Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:11 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

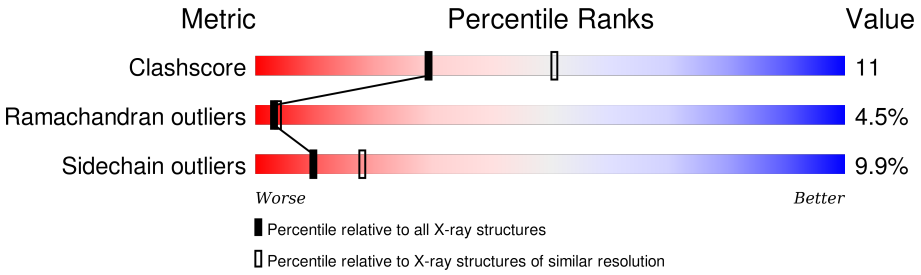
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	446	72% 24% • •
2	B	439	71% 22% • •
3	C	379	74% 20% • •
4	D	241	55% 33% 11% •
5	E	196	78% 20% • •
6	F	110	72% 15% 8% 5%
7	G	81	65% 20% 6% • 7%

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Mol	Chain	Length	Quality of chain
8	H	78	40% 40% 9% 10%
9	I	57	25% 39% 30% 7%
10	J	62	56% 32% 10%
11	K	56	75% 13% 7% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	UQ2	C	383	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 16896 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3458	2161	609	668	20	0	0	0

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

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

- Molecule 3 is a protein called Cytochrome b.

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

- Molecule 4 is a protein called cytochrome c1.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	105	Total	C	N	O	S	0	0	0
			911	576	165	168	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	0
			628	410	118	99	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			575	347	102	121	5			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			483	316	82	85			

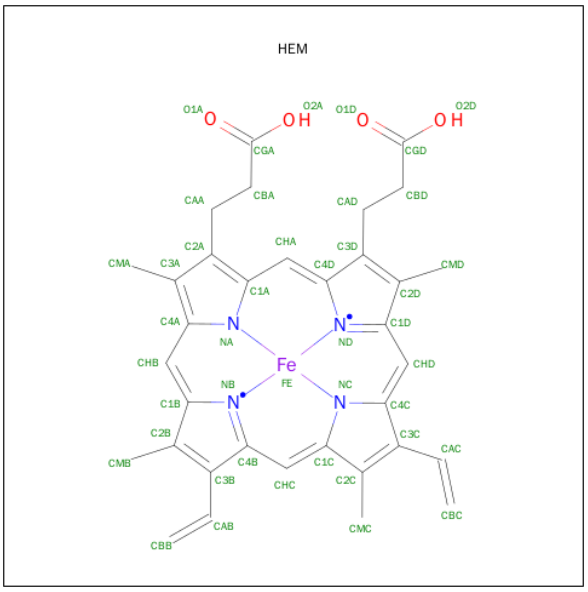
- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase complex 6.4 kDa protein.

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

There is a discrepancy between the modelled and reference sequences:

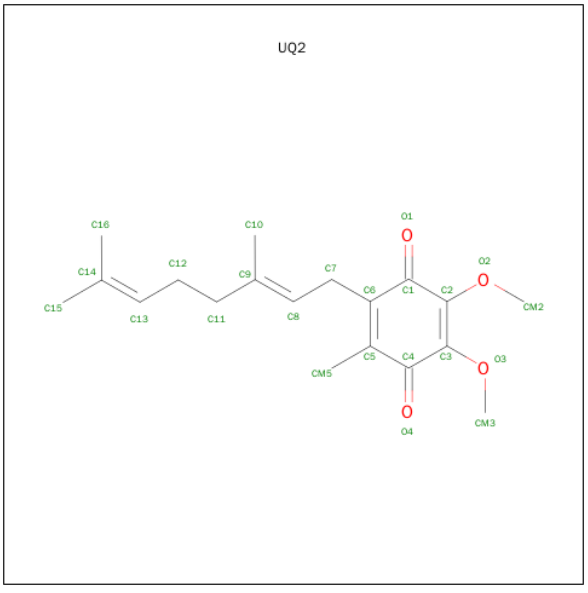
Chain	Residue	Modelled	Actual	Comment	Reference
K	22	GLN	SER	SEE REMARK 999	UNP P07552

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



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

- Molecule 13 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).



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

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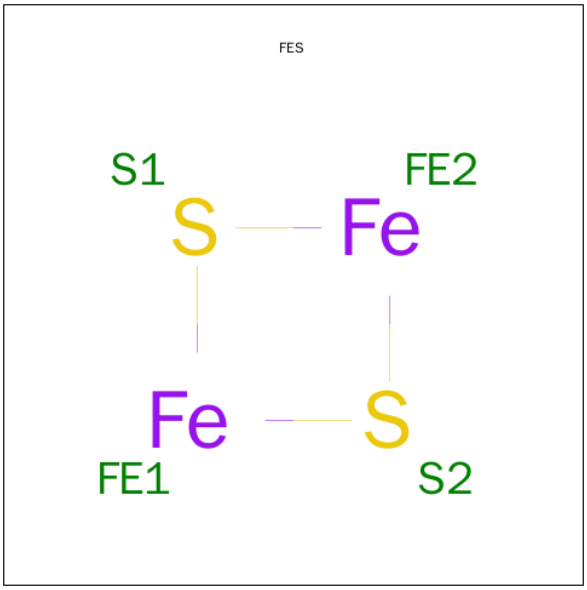
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C O 23 19 4	0	0

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



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

- Molecule 15 is water.

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

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

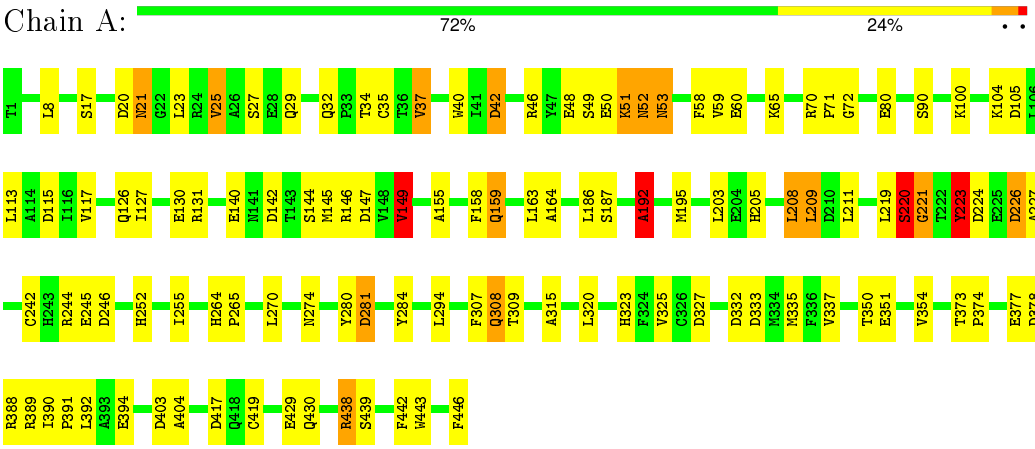
3 Residue-property plots (i)

These plots are drawn for all protein, RNA 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.

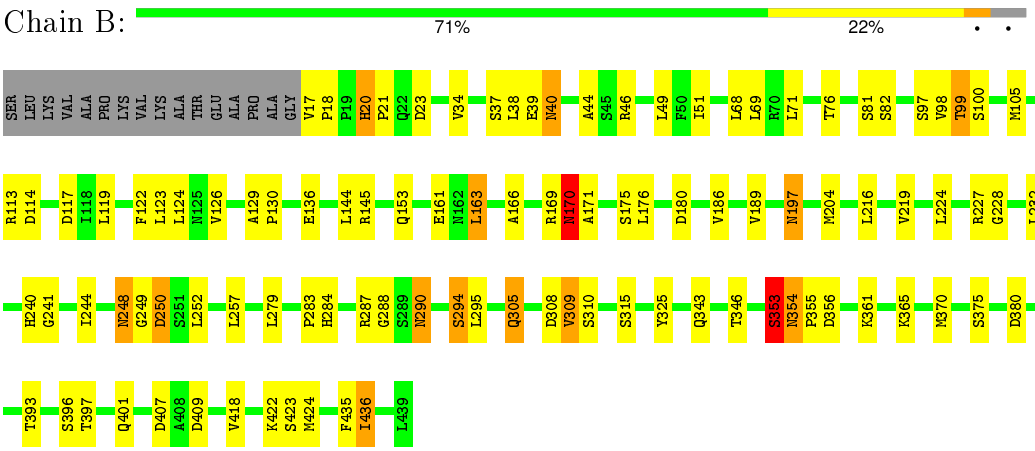
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Chain A:



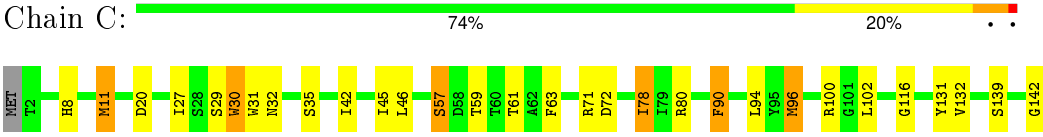
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

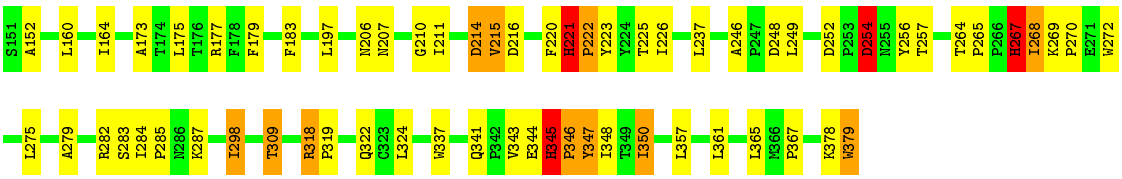
Chain B:



- Molecule 3: Cytochrome b

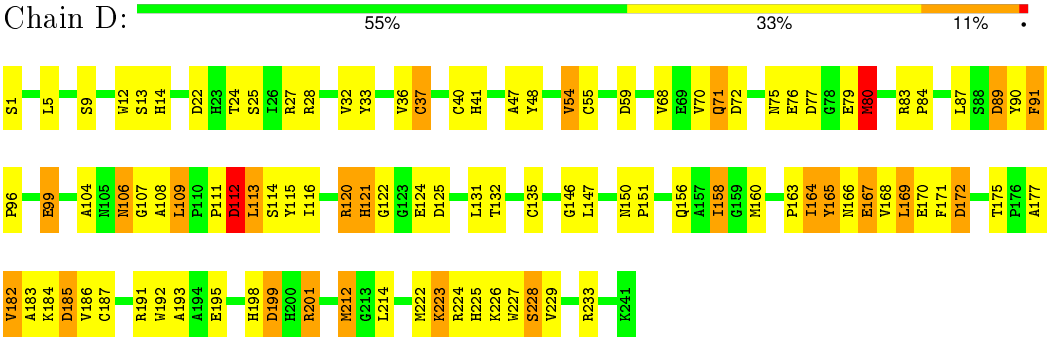
Chain C:





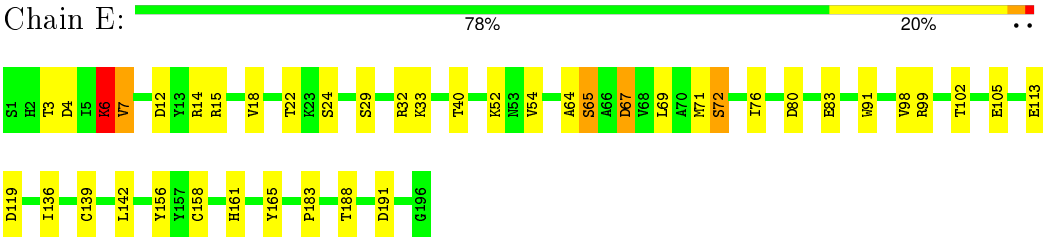
• Molecule 4: cytochrome c1

Chain D:



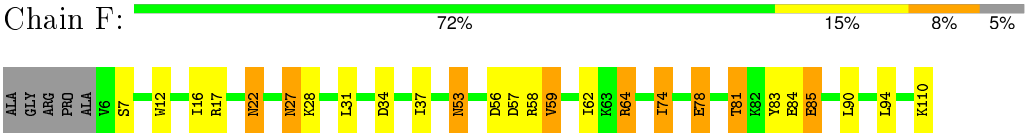
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT, mitochondrial

Chain E:



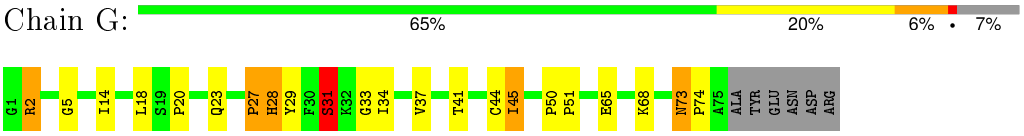
• Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F:



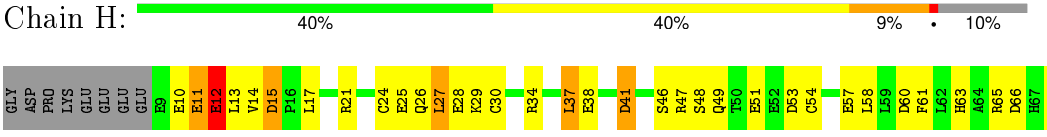
• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain G:



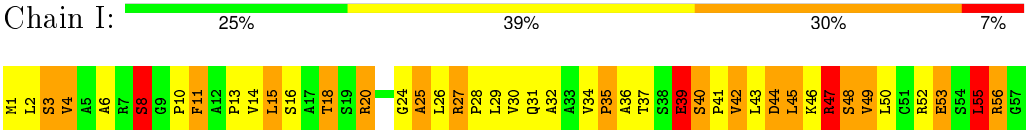
• Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H:



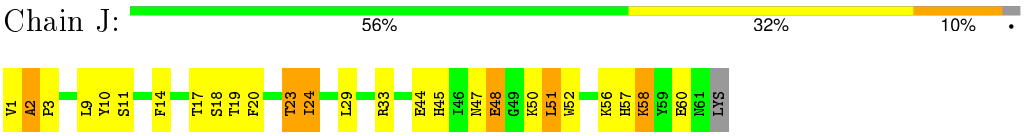
• Molecule 9: Ubiquinol-cytochrome C reductase 8 kDa protein

Chain I:



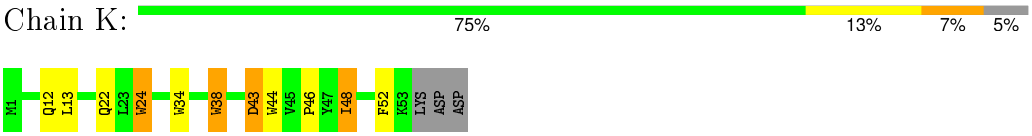
• Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:



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

Chain K:



