



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:53 AM GMT

PDB ID : 1NTM
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

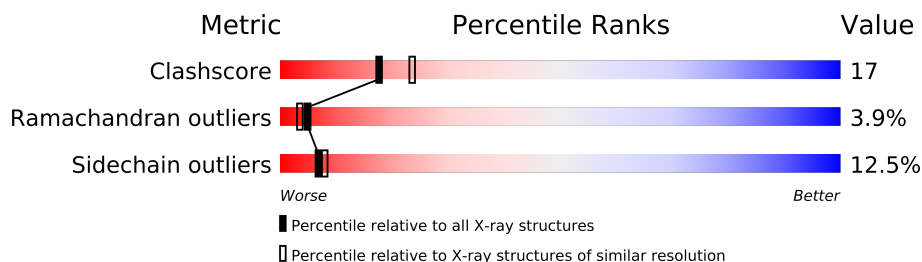
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	
2	B	439	
3	C	379	
4	D	241	
5	E	196	
6	F	110	
7	G	81	
8	H	78	
9	I	57	
10	J	62	
11	K	56	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 17049 atoms, of which 0 are hydrogen and 0 are deuterium.

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:

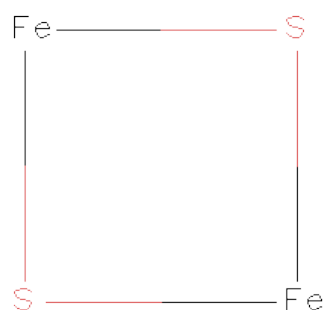
Chain	Residue	Modelled	Actual	Comment	Reference
K	22	GLN	SER	SEE REMARK 999	UNP P07552

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



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 (three-letter code: FES) (formula: Fe₂S₂).



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

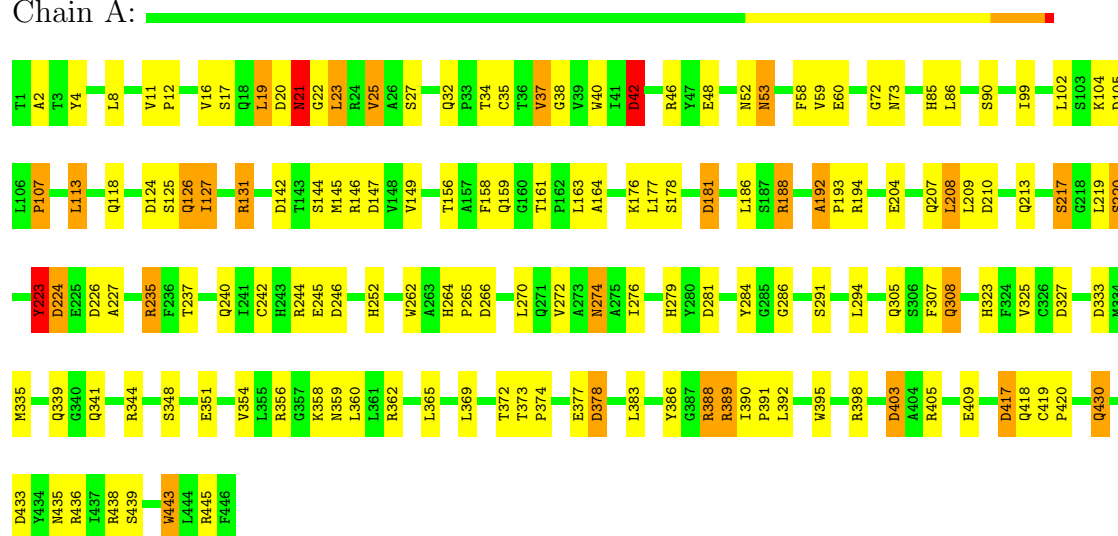
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

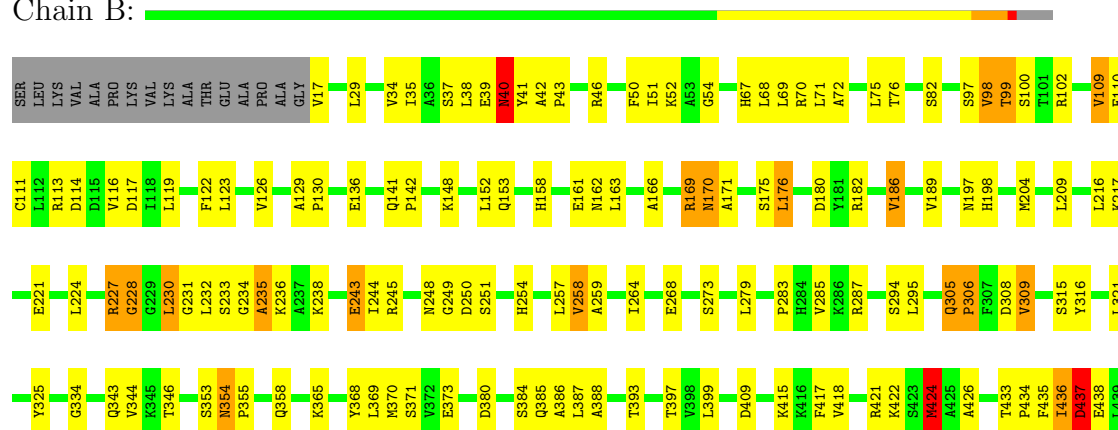
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Chain A:



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

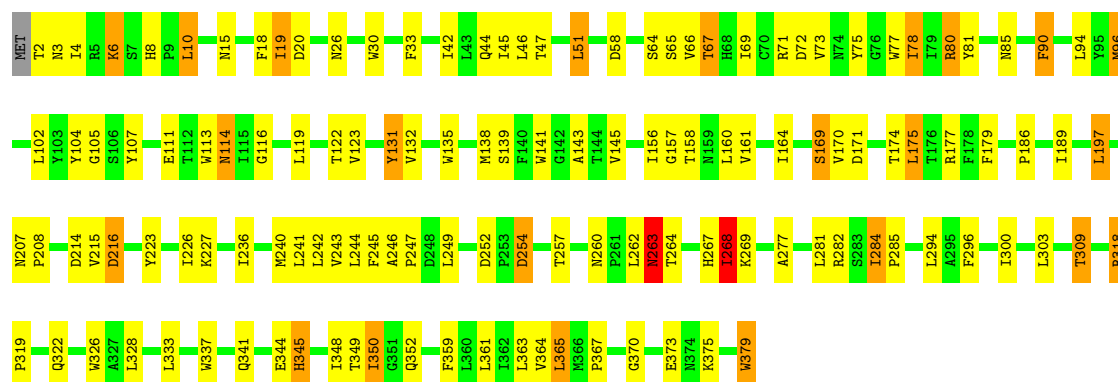
Chain B:



- Molecule 3: Cytochrome b

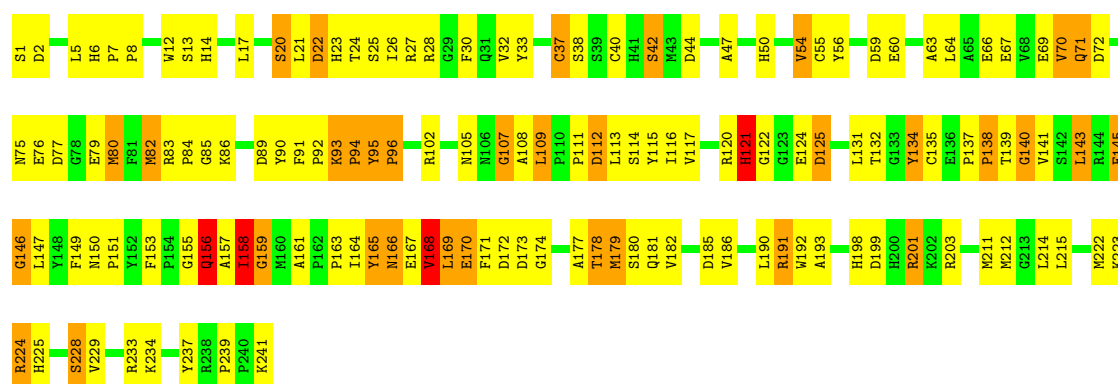
Chain C:





