



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:53 PM UTC

PDB ID : 1NTM / pdb_00001ntm
Title : Crystal Structure of Mitochondrial Cytochrome bc1 Complex at 2.4 Angstrom
Authors : Gao, X.; Wen, X.; Esser, L.; Quinn, B.; Yu, L.; Yu, C.; Xia, D.
Deposited on : 2003-01-30
Resolution : 2.40 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

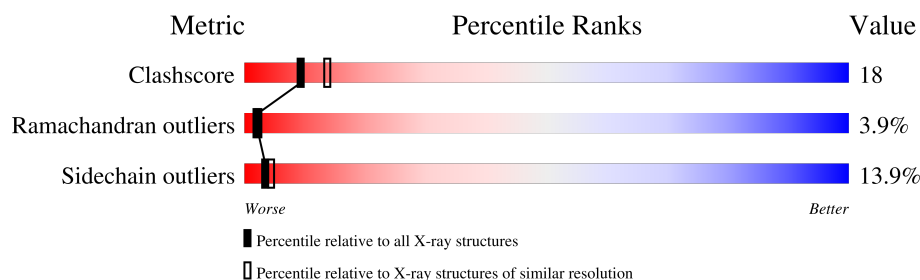
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	64% 28% 7%
2	B	439	61% 29% 5% . .
3	C	379	60% 31% 8% .
4	D	241	37% 43% 17% .
5	E	196	69% 24% . .
6	F	110	65% 21% 8% . 5%
7	G	81	62% 22% 6% . 7%
8	H	78	56% 22% 6% . 14%

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Mol	Chain	Length	Quality of chain
9	I	57	16% 44% 35% 5%
10	J	62	53% 31% 13%
11	K	56	59% 21% 9% • 9%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 17049 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
1	A	446	Total	C	N	O	S	0	0	0
			3458	2161	609	668	20			

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

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

- Molecule 3 is a protein called Cytochrome b.

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

- Molecule 4 is a protein called cytochrome c1.

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

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

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

- 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	67	Total	C	N	O	S	0	0	0
			548	332	99	112	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	60	Total	C	N	O	S	0	0	0
			478	313	81	84				

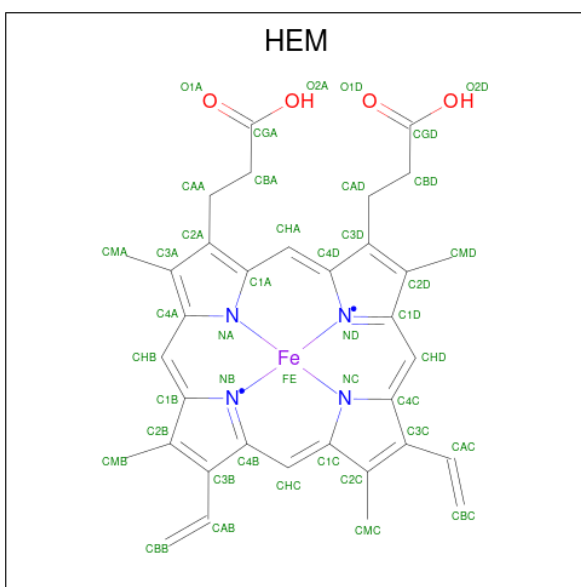
- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase complex 6.4 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	51	Total	C	N	O	S	0	0	0
			421	280	76	64	1			

There is a discrepancy between the modelled and reference sequences:

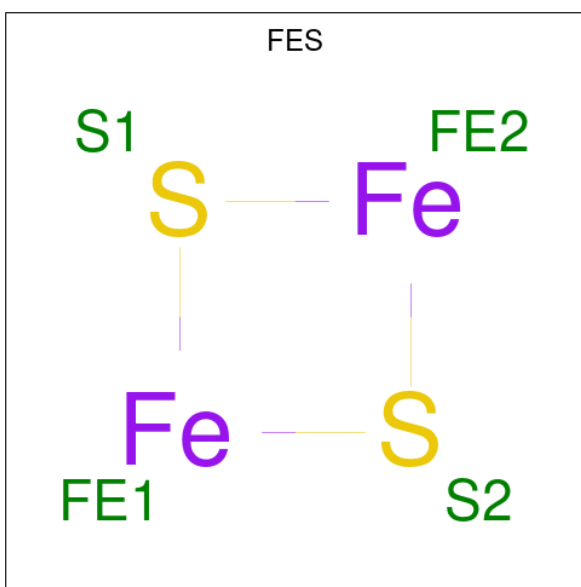
Chain	Residue	Modelled	Actual	Comment	Reference
K	22	GLN	SER	SEE REMARK 999	UNP P07552

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 14 is water.

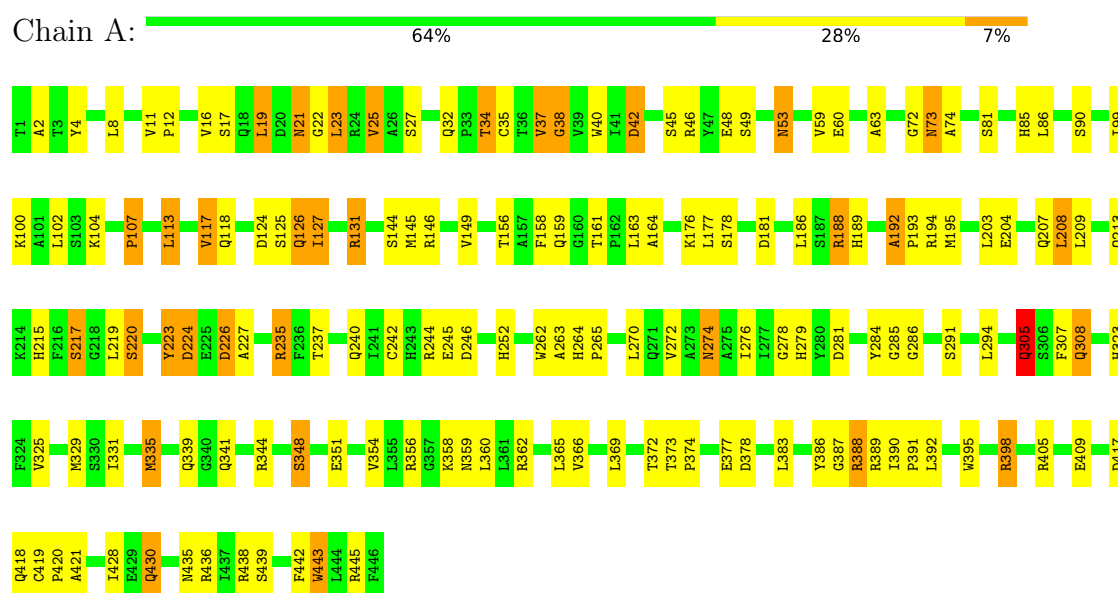
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	99	Total 99	O 99	0	0
14	B	152	Total 152	O 152	0	0
14	C	64	Total 64	O 64	0	0
14	D	43	Total 43	O 43	0	0
14	E	8	Total 8	O 8	0	0
14	F	37	Total 37	O 37	0	0
14	G	23	Total 23	O 23	0	0
14	H	7	Total 7	O 7	0	0
14	I	5	Total 5	O 5	0	0
14	J	6	Total 6	O 6	0	0
14	K	10	Total 10	O 10	0	0

3 Residue-property plots

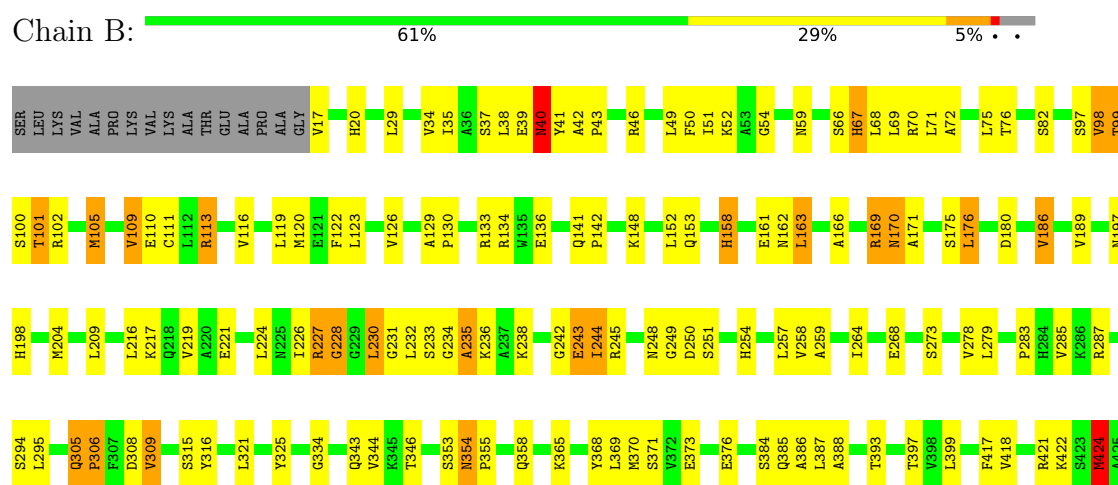
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



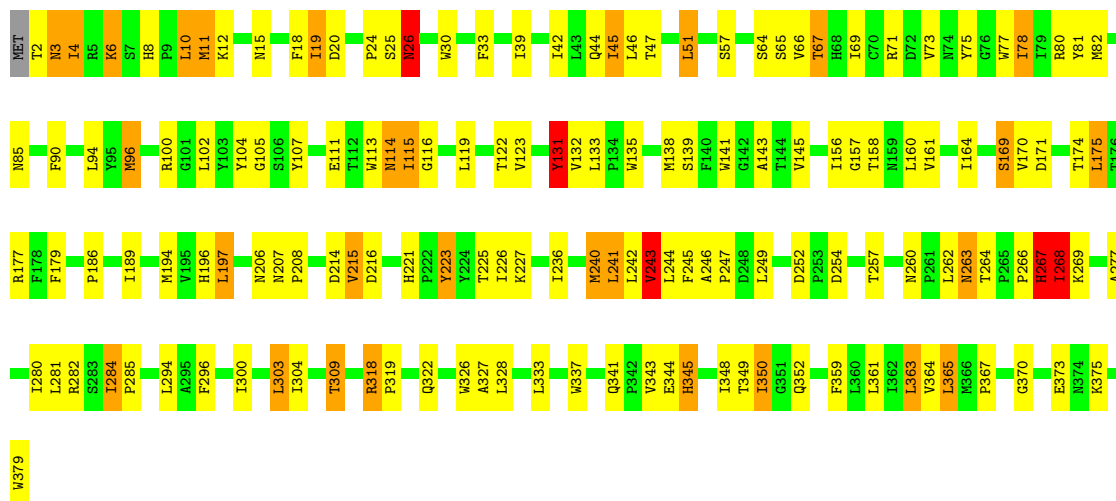
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial





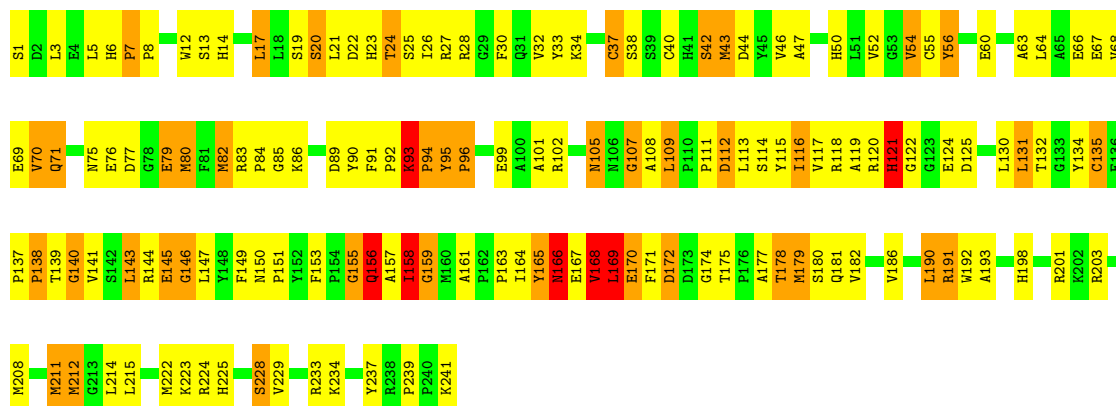
• Molecule 3: Cytochrome b

Chain C: 60% 31% 8%



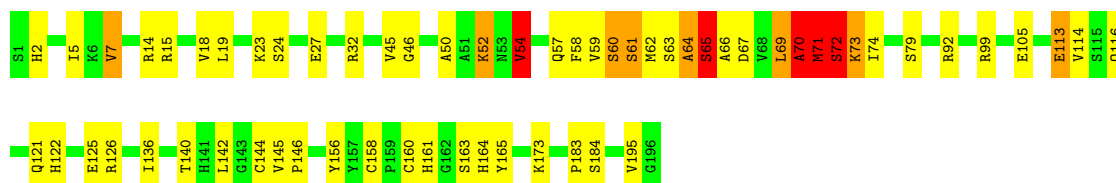
• Molecule 4: cytochrome c1

Chain D: 37% 43% 17%



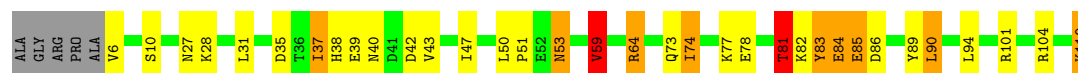
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, mitochondrial

Chain E: 69% 24%



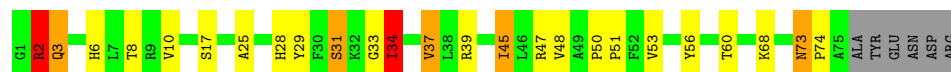
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F: 



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

Chain G: 

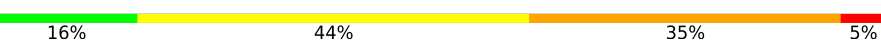


- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H: 