4 Data and refinement statistics (i)

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	153.83Å 153.83Å 596.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.99 – 2.60	Depositor
% Data completeness (in resolution range)	100.0 (28.99-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.247 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16896	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, UQ2, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.91	2/3531 (0.1%)	0.88	17/4792 (0.4%)
2	B	1.11	6/3232 (0.2%)	0.90	11/4386 (0.3%)
3	C	0.89	3/3100 (0.1%)	0.82	7/4242 (0.2%)
4	D	0.76	0/1977	0.89	8/2684 (0.3%)
5	E	0.75	1/1553 (0.1%)	0.81	5/2100 (0.2%)
6	F	1.11	2/930 (0.2%)	0.94	4/1246 (0.3%)
7	G	0.98	0/649	0.77	0/878
8	H	0.69	0/580	0.98	7/777 (0.9%)
9	I	1.29	2/411 (0.5%)	1.28	4/558 (0.7%)
10	J	0.78	0/495	0.79	1/672 (0.1%)
11	K	0.76	0/453	0.72	1/621 (0.2%)
All	All	0.93	16/16911 (0.1%)	0.88	65/22956 (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
1	A	1	0
2	B	1	0
3	C	1	2
4	D	2	0
7	G	1	0
8	H	1	0
9	I	1	0
10	J	1	0
All	All	9	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	379	TRP	CB-CG	-8.67	1.34	1.50
9	I	25	ALA	CA-CB	-7.45	1.36	1.52
2	B	424	MET	SD-CE	-7.45	1.36	1.77
2	B	309	VAL	CB-CG1	-7.40	1.37	1.52
1	A	281	ASP	CB-CG	-6.75	1.37	1.51
3	C	221	HIS	C-N	-6.33	1.22	1.34
2	B	248	ASN	CB-CG	-6.22	1.36	1.51
1	A	149	VAL	CB-CG2	-6.00	1.40	1.52
2	B	170	ASN	N-CA	-5.80	1.34	1.46
2	B	105	MET	SD-CE	-5.70	1.46	1.77
3	C	11	MET	SD-CE	5.63	2.09	1.77
2	B	197	ASN	CB-CG	-5.57	1.38	1.51
6	F	64	ARG	CG-CD	-5.27	1.38	1.51
6	F	59	VAL	CA-CB	5.25	1.65	1.54
9	I	42	VAL	CA-CB	5.04	1.65	1.54
5	E	6	LYS	CB-CG	5.03	1.66	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	221	HIS	N-CA-C	7.66	131.69	111.00
1	A	42	ASP	CB-CG-OD2	7.55	125.10	118.30
4	D	122	GLY	N-CA-C	-7.31	94.83	113.10
3	C	252	ASP	CB-CG-OD2	7.04	124.64	118.30
6	F	85	GLU	N-CA-C	-7.00	92.09	111.00
6	F	57	ASP	CB-CG-OD2	6.75	124.38	118.30
2	B	114	ASP	CB-CG-OD2	6.63	124.27	118.30
2	B	380	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	51	LYS	N-CA-C	-6.58	93.24	111.00
10	J	51	LEU	N-CA-C	6.56	128.72	111.00
6	F	34	ASP	CB-CG-OD2	6.43	124.09	118.30
4	D	112	ASP	CB-CG-OD2	6.33	123.99	118.30
2	B	250	ASP	CB-CG-OD2	6.23	123.90	118.30
6	F	56	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	105	ASP	CB-CG-OD2	6.16	123.84	118.30
8	H	53	ASP	N-CA-C	6.01	127.23	111.00
1	A	333	ASP	CB-CG-OD2	5.99	123.69	118.30
8	H	12	GLU	N-CA-C	5.97	127.11	111.00
1	A	327	ASP	CB-CG-OD2	5.95	123.66	118.30
8	H	66	ASP	CB-CG-OD2	5.90	123.61	118.30
2	B	234	GLY	N-CA-C	5.87	127.78	113.10
2	B	23	ASP	CB-CG-OD2	5.83	123.54	118.30
4	D	169	LEU	N-CA-C	5.82	126.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	142	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	246	ASP	CB-CG-OD2	5.79	123.51	118.30
2	B	163	LEU	CB-CG-CD2	5.77	120.80	111.00
3	C	214	ASP	CB-CG-OD2	5.76	123.48	118.30
2	B	180	ASP	CB-CG-OD2	5.75	123.47	118.30
11	K	43	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	281	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	20	ASP	CB-CG-OD2	5.69	123.42	118.30
3	C	248	ASP	CB-CG-OD2	5.67	123.40	118.30
9	I	44	ASP	CB-CG-OD2	5.66	123.40	118.30
8	H	53	ASP	CB-CG-OD2	5.64	123.38	118.30
9	I	44	ASP	N-CA-C	-5.64	95.76	111.00
4	D	185	ASP	CB-CG-OD2	5.62	123.36	118.30
4	D	89	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	417	ASP	CB-CG-OD2	5.59	123.33	118.30
3	C	254	ASP	CB-CG-OD2	5.58	123.32	118.30
2	B	409	ASP	CB-CG-OD2	5.55	123.29	118.30
4	D	72	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	332	ASP	CB-CG-OD2	5.53	123.28	118.30
8	H	60	ASP	CB-CG-OD2	5.46	123.22	118.30
3	C	20	ASP	CB-CG-OD2	5.44	123.20	118.30
4	D	59	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	159	GLN	N-CA-C	5.41	125.61	111.00
3	C	72	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	147	ASP	CB-CG-OD2	5.38	123.14	118.30
5	E	4	ASP	CB-CG-OD2	5.37	123.13	118.30
4	D	199	ASP	CB-CG-OD2	5.34	123.10	118.30
5	E	67	ASP	CB-CG-OD2	5.30	123.07	118.30
2	B	117	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	192	ALA	N-CA-C	5.26	125.20	111.00
8	H	27	LEU	N-CA-C	5.26	125.20	111.00
5	E	119	ASP	CB-CG-OD2	5.26	123.03	118.30
9	I	24	GLY	N-CA-C	5.26	126.24	113.10
1	A	37	VAL	CB-CA-C	-5.20	101.52	111.40
2	B	407	ASP	CB-CG-OD2	5.17	122.95	118.30
9	I	35	PRO	N-CA-C	-5.15	98.70	112.10
8	H	15	ASP	CB-CG-OD2	5.12	122.91	118.30
5	E	191	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	220	SER	N-CA-C	5.08	124.72	111.00
1	A	226	ASP	CB-CG-OD2	5.08	122.87	118.30
2	B	309	VAL	CB-CA-C	-5.07	101.77	111.40
5	E	80	ASP	CB-CG-OD2	5.05	122.85	118.30

All (9) chirality outliers are listed below:

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

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	69	0
2	B	3172	0	3152	69	0
3	C	3003	0	3065	76	0
4	D	1918	0	1870	65	0
5	E	1519	0	1504	20	0
6	F	911	0	904	15	0
7	G	628	0	636	15	0
8	H	575	0	550	14	0
9	I	406	0	437	61	0
10	J	483	0	465	20	0
11	K	437	0	439	7	0
12	C	86	0	60	5	0
12	D	43	0	30	3	0
13	C	46	0	52	19	0
14	E	4	0	0	0	0
15	A	29	0	0	3	0
15	B	39	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	78	0	0	6	0
15	D	30	0	0	1	0
15	E	3	0	0	0	0
15	F	14	0	0	3	0
15	G	4	0	0	0	0
15	H	1	0	0	0	0
15	I	4	0	0	1	0
15	J	2	0	0	0	0
15	K	3	0	0	0	0
All	All	16896	0	16520	376	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (376) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:MET:CE	3:C:11:MET:SD	2.09	1.41
4:D:37:CYS:SG	12:D:242:HEM:HAB	1.90	1.12
10:J:18:SER:HA	11:K:24:TRP:HZ3	1.19	1.03
1:A:325:VAL:HG21	9:I:43:LEU:HD12	1.44	0.98
3:C:221:HIS:CG	3:C:221:HIS:O	2.13	0.98
10:J:18:SER:HA	11:K:24:TRP:CZ3	2.00	0.96
7:G:73:ASN:HB3	7:G:74:PRO:HD3	1.43	0.96
2:B:76:THR:HG22	2:B:82:SER:H	1.28	0.94
2:B:385:GLN:HE22	2:B:393:THR:H	1.03	0.93
13:C:384:UQ2:H5M2	15:C:1010:HOH:O	1.70	0.90
3:C:221:HIS:CD2	3:C:221:HIS:O	2.26	0.87
3:C:146:ILE:HD11	13:C:383:UQ2:C4	2.06	0.85
2:B:169:ARG:HD3	2:B:240:HIS:HB2	1.62	0.80
4:D:37:CYS:SG	12:D:242:HEM:CAB	2.70	0.79
13:C:384:UQ2:H8	13:C:384:UQ2:H5M1	1.64	0.78
1:A:51:LYS:O	1:A:52:ASN:HB2	1.80	0.78
9:I:34:VAL:HB	9:I:35:PRO:HD3	1.65	0.78
2:B:325:TYR:CD2	9:I:28:PRO:HD2	2.19	0.77
1:A:446:PHE:OXT	10:J:17:THR:HB	1.85	0.77
2:B:99:THR:HB	9:I:14:VAL:HG22	1.66	0.77
3:C:45:ILE:HA	12:C:381:HEM:HAB	1.66	0.76
7:G:27:PRO:O	7:G:29:TYR:N	2.20	0.75
10:J:44:GLU:HG2	10:J:52:TRP:HZ2	1.52	0.74
2:B:161:GLU:OE1	2:B:175:SER:OG	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:47:ARG:HG2	9:I:48:SER:H	1.53	0.73
3:C:131:TYR:HA	12:C:381:HEM:HAD2	1.71	0.73
2:B:100:SER:O	9:I:13:PRO:HD2	1.87	0.73
4:D:164:ILE:HG22	4:D:179:MET:HG2	1.70	0.73
6:F:31:LEU:O	6:F:81:THR:HG21	1.89	0.73
3:C:211:ILE:HG21	6:F:62:ILE:HD12	1.71	0.72
1:A:48:GLU:OE2	15:A:471:HOH:O	2.06	0.72
13:C:384:UQ2:C8	13:C:384:UQ2:H5M1	2.20	0.72
4:D:195:GLU:OE1	4:D:201:ARG:NH1	2.23	0.71
3:C:322:GLN:NE2	15:C:1048:HOH:O	2.23	0.70
1:A:146:ARG:H	9:I:42:VAL:HG12	1.56	0.70
4:D:120:ARG:O	4:D:121:HIS:HB2	1.91	0.70
9:I:47:ARG:CG	9:I:48:SER:H	2.05	0.70
2:B:325:TYR:HB3	9:I:28:PRO:CD	2.22	0.69
2:B:385:GLN:HE22	2:B:393:THR:N	1.85	0.69
1:A:34:THR:HG21	2:B:370:MET:HG3	1.75	0.69
9:I:4:VAL:HG12	9:I:10:PRO:HG2	1.76	0.68
2:B:283:PRO:HG3	9:I:31:GLN:HG3	1.74	0.68
4:D:27:ARG:NH1	10:J:57:HIS:NE2	2.41	0.68
4:D:79:GLU:O	4:D:80:MET:HB2	1.94	0.68
6:F:58:ARG:NE	15:F:1902:HOH:O	2.27	0.68
2:B:435:PHE:O	2:B:436:ILE:HB	1.94	0.67
3:C:214:ASP:OD2	7:G:2:ARG:NH2	2.21	0.67
1:A:145:MET:O	1:A:149:VAL:HG23	1.94	0.67
6:F:58:ARG:NH2	15:F:1902:HOH:O	2.26	0.67
3:C:59:THR:O	15:C:1066:HOH:O	2.14	0.66
7:G:73:ASN:HB3	7:G:74:PRO:CD	2.23	0.65
2:B:310:SER:HB3	9:I:28:PRO:HG3	1.76	0.65
2:B:354:ASN:H	2:B:355:PRO:HD2	1.61	0.65
1:A:252:HIS:HD2	1:A:323:HIS:HE1	1.42	0.65
1:A:244:ARG:NH2	15:A:461:HOH:O	2.05	0.65
15:B:462:HOH:O	9:I:4:VAL:HG21	1.95	0.65
10:J:50:LYS:O	10:J:52:TRP:N	2.27	0.64
2:B:40:ASN:O	2:B:40:ASN:ND2	2.28	0.64
4:D:40:CYS:SG	12:D:242:HEM:HAC	2.37	0.64
9:I:6:ALA:C	9:I:8:SER:H	1.99	0.64
1:A:252:HIS:CD2	1:A:323:HIS:HE1	2.17	0.63
3:C:309:THR:HG21	3:C:367:PRO:O	1.99	0.63
3:C:322:GLN:OE1	15:C:1076:HOH:O	2.15	0.63
9:I:42:VAL:HG22	9:I:43:LEU:HD23	1.79	0.63
7:G:73:ASN:CB	7:G:74:PRO:HD3	2.23	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:THR:HG23	2:B:136:GLU:OE1	1.99	0.62
2:B:315:SER:O	9:I:4:VAL:HG13	2.00	0.62
1:A:244:ARG:NE	15:A:461:HOH:O	2.23	0.62
1:A:144:SER:HA	9:I:42:VAL:HB	1.80	0.61
1:A:51:LYS:O	1:A:52:ASN:CB	2.47	0.61
7:G:41:THR:O	7:G:45:ILE:HG12	1.99	0.61
4:D:165:TYR:O	4:D:165:TYR:CD2	2.54	0.61
5:E:18:VAL:O	5:E:18:VAL:HG12	1.99	0.61
3:C:222:PRO:HD2	3:C:223:TYR:H	1.65	0.61
2:B:385:GLN:NE2	2:B:393:THR:H	1.87	0.61
1:A:65:LYS:NZ	2:B:287:ARG:O	2.33	0.61
1:A:284:TYR:HE1	9:I:20:ARG:HG2	1.66	0.61
4:D:224:ARG:HD3	15:D:267:HOH:O	2.00	0.61
9:I:47:ARG:HG2	9:I:48:SER:N	2.16	0.60
1:A:237:THR:OG1	5:E:14:ARG:NH2	2.34	0.60
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.82	0.60
4:D:75:ASN:O	4:D:77:ASP:N	2.35	0.60
10:J:33:ARG:HD3	11:K:48:ILE:HA	1.83	0.60
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.83	0.59
6:F:27:ASN:HA	6:F:81:THR:HG23	1.83	0.59
6:F:28:LYS:HB3	6:F:74:ILE:HG12	1.83	0.59
4:D:165:TYR:O	4:D:165:TYR:HD2	1.86	0.59
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.21	0.59
3:C:206:ASN:ND2	3:C:207:ASN:H	2.00	0.59
2:B:290:ASN:HD22	2:B:290:ASN:N	2.00	0.59
3:C:345:HIS:O	3:C:347:TYR:N	2.36	0.59
1:A:351:GLU:H	11:K:12:GLN:NE2	2.00	0.59
2:B:325:TYR:HB3	9:I:28:PRO:HD3	1.84	0.59
9:I:44:ASP:O	9:I:46:LYS:HB2	2.03	0.58
2:B:71:LEU:HD23	9:I:15:LEU:HG	1.85	0.58
3:C:30:TRP:HZ3	3:C:96:MET:HG3	1.67	0.58
9:I:2:LEU:O	9:I:3:SER:HB3	2.03	0.58
4:D:90:TYR:C	4:D:92:PRO:HD3	2.24	0.58
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.39	0.58
3:C:132:VAL:HA	3:C:139:SER:HB3	1.86	0.58
9:I:46:LYS:HG2	9:I:47:ARG:H	1.68	0.58
4:D:83:ARG:NH2	4:D:89:ASP:OD1	2.36	0.58
3:C:282:ARG:NH2	3:C:341:GLN:O	2.38	0.57
4:D:180:SER:HB3	8:H:77:LEU:HD11	1.85	0.57
3:C:257:THR:HG22	4:D:115:TYR:HE1	1.69	0.56
10:J:19:THR:O	10:J:23:THR:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:SER:HB3	1:A:208:LEU:HD12	1.86	0.56
9:I:39:GLU:O	9:I:40:SER:HB3	2.05	0.56
1:A:388:ARG:NH2	1:A:394:GLU:OE2	2.39	0.56
4:D:93:LYS:H	4:D:94:PRO:HD2	1.71	0.56
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.88	0.56
9:I:11:PHE:HZ	9:I:27:ARG:HH21	1.53	0.56
3:C:146:ILE:HD11	13:C:383:UQ2:C5	2.36	0.56
3:C:142:GLY:HA2	13:C:383:UQ2:CM3	2.35	0.56
1:A:140:GLU:OE2	9:I:36:ALA:HB1	2.05	0.56
4:D:12:TRP:NE1	4:D:125:ASP:OD2	2.32	0.56
9:I:55:LEU:O	9:I:56:ARG:HB2	2.05	0.56
9:I:10:PRO:O	9:I:25:ALA:CB	2.54	0.55
9:I:8:SER:OG	9:I:26:LEU:HD13	2.05	0.55