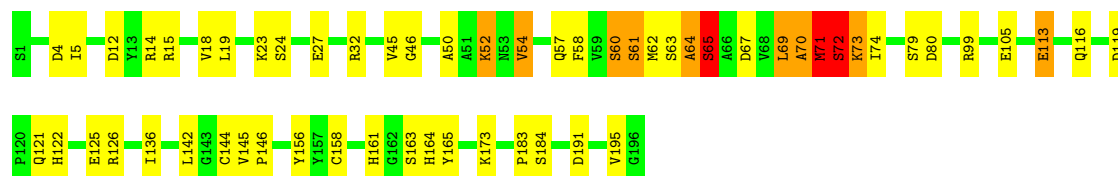
• Molecule 4: cytochrome c1

Chain D:



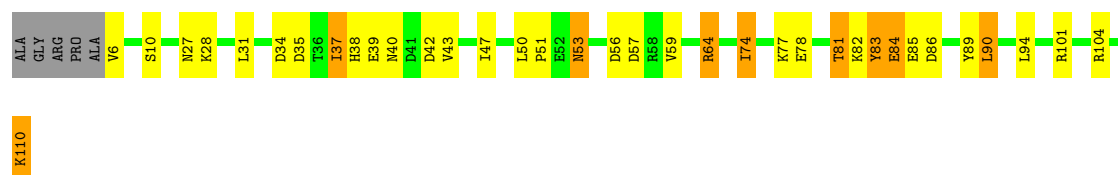
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, mitochondrial

Chain E:



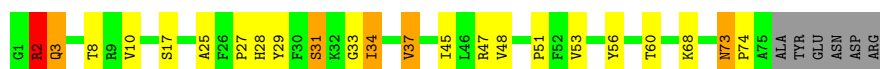
• Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F:



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

Chain G:



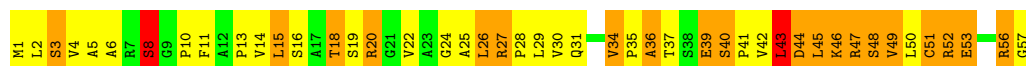
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H:



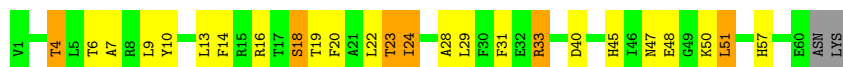
- Molecule 9: Ubiquinol-cytochrome C reductase 8 kDa protein

Chain I:



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

Chain J:



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

Chain K:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	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 i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.68	0/3531	0.91	16/4792 (0.3%)
2	B	0.85	2/3232 (0.1%)	0.93	10/4386 (0.2%)
3	C	0.64	1/3100 (0.0%)	0.84	6/4242 (0.1%)
4	D	0.56	0/1977	0.97	15/2684 (0.6%)
5	E	0.51	0/1553	0.90	10/2100 (0.5%)
6	F	0.79	0/930	0.93	3/1246 (0.2%)
7	G	0.67	0/649	0.78	0/878
8	H	0.47	0/553	0.90	5/741 (0.7%)
9	I	0.87	0/411	1.33	4/558 (0.7%)
10	J	0.59	0/490	0.82	1/665 (0.2%)
11	K	0.53	0/436	0.83	2/598 (0.3%)
All	All	0.68	3/16862 (0.0%)	0.91	72/22890 (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	1	0
4	D	1	0
7	G	1	0
9	I	2	0
All	All	6	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	424	MET	SD-CE	-6.85	1.39	1.77
2	B	258	VAL	CB-CG1	-6.53	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	379	TRP	CB-CG	-5.18	1.41	1.50

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	159	GLY	N-CA-C	8.66	134.76	113.10
5	E	71	MET	N-CA-C	8.40	133.67	111.00
6	F	34	ASP	CB-CG-OD2	7.77	125.29	118.30
2	B	114	ASP	CB-CG-OD2	7.47	125.02	118.30
4	D	122	GLY	N-CA-C	-7.27	94.92	113.10
5	E	73	LYS	N-CA-C	-7.18	91.62	111.00
1	A	266	ASP	CB-CG-OD2	6.93	124.54	118.30
4	D	158	ILE	N-CA-C	6.88	129.57	111.00
8	H	53	ASP	N-CA-C	6.43	128.37	111.00
2	B	170	ASN	N-CA-CB	-6.25	99.35	110.60
4	D	72	ASP	CB-CG-OD2	6.14	123.83	118.30
2	B	309	VAL	CB-CA-C	-6.08	99.84	111.40
4	D	107	GLY	N-CA-C	-6.08	97.91	113.10
4	D	185	ASP	CB-CG-OD2	6.06	123.76	118.30
1	A	403	ASP	CB-CG-OD2	6.04	123.74	118.30
10	J	40	ASP	CB-CG-OD2	6.02	123.71	118.30
3	C	268	ILE	N-CA-C	5.92	126.99	111.00
1	A	210	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	327	ASP	CB-CG-OD2	5.85	123.56	118.30
3	C	58	ASP	CB-CG-OD2	5.82	123.54	118.30
9	I	44	ASP	CB-CG-OD2	5.82	123.54	118.30
5	E	69	LEU	N-CA-C	-5.80	95.33	111.00
6	F	56	ASP	CB-CG-OD2	5.80	123.52	118.30
4	D	146	GLY	N-CA-C	-5.79	98.62	113.10
2	B	182	ARG	NE-CZ-NH1	-5.78	117.41	120.30
11	K	37	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	105	ASP	CB-CG-OD2	5.78	123.50	118.30
2	B	117	ASP	CB-CG-OD2	5.76	123.49	118.30
2	B	380	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	37	VAL	CB-CA-C	-5.68	100.61	111.40
1	A	333	ASP	CB-CG-OD2	5.68	123.41	118.30
2	B	409	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	378	ASP	CB-CG-OD2	5.66	123.39	118.30
4	D	59	ASP	CB-CG-OD2	5.66	123.39	118.30
9	I	26	LEU	N-CA-C	5.62	126.16	111.00
4	D	173	ASP	CB-CG-OD2	5.60	123.34	118.30
5	E	23	LYS	N-CA-C	5.59	126.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	60	ASP	CB-CG-OD2	5.59	123.33	118.30
4	D	125	ASP	CB-CG-OD2	5.58	123.32	118.30
8	H	27	LEU	N-CA-C	5.57	126.05	111.00
4	D	44	ASP	CB-CG-OD2	5.55	123.30	118.30
8	H	53	ASP	CB-CG-OD2	5.50	123.25	118.30
11	K	43	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	42	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	181	ASP	CB-CG-OD2	5.40	123.16	118.30
3	C	345	HIS	N-CA-C	5.40	125.58	111.00
1	A	417	ASP	CB-CG-OD2	5.39	123.15	118.30
5	E	72	SER	N-CA-C	5.38	125.54	111.00
1	A	20	ASP	CB-CG-OD2	5.37	123.13	118.30
2	B	235	ALA	N-CA-C	-5.35	96.56	111.00
4	D	2	ASP	CB-CG-OD2	5.34	123.11	118.30
9	I	46	LYS	N-CA-C	5.31	125.34	111.00
5	E	4	ASP	CB-CG-OD2	5.27	123.04	118.30
5	E	80	ASP	CB-CG-OD2	5.27	123.04	118.30
4	D	22	ASP	CB-CG-OD2	5.25	123.02	118.30
6	F	57	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	142	ASP	CB-CG-OD2	5.14	122.92	118.30
8	H	66	ASP	CB-CG-OD2	5.13	122.92	118.30
5	E	119	ASP	CB-CG-OD2	5.13	122.92	118.30
9	I	52	ARG	N-CA-C	5.13	124.86	111.00
2	B	234	GLY	N-CA-C	5.11	125.87	113.10
4	D	199	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	147	ASP	CB-CG-OD2	5.09	122.88	118.30
4	D	168	VAL	N-CA-C	-5.09	97.27	111.00
1	A	433	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	192	ALA	N-CA-C	5.06	124.67	111.00
2	B	40	ASN	N-CA-C	-5.05	97.36	111.00
3	C	254	ASP	CB-CG-OD2	5.04	122.83	118.30
5	E	191	ASP	CB-CG-OD2	5.04	122.83	118.30
3	C	72	ASP	CB-CG-OD2	5.02	122.82	118.30
5	E	12	ASP	CB-CG-OD2	5.00	122.80	118.30
3	C	216	ASP	CB-CG-OD2	5.00	122.80	118.30