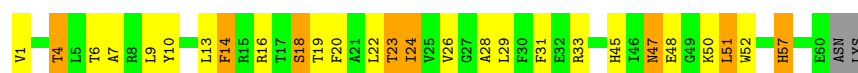
- Molecule 9: Ubiquinol-cytochrome C reductase 8 kDa protein

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

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.32Å 154.32Å 593.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	85.8 (20.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.237 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17049	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: 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	0.87	1/3531 (0.0%)	1.15	18/4792 (0.4%)
2	B	1.13	4/3232 (0.1%)	1.21	14/4386 (0.3%)
3	C	0.87	3/3100 (0.1%)	1.18	20/4242 (0.5%)
4	D	0.75	4/1977 (0.2%)	1.28	25/2684 (0.9%)
5	E	0.71	0/1553	1.28	15/2100 (0.7%)
6	F	0.96	1/930 (0.1%)	1.16	2/1246 (0.2%)
7	G	0.91	1/649 (0.2%)	1.21	4/878 (0.5%)
8	H	0.66	0/553	1.25	4/741 (0.5%)
9	I	1.16	1/411 (0.2%)	1.73	6/558 (1.1%)
10	J	0.77	0/490	1.17	4/665 (0.6%)
11	K	0.79	1/436 (0.2%)	1.12	2/598 (0.3%)
All	All	0.91	16/16862 (0.1%)	1.22	114/22890 (0.5%)

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	1	0
4	D	1	0
7	G	1	0
9	I	2	0
All	All	6	0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	424	MET	SD-CE	-16.02	1.39	1.79
7	G	34	ILE	CA-CB	11.40	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	18	VAL	CA-CB	9.30	1.59	1.54
9	I	1	MET	SD-CE	8.03	1.99	1.79
1	A	335	MET	SD-CE	-7.76	1.60	1.79
2	B	105	MET	SD-CE	-6.23	1.64	1.79
4	D	175	THR	CA-CB	6.06	1.62	1.53
4	D	158	ILE	CA-CB	5.88	1.62	1.54
3	C	240	MET	SD-CE	-5.77	1.65	1.79
4	D	212	MET	SD-CE	-5.69	1.65	1.79
2	B	436	ILE	N-CA	5.48	1.53	1.46
3	C	11	MET	SD-CE	5.38	1.93	1.79
2	B	163	LEU	CA-C	-5.30	1.46	1.52
4	D	211	MET	SD-CE	-5.19	1.66	1.79
6	F	81	THR	CA-CB	5.14	1.60	1.53
3	C	194	MET	SD-CE	5.01	1.92	1.79

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	71	MET	N-CA-C	15.77	133.67	108.76
5	E	69	LEU	N-CA-C	-14.14	95.33	111.03
2	B	235	ALA	N-CA-C	-13.45	96.56	113.23
8	H	53	ASP	N-CA-C	13.18	128.37	113.21
9	I	26	LEU	N-CA-C	10.59	126.16	108.90
5	E	23	LYS	N-CA-C	10.24	126.09	109.40
4	D	158	ILE	N-CA-C	9.73	129.57	109.34
5	E	66	ALA	N-CA-C	-9.70	102.07	112.93
9	I	7	ARG	N-CA-C	-9.61	102.17	112.93
9	I	52	ARG	N-CA-C	9.50	124.86	109.85
5	E	2	HIS	N-CA-C	-9.44	101.76	113.18
5	E	73	LYS	N-CA-C	-9.16	91.62	107.20
4	D	159	GLY	N-CA-C	9.11	134.76	113.18
9	I	46	LYS	N-CA-C	9.02	125.34	108.65
3	C	26	ASN	N-CA-C	8.60	121.89	111.40
5	E	114	VAL	N-CA-C	8.58	119.37	110.62
3	C	268	ILE	N-CA-C	8.49	126.99	109.34
4	D	52	VAL	N-CA-C	8.26	118.31	110.30
4	D	116	ILE	N-CA-C	8.19	118.96	110.36
10	J	57	HIS	N-CA-C	8.17	121.10	111.71
1	A	348	SER	N-CA-C	8.06	122.59	112.03
4	D	79	GLU	N-CA-C	8.04	120.91	108.12
2	B	40	ASN	N-CA-C	-7.77	97.36	109.25
4	D	122	GLY	N-CA-C	-7.70	94.92	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	18	VAL	N-CA-CB	7.66	116.43	110.45
2	B	170	ASN	N-CA-CB	-7.57	99.35	111.62
3	C	225	THR	N-CA-C	-7.38	101.42	112.04
2	B	435	PHE	N-CA-C	7.33	122.50	112.90
8	H	27	LEU	N-CA-C	7.16	126.05	110.80
3	C	345	HIS	N-CA-C	7.14	125.58	109.81
7	G	50	PRO	N-CA-C	7.10	119.37	110.70
4	D	107	GLY	N-CA-C	-7.04	97.91	110.86
1	A	45	SER	N-CA-C	-6.92	104.35	114.39
5	E	72	SER	N-CA-C	6.92	125.54	110.80
7	G	34	ILE	N-CA-CB	6.83	115.09	110.52
1	A	192	ALA	N-CA-C	6.72	124.67	109.81
1	A	285	GLY	N-CA-C	-6.64	103.08	112.37
8	H	54	CYS	N-CA-C	6.54	120.53	111.90
3	C	25	SER	N-CA-C	-6.54	105.16	113.01
10	J	14	PHE	N-CA-C	6.50	121.34	113.41
3	C	3	ASN	N-CA-C	6.48	119.12	109.59
1	A	74	ALA	N-CA-C	6.43	118.29	111.28
2	B	67	HIS	N-CA-C	-6.40	102.99	111.24
2	B	278	VAL	N-CA-C	-6.35	104.45	110.42
1	A	263	ALA	N-CA-C	6.34	120.27	112.54
9	I	23	ALA	N-CA-C	-6.33	97.75	108.26
1	A	37	VAL	CB-CA-C	-6.30	100.61	110.69
1	A	428	ILE	N-CA-C	6.29	117.51	111.91
3	C	57	SER	N-CA-C	6.29	120.80	112.25
2	B	309	VAL	CB-CA-C	-6.28	99.84	110.71
3	C	266	PRO	CA-C-N	6.20	128.50	120.44
3	C	266	PRO	C-N-CA	6.20	128.50	120.44
4	D	146	GLY	N-CA-C	-6.14	98.62	113.18
3	C	196	HIS	N-CA-C	-6.14	104.51	111.14
2	B	242	GLY	N-CA-C	-6.08	105.84	112.04
1	A	443	TRP	N-CA-C	6.06	119.36	109.06
3	C	133	LEU	N-CA-C	6.04	121.10	113.25
4	D	135	CYS	N-CA-C	6.04	117.37	108.86
1	A	189	HIS	N-CA-C	6.02	120.93	112.93
2	B	113	ARG	N-CA-C	5.95	119.64	112.38
4	D	119	ALA	N-CA-C	5.92	120.52	112.88
1	A	226	ASP	N-CA-C	5.91	119.54	110.20
3	C	221	HIS	N-CA-C	-5.91	101.40	110.32
9	I	11	PHE	N-CA-C	5.89	119.68	110.32
4	D	17	LEU	N-CA-C	5.88	117.38	110.97
3	C	115	ILE	N-CA-C	-5.88	104.62	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	24	THR	N-CA-C	-5.88	104.87	111.28
4	D	168	VAL	N-CA-C	-5.80	97.27	109.34
3	C	267	HIS	N-CA-C	5.77	117.25	111.07
5	E	72	SER	CA-C-N	5.77	129.40	121.33
5	E	72	SER	C-N-CA	5.77	129.40	121.33
2	B	243	GLU	N-CA-C	5.74	117.90	109.24
2	B	101	THR	N-CA-C	-5.73	100.42	108.96
1	A	387	GLY	N-CA-C	-5.70	108.18	115.42
4	D	93	LYS	N-CA-C	5.64	122.27	109.81
3	C	243	VAL	N-CA-C	5.58	116.32	110.62
4	D	144	ARG	N-CA-C	-5.58	104.72	112.03
3	C	327	ALA	N-CA-C	-5.54	105.24	111.28
4	D	101	ALA	N-CA-C	-5.54	105.15	111.14
1	A	421	ALA	N-CA-C	-5.53	99.51	108.52
6	F	59	VAL	N-CA-CB	5.53	118.05	110.54
3	C	4	ILE	N-CA-C	5.52	116.91	110.62
4	D	3	LEU	N-CA-C	-5.49	100.72	109.23
1	A	63	ALA	N-CA-C	5.45	117.92	111.33
6	F	85	GLU	N-CA-C	5.43	122.37	110.80
4	D	165	TYR	N-CA-CB	5.39	118.41	110.33
5	E	160	CYS	N-CA-C	5.36	117.12	111.28
8	H	66	ASP	N-CA-C	5.36	117.87	111.71
11	K	42	LEU	N-CA-C	5.36	117.87	111.71
2	B	234	GLY	N-CA-C	5.36	125.87	113.18
4	D	34	LYS	N-CA-C	5.34	117.79	111.33
4	D	191	ARG	N-CA-C	-5.33	105.11	111.03
1	A	81	SER	N-CA-C	5.32	117.83	111.71
3	C	206	ASN	N-CA-C	-5.32	102.12	110.36
3	C	223	TYR	N-CA-C	5.26	116.87	111.03
4	D	155	GLY	N-CA-C	-5.26	108.06	115.32
5	E	70	ALA	CA-C-N	-5.22	111.60	121.63
5	E	70	ALA	C-N-CA	-5.22	111.60	121.63
2	B	105	MET	N-CA-C	-5.21	100.91	109.40
10	J	47	ASN	N-CA-C	5.20	116.41	108.30
4	D	56	TYR	N-CA-C	5.16	117.49	109.60
4	D	19	SER	N-CA-C	5.16	117.13	108.73
5	E	7	VAL	CB-CA-C	-5.15	105.33	110.89
4	D	7	PRO	N-CA-C	5.13	116.97	110.70
1	A	305	GLN	N-CA-C	-5.13	107.15	113.41
1	A	278	GLY	N-CA-C	5.13	120.29	111.47
1	A	38	GLY	N-CA-C	5.10	118.14	110.18
2	B	158	HIS	CB-CA-C	-5.08	102.37	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	131	TYR	N-CA-C	5.06	119.08	113.01
7	G	45	ILE	N-CA-C	5.05	115.27	110.42
5	E	54	VAL	CB-CA-C	-5.05	105.50	111.97
10	J	52	TRP	N-CA-C	-5.04	107.10	113.20
4	D	166	ASN	N-CA-C	-5.04	100.06	110.80
7	G	34	ILE	N-CA-C	5.00	118.92	112.67

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	305	GLN	CA
3	C	345	HIS	CA
4	D	158	ILE	CA
7	G	2	ARG	CA
9	I	25	ALA	CA
9	I	42	VAL	CA