9:I:41:PRO:O	9:I:42:VAL:HG23	2.05	0.55
2:B:76:THR:HG22	2:B:82:SER:N	2.11	0.55
2:B:325:TYR:CG	9:I:28:PRO:HD2	2.41	0.55
2:B:39:GLU:OE2	2:B:113:ARG:NH2	2.38	0.55
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.89	0.55
2:B:129:ALA:N	2:B:130:PRO:HD3	2.21	0.55
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.42	0.55
10:J:44:GLU:HG2	10:J:52:TRP:CZ2	2.38	0.55
4:D:178:THR:O	4:D:182:VAL:HG12	2.07	0.55
1:A:46:ARG:HG3	1:A:163:LEU:HD13	1.89	0.55
3:C:116:GLY:C	12:C:382:HEM:HBC2	2.26	0.54
2:B:145:ARG:NH2	15:B:475:HOH:O	2.35	0.54
4:D:167:GLU:HG3	4:D:177:ALA:HB3	1.88	0.54
9:I:46:LYS:HG2	9:I:47:ARG:N	2.22	0.54
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.90	0.54
10:J:2:ALA:HB3	10:J:3:PRO:HD3	1.90	0.54
3:C:357:LEU:O	3:C:361:LEU:HB2	2.08	0.53
8:H:38:GLU:HA	8:H:41:ASP:HB2	1.90	0.53
2:B:153:GLN:NE2	9:I:46:LYS:HG3	2.23	0.53
5:E:6:LYS:HD3	5:E:6:LYS:H	1.71	0.53
1:A:309:THR:O	9:I:52:ARG:NH1	2.40	0.53
4:D:83:ARG:HG2	4:D:84:PRO:HD2	1.91	0.53
1:A:378:ASP:OD2	1:A:389:ARG:NH1	2.39	0.53
3:C:226:ILE:HG23	4:D:223:LYS:HB2	1.90	0.53
7:G:28:HIS:HB3	7:G:31:SER:HB2	1.91	0.53
3:C:272:TRP:HA	3:C:275:LEU:HG	1.90	0.53
2:B:204:MET:HE1	2:B:224:LEU:HD22	1.91	0.53
3:C:146:ILE:N	3:C:146:ILE:HD13	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:158:ILE:HG13	4:D:160:MET:H	1.72	0.53
10:J:58:LYS:C	10:J:60:GLU:H	2.13	0.52
3:C:146:ILE:HD11	13:C:383:UQ2:C3	2.38	0.52
9:I:34:VAL:HB	9:I:35:PRO:CD	2.36	0.52
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.91	0.52
4:D:54:VAL:HG21	4:D:192:TRP:CZ2	2.45	0.52
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.91	0.52
3:C:197:LEU:HD11	13:C:384:UQ2:H5M3	1.91	0.52
4:D:48:TYR:OH	4:D:93:LYS:NZ	2.36	0.52
6:F:64:ARG:HH11	6:F:64:ARG:HB3	1.73	0.52
4:D:109:LEU:O	4:D:111:PRO:HD3	2.10	0.51
6:F:83:TYR:CE1	6:F:84:GLU:HG3	2.46	0.51
4:D:165:TYR:O	4:D:167:GLU:N	2.43	0.51
4:D:124:GLU:HB3	4:D:187:CYS:HB3	1.92	0.51
6:F:12:TRP:O	6:F:16:ILE:HG12	2.10	0.51
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.92	0.50
3:C:223:TYR:HB3	4:D:227:TRP:CZ2	2.47	0.50
10:J:14:PHE:HD1	10:J:20:PHE:CD1	2.28	0.50
3:C:63:PHE:HB2	15:C:1042:HOH:O	2.10	0.50
3:C:270:PRO:HG3	13:C:383:UQ2:C4	2.41	0.50
6:F:58:ARG:CZ	15:F:1902:HOH:O	2.55	0.50
2:B:68:LEU:HD13	2:B:144:LEU:HD11	1.93	0.50
1:A:255:ILE:HD13	1:A:335:MET:HE1	1.92	0.50
8:H:25:GLU:HG3	8:H:61:PHE:HZ	1.77	0.50
9:I:44:ASP:O	9:I:45:LEU:C	2.50	0.49
4:D:222:MET:HG2	5:E:40:THR:HG22	1.93	0.49
4:D:112:ASP:OD1	4:D:112:ASP:N	2.36	0.49
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.94	0.49
1:A:255:ILE:HD13	1:A:335:MET:CE	2.42	0.49
2:B:170:ASN:HB3	2:B:171:ALA:H	1.41	0.49
6:F:53:ASN:HD22	6:F:53:ASN:N	2.11	0.49
1:A:429:GLU:OE2	7:G:5:GLY:N	2.35	0.49
2:B:308:ASP:HB2	9:I:32:ALA:HB2	1.95	0.48
3:C:29:SER:HA	3:C:32:ASN:HD22	1.78	0.48
6:F:78:GLU:HG3	6:F:78:GLU:H	1.42	0.48
4:D:28:ARG:O	4:D:32:VAL:HG23	2.13	0.48
4:D:91:PHE:N	4:D:92:PRO:HD3	2.28	0.48
1:A:187:SER:O	1:A:223:TYR:OH	2.28	0.48
4:D:70:VAL:O	4:D:71:GLN:HB3	2.14	0.48
1:A:146:ARG:HH12	1:A:308:GLN:NE2	2.11	0.48
1:A:145:MET:H	9:I:42:VAL:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:139:CYS:SG	5:E:165:TYR:OH	2.67	0.48
3:C:173:ALA:O	3:C:177:ARG:HB2	2.13	0.48
1:A:219:LEU:O	1:A:221:GLY:N	2.46	0.47
10:J:20:PHE:O	10:J:24:ILE:HG23	2.15	0.47
9:I:52:ARG:O	9:I:53:GLU:HB2	2.14	0.47
4:D:147:LEU:HA	4:D:158:ILE:O	2.15	0.47
1:A:255:ILE:HG21	1:A:335:MET:HE1	1.96	0.47
3:C:78:ILE:HG13	3:C:78:ILE:H	1.47	0.47
2:B:388:ALA:HB3	9:I:2:LEU:HD13	1.96	0.47
4:D:28:ARG:HD2	4:D:185:ASP:OD2	2.15	0.47
3:C:267:HIS:HE1	3:C:269:LYS:HE2	1.79	0.47
2:B:46:ARG:HD2	2:B:375:SER:HB3	1.95	0.47
1:A:308:GLN:HE21	1:A:323:HIS:HD2	1.62	0.47
1:A:48:GLU:HG3	1:A:53:ASN:HA	1.96	0.47
9:I:15:LEU:HA	9:I:15:LEU:HD22	1.49	0.47
10:J:9:LEU:HB3	10:J:14:PHE:HE2	1.79	0.47
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.97	0.47
2:B:44:ALA:HA	2:B:112:LEU:HA	1.97	0.47
5:E:29:SER:O	5:E:33:LYS:HG2	2.15	0.47
1:A:158:PHE:O	1:A:164:ALA:HB2	2.14	0.47
1:A:155:ALA:O	5:E:7:VAL:HG21	2.15	0.47
3:C:142:GLY:HA2	13:C:383:UQ2:H3M2	1.97	0.47
9:I:11:PHE:HZ	9:I:27:ARG:NH2	2.12	0.47
5:E:136:ILE:HD11	5:E:183:PRO:HB3	1.97	0.47
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.45	0.47
1:A:378:ASP:O	1:A:382:SER:OG	2.24	0.46
3:C:220:PHE:HE2	13:C:384:UQ2:C2	2.28	0.46
3:C:270:PRO:HB3	13:C:383:UQ2:C2	2.45	0.46
2:B:354:ASN:H	2:B:355:PRO:CD	2.27	0.46
9:I:6:ALA:C	9:I:8:SER:N	2.64	0.46
3:C:152:ALA:HB2	3:C:287:LYS:HG2	1.96	0.46
4:D:47:ALA:HA	4:D:90:TYR:HA	1.97	0.46
3:C:378:LYS:HE2	6:F:17:ARG:HD3	1.98	0.46
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.96	0.46
3:C:57:SER:O	3:C:57:SER:OG	2.32	0.46
4:D:99:GLU:HG2	4:D:99:GLU:H	1.23	0.46
9:I:20:ARG:NH1	15:I:58:HOH:O	2.44	0.46
8:H:73:LEU:O	8:H:75:ASN:N	2.48	0.46
4:D:22:ASP:HB3	4:D:25:SER:HB3	1.96	0.46
1:A:25:VAL:HG23	1:A:208:LEU:HD13	1.97	0.46
3:C:361:LEU:HA	3:C:365:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:THR:HG22	1:A:35:CYS:N	2.31	0.46
2:B:435:PHE:O	2:B:436:ILE:CB	2.63	0.46
2:B:39:GLU:CD	2:B:113:ARG:HH22	2.19	0.46
10:J:14:PHE:CD1	10:J:20:PHE:HD1	2.34	0.45
3:C:71:ARG:NH1	4:D:193:ALA:O	2.49	0.45
8:H:25:GLU:OE1	8:H:34:ARG:NH1	2.49	0.45
3:C:284:ILE:HA	3:C:285:PRO:HD3	1.82	0.45
8:H:37:LEU:HD11	8:H:58:LEU:HA	1.98	0.45
8:H:17:LEU:HG	8:H:21:ARG:HD2	1.99	0.45
3:C:142:GLY:HA2	13:C:383:UQ2:H3M1	1.97	0.45
9:I:46:LYS:CG	9:I:47:ARG:H	2.23	0.45
4:D:184:LYS:HB2	8:H:74:PHE:HE2	1.81	0.45
8:H:25:GLU:O	8:H:30:CYS:HB2	2.17	0.45
13:C:383:UQ2:H121	13:C:383:UQ2:H101	1.72	0.45
4:D:225:HIS:O	4:D:228:SER:HB2	2.16	0.45
4:D:33:TYR:HA	4:D:37:CYS:SG	2.57	0.45
3:C:222:PRO:CD	3:C:223:TYR:H	2.29	0.45
3:C:267:HIS:HB2	15:C:1068:HOH:O	2.16	0.45
3:C:8:HIS:CD2	3:C:11:MET:HG3	2.51	0.45
9:I:49:VAL:O	9:I:50:LEU:HB2	2.17	0.45
3:C:90:PHE:O	3:C:94:LEU:HB2	2.17	0.45
9:I:46:LYS:CG	9:I:47:ARG:N	2.77	0.45
9:I:47:ARG:CG	9:I:48:SER:N	2.75	0.45
2:B:250:ASP:C	2:B:252:LEU:H	2.19	0.45
13:C:383:UQ2:H72	13:C:383:UQ2:H5M1	1.72	0.44
