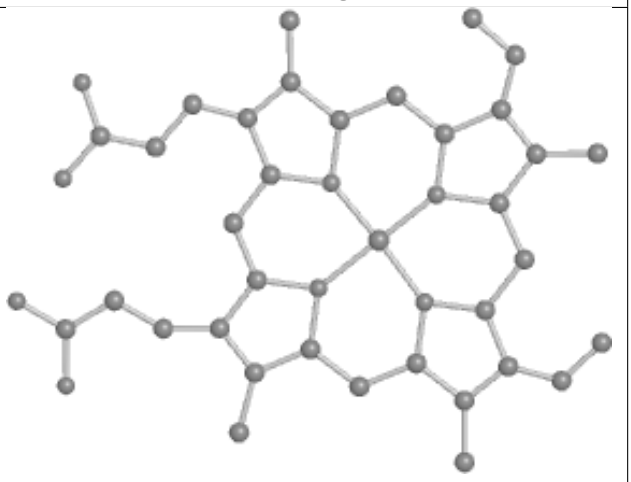
Bond lengths



Bond angles

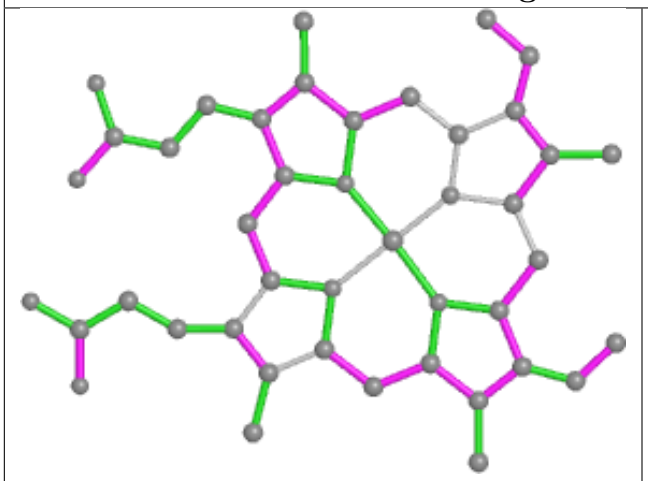


Torsions

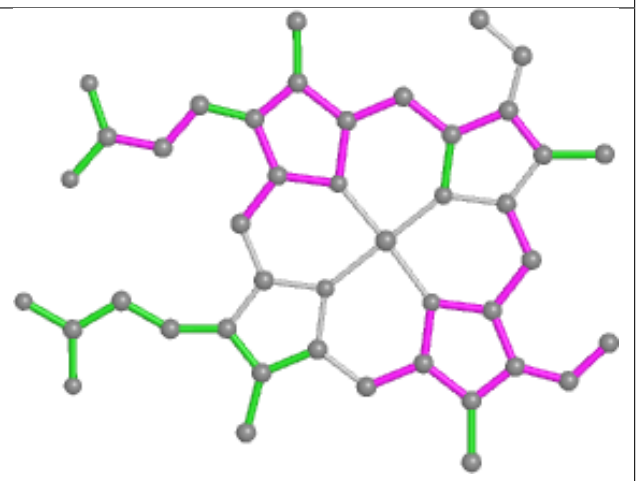


Rings

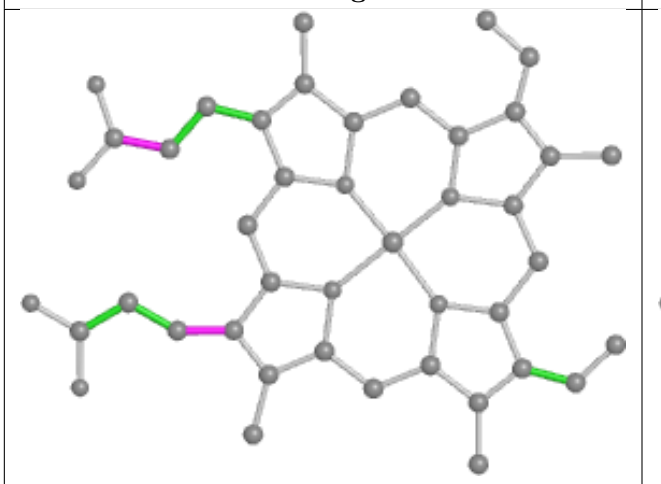
Ligand HEM D 242



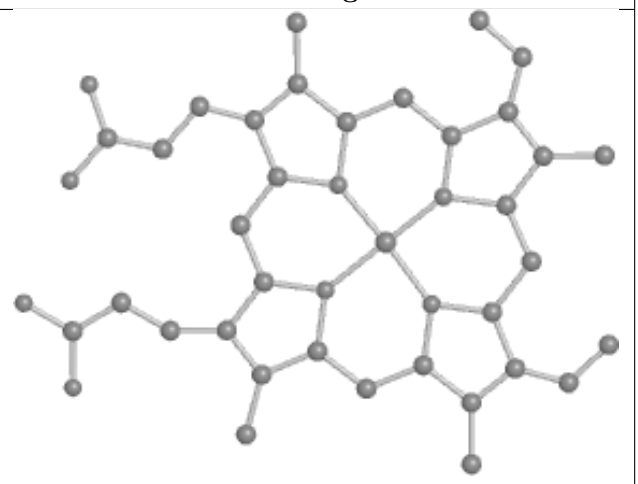