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	106	0
2	B	3172	0	3152	121	0
3	C	3003	0	3065	110	0
4	D	1918	0	1870	122	0
5	E	1519	0	1503	38	0
6	F	911	0	904	25	0
7	G	628	0	636	22	0
8	H	548	0	532	11	0
9	I	406	0	437	83	0
10	J	478	0	463	31	0
11	K	421	0	428	18	0
12	C	86	0	60	10	0
12	D	43	0	30	3	0
13	E	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	99	0	0	11	0
14	B	152	0	0	14	1
14	C	64	0	0	3	0
14	D	43	0	0	7	0
14	E	8	0	0	2	0
14	F	37	0	0	4	0
14	G	23	0	0	2	0
14	H	7	0	0	0	0
14	I	5	0	0	1	0
14	J	6	0	0	0	0
14	K	10	0	0	1	0
All	All	17049	0	16436	599	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (599) 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)
14:A:519:HOH:O	7:G:10:VAL:HB	1.40	1.18
1:A:244:ARG:HG2	14:A:519:HOH:O	1.46	1.15
2:B:227:ARG:HG2	14:B:479:HOH:O	1.48	1.14
4:D:169:LEU:HD11	4:D:177:ALA:HB3	1.22	1.12
4:D:169:LEU:HD11	4:D:177:ALA:CB	1.79	1.12
10:J:18:SER:HA	11:K:24:TRP:HZ3	1.16	1.09
9:I:46:LYS:HG2	9:I:47:ARG:H	1.02	1.07
2:B:99:THR:HB	9:I:14:VAL:HG22	1.38	1.05
4:D:234:LYS:NZ	14:D:1404:HOH:O	1.89	0.99
9:I:20:ARG:HG3	9:I:51:CYS:HB2	1.42	0.97
2:B:283:PRO:HG3	9:I:31:GLN:HG3	1.43	0.97
4:D:131:LEU:HG	4:D:164:ILE:HG13	1.45	0.96
1:A:46:ARG:HD2	1:A:163:LEU:HD13	1.46	0.96
4:D:161:ALA:O	4:D:163:PRO:HD3	1.64	0.95
10:J:18:SER:HA	11:K:24:TRP:CZ3	2.02	0.94
6:F:64:ARG:NH1	14:F:1914:HOH:O	2.00	0.94
2:B:385:GLN:HE22	2:B:393:THR:H	0.95	0.93
4:D:165:TYR:HD2	4:D:165:TYR:O	1.52	0.92
4:D:147:LEU:HB3	4:D:158:ILE:HG22	1.51	0.92
6:F:84:GLU:O	6:F:86:ASP:N	2.03	0.92
2:B:325:TYR:CD2	9:I:28:PRO:HD2	2.05	0.91
7:G:73:ASN:HB3	7:G:74:PRO:HD3	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:93:LYS:HB2	4:D:94:PRO:HD3	1.53	0.89
9:I:46:LYS:CG	9:I:47:ARG:H	1.80	0.89
4:D:169:LEU:CD1	4:D:177:ALA:HB3	2.02	0.88
2:B:385:GLN:NE2	2:B:393:THR:H	1.71	0.88
3:C:111:GLU:HG2	14:C:1052:HOH:O	1.71	0.88
9:I:46:LYS:HG2	9:I:47:ARG:N	1.88	0.88
4:D:166:ASN:HD22	4:D:166:ASN:H	1.22	0.86
1:A:244:ARG:NH2	14:A:461:HOH:O	1.93	0.85
1:A:124:ASP:HA	1:A:127:ILE:HG22	1.59	0.85
4:D:37:CYS:SG	12:D:242:HEM:CAB	2.66	0.83
2:B:71:LEU:HD23	9:I:15:LEU:HG	1.59	0.83
2:B:258:VAL:HG11	2:B:321:LEU:HB3	1.59	0.83
4:D:138:PRO:HG3	8:H:58:LEU:HD22	1.61	0.81
1:A:25:VAL:HG23	1:A:208:LEU:HD13	1.59	0.81
2:B:76:THR:HG22	2:B:82:SER:H	1.43	0.81
4:D:14:HIS:NE2	4:D:124:GLU:OE1	2.12	0.81
1:A:146:ARG:H	9:I:42:VAL:HG12	1.46	0.81
2:B:249:GLY:HA2	14:B:506:HOH:O	1.81	0.79
1:A:244:ARG:NE	14:A:461:HOH:O	2.11	0.79
3:C:15:ASN:HA	3:C:19:ILE:CG1	2.12	0.79
3:C:45:ILE:HA	12:C:381:HEM:HAB	1.63	0.79
10:J:14:PHE:HD1	10:J:20:PHE:HD1	1.30	0.78
4:D:47:ALA:H	4:D:50:HIS:HD2	1.30	0.78
14:B:532:HOH:O	9:I:4:VAL:HG21	1.81	0.78
9:I:34:VAL:HB	9:I:35:PRO:HD3	1.65	0.77
7:G:2:ARG:HA	14:G:103:HOH:O	1.84	0.77
4:D:120:ARG:O	4:D:121:HIS:HB2	1.84	0.77
6:F:82:LYS:C	6:F:83:TYR:O	2.23	0.77
3:C:240:MET:HE2	3:C:240:MET:HA	1.67	0.76
4:D:168:VAL:O	4:D:169:LEU:HB2	1.86	0.76
3:C:257:THR:HG22	4:D:115:TYR:HE1	1.50	0.76
9:I:20:ARG:HG3	9:I:51:CYS:CB	2.16	0.76
4:D:165:TYR:O	4:D:165:TYR:CD2	2.37	0.75
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.67	0.75
3:C:94:LEU:HD21	3:C:123:VAL:HG11	1.69	0.74
1:A:144:SER:HA	9:I:42:VAL:HB	1.70	0.74
4:D:169:LEU:CD1	4:D:177:ALA:CB	2.64	0.74
5:E:64:ALA:O	5:E:65:SER:HB2	1.85	0.74
5:E:18:VAL:HG12	5:E:18:VAL:O	1.86	0.74
2:B:294:SER:HB3	2:B:343:GLN:HE21	1.52	0.73
4:D:47:ALA:H	4:D:50:HIS:CD2	2.07	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:ASN:O	2:B:40:ASN:ND2	2.21	0.73
1:A:372:THR:OG1	2:B:373:GLU:OE1	2.06	0.73
1:A:419:CYS:SG	1:A:438:ARG:NH1	2.62	0.72
3:C:67:THR:HG22	3:C:71:ARG:HE	1.53	0.72
2:B:176:LEU:HG	9:I:13:PRO:CG	2.18	0.72
6:F:39:GLU:HG3	14:F:1024:HOH:O	1.89	0.72
9:I:2:LEU:O	9:I:3:SER:HB3	1.88	0.72
2:B:306:PRO:O	14:B:507:HOH:O	2.07	0.72
2:B:100:SER:O	9:I:13:PRO:HD2	1.89	0.72
2:B:315:SER:O	9:I:4:VAL:HG13	1.90	0.72
9:I:11:PHE:HZ	9:I:27:ARG:HH21	1.38	0.71
4:D:54:VAL:HG21	4:D:192:TRP:CZ2	2.26	0.71
10:J:19:THR:O	10:J:23:THR:HG22	1.91	0.71
2:B:305:GLN:HB3	2:B:306:PRO:HD3	1.72	0.71
3:C:257:THR:HG22	4:D:115:TYR:CE1	2.25	0.71
5:E:69:LEU:C	5:E:70:ALA:O	2.33	0.71
1:A:145:MET:O	1:A:149:VAL:HG23	1.90	0.71
1:A:117:VAL:HG11	1:A:195:MET:HE1	1.71	0.71
1:A:378:ASP:OD2	1:A:389:ARG:NH1	2.24	0.70
3:C:15:ASN:HA	3:C:19:ILE:HG13	1.73	0.70
1:A:85:HIS:CD2	2:B:370:MET:HE1	2.26	0.70
2:B:161:GLU:OE1	2:B:175:SER:OG	2.08	0.70
1:A:351:GLU:H	11:K:12:GLN:HE21	1.40	0.70
2:B:76:THR:HG23	2:B:136:GLU:OE1	1.92	0.70
6:F:28:LYS:HB3	6:F:74:ILE:HG12	1.73	0.70
7:G:73:ASN:HB3	7:G:74:PRO:CD	2.21	0.70
3:C:241:LEU:HD13	4:D:208:MET:HE1	1.74	0.69
9:I:6:ALA:C	9:I:8:SER:H	2.00	0.69
3:C:131:TYR:HA	12:C:381:HEM:HAD2	1.75	0.69
1:A:373:THR:HB	1:A:374:PRO:HD3	1.73	0.69
2:B:70:ARG:HG3	2:B:98:VAL:HG22	1.75	0.69
4:D:37:CYS:SG	12:D:242:HEM:HAB	2.32	0.68
3:C:105:GLY:HA2	3:C:107:TYR:CE1	2.28	0.68
4:D:93:LYS:HB2	4:D:94:PRO:CD	2.24	0.68
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.76	0.68
6:F:82:LYS:O	6:F:83:TYR:O	2.11	0.68
1:A:351:GLU:H	11:K:12:GLN:NE2	1.91	0.67
2:B:111:CYS:HB3	2:B:119:LEU:CD1	2.24	0.67
4:D:169:LEU:HD11	4:D:177:ALA:HB2	1.74	0.67
2:B:198:HIS:NE2	14:B:490:HOH:O	2.28	0.67
4:D:225:HIS:O	4:D:228:SER:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLN:HE21	1:A:323:HIS:HD2	1.43	0.66
4:D:75:ASN:O	4:D:77:ASP:N	2.28	0.66
4:D:102:ARG:HA	4:D:107:GLY:O	1.96	0.66
4:D:229:VAL:O	14:D:2102:HOH:O	2.13	0.66
4:D:66:GLU:HA	4:D:84:PRO:O	1.95	0.66
3:C:131:TYR:OH	3:C:138:MET:HB3	1.95	0.66
2:B:354:ASN:H	2:B:355:PRO:HD2	1.60	0.66
1:A:27:SER:HB3	1:A:208:LEU:HD12	1.78	0.65
4:D:224:ARG:HD3	14:D:1426:HOH:O	1.96	0.65
3:C:309:THR:HG21	3:C:367:PRO:O	1.96	0.65
4:D:90:TYR:C	4:D:92:PRO:HD3	2.22	0.65
2:B:111:CYS:SG	2:B:119:LEU:HD12	2.36	0.65
4:D:27:ARG:HH12	10:J:57:HIS:CD2	2.15	0.65
4:D:149:PHE:O	14:D:1443:HOH:O	2.15	0.65
1:A:305:GLN:HG3	9:I:46:LYS:O	1.97	0.65
2:B:153:GLN:HE22	9:I:46:LYS:HG3	1.62	0.65
6:F:6:VAL:N	6:F:10:SER:HG	1.96	0.64
2:B:46:ARG:HG3	2:B:46:ARG:HH11	1.62	0.64
2:B:245:ARG:NH2	2:B:433:THR:O	2.30	0.63
1:A:325:VAL:HG21	9:I:43:LEU:HD12	1.80	0.63
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.33	0.63
9:I:43:LEU:HD22	9:I:46:LYS:HD3	1.81	0.63
4:D:27:ARG:NH1	10:J:57:HIS:NE2	2.47	0.63
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.81	0.63
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.34	0.63
9:I:47:ARG:HD2	9:I:48:SER:H	1.64	0.63
2:B:227:ARG:NH2	2:B:230:LEU:O	2.32	0.62
4:D:30:PHE:HD2	4:D:56:TYR:HH	1.45	0.62
5:E:64:ALA:O	5:E:65:SER:CB	2.47	0.62
1:A:237:THR:OG1	5:E:14:ARG:NH2	2.33	0.62
6:F:59:VAL:HG21	7:G:10:VAL:HG13	1.81	0.62
1:A:291:SER:HB3	1:A:356:ARG:CZ	2.29	0.62
4:D:113:LEU:HG	4:D:190:LEU:HD11	1.81	0.62
1:A:188:ARG:HB3	1:A:188:ARG:HH11	1.63	0.62
3:C:15:ASN:HA	3:C:19:ILE:HG12	1.80	0.62
3:C:75:TYR:HB3	3:C:78:ILE:HD11	1.82	0.61
4:D:47:ALA:N	4:D:50:HIS:HD2	1.98	0.61
3:C:300:ILE:HD11	3:C:363:LEU:HD13	1.81	0.61
9:I:43:LEU:HA	9:I:46:LYS:HD3	1.82	0.61
2:B:243:GLU:HB2	2:B:424:MET:O	2.01	0.61
4:D:203:ARG:NH1	14:D:1427:HOH:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:83:ARG:HG2	4:D:84:PRO:HD2	1.81	0.61
5:E:121:GLN:OE1	5:E:126:ARG:NH1	2.32	0.61
1:A:19:LEU:HB3	1:A:21:ASN:HB2	1.83	0.60
4:D:28:ARG:O	4:D:32:VAL:HG23	2.00	0.60
5:E:69:LEU:O	5:E:70:ALA:O	2.18	0.60
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.33	0.60
1:A:274:ASN:ND2	14:A:466:HOH:O	2.33	0.60
2:B:161:GLU:CD	2:B:175:SER:HG	2.07	0.60
4:D:28:ARG:HB3	4:D:171:PHE:HE2	1.67	0.60
9:I:49:VAL:C	9:I:51:CYS:H	2.10	0.60
10:J:14:PHE:HD1	10:J:20:PHE:CD1	2.15	0.60
7:G:28:HIS:HB3	7:G:31:SER:HB2	1.84	0.60
3:C:114:ASN:N	3:C:114:ASN:HD22	1.98	0.59
4:D:23:HIS:CD2	10:J:50:LYS:HB2	2.37	0.59
2:B:258:VAL:CG1	2:B:259:ALA:N	2.65	0.59
3:C:119:LEU:HD22	12:C:382:HEM:HBB2	1.84	0.59
3:C:337:TRP:HZ3	3:C:350:ILE:HD11	1.66	0.59
2:B:102:ARG:NH2	2:B:161:GLU:OE2	2.36	0.59
2:B:176:LEU:HG	9:I:13:PRO:HG2	1.85	0.59
7:G:48:VAL:O	7:G:51:PRO:HD2	2.02	0.59
1:A:158:PHE:O	1:A:164:ALA:HB2	2.03	0.59
2:B:153:GLN:NE2	9:I:46:LYS:HG3	2.18	0.59
3:C:8:HIS:CD2	3:C:10:LEU:HB2	2.38	0.59
4:D:1:SER:N	4:D:156:GLN:HE22	2.01	0.58
2:B:122:PHE:O	2:B:126:VAL:HG23	2.03	0.58
2:B:249:GLY:CA	14:B:506:HOH:O	2.46	0.58
2:B:258:VAL:HG12	2:B:259:ALA:N	2.17	0.58
9:I:4:VAL:HG12	9:I:10:PRO:HG2	1.85	0.58
3:C:169:SER:OG	3:C:170:VAL:N	2.36	0.58
4:D:42:SER:HB2	4:D:112:ASP:HB3	1.86	0.58
3:C:94:LEU:HD21	3:C:123:VAL:CG1	2.32	0.58
1:A:240:GLN:NE2	1:A:242:CYS:SG	2.70	0.58
3:C:51:LEU:HD21	3:C:80:ARG:HA	1.86	0.58
11:K:48:ILE:O	11:K:48:ILE:HG22	2.04	0.58
1:A:272:VAL:O	1:A:276:ILE:HG13	2.03	0.57
3:C:309:THR:CG2	3:C:370:GLY:HA3	2.34	0.57
9:I:18:THR:OG1	9:I:53:GLU:OE2	2.11	0.57
4:D:60:GLU:O	4:D:64:LEU:HG	2.02	0.57
4:D:211:MET:HE1	10:J:31:PHE:CE2	2.39	0.57
1:A:156:THR:O	1:A:159:GLN:HG3	2.04	0.57
8:H:38:GLU:HA	8:H:41:ASP:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASP:OD1	1:A:438:ARG:NH2	2.33	0.57
6:F:104:ARG:NH2	14:F:1931:HOH:O	2.26	0.57
1:A:252:HIS:CE1	9:I:43:LEU:HB2	2.40	0.57
4:D:157:ALA:O	4:D:158:ILE:HG23	2.04	0.57
1:A:42:ASP:O	1:A:194:ARG:NH2	2.38	0.57
6:F:83:TYR:O	6:F:84:GLU:C	2.45	0.57
1:A:436:ARG:NH2	3:C:20:ASP:OD2	2.33	0.57
9:I:44:ASP:O	9:I:46:LYS:HB2	2.04	0.56
3:C:82:MET:HG2	3:C:240:MET:HE1	1.87	0.56
4:D:54:VAL:HG21	4:D:192:TRP:HZ2	1.70	0.56
4:D:79:GLU:HG3	4:D:80:MET:H	1.70	0.56
4:D:155:GLY:C	4:D:157:ALA:H	2.14	0.56
4:D:224:ARG:HB3	7:G:25:ALA:HB1	1.86	0.56
1:A:2:ALA:O	2:B:113:ARG:HD3	2.06	0.56
9:I:42:VAL:O	9:I:43:LEU:HB2	2.05	0.56
3:C:131:TYR:CA	12:C:381:HEM:HAD2	2.35	0.56
2:B:46:ARG:HG3	2:B:46:ARG:NH1	2.20	0.56
3:C:75:TYR:CE2	5:E:57:GLN:HG2	2.41	0.56
1:A:146:ARG:NH2	14:A:486:HOH:O	2.37	0.56
1:A:220:SER:HA	1:A:223:TYR:CB	2.36	0.56
3:C:44:GLN:HG3	12:C:381:HEM:HBC2	1.88	0.56
4:D:167:GLU:HG2	4:D:168:VAL:O	2.05	0.56
9:I:11:PHE:CE2	9:I:25:ALA:N	2.66	0.56
1:A:126:GLN:HA	1:A:126:GLN:HE21	1.70	0.56
4:D:165:TYR:O	4:D:166:ASN:C	2.47	0.56
6:F:37:ILE:HD12	6:F:43:VAL:HG21	1.87	0.56
6:F:53:ASN:N	6:F:53:ASN:HD22	2.03	0.56
3:C:348:ILE:HG22	3:C:352:GLN:NE2	2.21	0.56
5:E:5:ILE:HA	14:E:202:HOH:O	2.07	0.55
3:C:214:ASP:OD2	7:G:2:ARG:NH2	2.26	0.55
3:C:348:ILE:HG22	3:C:352:GLN:HE21	1.71	0.55
3:C:349:THR:HA	3:C:352:GLN:NE2	2.21	0.55
4:D:112:ASP:OD1	4:D:112:ASP:N	2.27	0.55
2:B:388:ALA:HB3	9:I:2:LEU:HD13	1.89	0.55
11:K:11:ARG:O	11:K:15:ARG:HD2	2.06	0.55
6:F:83:TYR:O	6:F:84:GLU:HG2	2.07	0.55
4:D:109:LEU:O	4:D:111:PRO:HD3	2.06	0.55
1:A:252:HIS:CD2	1:A:323:HIS:HE1	2.24	0.55
2:B:385:GLN:HA	9:I:2:LEU:HD12	1.88	0.55
1:A:365:LEU:HD11	9:I:56:ARG:HH21	1.72	0.54
4:D:171:PHE:O	4:D:174:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:TYR:CD1	9:I:1:MET:HG3	2.42	0.54
3:C:80:ARG:O	3:C:80:ARG:HD3	2.07	0.54
4:D:63:ALA:O	4:D:67:GLU:HG3	2.08	0.54
1:A:38:GLY:HA2	1:A:113:LEU:HD21	1.90	0.54
1:A:430:GLN:HG3	1:A:430:GLN:O	2.07	0.54
3:C:85:ASN:HD22	3:C:243:VAL:HG12	1.71	0.54
9:I:41:PRO:O	9:I:42:VAL:HG23	2.07	0.54
3:C:141:TRP:O	3:C:145:VAL:HG23	2.07	0.54
5:E:15:ARG:HD2	5:E:32:ARG:HD2	1.90	0.54
7:G:73:ASN:CB	7:G:74:PRO:HD3	2.30	0.54
1:A:86:LEU:HB3	2:B:285:VAL:HG22	1.89	0.54
1:A:220:SER:HA	1:A:223:TYR:HB2	1.89	0.54
2:B:101:THR:OG1	14:B:566:HOH:O	2.13	0.54
2:B:235:ALA:HA	14:B:539:HOH:O	2.08	0.54
3:C:116:GLY:C	12:C:382:HEM:HBC2	2.33	0.54
4:D:168:VAL:O	4:D:169:LEU:HD13	2.08	0.54
10:J:33:ARG:HG2	11:K:47:TYR:CE2	2.43	0.54
6:F:53:ASN:HD22	6:F:53:ASN:H	1.56	0.53
3:C:132:VAL:HA	3:C:139:SER:HB3	1.91	0.53
9:I:11:PHE:HZ	9:I:27:ARG:NH2	2.06	0.53
4:D:168:VAL:O	4:D:169:LEU:CB	2.53	0.53
5:E:158:CYS:HB3	5:E:163:SER:HB2	1.90	0.53
6:F:50:LEU:HD21	6:F:90:LEU:HD23	1.89	0.53
2:B:308:ASP:CG	9:I:28:PRO:HB3	2.34	0.53
5:E:99:ARG:NH2	5:E:105:GLU:OE2	2.40	0.53
2:B:34:VAL:HG11	2:B:386:ALA:HB1	1.91	0.53
5:E:113:GLU:OE1	5:E:116:GLN:HG2	2.09	0.53
4:D:12:TRP:NE1	4:D:125:ASP:OD2	2.33	0.53
11:K:18:VAL:HG12	11:K:19:PRO:HD3	1.91	0.53
2:B:170:ASN:HD22	2:B:238:LYS:HG3	1.74	0.53
4:D:166:ASN:HD22	4:D:166:ASN:N	2.00	0.53
9:I:47:ARG:HH11	9:I:47:ARG:HB3	1.75	0.52
1:A:335:MET:HE3	1:A:339:GLN:HG3	1.92	0.52
1:A:252:HIS:CE1	9:I:42:VAL:O	2.62	0.52
4:D:40:CYS:SG	12:D:242:HEM:HAC	2.49	0.52
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.39	0.52
9:I:34:VAL:HB	9:I:35:PRO:CD	2.35	0.52
7:G:56:TYR:C	7:G:56:TYR:CD1	2.87	0.52
3:C:337:TRP:CZ3	3:C:350:ILE:HD11	2.44	0.52
2:B:100:SER:O	9:I:13:PRO:CD	2.56	0.52
5:E:65:SER:O	14:E:200:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ARG:HG3	2:B:238:LYS:HB2	1.92	0.52
2:B:325:TYR:HB3	9:I:28:PRO:HD3	1.92	0.52
4:D:22:ASP:HB3	4:D:25:SER:HB3	1.92	0.52
9:I:44:ASP:O	9:I:45:LEU:C	2.53	0.52
7:G:3:GLN:N	14:G:103:HOH:O	2.31	0.52
3:C:281:LEU:HD22	3:C:294:LEU:HD22	1.92	0.51
10:J:29:LEU:HD13	11:K:34:TRP:HD1	1.75	0.51
2:B:308:ASP:OD1	9:I:28:PRO:HB3	2.10	0.51
1:A:341:GLN:HE22	1:A:344:ARG:HE	1.56	0.51
6:F:35:ASP:OD2	6:F:89:TYR:OH	2.19	0.51
1:A:386:TYR:C	1:A:388:ARG:H	2.17	0.51
4:D:215:LEU:HD21	5:E:46:GLY:HA3	1.93	0.51
4:D:33:TYR:HA	4:D:37:CYS:SG	2.51	0.51
5:E:70:ALA:O	5:E:71:MET:HG3	2.11	0.51
2:B:40:ASN:C	2:B:42:ALA:H	2.19	0.51
3:C:216:ASP:OD2	4:D:233:ARG:NH2	2.38	0.51
3:C:3:ASN:HB3	3:C:6:LYS:HG3	1.94	0.50
10:J:29:LEU:HG	11:K:48:ILE:HD13	1.93	0.50
2:B:385:GLN:HE22	2:B:393:THR:N	1.81	0.50
9:I:16:SER:HB3	9:I:19:SER:O	2.12	0.50
2:B:66:SER:HB2	2:B:105:MET:HE2	1.93	0.50
2:B:325:TYR:HB3	9:I:28:PRO:CD	2.42	0.50
6:F:40:ASN:H	6:F:43:VAL:HB	1.76	0.50
1:A:178:SER:O	1:A:181:ASP:HB2	2.11	0.50
1:A:281:ASP:OD2	9:I:47:ARG:HG2	2.12	0.50
3:C:33:PHE:CZ	3:C:96:MET:HG2	2.47	0.50