2:B:325:TYR:HB3	9:I:28:PRO:HD2	1.97	0.44
9:I:44:ASP:O	9:I:46:LYS:N	2.50	0.44
1:A:29:GLN:HG2	2:B:18:PRO:HG3	1.99	0.44
4:D:5:LEU:HD11	8:H:63:HIS:HB2	1.99	0.44
4:D:92:PRO:C	4:D:93:LYS:HG2	2.36	0.44
5:E:6:LYS:CD	5:E:6:LYS:H	2.29	0.44
5:E:15:ARG:HH11	5:E:32:ARG:HG2	1.83	0.44
2:B:393:THR:HG21	2:B:401:GLN:HE22	1.82	0.44
6:F:22:ASN:HA	6:F:27:ASN:HD21	1.81	0.44
4:D:120:ARG:HD3	4:D:120:ARG:HA	1.60	0.44
2:B:34:VAL:HG11	2:B:386:ALA:HB1	2.00	0.44
7:G:18:LEU:HB3	7:G:23:GLN:NE2	2.32	0.44
2:B:283:PRO:HG3	9:I:31:GLN:CG	2.46	0.44
9:I:18:THR:OG1	9:I:53:GLU:OE2	2.24	0.44
3:C:318:ARG:HA	3:C:319:PRO:HD3	1.73	0.44
2:B:288:GLY:O	2:B:290:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:114:VAL:HA	5:E:117:LEU:HD12	2.00	0.44
3:C:279:ALA:O	3:C:283:SER:OG	2.30	0.44
2:B:385:GLN:HG2	9:I:2:LEU:HD12	2.00	0.44
2:B:49:LEU:HD11	2:B:204:MET:HE3	1.99	0.44
4:D:79:GLU:HB2	4:D:80:MET:H	1.62	0.44
2:B:126:VAL:O	2:B:130:PRO:HG3	2.18	0.44
4:D:28:ARG:HB3	4:D:171:PHE:CE2	2.53	0.44
9:I:39:GLU:O	9:I:40:SER:CB	2.65	0.44
4:D:223:LYS:HD2	4:D:227:TRP:CD1	2.53	0.43
3:C:237:LEU:HD13	4:D:212:MET:HG2	1.99	0.43
8:H:11:GLU:O	8:H:12:GLU:HB2	2.18	0.43
3:C:8:HIS:HD2	3:C:11:MET:HG3	1.83	0.43
3:C:197:LEU:HD12	3:C:197:LEU:HA	1.86	0.43
3:C:346:PRO:HG3	7:G:65:GLU:HB3	1.99	0.43
4:D:14:HIS:NE2	4:D:124:GLU:OE1	2.45	0.43
4:D:183:ALA:HA	4:D:186:VAL:HG12	2.00	0.43
2:B:124:LEU:HD11	2:B:219:VAL:HG13	2.01	0.43
1:A:419:CYS:SG	1:A:438:ARG:NH1	2.92	0.43
5:E:64:ALA:O	5:E:65:SER:OG	2.28	0.43
3:C:27:ILE:HD12	13:C:384:UQ2:H2M1	2.00	0.43
10:J:29:LEU:HA	11:K:34:TRP:CD1	2.54	0.43
10:J:14:PHE:CD1	10:J:20:PHE:CD1	3.06	0.43
1:A:126:GLN:O	1:A:130:GLU:HG2	2.19	0.43
4:D:131:LEU:HD13	4:D:164:ILE:HD11	2.01	0.43
1:A:219:LEU:HB3	1:A:220:SER:H	1.65	0.43
2:B:76:THR:HB	2:B:81:SER:HA	2.00	0.43
10:J:29:LEU:HD13	11:K:34:TRP:HB2	2.00	0.43
5:E:99:ARG:NH2	5:E:105:GLU:OE2	2.51	0.43
3:C:31:TRP:HB3	13:C:384:UQ2:H2M1	2.01	0.43
1:A:373:THR:HB	1:A:374:PRO:HD3	2.01	0.43
5:E:72:SER:HB3	5:E:91:TRP:CD1	2.54	0.43
1:A:209:LEU:HD23	1:A:209:LEU:HA	1.81	0.43
7:G:34:ILE:HA	7:G:37:VAL:HG13	2.01	0.42
1:A:104:LYS:O	1:A:107:PRO:HD2	2.19	0.42
3:C:35:SER:HB3	13:C:384:UQ2:H71	2.00	0.42
3:C:215:VAL:HG21	6:F:59:VAL:HB	2.00	0.42
1:A:294:LEU:HG	1:A:307:PHE:CE1	2.55	0.42
1:A:17:SER:HB3	1:A:205:HIS:NE2	2.34	0.42
7:G:29:TYR:O	7:G:33:GLY:HA3	2.20	0.42
3:C:254:ASP:C	3:C:256:TYR:H	2.22	0.42
3:C:150:LEU:HB3	3:C:160:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HG2	2:B:284:HIS:HB2	2.00	0.42
2:B:20:HIS:CD2	2:B:20:HIS:H	2.37	0.42
1:A:252:HIS:HE1	9:I:43:LEU:HB2	1.85	0.42
3:C:265:PRO:HD2	3:C:268:ILE:HD11	2.02	0.42
4:D:28:ARG:HD3	4:D:171:PHE:CD2	2.55	0.42
1:A:220:SER:HA	1:A:223:TYR:HB3	2.01	0.42
4:D:41:HIS:ND1	4:D:113:LEU:HD13	2.34	0.42
2:B:353:SER:HB3	2:B:356:ASP:H	1.85	0.42
1:A:70:ARG:NH1	1:A:115:ASP:OD2	2.52	0.42
3:C:345:HIS:ND1	3:C:346:PRO:HD3	2.34	0.41
1:A:270:LEU:HD22	1:A:320:LEU:HD21	2.02	0.41
3:C:298:ILE:HA	3:C:298:ILE:HD13	1.59	0.41
3:C:179:PHE:HE2	12:C:381:HEM:HMA1	1.85	0.41
2:B:308:ASP:OD2	9:I:31:GLN:HB2	2.19	0.41
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.90	0.41
2:B:122:PHE:O	2:B:126:VAL:HG23	2.19	0.41
3:C:100:ARG:NH2	12:C:382:HEM:HBD1	2.36	0.41
3:C:267:HIS:HB3	3:C:268:ILE:H	1.34	0.41
5:E:65:SER:C	5:E:67:ASP:H	2.23	0.41
4:D:106:ASN:O	4:D:108:ALA:N	2.52	0.41
3:C:216:ASP:OD2	4:D:233:ARG:NH2	2.45	0.41
3:C:343:VAL:HG12	3:C:348:ILE:HG12	2.03	0.41
2:B:418:VAL:O	2:B:422:LYS:NZ	2.54	0.41
3:C:337:TRP:CZ3	3:C:350:ILE:HD11	2.55	0.41
2:B:361:LYS:O	2:B:365:LYS:HG3	2.20	0.41
8:H:54:CYS:HA	8:H:57:GLU:OE1	2.21	0.41
2:B:294:SER:CB	2:B:343:GLN:HE21	2.33	0.41
1:A:378:ASP:OD2	9:I:56:ARG:NH2	2.53	0.41
1:A:294:LEU:HD13	1:A:337:VAL:HG12	2.02	0.41
2:B:216:LEU:HD23	2:B:216:LEU:HA	1.90	0.41
1:A:390:ILE:HA	1:A:391:PRO:HD3	1.91	0.41
4:D:116:ILE:HA	4:D:116:ILE:HD13	1.92	0.41
2:B:241:GLY:HA2	2:B:423:SER:OG	2.20	0.41
9:I:2:LEU:HG	9:I:2:LEU:H	1.71	0.41
8:H:77:LEU:HA	8:H:77:LEU:HD23	1.81	0.41
2:B:294:SER:HB3	2:B:343:GLN:HE21	1.85	0.41
1:A:280:TYR:CG	1:A:281:ASP:N	2.89	0.41
1:A:59:VAL:HG11	1:A:186:LEU:HD21	2.03	0.41
4:D:170:GLU:C	4:D:172:ASP:H	2.24	0.41
3:C:270:PRO:HG3	13:C:383:UQ2:C3	2.51	0.41
9:I:47:ARG:CD	9:I:48:SER:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:345:HIS:O	3:C:346:PRO:C	2.59	0.41
5:E:72:SER:HB3	5:E:91:TRP:HD1	1.86	0.41
4:D:113:LEU:HA	4:D:113:LEU:HD12	1.84	0.41
3:C:344:GLU:O	3:C:348:ILE:HG13	2.20	0.41
4:D:150:ASN:HA	4:D:151:PRO:HD3	1.93	0.41
2:B:387:LEU:HD12	2:B:387:LEU:HA	1.87	0.41
10:J:47:ASN:O	10:J:48:GLU:HB2	2.21	0.41
1:A:21:ASN:HB3	1:A:192:ALA:HB1	2.03	0.41
4:D:93:LYS:O	4:D:94:PRO:C	2.60	0.41
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.74	0.41
1:A:110:VAL:HG11	1:A:211:LEU:HB3	2.03	0.41
11:K:13:LEU:HA	11:K:13:LEU:HD23	1.94	0.40
3:C:324:LEU:HA	3:C:324:LEU:HD23	1.89	0.40
8:H:47:ARG:HB3	8:H:48:SER:H	1.76	0.40
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.56	0.40
2:B:37:SER:HB3	2:B:216:LEU:HD12	2.04	0.40
4:D:198:HIS:ND1	4:D:199:ASP:OD1	2.48	0.40
3:C:206:ASN:HD21	3:C:210:GLY:HA2	1.85	0.40
1:A:8:LEU:HD22	1:A:392:LEU:HB3	2.04	0.40
1:A:442:PHE:C	1:A:442:PHE:CD2	2.94	0.40
1:A:242:CYS:O	7:G:14:ILE:HA	2.21	0.40
2:B:290:ASN:OD1	9:I:31:GLN:NE2	2.54	0.40
4:D:170:GLU:O	4:D:172:ASP:N	2.45	0.40
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	444/446 (100%)	409 (92%)	21 (5%)	14 (3%)	5 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	421/439 (96%)	393 (93%)	20 (5%)	8 (2%)	10 19
3	C	376/379 (99%)	349 (93%)	18 (5%)	9 (2%)	7 13
4	D	239/241 (99%)	183 (77%)	36 (15%)	20 (8%)	1 1
5	E	194/196 (99%)	175 (90%)	15 (8%)	4 (2%)	9 16
6	F	103/110 (94%)	98 (95%)	3 (3%)	2 (2%)	10 19
7	G	73/81 (90%)	65 (89%)	3 (4%)	5 (7%)	1 1
8	H	68/78 (87%)	49 (72%)	10 (15%)	9 (13%)	0 0
9	I	55/57 (96%)	26 (47%)	16 (29%)	13 (24%)	0 0
10	J	59/62 (95%)	45 (76%)	9 (15%)	5 (8%)	1 1
11	K	51/56 (91%)	42 (82%)	4 (8%)	5 (10%)	1 0
All	All	2083/2145 (97%)	1834 (88%)	155 (7%)	94 (4%)	3 4