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

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Mol	Chain	Res	Type	Atom
7	G	2	ARG	CA
9	I	25	ALA	CA
9	I	42	VAL	CA

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	99	0
2	B	3172	0	3152	114	0
3	C	3003	0	3065	106	0
4	D	1918	0	1870	114	0
5	E	1519	0	1503	37	0
6	F	911	0	904	25	0
7	G	628	0	636	21	0
8	H	548	0	532	11	0
9	I	406	0	437	80	0
10	J	478	0	463	28	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
14	A	99	0	0	11	0
14	B	152	0	0	13	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	571	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (571) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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:O	4:D:165:TYR:HD2	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
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
9:I:46:LYS:HG2	9:I:47:ARG:N	1.88	0.88
3:C:111:GLU:HG2	14:C:1052:HOH:O	1.71	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:234:LYS:NZ	14:D:1404:HOH:O	1.89	0.82
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
4:D:168:VAL:O	4:D:169:LEU:HB2	1.86	0.76
9:I:20:ARG:HG3	9:I:51:CYS:CB	2.16	0.76
3:C:257:THR:HG22	4:D:115:TYR:HE1	1.50	0.76
4:D:165:TYR:O	4:D:165:TYR:CD2	2.37	0.75
5:E:18:VAL:O	5:E:18:VAL:HG12	1.86	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
4:D:169:LEU:CD1	4:D:177:ALA:CB	2.64	0.74
1:A:144:SER:HA	9:I:42:VAL:HB	1.70	0.74
5:E:64:ALA:O	5:E:65:SER:HB2	1.85	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
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:82:LYS:C	6:F:83:TYR:O	2.23	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:315:SER:O	9:I:4:VAL:HG13	1.90	0.72
2:B:100:SER:O	9:I:13:PRO:HD2	1.89	0.72
9:I:11:PHE:HZ	9:I:27:ARG:HH21	1.38	0.71
10:J:19:THR:O	10:J:23:THR:HG22	1.91	0.71
4:D:54:VAL:HG21	4:D:192:TRP:CZ2	2.26	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
1:A:145:MET:O	1:A:149:VAL:HG23	1.90	0.71
3:C:15:ASN:HA	3:C:19:ILE:HG13	1.73	0.70
1:A:378:ASP:OD2	1:A:389:ARG:NH1	2.24	0.70
2:B:161:GLU:OE1	2:B:175:SER:OG	2.08	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:76:THR:HG23	2:B:136:GLU:OE1	1.92	0.70
1:A:351:GLU:H	11:K:12:GLN:HE21	1.40	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: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
4:D:169:LEU:HD11	4:D:177:ALA:HB2	1.74	0.67
2:B:111:CYS:HB3	2:B:119:LEU:CD1	2.24	0.67
4:D:225:HIS:O	4:D:228:SER:HB2	1.94	0.67
2:B:198:HIS:NE2	14:B:490:HOH:O	2.28	0.67
1:A:308:GLN:HE21	1:A:323:HIS:HD2	1.43	0.66
5:E:69:LEU:C	5:E:70:ALA:O	2.33	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
9:I:6:ALA:C	9:I:8:SER:H	2.00	0.65
9:I:18:THR:OG1	9:I:53:GLU:OE2	2.11	0.65
2:B:111:CYS:SG	2:B:119:LEU:HD12	2.36	0.65
4:D:149:PHE:O	14:D:1443:HOH:O	2.15	0.65
4:D:27:ARG:HH12	10:J:57:HIS:CD2	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:HH11	2:B:46:ARG:HG3	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.81	0.63
9:I:47:ARG:HD2	9:I:48:SER:H	1.64	0.63
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.34	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:HH11	1:A:188:ARG:HB3	1.63	0.62
3:C:15:ASN:HA	3:C:19:ILE:HG12	1.80	0.62
4:D:47:ALA:N	4:D:50:HIS:HD2	1.98	0.61
3:C:75:TYR:HB3	3:C:78:ILE:HD11	1.82	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
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
4:D:28:ARG:O	4:D:32:VAL:HG23	2.00	0.60
1:A:19:LEU:HB3	1:A:21:ASN:HB2	1.83	0.60
4:D:90:TYR:C	4:D:92:PRO:HD3	2.22	0.60
5:E:69:LEU:O	5:E:70:ALA:O	2.18	0.60
1:A:274:ASN:ND2	14:A:466:HOH:O	2.33	0.60
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.33	0.60
4:D:28:ARG:HB3	4:D:171:PHE:HE2	1.67	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:337:TRP:HZ3	3:C:350:ILE:HD11	1.66	0.59
3:C:119:LEU:HD22	12:C:382:HEM:HBB2	1.84	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
2:B:153:GLN:NE2	9:I:46:LYS:HG3	2.18	0.59
1:A:158:PHE:O	1:A:164:ALA:HB2	2.03	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:258:VAL:HG12	2:B:259:ALA:N	2.17	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:249:GLY:CA	14:B:506:HOH:O	2.46	0.58
9:I:4:VAL:HG12	9:I:10:PRO:HG2	1.85	0.58
2:B:122:PHE:O	2:B:126:VAL:HG23	2.03	0.58
3:C:240:MET:HE2	3:C:240:MET:HA	1.86	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
2:B:161:GLU:CD	2:B:175:SER:HG	2.04	0.58
3:C:51:LEU:HD21	3:C:80:ARG:HA	1.86	0.58
11:K:48:ILE:HG22	11:K:48:ILE:O	2.04	0.58
1:A:240:GLN:NE2	1:A:242:CYS:SG	2.70	0.58
3:C:309:THR:CG2	3:C:370:GLY:HA3	2.34	0.57
1:A:272:VAL:O	1:A:276:ILE:HG13	2.03	0.57
4:D:60:GLU:O	4:D:64:LEU:HG	2.02	0.57
8:H:38:GLU:HA	8:H:41:ASP:HB2	1.86	0.57
1:A:156:THR:O	1:A:159:GLN:HG3	2.04	0.57
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
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
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:224:ARG:HB3	7:G:25:ALA:HB1	1.86	0.56
9:I:42:VAL:O	9:I:43:LEU:HB2	2.05	0.56
1:A:2:ALA:O	2:B:113:ARG:HD3	2.06	0.56
3:C:131:TYR:CA	12:C:381:HEM:HAD2	2.35	0.56
2:B:46:ARG:NH1	2:B:46:ARG:HG3	2.20	0.56
3:C:75:TYR:CE2	5:E:57:GLN:HG2	2.41	0.56
4:D:167:GLU:HG2	4:D:168:VAL:O	2.05	0.56
1:A:146:ARG:NH2	14:A:486:HOH:O	2.37	0.56
3:C:44:GLN:HG3	12:C:381:HEM:HBC2	1.88	0.56
9:I:11:PHE:CE2	9:I:25:ALA:N	2.66	0.56
1:A:220:SER:HA	1:A:223:TYR:CB	2.36	0.56
1:A:126:GLN:HE21	1:A:126:GLN:HA	1.70	0.56
6:F:53:ASN:HD22	6:F:53:ASN:N	2.03	0.56
6:F:37:ILE:HD12	6:F:43:VAL:HG21	1.87	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:348:ILE:HG22	3:C:352:GLN:HE21	1.71	0.55
9:I:49:VAL:C	9:I:51:CYS:H	2.10	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
4:D:171:PHE:O	4:D:174:GLY:N	2.40	0.54
1:A:365:LEU:HD11	9:I:56:ARG:HH21	1.72	0.54
3:C:80:ARG:HD3	3:C:80:ARG:O	2.07	0.54
2:B:368:TYR:CD1	9:I:1:MET:HG3	2.42	0.54
4:D:63:ALA:O	4:D:67:GLU:HG3	2.08	0.54
9:I:41:PRO:O	9:I:42:VAL:HG23	2.07	0.54
1:A:38:GLY:HA2	1:A:113:LEU:HD21	1.90	0.54
3:C:85:ASN:HD22	3:C:243:VAL:HG12	1.71	0.54
1:A:430:GLN:O	1:A:430:GLN:HG3	2.07	0.54
7:G:73:ASN:CB	7:G:74:PRO:HD3	2.30	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
1:A:220:SER:HA	1:A:223:TYR:HB2	1.89	0.54
1:A:86:LEU:HB3	2:B:285:VAL:HG22	1.89	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