1:A:19:LEU:HD22	1:A:23:LEU:HD12	1.94	0.50
1:A:213:GLN:O	1:A:217:SER:HB3	2.11	0.50
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.92	0.50
9:I:24:GLY:O	9:I:25:ALA:HB2	2.12	0.50
3:C:8:HIS:CD2	3:C:10:LEU:H	2.29	0.50
4:D:83:ARG:NH2	4:D:89:ASP:OD1	2.45	0.50
8:H:21:ARG:HD3	8:H:65:ARG:HH21	1.77	0.50
9:I:2:LEU:O	9:I:3:SER:CB	2.57	0.50
1:A:104:LYS:O	1:A:107:PRO:HD2	2.12	0.49
1:A:279:HIS:HB2	9:I:20:ARG:NH2	2.26	0.49
2:B:368:TYR:O	2:B:369:LEU:C	2.54	0.49
3:C:119:LEU:HD22	12:C:382:HEM:CBB	2.41	0.49
4:D:75:ASN:HB3	4:D:79:GLU:OE2	2.12	0.49
5:E:71:MET:HE3	5:E:92:ARG:HA	1.93	0.49
6:F:43:VAL:O	6:F:47:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:59:VAL:CG2	7:G:10:VAL:HG13	2.42	0.49
3:C:47:THR:HG22	5:E:58:PHE:HZ	1.77	0.49
2:B:99:THR:CB	9:I:14:VAL:HG22	2.27	0.49
10:J:14:PHE:CD1	10:J:20:PHE:HD1	2.20	0.49
2:B:305:GLN:NE2	9:I:35:PRO:HB3	2.27	0.49
3:C:170:VAL:HG13	3:C:174:THR:HG21	1.95	0.49
4:D:66:GLU:HG3	4:D:85:GLY:O	2.12	0.49
1:A:252:HIS:HE1	9:I:43:LEU:HB2	1.76	0.49
2:B:109:VAL:HG22	2:B:119:LEU:HD22	1.95	0.49
4:D:166:ASN:H	4:D:166:ASN:ND2	2.01	0.49
3:C:243:VAL:O	3:C:247:PRO:HG3	2.13	0.49
4:D:139:THR:HG22	4:D:140:GLY:H	1.77	0.49
5:E:70:ALA:O	5:E:71:MET:CB	2.54	0.49
14:A:519:HOH:O	7:G:10:VAL:CB	2.21	0.49
2:B:243:GLU:HG3	14:B:574:HOH:O	2.11	0.49
4:D:27:ARG:NH1	10:J:57:HIS:CE1	2.81	0.49
2:B:71:LEU:CD2	9:I:15:LEU:HG	2.36	0.48
9:I:1:MET:HE2	9:I:7:ARG:HG3	1.94	0.48
9:I:11:PHE:HE2	9:I:25:ALA:H	1.54	0.48
1:A:48:GLU:OE1	1:A:53:ASN:HA	2.13	0.48
1:A:252:HIS:HD2	1:A:323:HIS:HE1	1.61	0.48
3:C:268:ILE:HG23	3:C:268:ILE:O	2.13	0.48
4:D:120:ARG:O	4:D:121:HIS:CB	2.59	0.48
8:H:66:ASP:HA	8:H:69:VAL:HB	1.95	0.48
1:A:158:PHE:HB3	1:A:161:THR:OG1	2.13	0.48
2:B:129:ALA:N	2:B:130:PRO:HD3	2.28	0.48
3:C:373:GLU:HB2	14:C:1061:HOH:O	2.13	0.48
3:C:348:ILE:O	3:C:352:GLN:HG3	2.14	0.48
4:D:47:ALA:N	4:D:50:HIS:CD2	2.78	0.48
10:J:4:THR:HA	10:J:7:ALA:HB3	1.96	0.48
10:J:14:PHE:CD1	10:J:20:PHE:CD1	3.00	0.48
2:B:72:ALA:HB1	2:B:75:LEU:HG	1.94	0.48
4:D:86:LYS:N	4:D:89:ASP:OD2	2.33	0.48
4:D:180:SER:OG	8:H:17:LEU:HB2	2.13	0.48
3:C:245:PHE:C	3:C:247:PRO:HD3	2.39	0.48
4:D:1:SER:H1	4:D:156:GLN:HE22	1.62	0.48
4:D:20:SER:HB3	10:J:47:ASN:CG	2.39	0.48
10:J:20:PHE:O	10:J:24:ILE:HG23	2.14	0.48
3:C:282:ARG:NH2	3:C:341:GLN:O	2.45	0.47
3:C:179:PHE:CE2	12:C:381:HEM:HMA3	2.49	0.47
1:A:118:GLN:HG2	1:A:219:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:NH2	1:A:177:LEU:O	2.47	0.47
2:B:305:GLN:HE22	9:I:35:PRO:HB3	1.79	0.47
4:D:178:THR:HG23	4:D:181:GLN:HB2	1.96	0.47
5:E:65:SER:C	5:E:67:ASP:H	2.22	0.47
9:I:20:ARG:NH1	9:I:48:SER:OG	2.46	0.47
4:D:150:ASN:O	4:D:156:GLN:HA	2.14	0.47
4:D:157:ALA:C	4:D:158:ILE:HG23	2.40	0.47
2:B:243:GLU:OE2	2:B:435:PHE:O	2.32	0.47
14:A:519:HOH:O	7:G:10:VAL:CG1	2.55	0.47
3:C:77:TRP:CZ3	4:D:201:ARG:HB3	2.50	0.47
4:D:164:ILE:HB	4:D:179:MET:HE2	1.97	0.47
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.97	0.47
2:B:39:GLU:OE2	2:B:113:ARG:NH2	2.48	0.47
2:B:435:PHE:O	2:B:436:ILE:HB	2.14	0.47
3:C:30:TRP:HZ3	3:C:96:MET:HG3	1.80	0.47
4:D:211:MET:HE1	10:J:31:PHE:CZ	2.49	0.47
2:B:37:SER:HB3	2:B:216:LEU:HD12	1.96	0.47
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.45	0.47
5:E:60:SER:C	5:E:62:MET:H	2.23	0.47
3:C:207:ASN:HB2	3:C:208:PRO:HD2	1.96	0.46
3:C:349:THR:HA	3:C:352:GLN:HE21	1.80	0.46
1:A:85:HIS:O	1:A:99:ILE:HA	2.15	0.46
4:D:71:GLN:HE21	4:D:80:MET:HG3	1.80	0.46
4:D:134:TYR:HD2	14:D:1443:HOH:O	1.96	0.46
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.95	0.46
7:G:34:ILE:HA	7:G:37:VAL:HG13	1.98	0.46
2:B:49:LEU:HD11	2:B:204:MET:HE3	1.97	0.46
2:B:294:SER:HB3	2:B:343:GLN:NE2	2.27	0.46
3:C:24:PRO:C	3:C:26:ASN:H	2.22	0.46
3:C:157:GLY:O	3:C:161:VAL:HG23	2.14	0.46
3:C:267:HIS:CE1	3:C:269:LYS:HG2	2.50	0.46
5:E:18:VAL:O	5:E:18:VAL:CG1	2.58	0.46
2:B:437:ASP:HB3	2:B:438:GLU:HG3	1.98	0.46
14:B:520:HOH:O	9:I:11:PHE:HB2	2.15	0.46
4:D:117:VAL:HG11	4:D:191:ARG:HH11	1.79	0.46
2:B:68:LEU:HD23	2:B:186:VAL:HG22	1.98	0.46
3:C:170:VAL:HG12	3:C:170:VAL:O	2.15	0.46
3:C:296:PHE:O	3:C:300:ILE:HB	2.16	0.46
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.98	0.46
5:E:72:SER:HB3	5:E:73:LYS:H	1.24	0.46
4:D:43:MET:HE3	4:D:46:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:HIS:O	2:B:68:LEU:C	2.59	0.46
2:B:325:TYR:CG	9:I:28:PRO:HD2	2.50	0.46
2:B:385:GLN:NE2	14:B:584:HOH:O	2.44	0.46
14:B:565:HOH:O	9:I:18:THR:HG23	2.15	0.46
3:C:344:GLU:O	3:C:348:ILE:HG13	2.16	0.46
8:H:73:LEU:HB3	8:H:74:PHE:H	1.59	0.46
9:I:41:PRO:C	9:I:42:VAL:HG23	2.41	0.45
10:J:29:LEU:HD13	11:K:34:TRP:CD1	2.50	0.45
1:A:124:ASP:HA	1:A:127:ILE:CG2	2.37	0.45
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.74	0.45
14:A:480:HOH:O	9:I:42:VAL:HG21	2.15	0.45
2:B:126:VAL:O	2:B:130:PRO:HG3	2.16	0.45
6:F:64:ARG:HH11	6:F:64:ARG:HB3	1.81	0.45
3:C:375:LYS:HA	3:C:375:LYS:HD3	1.77	0.45
2:B:111:CYS:CB	2:B:119:LEU:HD12	2.46	0.45
5:E:52:LYS:HD2	11:K:34:TRP:CZ2	2.51	0.45
10:J:18:SER:CA	11:K:24:TRP:HZ3	2.07	0.45
2:B:268:GLU:N	14:B:517:HOH:O	2.47	0.45
5:E:136:ILE:HD11	5:E:183:PRO:HB3	1.99	0.45
9:I:20:ARG:NH1	14:I:62:HOH:O	2.24	0.45
9:I:41:PRO:HB3	9:I:44:ASP:CG	2.42	0.45
1:A:252:HIS:CD2	1:A:323:HIS:CE1	3.05	0.45
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.98	0.45
9:I:15:LEU:HA	9:I:15:LEU:HD22	1.29	0.45
10:J:50:LYS:O	10:J:51:LEU:HB2	2.16	0.45
3:C:260:ASN:HB3	3:C:263:ASN:HB2	1.97	0.45
2:B:204:MET:HE1	2:B:224:LEU:HD22	1.99	0.45
3:C:132:VAL:HG22	3:C:143:ALA:HB2	1.98	0.45
4:D:156:GLN:HE21	4:D:156:GLN:HB2	1.50	0.45
1:A:252:HIS:HD2	1:A:323:HIS:CE1	2.35	0.44
3:C:100:ARG:HD2	3:C:100:ARG:C	2.42	0.44
5:E:50:ALA:O	5:E:54:VAL:HG23	2.17	0.44
7:G:29:TYR:O	7:G:33:GLY:HA3	2.17	0.44
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.52	0.44
1:A:146:ARG:HH12	1:A:308:GLN:NE2	2.15	0.44
4:D:143:LEU:H	4:D:143:LEU:HG	1.57	0.44
4:D:145:GLU:O	4:D:145:GLU:HG3	2.17	0.44
4:D:165:TYR:O	4:D:167:GLU:N	2.50	0.44
8:H:69:VAL:O	8:H:73:LEU:HB2	2.17	0.44
10:J:16:ARG:C	10:J:18:SER:N	2.72	0.44
1:A:73:ASN:OD1	1:A:73:ASN:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASP:HB3	1:A:284:TYR:CD1	2.52	0.44
2:B:227:ARG:HG3	14:B:446:HOH:O	2.16	0.44
3:C:8:HIS:HD2	3:C:10:LEU:HB2	1.83	0.44
1:A:149:VAL:HG21	1:A:252:HIS:CB	2.45	0.44
2:B:148:LYS:NZ	2:B:180:ASP:OD1	2.40	0.44
3:C:227:LYS:HD2	14:D:1043:HOH:O	2.17	0.44
5:E:69:LEU:HD23	5:E:69:LEU:HA	1.84	0.44
8:H:39:LEU:O	8:H:43:ARG:HG3	2.18	0.44
2:B:133:ARG:O	2:B:134:ARG:C	2.61	0.44
4:D:28:ARG:HB3	4:D:171:PHE:CE2	2.51	0.44
3:C:240:MET:HB3	3:C:244:LEU:HD12	1.99	0.44
4:D:32:VAL:HG11	4:D:186:VAL:HB	2.00	0.44
5:E:70:ALA:O	5:E:71:MET:CG	2.66	0.44
3:C:322:GLN:HE21	3:C:322:GLN:HB3	1.54	0.44
4:D:47:ALA:HA	4:D:90:TYR:HA	2.00	0.44
3:C:116:GLY:HA3	12:C:382:HEM:C3C	2.53	0.43
4:D:237:TYR:CE2	4:D:239:PRO:HG3	2.53	0.43
9:I:24:GLY:O	9:I:25:ALA:CB	2.64	0.43
1:A:246:ASP:OD2	14:A:461:HOH:O	2.21	0.43
1:A:2:ALA:O	2:B:113:ARG:CD	2.67	0.43
2:B:316:TYR:OH	9:I:10:PRO:HB3	2.19	0.43
9:I:39:GLU:O	9:I:40:SER:CB	2.66	0.43
1:A:59:VAL:HG11	1:A:186:LEU:HD21	2.01	0.43
1:A:442:PHE:CD2	1:A:442:PHE:C	2.96	0.43
6:F:110:LYS:H	6:F:110:LYS:HG2	1.57	0.43
2:B:369:LEU:HD11	2:B:399:LEU:HD11	1.99	0.43
2:B:418:VAL:O	2:B:422:LYS:NZ	2.51	0.43
3:C:135:TRP:HH2	3:C:170:VAL:HG12	1.84	0.43
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.53	0.43
3:C:318:ARG:HB2	3:C:373:GLU:OE1	2.19	0.43
4:D:30:PHE:O	4:D:33:TYR:N	2.51	0.43
4:D:70:VAL:O	4:D:71:GLN:HB2	2.19	0.43
4:D:117:VAL:CG1	4:D:191:ARG:HH11	2.32	0.43
1:A:145:MET:H	9:I:42:VAL:HA	1.84	0.43
2:B:40:ASN:O	2:B:42:ALA:N	2.47	0.43
3:C:113:TRP:HA	12:C:382:HEM:HH1	2.01	0.43
9:I:6:ALA:C	9:I:8:SER:N	2.73	0.43
1:A:11:VAL:HA	1:A:12:PRO:HD3	1.90	0.43
2:B:42:ALA:HA	2:B:43:PRO:HD3	1.93	0.43
2:B:111:CYS:HB3	2:B:119:LEU:HD12	2.00	0.43
2:B:433:THR:HA	2:B:434:PRO:HD2	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.89	0.43
2:B:120:MET:HE2	2:B:120:MET:HB2	1.74	0.42
4:D:137:PRO:HA	4:D:138:PRO:HD3	1.82	0.42
1:A:25:VAL:CG2	1:A:208:LEU:HD13	2.41	0.42
1:A:419:CYS:HA	1:A:420:PRO:HD3	1.84	0.42
2:B:170:ASN:ND2	2:B:238:LYS:HG3	2.32	0.42
3:C:66:VAL:O	3:C:69:ILE:HB	2.19	0.42
5:E:60:SER:O	5:E:62:MET:N	2.51	0.42
9:I:46:LYS:CG	9:I:47:ARG:N	2.58	0.42
1:A:204:GLU:O	1:A:207:GLN:HB2	2.19	0.42
2:B:279:LEU:HD23	2:B:279:LEU:HA	1.87	0.42
4:D:150:ASN:HA	4:D:151:PRO:HD3	1.91	0.42
4:D:191:ARG:HH11	4:D:191:ARG:HD2	1.72	0.42
2:B:141:GLN:HB2	2:B:142:PRO:HD3	2.00	0.42
2:B:162:ASN:HD22	2:B:162:ASN:HA	1.64	0.42
3:C:122:THR:HG22	3:C:189:ILE:CG1	2.50	0.42
1:A:11:VAL:HG21	1:A:392:LEU:HD12	2.01	0.42
1:A:100:LYS:HE3	2:B:370:MET:HE3	2.00	0.42
3:C:197:LEU:HD12	3:C:197:LEU:HA	1.86	0.42
3:C:303:LEU:HD23	3:C:303:LEU:HA	1.84	0.42
9:I:26:LEU:C	9:I:27:ARG:HG3	2.45	0.42
10:J:13:LEU:HD22	10:J:23:THR:HB	2.00	0.42
1:A:294:LEU:HG	1:A:307:PHE:CE1	2.55	0.42
2:B:365:LYS:HG2	2:B:399:LEU:HD22	2.01	0.42
3:C:8:HIS:HD2	3:C:10:LEU:H	1.67	0.42
5:E:122:HIS:O	5:E:125:GLU:HG2	2.20	0.42
10:J:50:LYS:HG3	10:J:51:LEU:N	2.33	0.42
2:B:227:ARG:HD3	2:B:228:GLY:N	2.34	0.42
3:C:80:ARG:HD2	3:C:81:TYR:CE1	2.55	0.42
3:C:284:ILE:HA	3:C:285:PRO:HD3	1.82	0.42
4:D:116:ILE:HD13	4:D:116:ILE:HA	1.79	0.42
5:E:45:VAL:HG13	10:J:28:ALA:HA	2.02	0.42
6:F:50:LEU:HA	6:F:51:PRO:HD3	1.93	0.42
1:A:359:ASN:ND2	1:A:362:ARG:HH11	2.17	0.42
1:A:398:ARG:HG2	14:A:522:HOH:O	2.20	0.42
2:B:354:ASN:H	2:B:355:PRO:CD	2.31	0.42
3:C:122:THR:HG22	3:C:189:ILE:HG12	2.01	0.42
4:D:21:LEU:HD13	4:D:26:ILE:HD11	2.00	0.42
4:D:69:GLU:HB3	4:D:82:MET:HG2	2.01	0.42
4:D:153:PHE:CE2	4:D:158:ILE:HG12	2.55	0.42
10:J:9:LEU:HD12	10:J:9:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:22:LEU:HA	11:K:27:VAL:HG22	2.01	0.42
11:K:41:ILE:H	11:K:41:ILE:HG12	1.70	0.42
1:A:34:THR:CG2	1:A:35:CYS:N	2.83	0.42
1:A:235:ARG:HE	1:A:235:ARG:HB3	1.63	0.42
3:C:69:ILE:O	3:C:73:VAL:HB	2.20	0.42
2:B:227:ARG:HH22	2:B:231:GLY:HA2	1.85	0.42
4:D:112:ASP:O	4:D:116:ILE:HG12	2.20	0.42
8:H:62:LEU:HD23	8:H:65:ARG:NH1	2.35	0.42
2:B:59:ASN:OD1	2:B:59:ASN:C	2.62	0.41
2:B:295:LEU:HD23	2:B:295:LEU:HA	1.84	0.41
3:C:361:LEU:HA	3:C:365:LEU:HB2	2.01	0.41
4:D:155:GLY:C	4:D:157:ALA:N	2.76	0.41
1:A:22:GLY:HA3	1:A:193:PRO:HG3	2.02	0.41
1:A:307:PHE:C	1:A:307:PHE:CD2	2.97	0.41
3:C:90:PHE:HD1	3:C:90:PHE:O	2.03	0.41
3:C:226:ILE:HD11	4:D:222:MET:HB3	2.01	0.41
2:B:52:LYS:HZ3	2:B:233:SER:HG	1.63	0.41
3:C:94:LEU:CD2	3:C:123:VAL:HG11	2.43	0.41
6:F:31:LEU:O	6:F:81:THR:HG21	2.21	0.41
1:A:435:ASN:ND2	3:C:223:TYR:OH	2.53	0.41
2:B:217:LYS:O	2:B:221:GLU:HG3	2.20	0.41
2:B:264:ILE:HD11	9:I:2:LEU:HA	2.02	0.41
4:D:6:HIS:HA	4:D:7:PRO:HD3	1.86	0.41
1:A:360:LEU:HD23	1:A:360:LEU:HA	1.82	0.41
3:C:337:TRP:HZ3	3:C:350:ILE:CD1	2.33	0.41
4:D:171:PHE:O	4:D:172:ASP:C	2.64	0.41
7:G:73:ASN:CB	7:G:74:PRO:CD	2.95	0.41
1:A:369:LEU:HD12	1:A:392:LEU:HD21	2.03	0.41
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.79	0.41
4:D:211:MET:HE1	10:J:31:PHE:HE2	1.82	0.41
1:A:390:ILE:HA	1:A:391:PRO:HD3	1.81	0.41
3:C:326:TRP:NE1	7:G:48:VAL:HG22	2.36	0.41
3:C:361:LEU:HA	3:C:361:LEU:HD12	1.79	0.41
6:F:38:HIS:HB3	14:F:1916:HOH:O	2.20	0.41
8:H:21:ARG:HG2	8:H:65:ARG:HE	1.86	0.41
8:H:73:LEU:O	8:H:75:ASN:N	2.54	0.41
1:A:443:TRP:CZ2	1:A:445:ARG:NH1	2.89	0.41
2:B:344:VAL:HG11	2:B:417:PHE:CD2	2.55	0.41
4:D:165:TYR:HD2	4:D:165:TYR:C	2.25	0.41
5:E:52:LYS:HB2	5:E:52:LYS:HE2	1.73	0.41
9:I:49:VAL:HG12	9:I:50:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:52:ARG:O	9:I:53:GLU:HB2	2.20	0.41
11:K:48:ILE:O	11:K:48:ILE:CG2	2.69	0.41
1:A:102:LEU:HD23	1:A:104:LYS:HE3	2.02	0.41
1:A:223:TYR:HB3	1:A:224:ASP:H	1.56	0.41
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.78	0.41
2:B:50:PHE:HB3	2:B:387:LEU:HD22	2.02	0.41
2:B:152:LEU:HG	2:B:158:HIS:CD2	2.56	0.41
2:B:435:PHE:O	2:B:436:ILE:CB	2.68	0.41
3:C:71:ARG:NH1	4:D:193:ALA:O	2.50	0.41
3:C:81:TYR:HD2	14:C:1440:HOH:O	2.04	0.41
3:C:319:PRO:HG3	7:G:47:ARG:HH12	1.85	0.41
4:D:7:PRO:HA	4:D:8:PRO:HD3	1.85	0.41
4:D:95:TYR:HA	4:D:96:PRO:HD3	1.94	0.41
4:D:120:ARG:HD3	4:D:120:ARG:HA	1.84	0.41
6:F:42:ASP:OD2	6:F:101:ARG:NH2	2.54	0.41
9:I:34:VAL:O	9:I:36:ALA:N	2.52	0.41
11:K:38:TRP:HD1	11:K:39:ARG:HG3	1.85	0.41
1:A:354:VAL:O	1:A:358:LYS:HG3	2.21	0.41
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.61	0.41
11:K:44:TRP:HD1	14:K:2610:HOH:O	2.03	0.41
2:B:29:LEU:HD23	2:B:29:LEU:HA	1.79	0.40
3:C:186:PRO:HA	3:C:189:ILE:HD12	2.03	0.40
4:D:178:THR:OG1	4:D:179:MET:N	2.53	0.40
10:J:24:ILE:HD12	10:J:24:ILE:C	2.46	0.40
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.68	0.40
1:A:329:MET:HE2	7:G:6:HIS:CE1	2.56	0.40
3:C:2:THR:HB	3:C:3:ASN:H	1.65	0.40
3:C:11:MET:O	3:C:12:LYS:C	2.64	0.40
3:C:77:TRP:CH2	4:D:201:ARG:HB3	2.55	0.40
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.96	0.40
1:A:395:TRP:CZ3	9:I:57:GLY:HA3	2.57	0.40
2:B:254:HIS:O	2:B:426:ALA:HA	2.21	0.40
3:C:65:SER:O	3:C:69:ILE:HG13	2.22	0.40
3:C:104:TYR:CE2	3:C:208:PRO:HA	2.56	0.40
3:C:215:VAL:HG23	7:G:8:THR:HG21	2.04	0.40
3:C:135:TRP:CE3	3:C:175:LEU:HG	2.57	0.40
3:C:236:ILE:HA	3:C:236:ILE:HD13	1.80	0.40
4:D:91:PHE:N	4:D:92:PRO:HD3	2.35	0.40
1:A:405:ARG:O	1:A:409:GLU:HB2	2.20	0.40
2:B:250:ASP:O	2:B:251:SER:HB3	2.20	0.40
3:C:122:THR:CG2	3:C:189:ILE:HG12	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:296:PHE:HD1	3:C:359:PHE:CE1	2.40	0.40
5:E:74:ILE:HG22	5:E:195:VAL:HB	2.03	0.40
9:I:56:ARG:HB3	9:I:57:GLY:H	1.72	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:549:HOH:O	14:B:586:HOH:O[6_565]	1.68	0.52