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	220	SER
1	A	227	ALA
2	B	305	GLN
3	C	222	PRO
3	C	254	ASP
3	C	267	HIS
3	C	345	HIS
3	C	346	PRO
3	C	347	TYR
4	D	71	GLN
4	D	76	GLU
4	D	80	MET
4	D	96	PRO
4	D	121	HIS
4	D	169	LEU
4	D	172	ASP
5	E	65	SER
5	E	69	LEU
7	G	2	ARG
7	G	27	PRO
7	G	28	HIS
7	G	73	ASN

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Mol	Chain	Res	Type
8	H	12	GLU
8	H	27	LEU
8	H	73	LEU
8	H	74	PHE
9	I	29	LEU
9	I	37	THR
9	I	39	GLU
9	I	40	SER
9	I	45	LEU
9	I	53	GLU
9	I	55	LEU
9	I	56	ARG
10	J	48	GLU
10	J	51	LEU
11	K	52	PHE
1	A	50	GLU
1	A	52	ASN
1	A	72	GLY
2	B	21	PRO
3	C	30	TRP
4	D	107	GLY
8	H	11	GLU
8	H	26	GLN
8	H	28	GLU
8	H	49	GLN
9	I	8	SER
9	I	47	ARG
10	J	58	LYS
11	K	48	ILE
1	A	21	ASN
1	A	223	TYR
1	A	315	ALA
2	B	228	GLY
4	D	36	VAL
4	D	87	LEU
4	D	93	LYS
4	D	94	PRO
4	D	167	GLU
5	E	71	MET
5	E	72	SER
6	F	7	SER
6	F	85	GLU

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Mol	Chain	Res	Type
9	I	3	SER
9	I	48	SER
10	J	2	ALA
10	J	56	LYS
11	K	38	TRP
1	A	192	ALA
1	A	224	ASP
2	B	236	LYS
2	B	353	SER
4	D	104	ALA
4	D	146	GLY
4	D	166	ASN
7	G	31	SER
8	H	46	SER
9	I	4	VAL
1	A	49	SER
2	B	354	ASN
4	D	54	VAL
4	D	106	ASN
11	K	43	ASP
3	C	268	ILE
11	K	46	PRO
1	A	71	PRO
2	B	249	GLY
4	D	91	PHE
4	D	163	PRO
2	B	436	ILE
1	A	221	GLY
3	C	221	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	370/370 (100%)	339 (92%)	31 (8%)	14 26
2	B	332/343 (97%)	301 (91%)	31 (9%)	11 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	326/327 (100%)	305 (94%)	21 (6%)	22 43
4	D	206/206 (100%)	173 (84%)	33 (16%)	3 5
5	E	168/168 (100%)	157 (94%)	11 (6%)	21 42
6	F	96/98 (98%)	86 (90%)	10 (10%)	9 16
7	G	66/71 (93%)	62 (94%)	4 (6%)	23 46
8	H	67/74 (90%)	55 (82%)	12 (18%)	2 3
9	I	44/44 (100%)	31 (70%)	13 (30%)	0 1
10	J	46/52 (88%)	41 (89%)	5 (11%)	8 14
11	K	42/46 (91%)	38 (90%)	4 (10%)	11 20
All	All	1763/1799 (98%)	1588 (90%)	175 (10%)	10 18

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	25	VAL
1	A	32	GLN
1	A	37	VAL
1	A	42	ASP
1	A	53	ASN
1	A	58	PHE
1	A	90	SER
1	A	100	LYS
1	A	113	LEU
1	A	117	VAL
1	A	127	ILE
1	A	131	ARG
1	A	149	VAL
1	A	195	MET
1	A	203	LEU
1	A	208	LEU
1	A	209	LEU
1	A	223	TYR
1	A	226	ASP
1	A	230	THR
1	A	245	GLU
1	A	274	ASN
1	A	308	GLN
1	A	350	THR

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Mol	Chain	Res	Type
1	A	383	LEU
1	A	403	ASP
1	A	430	GLN
1	A	438	ARG
1	A	439	SER
1	A	443	TRP
2	B	17	VAL
2	B	20	HIS
2	B	38	LEU
2	B	40	ASN
2	B	69	LEU
2	B	97	SER
2	B	98	VAL
2	B	99	THR
2	B	109	VAL
2	B	110	GLU
2	B	119	LEU
2	B	123	LEU
2	B	163	LEU
2	B	170	ASN
2	B	176	LEU
2	B	186	VAL
2	B	189	VAL
2	B	197	ASN
2	B	227	ARG
2	B	232	LEU
2	B	248	ASN
2	B	257	LEU
2	B	290	ASN
2	B	294	SER
2	B	305	GLN
2	B	309	VAL
2	B	346	THR
2	B	353	SER
2	B	387	LEU
2	B	396	SER
2	B	397	THR
3	C	42	ILE
3	C	46	LEU
3	C	57	SER
3	C	61	THR
3	C	78	ILE

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Mol	Chain	Res	Type
3	C	80	ARG
3	C	90	PHE
3	C	96	MET
3	C	102	LEU
3	C	164	ILE
3	C	175	LEU
3	C	183	PHE
3	C	215	VAL
3	C	225	THR
3	C	264	THR
3	C	267	HIS
3	C	298	ILE
3	C	309	THR
3	C	318	ARG
3	C	350	ILE
3	C	379	TRP
4	D	1	SER
4	D	9	SER
4	D	13	SER
4	D	24	THR
4	D	37	CYS
4	D	55	CYS
4	D	68	VAL
4	D	80	MET
4	D	93	LYS
4	D	95	TYR
4	D	99	GLU
4	D	109	LEU
4	D	112	ASP
4	D	113	LEU
4	D	114	SER
4	D	120	ARG
4	D	132	THR
4	D	135	CYS
4	D	156	GLN
4	D	158	ILE
4	D	164	ILE
4	D	165	TYR
4	D	168	VAL
4	D	175	THR
4	D	179	MET
4	D	182	VAL