2:B:235:ALA:HA	14:B:539:HOH:O	2.08	0.54
6:F:53:ASN:H	6:F:53:ASN:HD22	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
5:E:99:ARG:NH2	5:E:105:GLU:OE2	2.40	0.53
5:E:113:GLU:OE1	5:E:116:GLN:HG2	2.09	0.53
2:B:34:VAL:HG11	2:B:386:ALA:HB1	1.91	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:HB3	9:I:47:ARG:HH11	1.75	0.52
1:A:252:HIS:CE1	9:I:42:VAL:O	2.62	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:40:CYS:SG	12:D:242:HEM:HAC	2.49	0.52
6:F:83:TYR:O	6:F:84:GLU:C	2.45	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
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
2:B:325:TYR:HB3	9:I:28:PRO:HD3	1.92	0.52
2:B:169:ARG:HG3	2:B:238:LYS:HB2	1.92	0.52
4:D:22:ASP:HB3	4:D:25:SER:HB3	1.92	0.52
7:G:3:GLN:N	14:G:103:HOH:O	2.31	0.52
10:J:29:LEU:HD13	11:K:34:TRP:HD1	1.75	0.51
3:C:281:LEU:HD22	3:C:294:LEU:HD22	1.92	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
4:D:165:TYR:O	4:D:166:ASN:C	2.47	0.51
4:D:215:LEU:HD21	5:E:46:GLY:HA3	1.93	0.51
2:B:204:MET:HE1	2:B:224:LEU:HD22	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
4:D:155:GLY:C	4:D:157:ALA:H	2.14	0.51
3:C:216:ASP:OD2	4:D:233:ARG:NH2	2.38	0.51
10:J:29:LEU:HG	11:K:48:ILE:HD13	1.93	0.50
3:C:3:ASN:HB3	3:C:6:LYS:HG3	1.94	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: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: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:178:SER:O	1:A:181:ASP:HB2	2.11	0.50
1:A:19:LEU:HD22	1:A:23:LEU:HD12	1.94	0.50
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.92	0.50
1:A:213:GLN:O	1:A:217:SER:HB3	2.11	0.50
9:I:24:GLY:O	9:I:25:ALA:HB2	2.12	0.50
9:I:2:LEU:O	9:I:3:SER:CB	2.57	0.50
4:D:83:ARG:NH2	4:D:89:ASP:OD1	2.45	0.50
3:C:8:HIS:CD2	3:C:10:LEU:H	2.29	0.50
8:H:21:ARG:HD3	8:H:65:ARG:HH21	1.77	0.50
6:F:59:VAL:CG2	7:G:10:VAL:HG13	2.42	0.49
1:A:279:HIS:HB2	9:I:20:ARG:NH2	2.26	0.49
4:D:75:ASN:HB3	4:D:79:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:119:LEU:HD22	12:C:382:HEM:CBB	2.41	0.49
6:F:43:VAL:O	6:F:47:ILE:HG12	2.12	0.49
1:A:104:LYS:O	1:A:107:PRO:HD2	2.12	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
4:D:166:ASN:ND2	4:D:166:ASN:H	2.01	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
3:C:116:GLY:C	12:C:382:HEM:HBC2	2.33	0.49
5:E:70:ALA:O	5:E:71:MET:CB	2.54	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
14:A:519:HOH:O	7:G:10:VAL:CB	2.21	0.49
4:D:27:ARG:NH1	10:J:57:HIS:CE1	2.81	0.49
2:B:243:GLU:HG3	14:B:574:HOH:O	2.11	0.49
2:B:71:LEU:CD2	9:I:15:LEU:HG	2.36	0.48
9:I:11:PHE:HE2	9:I:25:ALA:H	1.54	0.48
1:A:252:HIS:HD2	1:A:323:HIS:HE1	1.61	0.48
4:D:120:ARG:O	4:D:121:HIS:CB	2.59	0.48
1:A:48:GLU:OE1	1:A:53:ASN:HA	2.13	0.48
3:C:268:ILE:O	3:C:268:ILE:HG23	2.13	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
2:B:308:ASP:CG	9:I:28:PRO:HB3	2.34	0.48
3:C:348:ILE:O	3:C:352:GLN:HG3	2.14	0.48
10:J:14:PHE:CD1	10:J:20:PHE:CD1	3.00	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
1:A:335:MET:HE3	1:A:339:GLN:HG3	1.95	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
2:B:72:ALA:HB1	2:B:75:LEU:HG	1.94	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	Distance(Å)	Clash(Å)
7:G:56:TYR:C	7:G:56:TYR:CD1	2.87	0.47
9:I:20:ARG:NH1	9:I:48:SER:OG	2.46	0.47
2:B:305:GLN:HE22	9:I:35:PRO:HB3	1.79	0.47
1:A:131:ARG:NH2	1:A:177:LEU:O	2.47	0.47
4:D:178:THR:HG23	4:D:181:GLN:HB2	1.96	0.47
4:D:150:ASN:O	4:D:156:GLN:HA	2.14	0.47
2:B:243:GLU:OE2	2:B:435:PHE:O	2.32	0.47
4:D:1:SER:H1	4:D:156:GLN:HE22	1.63	0.47
14:A:519:HOH:O	7:G:10:VAL:CG1	2.55	0.47
9:I:44:ASP:O	9:I:45:LEU:C	2.53	0.47
2:B:435:PHE:O	2:B:436:ILE:HB	2.14	0.47
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.97	0.47
3:C:77:TRP:CZ3	4:D:201:ARG:HB3	2.50	0.47
2:B:39:GLU:OE2	2:B:113:ARG:NH2	2.48	0.47
3:C:30:TRP:HZ3	3:C:96:MET:HG3	1.80	0.47
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.45	0.47
1:A:386:TYR:C	1:A:388:ARG:H	2.17	0.47
2:B:37:SER:HB3	2:B:216:LEU:HD12	1.96	0.47
3:C:349:THR:HA	3:C:352:GLN:HE21	1.80	0.46
3:C:207:ASN:HB2	3:C:208:PRO:HD2	1.96	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
7:G:34:ILE:HA	7:G:37:VAL:HG13	1.98	0.46
1:A:85:HIS:O	1:A:99:ILE:HA	2.15	0.46
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.95	0.46
5:E:18:VAL:CG1	5:E:18:VAL:O	2.58	0.46
2:B:294:SER:HB3	2:B:343:GLN:NE2	2.27	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
14:B:520:HOH:O	9:I:11:PHE:HB2	2.15	0.46
2:B:437:ASP:HB3	2:B:438:GLU:HG3	1.98	0.46
4:D:117:VAL:HG11	4:D:191:ARG:HH11	1.79	0.46
2:B:40:ASN:C	2:B:42:ALA:H	2.19	0.46
3:C:296:PHE:O	3:C:300:ILE:HB	2.16	0.46
3:C:170:VAL:O	3:C:170:VAL:HG12	2.15	0.46
2:B:68:LEU:HD23	2:B:186:VAL:HG22	1.98	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
2:B:385:GLN:NE2	14:B:584:HOH:O	2.44	0.46
2:B:325:TYR:CG	9:I:28:PRO:HD2	2.50	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:73:LEU:HB3	8:H:74:PHE:H	1.59	0.46
10:J:29:LEU:HD13	11:K:34:TRP:CD1	2.50	0.45
14:A:480:HOH:O	9:I:42:VAL:HG21	2.15	0.45
6:F:64:ARG:HH11	6:F:64:ARG:HB3	1.81	0.45
1:A:124:ASP:HA	1:A:127:ILE:CG2	2.37	0.45
2:B:126:VAL:O	2:B:130:PRO:HG3	2.16	0.45
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.74	0.45
6:F:35:ASP:OD2	6:F:89:TYR:OH	2.19	0.45
3:C:375:LYS:HD3	3:C:375:LYS:HA	1.77	0.45
2:B:111:CYS:CB	2:B:119:LEU:HD12	2.46	0.45
10:J:50:LYS:O	10:J:51:LEU:HB2	2.16	0.45
10:J:18:SER:CA	11:K:24:TRP:HZ3	2.07	0.45
5:E:52:LYS:HD2	11:K:34:TRP:CZ2	2.51	0.45
9:I:20:ARG:NH1	14:I:62:HOH:O	2.24	0.45
2:B:368:TYR:O	2:B:369:LEU:C	2.54	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
1:A:252:HIS:CD2	1:A:323:HIS:CE1	3.05	0.45
9:I:15:LEU:HA	9:I:15:LEU:HD22	1.29	0.45
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.98	0.45
3:C:260:ASN:HB3	3:C:263:ASN:HB2	1.97	0.45
4:D:156:GLN:HE21	4:D:156:GLN:HB2	1.50	0.45
3:C:132:VAL:HG22	3:C:143:ALA:HB2	1.98	0.45
1:A:252:HIS:HD2	1:A:323:HIS:CE1	2.35	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:146:ARG:HH12	1:A:308:GLN:NE2	2.15	0.44
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.52	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
2:B:227:ARG:HG3	14:B:446:HOH:O	2.16	0.44
1:A:281:ASP:HB3	1:A:284:TYR:CD1	2.52	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
5:E:69:LEU:HD23	5:E:69:LEU:HA	1.84	0.44