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	444/446 (100%)	408 (92%)	26 (6%)	10 (2%)	5	6
2	B	421/439 (96%)	386 (92%)	24 (6%)	11 (3%)	4	4
3	C	376/379 (99%)	330 (88%)	41 (11%)	5 (1%)	9	14
4	D	239/241 (99%)	185 (77%)	30 (13%)	24 (10%)	0	0
5	E	194/196 (99%)	175 (90%)	14 (7%)	5 (3%)	4	4
6	F	103/110 (94%)	98 (95%)	3 (3%)	2 (2%)	6	8
7	G	73/81 (90%)	64 (88%)	6 (8%)	3 (4%)	2	2
8	H	65/78 (83%)	53 (82%)	7 (11%)	5 (8%)	1	0
9	I	55/57 (96%)	22 (40%)	19 (34%)	14 (26%)	0	0
10	J	58/62 (94%)	45 (78%)	11 (19%)	2 (3%)	3	2
11	K	49/56 (88%)	41 (84%)	7 (14%)	1 (2%)	6	7
All	All	2077/2145 (97%)	1807 (87%)	188 (9%)	82 (4%)	2	2

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	GLY
1	A	227	ALA
2	B	171	ALA
2	B	305	GLN
2	B	436	ILE
3	C	268	ILE
3	C	345	HIS
4	D	71	GLN
4	D	76	GLU
4	D	80	MET
4	D	93	LYS
4	D	94	PRO
4	D	121	HIS
4	D	156	GLN
4	D	158	ILE
4	D	169	LEU
5	E	64	ALA
5	E	65	SER
5	E	70	ALA
5	E	72	SER
6	F	83	TYR
6	F	85	GLU
7	G	2	ARG
7	G	73	ASN
8	H	27	LEU
8	H	73	LEU
8	H	74	PHE
9	I	8	SER
9	I	51	CYS
9	I	53	GLU
1	A	21	ASN
1	A	224	ASP
4	D	96	PRO
4	D	108	ALA
4	D	145	GLU
4	D	159	GLY
4	D	170	GLU
7	G	3	GLN
9	I	3	SER
9	I	29	LEU
9	I	36	ALA
9	I	37	THR
9	I	39	GLU