Bond lengths



Bond angles

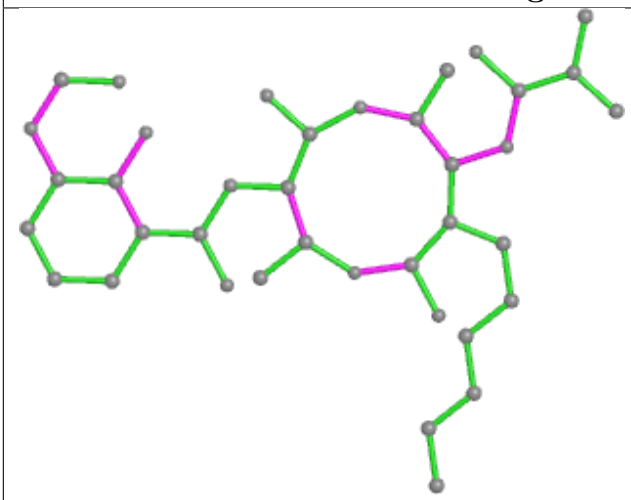


Torsions

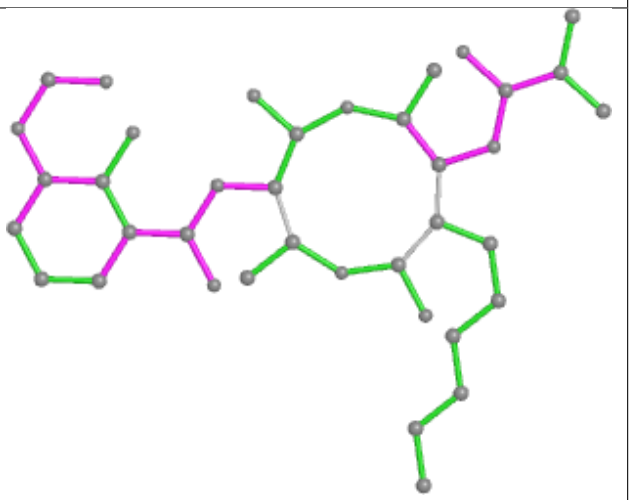


Rings

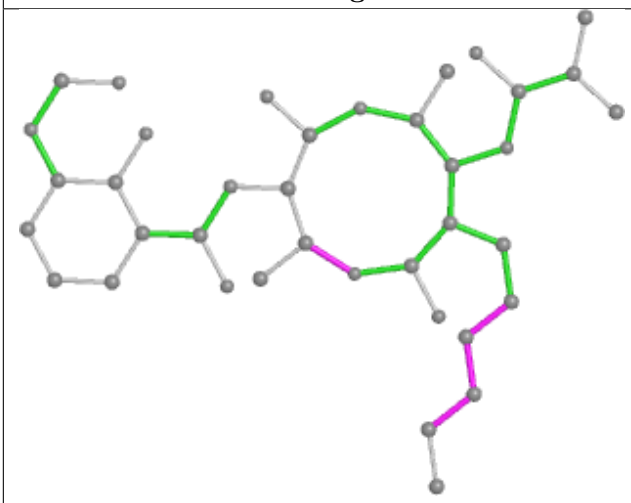
Ligand AY1 C 383



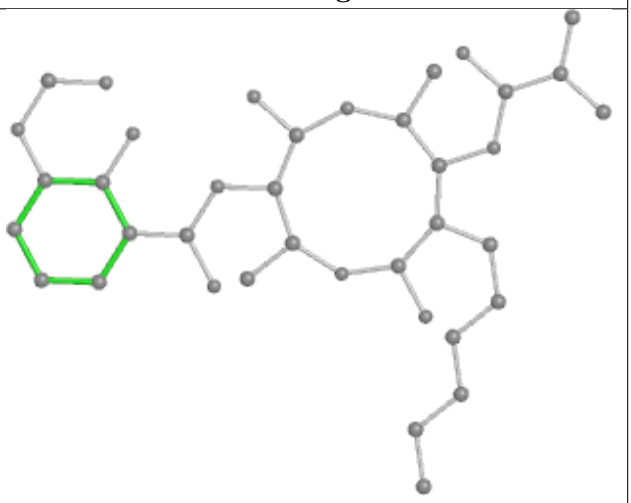
Bond lengths