3:C:227:LYS:HD2	14:D:1043:HOH:O	2.17	0.44
8:H:39:LEU:O	8:H:43:ARG:HG3	2.18	0.44
4:D:28:ARG:HB3	4:D:171:PHE:CE2	2.51	0.44
2:B:148:LYS:NZ	2:B:180:ASP:OD1	2.40	0.44
2:B:370:MET:HB3	2:B:370:MET:HE2	1.84	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:70:ALA:O	5:E:71:MET:CG	2.66	0.44
4:D:32:VAL:HG11	4:D:186:VAL:HB	2.00	0.44
3:C:240:MET:HB3	3:C:244:LEU:HD12	1.99	0.44
4:D:47:ALA:HA	4:D:90:TYR:HA	2.00	0.44
3:C:322:GLN:HE21	3:C:322:GLN:HB3	1.54	0.44
9:I:24:GLY:O	9:I:25:ALA:CB	2.64	0.43
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
1:A:246:ASP:OD2	14:A:461:HOH:O	2.21	0.43
2:B:316:TYR:OH	9:I:10:PRO:HB3	2.19	0.43
1:A:2:ALA:O	2:B:113:ARG:CD	2.67	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
6:F:110:LYS:HG2	6:F:110:LYS:H	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
3:C:245:PHE:C	3:C:247:PRO:HD3	2.39	0.43
4:D:30:PHE:O	4:D:33:TYR:N	2.51	0.43
3:C:318:ARG:HB2	3:C:373:GLU:OE1	2.19	0.43
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.53	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
2:B:52:LYS:HZ3	2:B:233:SER:HG	1.63	0.43
4:D:20:SER:HB3	10:J:47:ASN:CG	2.39	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:HHH	2.01	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
1:A:11:VAL:HA	1:A:12:PRO:HD3	1.90	0.43
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.89	0.43
4:D:137:PRO:HA	4:D:138:PRO:HD3	1.82	0.42
5:E:65:SER:C	5:E:67:ASP:H	2.22	0.42
9:I:46:LYS:CG	9:I:47:ARG:N	2.58	0.42
4:D:157:ALA:C	4:D:158:ILE:HG23	2.40	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
5:E:60:SER:O	5:E:62:MET:N	2.51	0.42
3:C:66:VAL:O	3:C:69:ILE:HB	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:204:GLU:O	1:A:207:GLN:HB2	2.19	0.42
2:B:279:LEU:HA	2:B:279:LEU:HD23	1.87	0.42
3:C:122:THR:HG22	3:C:189:ILE:CG1	2.50	0.42
2:B:162:ASN:HA	2:B:162:ASN:HD22	1.64	0.42
2:B:141:GLN:HB2	2:B:142:PRO:HD3	2.00	0.42
10:J:13:LEU:HD22	10:J:23:THR:HB	2.00	0.42
1:A:11:VAL:HG21	1:A:392:LEU:HD12	2.01	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
10:J:50:LYS:HG3	10:J:51:LEU:N	2.33	0.42
3:C:8:HIS:HD2	3:C:10:LEU:H	1.67	0.42
2:B:365:LYS:HG2	2:B:399:LEU:HD22	2.01	0.42
1:A:294:LEU:HG	1:A:307:PHE:CE1	2.55	0.42
5:E:122:HIS:O	5:E:125:GLU:HG2	2.20	0.42
2:B:227:ARG:HD3	2:B:228:GLY:N	2.34	0.42
4:D:116:ILE:HD13	4:D:116:ILE:HA	1.79	0.42
3:C:80:ARG:HD2	3:C:81:TYR:CE1	2.55	0.42
6:F:50:LEU:HA	6:F:51:PRO:HD3	1.93	0.42
5:E:60:SER:C	5:E:62:MET:H	2.23	0.42
3:C:284:ILE:HA	3:C:285:PRO:HD3	1.82	0.42
5:E:45:VAL:HG13	10:J:28:ALA:HA	2.02	0.42
4:D:153:PHE:CE2	4:D:158:ILE:HG12	2.55	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
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
10:J:22:LEU:HA	11:K:27:VAL:HG22	2.01	0.42
10:J:9:LEU:HD12	10:J:9:LEU:HA	1.86	0.42
11:K:41:ILE:HG12	11:K:41:ILE:H	1.70	0.42
4:D:69:GLU:HB3	4:D:82:MET:HG2	2.01	0.42
3:C:69:ILE:O	3:C:73:VAL:HB	2.20	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
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
4:D:211:MET:HE3	10:J:31:PHE:HE2	1.85	0.41
3:C:361:LEU:HA	3:C:365:LEU:HB2	2.01	0.41
2:B:295:LEU:HD23	2:B:295:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:22:GLY:HA3	1:A:193:PRO:HG3	2.02	0.41
3:C:90:PHE:O	3:C:90:PHE:HD1	2.03	0.41
3:C:226:ILE:HD11	4:D:222:MET:HB3	2.01	0.41
3:C:94:LEU:CD2	3:C:123:VAL:HG11	2.43	0.41
2:B:435:PHE:O	2:B:436:ILE:CB	2.68	0.41
6:F:31:LEU:O	6:F:81:THR:HG21	2.21	0.41
9:I:41:PRO:C	9:I:42:VAL:HG23	2.41	0.41
2:B:264:ILE:HD11	9:I:2:LEU:HA	2.02	0.41
2:B:217:LYS:O	2:B:221:GLU:HG3	2.20	0.41
4:D:6:HIS:HA	4:D:7:PRO:HD3	1.86	0.41
1:A:435:ASN:ND2	3:C:223:TYR:OH	2.53	0.41
7:G:73:ASN:CB	7:G:74:PRO:CD	2.95	0.41
3:C:337:TRP:HZ3	3:C:350:ILE:CD1	2.33	0.41
1:A:360:LEU:HA	1:A:360:LEU:HD23	1.82	0.41
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.79	0.41
1:A:369:LEU:HD12	1:A:392:LEU:HD21	2.03	0.41
3:C:326:TRP:NE1	7:G:48:VAL:HG22	2.36	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
3:C:361:LEU:HD12	3:C:361:LEU:HA	1.79	0.41
1:A:390:ILE:HA	1:A:391:PRO:HD3	1.81	0.41
6:F:38:HIS:HB3	14:F:1916:HOH:O	2.20	0.41
9:I:49:VAL:HG12	9:I:50:LEU:H	1.86	0.41
9:I:52:ARG:O	9:I:53:GLU:HB2	2.20	0.41
5:E:52:LYS:HE2	5:E:52:LYS:HB2	1.73	0.41
11:K:48:ILE:CG2	11:K:48:ILE:O	2.69	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
9:I:34:VAL:O	9:I:36:ALA:N	2.52	0.41
4:D:120:ARG:HD3	4:D:120:ARG:HA	1.84	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
1:A:223:TYR:HB3	1:A:224:ASP:H	1.56	0.41
1:A:102:LEU:HD23	1:A:104:LYS:HE3	2.02	0.41
2:B:67:HIS:O	2:B:68:LEU:C	2.59	0.41
4:D:7:PRO:HA	4:D:8:PRO:HD3	1.85	0.41
2:B:152:LEU:HG	2:B:158:HIS:CD2	2.56	0.41
6:F:42:ASP:OD2	6:F:101:ARG:NH2	2.54	0.41
4:D:95:TYR:HA	4:D:96:PRO:HD3	1.94	0.41
2:B:50:PHE:HB3	2:B:387:LEU:HD22	2.02	0.41
1:A:270:LEU:HD23	1:A:270:LEU:HA	1.78	0.41
11:K:38:TRP:HD1	11:K:39:ARG:HG3	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:319:PRO:HG3	7:G:47:ARG:HH12	1.85	0.41
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.61	0.41
1:A:354:VAL:O	1:A:358:LYS:HG3	2.21	0.41
11:K:44:TRP:HD1	14:K:2610:HOH:O	2.03	0.41
10:J:16:ARG:C	10:J:18:SER:N	2.72	0.40
4:D:178:THR:OG1	4:D:179:MET:N	2.53	0.40
3:C:186:PRO:HA	3:C:189:ILE:HD12	2.03	0.40
2:B:29:LEU:HD23	2:B:29:LEU:HA	1.79	0.40
1:A:274:ASN:HA	1:A:274:ASN:HD22	1.68	0.40
3:C:240:MET:CE	3:C:240:MET:HA	2.50	0.40
3:C:2:THR:HB	3:C:3:ASN:H	1.65	0.40
3:C:77:TRP:CH2	4:D:201:ARG:HB3	2.55	0.40
1:A:395:TRP:CZ3	9:I:57:GLY:HA3	2.57	0.40
3:C:104:TYR:CE2	3:C:208:PRO:HA	2.56	0.40
3:C:65:SER:O	3:C:69:ILE:HG13	2.22	0.40
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.96	0.40
2:B:254:HIS:O	2:B:426:ALA:HA	2.21	0.40
3:C:215:VAL:HG23	7:G:8:THR:HG21	2.04	0.40
9:I:41:PRO:HB3	9:I:44:ASP:CG	2.42	0.40
4:D:91:PHE:N	4:D:92:PRO:HD3	2.35	0.40
3:C:135:TRP:CE3	3:C:175:LEU:HG	2.57	0.40
3:C:236:ILE:HD13	3:C:236:ILE:HA	1.80	0.40
3:C:296:PHE:HD1	3:C:359:PHE:CE1	2.40	0.40
9:I:56:ARG:HB3	9:I:57:GLY:H	1.72	0.40
3:C:122:THR:CG2	3:C:189:ILE:HG12	2.52	0.40
2:B:250:ASP:O	2:B:251:SER:HB3	2.20	0.40
5:E:74:ILE:HG22	5:E:195:VAL:HB	2.03	0.40
1:A:405:ARG:O	1:A:409:GLU:HB2	2.20	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	Distance(Å)	Clash(Å)
14:B:549:HOH:O	14:B:586:HOH:O[6.565]	1.68	0.52