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Mol	Chain	Res	Type
9	I	45	LEU
9	I	48	SER
10	J	51	LEU
1	A	220	SER
1	A	262	TRP
2	B	228	GLY
2	B	437	ASP
3	C	263	ASN
4	D	105	ASN
4	D	138	PRO
4	D	140	GLY
5	E	61	SER
9	I	5	ALA
9	I	43	LEU
1	A	107	PRO
1	A	192	ALA
2	B	41	TYR
2	B	236	LYS
4	D	38	SER
4	D	198	HIS
11	K	38	TRP
1	A	223	TYR
2	B	306	PRO
2	B	353	SER
2	B	354	ASN
4	D	146	GLY
4	D	172	ASP
8	H	49	GLN
3	C	264	THR
4	D	168	VAL
8	H	26	GLN
9	I	40	SER
10	J	48	GLU
4	D	70	VAL
2	B	54	GLY
1	A	286	GLY
4	D	54	VAL
9	I	34	VAL
3	C	364	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	329 (89%)	41 (11%)	6	9
2	B	332/343 (97%)	292 (88%)	40 (12%)	5	7
3	C	326/327 (100%)	276 (85%)	50 (15%)	3	3
4	D	206/206 (100%)	166 (81%)	40 (19%)	1	2
5	E	168/168 (100%)	152 (90%)	16 (10%)	8	13
6	F	96/98 (98%)	82 (85%)	14 (15%)	3	4
7	G	66/71 (93%)	56 (85%)	10 (15%)	3	3
8	H	64/74 (86%)	57 (89%)	7 (11%)	6	9
9	I	44/44 (100%)	33 (75%)	11 (25%)	0	1
10	J	46/52 (88%)	38 (83%)	8 (17%)	2	2
11	K	41/46 (89%)	33 (80%)	8 (20%)	1	2
All	All	1759/1799 (98%)	1514 (86%)	245 (14%)	3	4

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	17	SER
1	A	19	LEU
1	A	23	LEU
1	A	25	VAL
1	A	32	GLN
1	A	34	THR
1	A	37	VAL
1	A	42	ASP
1	A	49	SER
1	A	53	ASN
1	A	73	ASN
1	A	90	SER
1	A	113	LEU
1	A	117	VAL

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Mol	Chain	Res	Type
1	A	125	SER
1	A	126	GLN
1	A	127	ILE
1	A	131	ARG
1	A	176	LYS
1	A	188	ARG
1	A	203	LEU
1	A	208	LEU
1	A	209	LEU
1	A	215	HIS
1	A	217	SER
1	A	226	ASP
1	A	235	ARG
1	A	245	GLU
1	A	274	ASN
1	A	305	GLN
1	A	308	GLN
1	A	331	ILE
1	A	348	SER
1	A	366	VAL
1	A	383	LEU
1	A	388	ARG
1	A	398	ARG
1	A	418	GLN
1	A	430	GLN
1	A	439	SER
2	B	17	VAL
2	B	20	HIS
2	B	35	ILE
2	B	38	LEU
2	B	40	ASN
2	B	69	LEU
2	B	97	SER
2	B	98	VAL
2	B	99	THR
2	B	109	VAL
2	B	110	GLU
2	B	116	VAL
2	B	123	LEU
2	B	163	LEU
2	B	169	ARG
2	B	176	LEU

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Mol	Chain	Res	Type
2	B	186	VAL
2	B	189	VAL
2	B	197	ASN
2	B	209	LEU
2	B	219	VAL
2	B	226	ILE
2	B	227	ARG
2	B	230	LEU
2	B	232	LEU
2	B	244	ILE
2	B	248	ASN
2	B	257	LEU
2	B	273	SER
2	B	309	VAL
2	B	346	THR
2	B	358	GLN
2	B	371	SER
2	B	376	GLU
2	B	384	SER
2	B	397	THR
2	B	421	ARG
2	B	424	MET
2	B	436	ILE
2	B	437	ASP
3	C	4	ILE
3	C	6	LYS
3	C	10	LEU
3	C	18	PHE
3	C	19	ILE
3	C	26	ASN
3	C	39	ILE
3	C	42	ILE
3	C	45	ILE
3	C	46	LEU
3	C	51	LEU
3	C	64	SER
3	C	67	THR
3	C	78	ILE
3	C	96	MET
3	C	102	LEU
3	C	114	ASN
3	C	115	ILE

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Mol	Chain	Res	Type
3	C	131	TYR
3	C	156	ILE
3	C	158	THR
3	C	160	LEU
3	C	164	ILE
3	C	169	SER
3	C	171	ASP
3	C	175	LEU
3	C	177	ARG
3	C	197	LEU
3	C	215	VAL
3	C	241	LEU
3	C	242	LEU
3	C	243	VAL
3	C	252	ASP
3	C	254	ASP
3	C	262	LEU
3	C	267	HIS
3	C	268	ILE
3	C	280	ILE
3	C	284	ILE
3	C	303	LEU
3	C	304	ILE
3	C	309	THR
3	C	318	ARG
3	C	328	LEU
3	C	333	LEU
3	C	343	VAL
3	C	350	ILE
3	C	363	LEU
3	C	365	LEU
3	C	379	TRP
4	D	5	LEU
4	D	13	SER
4	D	17	LEU
4	D	20	SER
4	D	24	THR
4	D	37	CYS
4	D	42	SER
4	D	43	MET
4	D	44	ASP
4	D	55	CYS

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Mol	Chain	Res	Type
4	D	68	VAL
4	D	82	MET
4	D	95	TYR
4	D	99	GLU
4	D	105	ASN
4	D	109	LEU
4	D	112	ASP
4	D	114	SER
4	D	118	ARG
4	D	121	HIS
4	D	130	LEU
4	D	131	LEU
4	D	132	THR
4	D	135	CYS
4	D	141	VAL
4	D	143	LEU
4	D	156	GLN
4	D	158	ILE
4	D	166	ASN
4	D	169	LEU
4	D	170	GLU
4	D	178	THR
4	D	179	MET
4	D	182	VAL
4	D	190	LEU
4	D	212	MET
4	D	214	LEU
4	D	223	LYS
4	D	228	SER
4	D	241	LYS
5	E	7	VAL
5	E	19	LEU
5	E	24	SER
5	E	27	GLU
5	E	52	LYS
5	E	54	VAL
5	E	59	VAL
5	E	60	SER
5	E	61	SER
5	E	63	SER
5	E	65	SER
5	E	71	MET

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Mol	Chain	Res	Type
5	E	79	SER
5	E	113	GLU
5	E	140	THR
5	E	184	SER
6	F	27	ASN
6	F	37	ILE
6	F	53	ASN
6	F	59	VAL
6	F	64	ARG
6	F	73	GLN
6	F	74	ILE
6	F	77	LYS
6	F	78	GLU
6	F	81	THR
6	F	84	GLU
6	F	90	LEU
6	F	94	LEU
6	F	110	LYS
7	G	2	ARG
7	G	17	SER
7	G	31	SER
7	G	34	ILE
7	G	37	VAL
7	G	39	ARG
7	G	45	ILE
7	G	53	VAL
7	G	60	THR
7	G	68	LYS
8	H	37	LEU
8	H	49	GLN
8	H	52	GLU
8	H	65	ARG
8	H	68	CYS
8	H	73	LEU
8	H	77	LEU
9	I	8	SER
9	I	15	LEU
9	I	18	THR
9	I	20	ARG
9	I	22	VAL
9	I	26	LEU
9	I	27	ARG