Bond angles

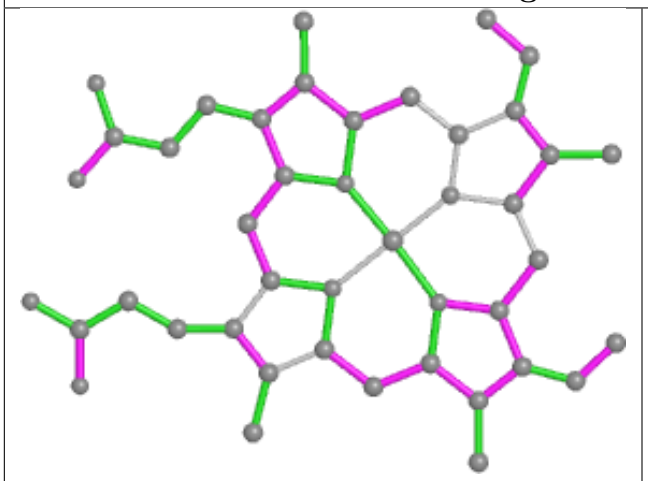


Torsions

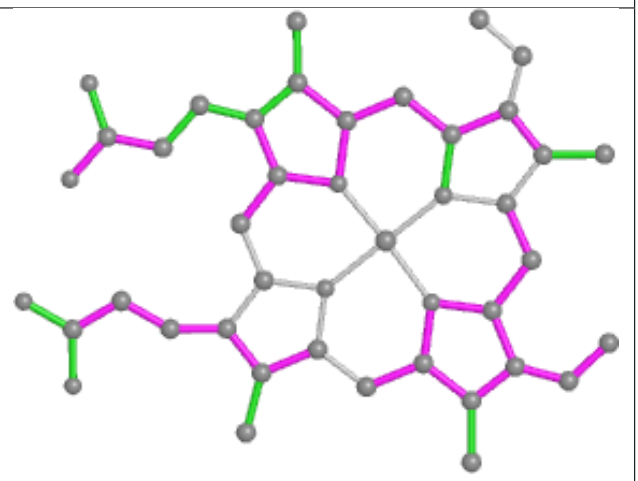


Rings

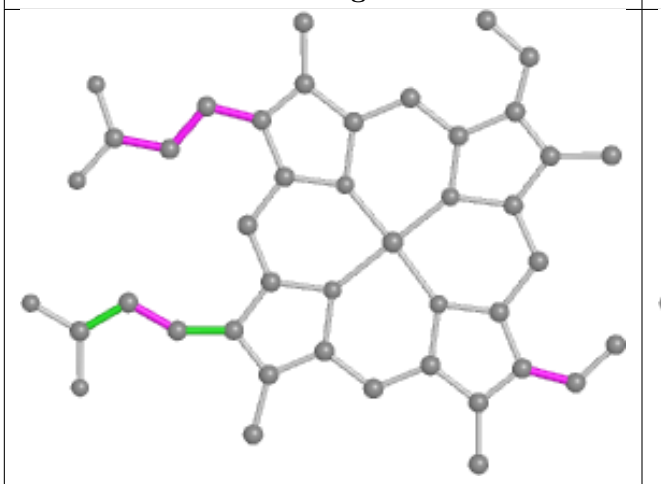
Ligand HEM C 381



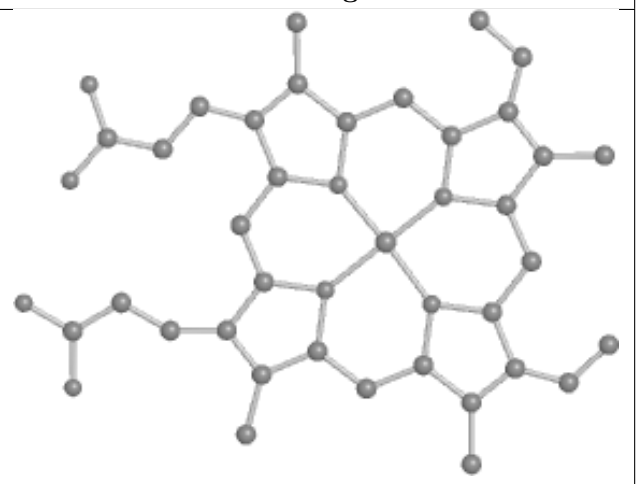
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.