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	10	10
2	B	421/439 (96%)	386 (92%)	24 (6%)	11 (3%)	8	8
3	C	376/379 (99%)	330 (88%)	41 (11%)	5 (1%)	18	24
4	D	239/241 (99%)	185 (77%)	30 (13%)	24 (10%)	1	0
5	E	194/196 (99%)	175 (90%)	14 (7%)	5 (3%)	8	8
6	F	103/110 (94%)	98 (95%)	3 (3%)	2 (2%)	12	14
7	G	73/81 (90%)	64 (88%)	6 (8%)	3 (4%)	4	3
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%)	6	4
11	K	49/56 (88%)	41 (84%)	7 (14%)	1 (2%)	11	13
All	All	2077/2145 (97%)	1807 (87%)	188 (9%)	82 (4%)	5	3

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	331 (90%)	39 (10%)	10	14
2	B	332/343 (97%)	296 (89%)	36 (11%)	9	13
3	C	326/327 (100%)	285 (87%)	41 (13%)	7	8
4	D	206/206 (100%)	171 (83%)	35 (17%)	3	3
5	E	168/168 (100%)	155 (92%)	13 (8%)	18	28
6	F	96/98 (98%)	84 (88%)	12 (12%)	7	8
7	G	66/71 (93%)	56 (85%)	10 (15%)	4	5
8	H	64/74 (86%)	58 (91%)	6 (9%)	13	18
9	I	44/44 (100%)	32 (73%)	12 (27%)	0	0
10	J	46/52 (88%)	39 (85%)	7 (15%)	4	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	41/46 (89%)	33 (80%)	8 (20%)	2	2
All	All	1759/1799 (98%)	1540 (88%)	219 (12%)	7	8

All (219) 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	21	ASN
1	A	23	LEU
1	A	25	VAL
1	A	32	GLN
1	A	37	VAL
1	A	42	ASP
1	A	52	ASN
1	A	53	ASN
1	A	58	PHE
1	A	73	ASN
1	A	90	SER
1	A	113	LEU
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	208	LEU
1	A	209	LEU
1	A	217	SER
1	A	223	TYR
1	A	226	ASP
1	A	235	ARG
1	A	245	GLU
1	A	274	ASN
1	A	308	GLN
1	A	348	SER
1	A	383	LEU
1	A	388	ARG
1	A	389	ARG
1	A	403	ASP
1	A	418	GLN

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Mol	Chain	Res	Type
1	A	430	GLN
1	A	439	SER
1	A	443	TRP
2	B	17	VAL
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
2	B	186	VAL
2	B	189	VAL
2	B	197	ASN
2	B	209	LEU
2	B	227	ARG
2	B	230	LEU
2	B	232	LEU
2	B	243	GLU
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	384	SER
2	B	397	THR
2	B	415	LYS
2	B	421	ARG
2	B	424	MET
2	B	437	ASP
3	C	4	ILE
3	C	6	LYS
3	C	10	LEU