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Mol	Chain	Res	Type
9	I	30	VAL
9	I	43	LEU
9	I	47	ARG
9	I	49	VAL
10	J	1	VAL
10	J	4	THR
10	J	6	THR
10	J	18	SER
10	J	23	THR
10	J	24	ILE
10	J	26	VAL
10	J	45	HIS
11	K	4	ARG
11	K	12	GLN
11	K	18	VAL
11	K	20	THR
11	K	23	LEU
11	K	24	TRP
11	K	39	ARG
11	K	41	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	29	GLN
1	A	32	GLN
1	A	52	ASN
1	A	85	HIS
1	A	94	HIS
1	A	118	GLN
1	A	136	GLN
1	A	141	ASN
1	A	173	ASN
1	A	252	HIS
1	A	274	ASN
1	A	305	GLN
1	A	308	GLN
1	A	323	HIS
1	A	328	HIS
1	A	341	GLN
1	A	359	ASN

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Mol	Chain	Res	Type
1	A	368	HIS
1	A	418	GLN
1	A	430	GLN
1	A	435	ASN
2	B	104	ASN
2	B	143	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	305	GLN
2	B	313	ASN
2	B	342	ASN
2	B	343	GLN
2	B	362	ASN
2	B	385	GLN
2	B	412	ASN
2	B	432	HIS
3	C	8	HIS
3	C	32	ASN
3	C	44	GLN
3	C	85	ASN
3	C	114	ASN
3	C	159	ASN
3	C	206	ASN
3	C	312	GLN
3	C	322	GLN
3	C	345	HIS
3	C	352	GLN
4	D	23	HIS
4	D	71	GLN
4	D	75	ASN
4	D	97	ASN
4	D	105	ASN
4	D	106	ASN
4	D	121	HIS
4	D	156	GLN
4	D	166	ASN
5	E	53	ASN
5	E	57	GLN

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Mol	Chain	Res	Type
5	E	149	ASN
6	F	53	ASN
7	G	6	HIS
7	G	64	GLN
8	H	63	HIS
8	H	75	ASN
11	K	12	GLN
11	K	16	ASN
11	K	22	GLN
11	K	49	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	HEM	D	242	4	50,50,50	3.45	26 (52%)	67,82,82	2.65	31 (46%)
12	HEM	C	382	3	50,50,50	3.38	22 (44%)	67,82,82	2.47	26 (38%)
13	FES	E	197	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	HEM	C	381	3	50,50,50	3.46	27 (54%)	67,82,82	2.70	26 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HEM	D	242	4	-	4/14/54/54	-
12	HEM	C	382	3	-	9/14/54/54	-
13	FES	E	197	5	-	-	0/1/1/1
12	HEM	C	381	3	-	8/14/54/54	-

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	C4D-C3D	-7.71	1.32	1.45
12	C	382	HEM	C3C-C4C	-7.55	1.32	1.46
12	C	381	HEM	C3C-C4C	-7.13	1.33	1.46
12	D	242	HEM	C4D-C3D	-6.96	1.33	1.45
12	D	242	HEM	C3C-C4C	-6.88	1.34	1.46
12	C	381	HEM	C1C-C2C	-6.36	1.32	1.45
12	D	242	HEM	C1C-C2C	-6.32	1.32	1.45
12	C	382	HEM	C1C-C2C	-6.26	1.32	1.45
12	D	242	HEM	C1B-C2B	-6.26	1.31	1.44
12	D	242	HEM	CHC-C1C	6.10	1.50	1.38
12	C	381	HEM	CHD-C4C	6.08	1.50	1.38
12	C	381	HEM	FE-NA	6.07	2.15	1.95
12	D	242	HEM	CHD-C4C	6.03	1.50	1.38
12	C	382	HEM	C3B-C4B	-5.97	1.33	1.44
12	C	382	HEM	C4D-C3D	-5.97	1.34	1.45
12	C	382	HEM	C1B-C2B	-5.89	1.32	1.44
12	C	382	HEM	CHD-C4C	5.81	1.49	1.38
12	D	242	HEM	FE-NA	5.81	2.14	1.95
12	D	242	HEM	C3B-C4B	-5.78	1.33	1.44
12	C	382	HEM	CHA-C4D	5.75	1.50	1.38
12	C	382	HEM	CHC-C1C	5.74	1.49	1.38
12	C	381	HEM	C3B-C4B	-5.68	1.33	1.44
12	C	382	HEM	FE-NA	5.62	2.13	1.95
12	C	382	HEM	C1D-C2D	-5.59	1.33	1.44
12	D	242	HEM	C1D-C2D	-5.26	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	CHA-C4D	5.14	1.48	1.38
12	C	381	HEM	CHC-C1C	5.09	1.48	1.38
12	C	381	HEM	C1D-C2D	-5.05	1.34	1.44
12	C	381	HEM	CHC-C4B	4.95	1.50	1.39
12	D	242	HEM	CBC-CAC	4.93	1.54	1.30
12	C	381	HEM	CHB-C1B	4.90	1.48	1.38
12	D	242	HEM	CHB-C1B	4.89	1.48	1.38
12	C	381	HEM	C1B-C2B	-4.84	1.34	1.44
12	D	242	HEM	CBB-CAB	4.79	1.53	1.30
12	C	382	HEM	CBB-CAB	4.75	1.53	1.30
12	C	382	HEM	CHB-C4A	4.64	1.49	1.39
12	D	242	HEM	CHC-C4B	4.60	1.49	1.39
12	C	381	HEM	CBC-CAC	4.59	1.52	1.30
12	D	242	HEM	CHA-C4D	4.57	1.47	1.38
12	C	381	HEM	CBB-CAB	4.57	1.52	1.30
12	C	382	HEM	CBC-CAC	4.53	1.52	1.30
12	C	382	HEM	CHD-C1D	4.53	1.49	1.39
12	C	382	HEM	CHA-C1A	4.53	1.49	1.39
12	D	242	HEM	CHD-C1D	4.47	1.49	1.39
12	C	382	HEM	CHB-C1B	4.39	1.47	1.38
12	C	381	HEM	CHD-C1D	4.28	1.48	1.39
12	D	242	HEM	CHB-C4A	4.25	1.48	1.39
12	C	381	HEM	CHA-C1A	4.24	1.48	1.39
12	C	381	HEM	CHB-C4A	3.96	1.48	1.39
12	C	382	HEM	CHC-C4B	3.90	1.48	1.39
12	D	242	HEM	CHA-C1A	3.87	1.48	1.39
12	D	242	HEM	C2A-C3A	3.14	1.47	1.38
12	C	381	HEM	C2A-C3A	3.02	1.46	1.38
12	C	382	HEM	O2A-CGA	-2.98	1.21	1.30
12	C	381	HEM	C3C-C2C	-2.94	1.31	1.37
12	C	381	HEM	C1A-C2A	2.86	1.50	1.44
12	C	382	HEM	C2A-C3A	2.83	1.46	1.38
12	D	242	HEM	O2D-CGD	-2.71	1.21	1.30
12	D	242	HEM	O2A-CGA	-2.63	1.22	1.30
12	C	381	HEM	C4B-NB	2.58	1.43	1.38
12	C	381	HEM	C3B-C2B	-2.55	1.32	1.37
12	C	381	HEM	O2A-CGA	-2.54	1.22	1.30
12	C	381	HEM	C1C-NC	2.50	1.44	1.39
12	C	382	HEM	O2D-CGD	-2.46	1.22	1.30
12	D	242	HEM	C3D-C2D	-2.44	1.31	1.36
12	C	382	HEM	C4A-NA	-2.35	1.35	1.39
12	D	242	HEM	C3C-C2C	-2.28	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	O2D-CGD	-2.28	1.23	1.30
12	C	382	HEM	C1A-C2A	2.28	1.49	1.44
12	D	242	HEM	C1A-NA	-2.27	1.35	1.39
12	C	381	HEM	C4A-C3A	2.22	1.48	1.43
12	D	242	HEM	C4A-C3A	2.20	1.48	1.43
12	D	242	HEM	CAC-C3C	2.05	1.52	1.47
12	C	381	HEM	C1D-ND	2.04	1.42	1.38
12	D	242	HEM	C1C-NC	2.01	1.43	1.39

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	382	HEM	C4C-CHD-C1D	-7.15	110.82	126.02
12	C	381	HEM	C1C-CHC-C4B	-6.92	111.32	126.02
12	D	242	HEM	C1C-CHC-C4B	-6.53	112.14	126.02
12	C	381	HEM	C4C-CHD-C1D	-6.29	112.65	126.02
12	D	242	HEM	C4C-CHD-C1D	-6.11	113.03	126.02
12	C	382	HEM	C1C-CHC-C4B	-6.07	113.12	126.02
12	C	382	HEM	C4A-CHB-C1B	-5.53	113.24	126.25
12	C	381	HEM	C4D-ND-C1D	-5.51	98.68	105.21
12	D	242	HEM	C4A-CHB-C1B	-5.46	113.40	126.25
12	C	382	HEM	CHB-C4A-NA	5.30	133.47	123.86
12	C	381	HEM	C4A-CHB-C1B	-5.18	114.08	126.25
12	C	381	HEM	C1A-CHA-C4D	-5.06	114.35	126.25
12	D	242	HEM	CHB-C4A-NA	5.02	132.97	123.86
12	D	242	HEM	CHA-C1A-NA	5.00	132.94	123.86
12	D	242	HEM	C1A-CHA-C4D	-4.96	114.59	126.25
12	C	381	HEM	CHB-C4A-NA	4.86	132.68	123.86
12	C	381	HEM	CHC-C4B-NB	4.71	129.50	124.42
12	D	242	HEM	CHB-C1B-NB	4.69	130.17	124.37
12	C	381	HEM	C1B-NB-C4B	-4.66	99.69	105.21
12	C	382	HEM	C4A-NA-C1A	4.64	113.38	105.82
12	D	242	HEM	C4D-ND-C1D	-4.41	99.98	105.21
12	D	242	HEM	CHC-C1C-NC	4.27	129.10	124.45
12	D	242	HEM	C1B-NB-C4B	-3.98	100.50	105.21
12	D	242	HEM	C4A-NA-C1A	3.93	112.22	105.82
12	C	382	HEM	CAA-C2A-C1A	3.91	132.57	124.94
12	C	381	HEM	C4C-C3C-C2C	3.90	110.20	106.81
12	C	381	HEM	CBB-CAB-C3B	-3.89	108.08	127.53
12	C	381	HEM	C4A-NA-C1A	3.84	112.08	105.82
12	C	381	HEM	C4C-NC-C1C	-3.81	99.60	105.82
12	C	381	HEM	CHA-C4D-C3D	-3.79	118.25	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	382	HEM	C1A-CHA-C4D	-3.76	117.41	126.25
12	C	381	HEM	CHA-C4D-ND	3.73	128.98	124.37
12	C	381	HEM	CBC-CAC-C3C	-3.70	109.02	127.53
12	C	381	HEM	C4B-C3B-C2B	3.59	110.58	107.28
12	C	382	HEM	CHC-C1C-NC	3.56	128.33	124.45
12	C	382	HEM	CHB-C1B-NB	3.43	128.62	124.37
12	C	382	HEM	CHC-C4B-NB	3.35	128.02	124.42
12	C	382	HEM	CHA-C1A-NA	3.34	129.93	123.86
12	D	242	HEM	CHC-C4B-NB	3.33	128.01	124.42
12	D	242	HEM	CBC-CAC-C3C	-3.29	111.08	127.53
12	C	381	HEM	CHB-C1B-NB	3.26	128.40	124.37
12	C	382	HEM	CHD-C1D-ND	3.26	127.93	124.42
12	C	381	HEM	CHA-C1A-NA	3.26	129.77	123.86
12	C	382	HEM	C4C-NC-C1C	-3.23	100.56	105.82
12	D	242	HEM	CHA-C1A-C2A	-3.20	118.30	125.30
12	C	382	HEM	C1B-NB-C4B	-3.10	101.53	105.21
12	D	242	HEM	C4C-NC-C1C	-3.10	100.77	105.82
12	D	242	HEM	C3B-C2B-C1B	3.07	108.72	106.41
12	D	242	HEM	CHB-C1B-C2B	-3.05	118.27	126.95
12	C	381	HEM	CHB-C4A-C3A	-3.05	118.57	127.43
12	D	242	HEM	CHA-C4D-ND	3.03	128.11	124.37
12	D	242	HEM	CHB-C4A-C3A	-3.01	118.70	127.43
12	C	382	HEM	CHB-C4A-C3A	-2.99	118.75	127.43
12	D	242	HEM	CHD-C4C-NC	2.93	127.64	124.45
12	C	381	HEM	CHD-C4C-NC	2.90	127.61	124.45
12	D	242	HEM	C3C-C2C-C1C	2.87	109.76	107.05
12	C	382	HEM	CBB-CAB-C3B	-2.84	113.35	127.53
12	C	382	HEM	CBC-CAC-C3C	-2.81	113.49	127.53
12	D	242	HEM	CHA-C4D-C3D	-2.81	120.05	125.23
12	D	242	HEM	CHD-C1D-ND	2.79	127.42	124.42
12	C	381	HEM	CHC-C1C-NC	2.72	127.41	124.45
12	C	382	HEM	C1D-C2D-C3D	2.63	109.75	106.98
12	C	382	HEM	O2A-CGA-CBA	2.59	122.19	114.00
12	C	381	HEM	CHB-C1B-C2B	-2.59	119.60	126.95
12	C	382	HEM	C3B-C2B-C1B	2.57	108.34	106.41
12	D	242	HEM	C1D-C2D-C3D	2.50	109.61	106.98
12	C	382	HEM	CHC-C1C-C2C	-2.49	120.31	125.49
12	C	382	HEM	C2A-C1A-NA	-2.49	107.39	110.15
12	C	381	HEM	CHC-C4B-C3B	-2.47	120.15	125.07
12	D	242	HEM	C4C-C3C-C2C	2.41	108.90	106.81
12	D	242	HEM	CHC-C1C-C2C	-2.35	120.59	125.49
12	C	382	HEM	CHB-C1B-C2B	-2.30	120.42	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	382	HEM	C4B-C3B-C2B	2.27	109.36	107.28
12	D	242	HEM	CBB-CAB-C3B	-2.23	116.40	127.53
12	D	242	HEM	CAA-CBA-CGA	-2.21	107.80	113.67
12	C	381	HEM	CAA-C2A-C1A	2.20	129.24	124.94
12	C	382	HEM	CAA-C2A-C3A	-2.16	122.22	127.07
12	C	381	HEM	CHD-C1D-C2D	-2.09	121.73	125.03
12	C	381	HEM	CHC-C1C-C2C	-2.08	121.15	125.49
12	D	242	HEM	CHD-C1D-C2D	-2.03	121.82	125.03
12	D	242	HEM	O2D-CGD-CBD	2.02	120.38	114.00
12	C	382	HEM	CHA-C4D-ND	2.02	126.86	124.37
12	D	242	HEM	CHD-C4C-C3C	-2.02	121.81	125.21

There are no chirality outliers.

All (21) torsion outliers are listed below:

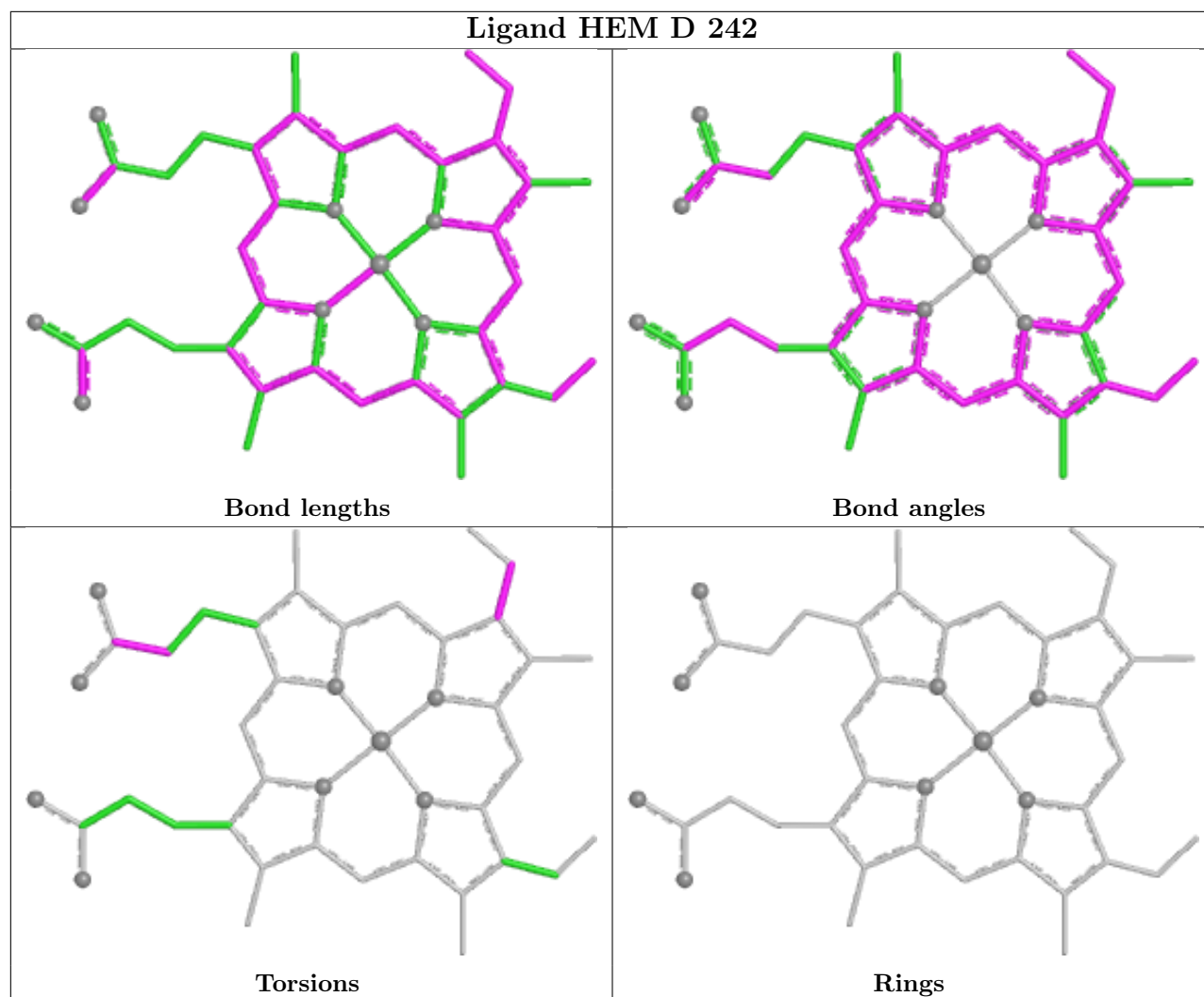
Mol	Chain	Res	Type	Atoms
12	C	381	HEM	C2B-C3B-CAB-CBB
12	C	381	HEM	C4B-C3B-CAB-CBB
12	C	381	HEM	C2C-C3C-CAC-CBC
12	C	381	HEM	C4C-C3C-CAC-CBC
12	C	382	HEM	C1A-C2A-CAA-CBA
12	C	382	HEM	C3A-C2A-CAA-CBA
12	C	382	HEM	C2B-C3B-CAB-CBB
12	D	242	HEM	C2C-C3C-CAC-CBC
12	D	242	HEM	C4C-C3C-CAC-CBC
12	C	382	HEM	C4B-C3B-CAB-CBB
12	C	382	HEM	C2A-CAA-CBA-CGA
12	C	381	HEM	C3D-CAD-CBD-CGD
12	C	382	HEM	C2C-C3C-CAC-CBC
12	C	381	HEM	C2A-CAA-CBA-CGA
12	C	381	HEM	CAD-CBD-CGD-O1D
12	C	381	HEM	CAD-CBD-CGD-O2D
12	D	242	HEM	CAD-CBD-CGD-O1D
12	D	242	HEM	CAD-CBD-CGD-O2D
12	C	382	HEM	CAD-CBD-CGD-O2D
12	C	382	HEM	C4C-C3C-CAC-CBC
12	C	382	HEM	CAD-CBD-CGD-O1D

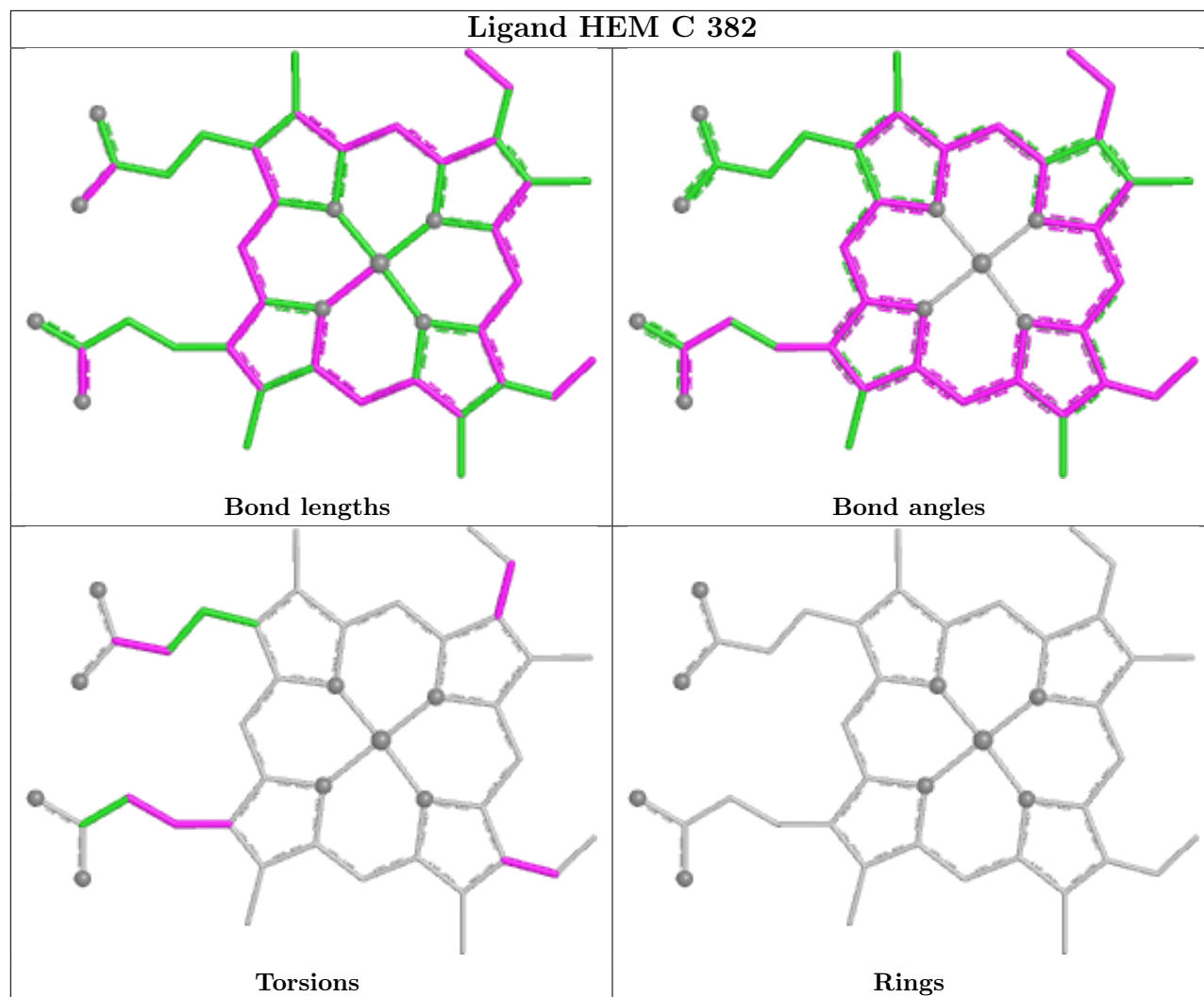
There are no ring outliers.

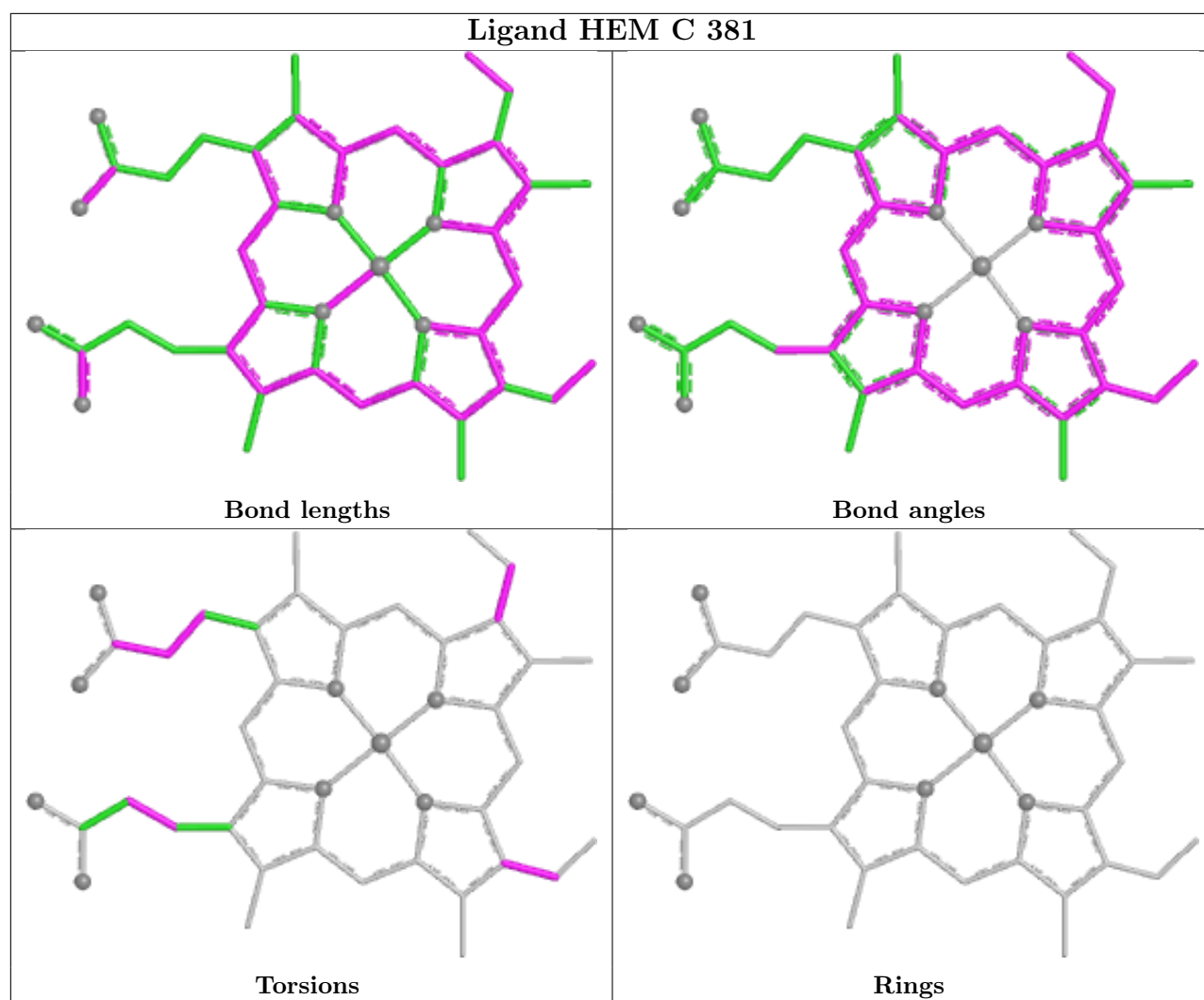
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	242	HEM	3	0
12	C	382	HEM	5	0
12	C	381	HEM	5	0

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







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.