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Mol	Chain	Res	Type
3	C	18	PHE
3	C	19	ILE
3	C	26	ASN
3	C	42	ILE
3	C	46	LEU
3	C	51	LEU
3	C	64	SER
3	C	67	THR
3	C	78	ILE
3	C	80	ARG
3	C	90	PHE
3	C	96	MET
3	C	102	LEU
3	C	114	ASN
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	241	LEU
3	C	242	LEU
3	C	252	ASP
3	C	254	ASP
3	C	262	LEU
3	C	263	ASN
3	C	284	ILE
3	C	309	THR
3	C	318	ARG
3	C	328	LEU
3	C	333	LEU
3	C	350	ILE
3	C	365	LEU
3	C	379	TRP
4	D	5	LEU
4	D	13	SER
4	D	17	LEU
4	D	20	SER

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Mol	Chain	Res	Type
4	D	24	THR
4	D	37	CYS
4	D	42	SER
4	D	55	CYS
4	D	82	MET
4	D	95	TYR
4	D	109	LEU
4	D	112	ASP
4	D	114	SER
4	D	121	HIS
4	D	132	THR
4	D	134	TYR
4	D	135	CYS
4	D	141	VAL
4	D	143	LEU
4	D	156	GLN
4	D	158	ILE
4	D	165	TYR
4	D	166	ASN
4	D	170	GLU
4	D	178	THR
4	D	179	MET
4	D	182	VAL
4	D	191	ARG
4	D	201	ARG
4	D	212	MET
4	D	214	LEU
4	D	223	LYS
4	D	224	ARG
4	D	228	SER
4	D	241	LYS
5	E	19	LEU
5	E	24	SER
5	E	27	GLU
5	E	52	LYS
5	E	54	VAL
5	E	60	SER
5	E	61	SER
5	E	63	SER
5	E	65	SER
5	E	71	MET
5	E	79	SER

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Mol	Chain	Res	Type
5	E	113	GLU
5	E	184	SER
6	F	27	ASN
6	F	37	ILE
6	F	53	ASN
6	F	64	ARG
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	27	PRO
7	G	31	SER
7	G	34	ILE
7	G	37	VAL
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
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
9	I	30	VAL
9	I	43	LEU
9	I	47	ARG
9	I	49	VAL
9	I	56	ARG

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Mol	Chain	Res	Type
10	J	4	THR
10	J	6	THR
10	J	18	SER
10	J	23	THR
10	J	24	ILE
10	J	33	ARG
10	J	45	HIS
11	K	4	ARG
11	K	15	ARG
11	K	18	VAL
11	K	20	THR
11	K	23	LEU
11	K	24	TRP
11	K	39	ARG
11	K	44	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	52	ASN
1	A	85	HIS
1	A	94	HIS
1	A	119	ASN
1	A	136	GLN
1	A	141	ASN
1	A	173	ASN
1	A	252	HIS
1	A	271	GLN
1	A	274	ASN
1	A	305	GLN
1	A	308	GLN
1	A	323	HIS
1	A	341	GLN
1	A	359	ASN
1	A	368	HIS
1	A	418	GLN
1	A	435	ASN
2	B	104	ASN
2	B	143	GLN
2	B	162	ASN
2	B	170	ASN

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Mol	Chain	Res	Type
2	B	174	ASN
2	B	197	ASN
2	B	248	ASN
2	B	305	GLN
2	B	342	ASN
2	B	343	GLN
2	B	362	ASN
2	B	385	GLN
2	B	412	ASN
3	C	8	HIS
3	C	32	ASN
3	C	85	ASN
3	C	114	ASN
3	C	206	ASN
3	C	322	GLN
3	C	345	HIS
3	C	352	GLN
4	D	23	HIS
4	D	71	GLN
4	D	105	ASN
4	D	121	HIS
4	D	156	GLN
4	D	166	ASN
5	E	57	GLN
6	F	53	ASN
7	G	64	GLN
9	I	31	GLN
10	J	45	HIS
11	K	12	GLN
11	K	16	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	C	381	3	49,50,50	11.57	29 (59%)	46,82,82	3.55	19 (41%)
12	HEM	C	382	3	49,50,50	11.58	28 (57%)	46,82,82	3.38	22 (47%)
12	HEM	D	242	4	49,50,50	12.15	28 (57%)	46,82,82	3.61	21 (45%)
13	FES	E	197	5	0,4,4	0.00	-	0,4,4	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HEM	C	381	3	-	0/14/114/114	0/0/8/8
12	HEM	C	382	3	-	0/14/114/114	0/0/8/8
12	HEM	D	242	4	-	0/14/114/114	0/0/8/8
13	FES	E	197	5	-	0/0/4/4	0/0/1/1

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	242	HEM	C2B-C1B	-51.01	1.31	1.44
12	C	381	HEM	C3D-C4D	-50.44	1.32	1.44
12	C	382	HEM	C2B-C1B	-48.02	1.32	1.44
12	C	382	HEM	C2D-C1D	-45.60	1.33	1.44
12	D	242	HEM	C3D-C4D	-45.40	1.33	1.44
12	D	242	HEM	C2D-C1D	-42.89	1.33	1.44
12	C	381	HEM	C2D-C1D	-41.17	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	C2B-C1B	-39.46	1.34	1.44
12	C	382	HEM	C3D-C4D	-38.64	1.34	1.44
12	C	382	HEM	CHA-C4D	9.98	1.50	1.35
12	C	382	HEM	C3B-C4B	-9.32	1.33	1.44
12	C	381	HEM	CHA-C4D	9.12	1.48	1.35
12	D	242	HEM	C3B-C4B	-9.01	1.33	1.44
12	C	381	HEM	C3B-C4B	-8.83	1.33	1.44
12	C	381	HEM	CHB-C1B	8.78	1.48	1.35
12	D	242	HEM	CHB-C1B	8.76	1.48	1.35
12	D	242	HEM	CHA-C4D	8.31	1.47	1.35
12	C	382	HEM	CHB-C1B	8.06	1.47	1.35
12	D	242	HEM	CHC-C1C	7.37	1.50	1.36
12	C	381	HEM	CHD-C4C	7.34	1.50	1.36
12	D	242	HEM	CHD-C4C	7.30	1.50	1.36
12	C	381	HEM	C3C-C2C	-7.18	1.31	1.43
12	C	382	HEM	CHD-C4C	7.08	1.49	1.36
12	D	242	HEM	C3D-C2D	-7.00	1.31	1.43
12	C	382	HEM	CHC-C1C	7.00	1.49	1.36
12	C	381	HEM	C3B-C2B	-6.74	1.32	1.43
12	C	381	HEM	C4A-C3A	6.54	1.48	1.40
12	D	242	HEM	C4A-C3A	6.50	1.48	1.40
12	C	381	HEM	C3D-C2D	-6.45	1.32	1.43
12	D	242	HEM	C3C-C2C	-6.43	1.32	1.43
12	C	381	HEM	CHC-C1C	6.35	1.48	1.36
12	C	382	HEM	C3B-C2B	-6.02	1.33	1.43
12	C	382	HEM	C4A-C3A	5.99	1.47	1.40
12	D	242	HEM	C3B-C2B	-5.78	1.33	1.43
12	C	382	HEM	C3C-C2C	-5.51	1.34	1.43
12	C	382	HEM	C3D-C2D	-5.47	1.34	1.43
12	C	381	HEM	FE-NA	5.29	2.15	1.92
12	D	242	HEM	FE-NA	5.09	2.14	1.92
12	C	382	HEM	FE-NA	4.94	2.13	1.92
12	C	381	HEM	CHC-C4B	4.74	1.50	1.39
12	C	381	HEM	C1C-NC	4.44	1.44	1.38
12	D	242	HEM	CHC-C4B	4.41	1.49	1.39
12	C	382	HEM	CHD-C1D	4.34	1.49	1.39
12	D	242	HEM	CBC-CAC	4.32	1.54	1.28
12	D	242	HEM	CHD-C1D	4.28	1.49	1.39
12	D	242	HEM	CBB-CAB	4.21	1.53	1.28
12	C	382	HEM	CBB-CAB	4.18	1.53	1.28
12	C	381	HEM	CHD-C1D	4.09	1.48	1.39
12	C	381	HEM	CBC-CAC	4.05	1.52	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	CBB-CAB	4.03	1.52	1.28
12	C	382	HEM	CBC-CAC	4.00	1.52	1.28
12	C	381	HEM	C1A-C2A	4.00	1.50	1.43
12	D	242	HEM	C3C-CAC	3.97	1.52	1.40
12	D	242	HEM	C1C-NC	3.80	1.43	1.38
12	C	382	HEM	CHC-C4B	3.73	1.48	1.39
12	C	382	HEM	C3C-CAC	3.73	1.52	1.40
12	D	242	HEM	C4C-NC	3.67	1.43	1.38
12	D	242	HEM	C3B-CAB	3.64	1.51	1.40
12	C	382	HEM	C4A-CHB	3.62	1.49	1.39
12	C	382	HEM	C3B-CAB	3.54	1.51	1.40
12	C	382	HEM	C1A-CHA	3.53	1.49	1.39
12	C	381	HEM	C2C-C1C	-3.44	1.32	1.43
12	D	242	HEM	C2C-C1C	-3.41	1.32	1.43
12	C	382	HEM	C2C-C1C	-3.38	1.32	1.43
12	C	381	HEM	C4C-NC	3.34	1.42	1.38
12	C	381	HEM	C3C-CAC	3.32	1.50	1.40
12	C	382	HEM	C1A-C2A	3.31	1.49	1.43
12	D	242	HEM	C4A-CHB	3.30	1.48	1.39
12	C	381	HEM	C1A-CHA	3.30	1.48	1.39
12	D	242	HEM	C2A-C3A	3.18	1.47	1.37
12	C	381	HEM	C3B-CAB	3.13	1.50	1.40
12	C	381	HEM	C2A-C3A	3.07	1.46	1.37
12	C	381	HEM	C4A-CHB	3.06	1.48	1.39
12	D	242	HEM	C1A-CHA	2.99	1.48	1.39
12	C	382	HEM	C2A-C3A	2.91	1.46	1.37
12	C	382	HEM	C4C-NC	2.82	1.42	1.38
12	C	382	HEM	C1C-NC	2.64	1.41	1.38
12	C	382	HEM	O2A-CGA	-2.63	1.21	1.30
12	D	242	HEM	C1A-C2A	2.62	1.48	1.43
12	C	381	HEM	C4B-NB	2.50	1.43	1.37
12	D	242	HEM	O2D-CGD	-2.39	1.21	1.30
12	D	242	HEM	O2A-CGA	-2.31	1.22	1.30
12	C	381	HEM	O2A-CGA	-2.23	1.22	1.30
12	C	382	HEM	O2D-CGD	-2.16	1.22	1.30
12	C	381	HEM	C1D-ND	2.06	1.42	1.37

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	382	HEM	C4A-CHB-C1B	-10.81	113.24	127.47
12	D	242	HEM	C4A-CHB-C1B	-10.69	113.40	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	381	HEM	C4A-CHB-C1B	-10.18	114.08	127.47
12	C	381	HEM	C1A-CHA-C4D	-9.97	114.35	127.47
12	D	242	HEM	C1A-CHA-C4D	-9.79	114.59	127.47
12	C	382	HEM	C1A-CHA-C4D	-7.65	117.41	127.47
12	C	381	HEM	C4D-ND-C1D	-6.34	98.68	105.16
12	C	382	HEM	C1D-CHD-C4C	-5.98	110.82	126.57
12	C	381	HEM	CHC-C4B-NB	5.91	129.50	124.58
12	C	381	HEM	C4B-CHC-C1C	-5.79	111.32	126.57
12	C	382	HEM	C3B-C4B-NB	-5.77	109.87	114.00
12	C	381	HEM	C4C-NC-C1C	-5.70	99.60	105.53
12	C	381	HEM	C3B-C4B-NB	-5.50	110.06	114.00
12	D	242	HEM	C3B-C4B-NB	-5.49	110.07	114.00
12	D	242	HEM	C4B-CHC-C1C	-5.48	112.14	126.57
12	C	381	HEM	C1B-NB-C4B	-5.35	99.69	105.16
12	C	382	HEM	CHB-C4A-NA	5.32	133.47	124.58
12	C	381	HEM	C1D-CHD-C4C	-5.29	112.65	126.57
12	D	242	HEM	C1D-CHD-C4C	-5.14	113.03	126.57
12	C	382	HEM	C4B-CHC-C1C	-5.11	113.12	126.57
12	D	242	HEM	C4D-ND-C1D	-5.06	99.98	105.16
12	D	242	HEM	CHC-C1C-NC	5.03	129.10	124.73
12	C	382	HEM	C4A-NA-C1A	5.02	113.38	106.76
12	D	242	HEM	CHB-C4A-NA	5.02	132.97	124.58
12	D	242	HEM	CHA-C1A-NA	5.00	132.94	124.58
12	C	381	HEM	CHB-C4A-NA	4.85	132.68	124.58
12	C	382	HEM	C4C-NC-C1C	-4.78	100.56	105.53
12	D	242	HEM	C4C-NC-C1C	-4.58	100.77	105.53
12	D	242	HEM	C1B-NB-C4B	-4.56	100.50	105.16
12	D	242	HEM	CHB-C1B-NB	4.27	130.17	124.31
12	D	242	HEM	C4A-NA-C1A	4.14	112.22	106.76
12	C	382	HEM	CHC-C1C-NC	4.14	128.33	124.73
12	C	382	HEM	CHC-C4B-NB	4.14	128.02	124.58
12	D	242	HEM	CHC-C4B-NB	4.12	128.01	124.58
12	D	242	HEM	C2A-C1A-CHA	-4.06	118.30	126.00
12	C	381	HEM	C4A-NA-C1A	4.04	112.08	106.76
12	C	382	HEM	CHD-C1D-ND	4.03	127.93	124.58
12	C	381	HEM	C3A-C4A-CHB	-3.92	118.57	126.00
12	D	242	HEM	C3A-C4A-CHB	-3.85	118.70	126.00
12	C	382	HEM	C3A-C4A-CHB	-3.82	118.75	126.00
12	C	382	HEM	C1B-NB-C4B	-3.54	101.53	105.16
12	D	242	HEM	CHD-C1D-ND	3.42	127.42	124.58
12	C	381	HEM	CHA-C4D-ND	3.40	128.98	124.31
12	D	242	HEM	CHD-C4C-NC	3.35	127.64	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	381	HEM	CHD-C4C-NC	3.31	127.61	124.73
12	C	382	HEM	CHA-C1A-NA	3.20	129.93	124.58
12	C	382	HEM	CHB-C1B-NB	3.14	128.62	124.31
12	C	381	HEM	CHA-C1A-NA	3.11	129.77	124.58
12	C	381	HEM	CHC-C1C-NC	3.09	127.41	124.73
12	C	381	HEM	CHB-C1B-NB	2.98	128.40	124.31
12	D	242	HEM	CHA-C4D-ND	2.77	128.11	124.31
12	C	382	HEM	C2D-C1D-ND	-2.75	109.68	112.93
12	C	382	HEM	CBD-CAD-C3D	-2.64	108.60	114.37
12	C	382	HEM	CAA-C2A-C3A	-2.38	122.22	129.00
12	C	382	HEM	CAA-C2A-C1A	2.34	132.57	125.50
12	D	242	HEM	C4A-C3A-C2A	-2.34	105.37	107.00
12	D	242	HEM	C2D-C1D-ND	-2.30	110.21	112.93
12	C	381	HEM	C2A-C1A-CHA	-2.28	121.67	126.00
12	C	382	HEM	O2A-CGA-CBA	2.26	122.19	114.22
12	C	382	HEM	C4D-ND-C1D	-2.24	102.87	105.16
12	C	382	HEM	C3A-C4A-NA	-2.21	107.74	109.41
12	C	381	HEM	C1A-C2A-C3A	-2.12	104.73	106.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.