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Mol	Chain	Res	Type
4	D	191	ARG
4	D	201	ARG
4	D	212	MET
4	D	214	LEU
4	D	223	LYS
4	D	226	LYS
4	D	228	SER
5	E	3	THR
5	E	6	LYS
5	E	7	VAL
5	E	12	ASP
5	E	22	THR
5	E	24	SER
5	E	52	LYS
5	E	54	VAL
5	E	113	GLU
5	E	158	CYS
5	E	188	THR
6	F	22	ASN
6	F	27	ASN
6	F	37	ILE
6	F	53	ASN
6	F	74	ILE
6	F	78	GLU
6	F	81	THR
6	F	90	LEU
6	F	94	LEU
6	F	110	LYS
7	G	31	SER
7	G	44	CYS
7	G	45	ILE
7	G	68	LYS
8	H	10	GLU
8	H	13	LEU
8	H	14	VAL
8	H	15	ASP
8	H	24	CYS
8	H	29	LYS
8	H	37	LEU
8	H	41	ASP
8	H	51	GLU
8	H	65	ARG

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Mol	Chain	Res	Type
8	H	68	CYS
8	H	71	HIS
9	I	1	MET
9	I	8	SER
9	I	11	PHE
9	I	15	LEU
9	I	16	SER
9	I	18	THR
9	I	20	ARG
9	I	27	ARG
9	I	30	VAL
9	I	39	GLU
9	I	47	ARG
9	I	49	VAL
9	I	55	LEU
10	J	1	VAL
10	J	11	SER
10	J	23	THR
10	J	24	ILE
10	J	45	HIS
11	K	22	GLN
11	K	24	TRP
11	K	38	TRP
11	K	44	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	73	ASN
1	A	119	ASN
1	A	126	GLN
1	A	141	ASN
1	A	173	ASN
1	A	189	HIS
1	A	252	HIS
1	A	271	GLN
1	A	274	ASN
1	A	305	GLN
1	A	323	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
2	B	20	HIS
2	B	143	GLN
2	B	153	GLN
2	B	162	ASN
2	B	174	ASN
2	B	197	ASN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	342	ASN
2	B	343	GLN
2	B	362	ASN
2	B	385	GLN
2	B	401	GLN
3	C	8	HIS
3	C	32	ASN
3	C	68	HIS
3	C	114	ASN
3	C	206	ASN
3	C	267	HIS
3	C	341	GLN
3	C	352	GLN
4	D	71	GLN
4	D	105	ASN
4	D	121	HIS
4	D	156	GLN
4	D	200	HIS
5	E	53	ASN
5	E	57	GLN
5	E	161	HIS
6	F	38	HIS
6	F	53	ASN
6	F	72	GLN
9	I	31	GLN
11	K	12	GLN
11	K	16	ASN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	HEM	C	381	3	30,50,50	5.58	17 (56%)	24,82,82	4.01	11 (45%)
12	HEM	C	382	3	30,50,50	5.70	18 (60%)	24,82,82	3.72	12 (50%)
13	UQ2	C	383	-	23,23,23	2.08	7 (30%)	28,31,31	1.58	5 (17%)
13	UQ2	C	384	-	23,23,23	2.22	6 (26%)	28,31,31	1.50	6 (21%)
12	HEM	D	242	4	30,50,50	5.92	17 (56%)	24,82,82	3.82	11 (45%)
14	FES	E	200	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	-	0/10/54/54	0/0/8/8
12	HEM	C	382	3	-	0/10/54/54	0/0/8/8
13	UQ2	C	383	-	-	0/15/39/39	0/1/1/1
13	UQ2	C	384	-	-	0/15/39/39	0/1/1/1
12	HEM	D	242	4	-	0/10/54/54	0/0/8/8
14	FES	E	200	5	-	0/0/4/4	0/1/1/1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	382	HEM	C3B-C4B	-20.57	1.33	1.51
12	D	242	HEM	C3B-C4B	-20.11	1.33	1.51
12	C	381	HEM	C3B-C4B	-18.67	1.35	1.51
12	D	242	HEM	C3D-C4D	-14.75	1.32	1.51
12	C	381	HEM	C3D-C4D	-12.94	1.34	1.51
12	C	382	HEM	C3D-C4D	-11.40	1.36	1.51
12	C	382	HEM	C2C-C1C	-10.97	1.31	1.52
12	C	381	HEM	C2C-C1C	-10.03	1.33	1.52
12	D	242	HEM	C2C-C1C	-9.85	1.33	1.52
12	D	242	HEM	C2D-C3D	-7.60	1.31	1.54
12	C	382	HEM	C2D-C3D	-7.01	1.33	1.54
12	C	381	HEM	C2D-C3D	-6.86	1.33	1.54
12	D	242	HEM	C2B-C1B	-6.24	1.31	1.51
12	C	382	HEM	C2B-C1B	-5.71	1.33	1.51
12	D	242	HEM	C2D-C1D	-5.55	1.33	1.51
12	C	381	HEM	C2B-C1B	-5.18	1.34	1.51
12	C	382	HEM	C2D-C1D	-4.75	1.36	1.51
12	C	381	HEM	C2D-C1D	-4.67	1.36	1.51
12	C	382	HEM	CMA-C3A	-2.12	1.47	1.51
13	C	384	UQ2	C7-C8	2.00	1.53	1.50
13	C	383	UQ2	C7-C6	2.02	1.55	1.51
13	C	384	UQ2	C7-C6	2.04	1.55	1.51
13	C	383	UQ2	C7-C8	2.25	1.54	1.50
13	C	383	UQ2	C6-C1	2.28	1.52	1.46
12	C	381	HEM	C2A-C3A	2.46	1.45	1.37
12	C	382	HEM	C2A-C3A	2.49	1.45	1.37
12	D	242	HEM	C1A-CHA	2.66	1.47	1.39
13	C	384	UQ2	C13-C14	2.80	1.40	1.32
12	D	242	HEM	C4A-CHB	2.90	1.47	1.39
12	C	382	HEM	CHC-C4B	2.95	1.47	1.38
13	C	383	UQ2	C13-C14	2.98	1.41	1.32
12	D	242	HEM	C2A-C3A	3.02	1.46	1.37
12	C	382	HEM	C4A-CHB	3.04	1.48	1.39
12	C	381	HEM	C4A-CHB	3.12	1.48	1.39
12	C	381	HEM	CHD-C1D	3.16	1.47	1.38
13	C	384	UQ2	C3-C2	3.28	1.49	1.35
12	D	242	HEM	CHC-C4B	3.33	1.48	1.38
12	C	382	HEM	C1A-CHA	3.47	1.49	1.39
12	D	242	HEM	CHD-C1D	3.48	1.48	1.38
13	C	383	UQ2	C3-C2	3.50	1.50	1.35
12	C	382	HEM	CHD-C1D	3.54	1.48	1.38
13	C	383	UQ2	C8-C9	3.54	1.39	1.33
12	C	382	HEM	CBC-CAC	3.84	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	384	UQ2	C8-C9	3.91	1.40	1.33
12	C	381	HEM	CBB-CAB	3.97	1.52	1.29
12	C	381	HEM	C1A-CHA	3.98	1.50	1.39
12	D	242	HEM	CBB-CAB	4.03	1.52	1.29
12	C	381	HEM	CBC-CAC	4.04	1.52	1.29
12	C	382	HEM	CBB-CAB	4.11	1.53	1.29
12	C	381	HEM	CHC-C4B	4.12	1.50	1.38
12	C	382	HEM	C1C-NC	4.12	1.41	1.36
12	D	242	HEM	CBC-CAC	4.33	1.54	1.29
12	C	381	HEM	CHC-C1C	4.91	1.47	1.36
12	D	242	HEM	C1C-NC	5.27	1.42	1.36
12	C	382	HEM	C4C-NC	5.28	1.42	1.36
12	C	382	HEM	CHC-C1C	5.32	1.48	1.36
12	D	242	HEM	C4C-NC	5.37	1.42	1.36
12	C	382	HEM	CHD-C4C	5.48	1.49	1.36
12	D	242	HEM	CHC-C1C	5.53	1.49	1.36
12	C	381	HEM	CHD-C4C	5.64	1.49	1.36
12	D	242	HEM	CHD-C4C	5.69	1.49	1.36
12	C	381	HEM	C4C-NC	5.89	1.43	1.36
12	C	381	HEM	C1C-NC	6.07	1.43	1.36
13	C	383	UQ2	C6-C5	6.19	1.49	1.35
13	C	384	UQ2	C6-C5	7.73	1.53	1.35

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	381	HEM	C3C-CAC-CBC	-9.61	109.71	124.46
12	C	381	HEM	C3B-CAB-CBB	-9.24	110.29	124.46
12	D	242	HEM	C3C-CAC-CBC	-9.06	110.56	124.46
12	C	382	HEM	C1D-CHD-C4C	-8.59	111.47	125.82
12	C	382	HEM	C3C-CAC-CBC	-7.83	112.44	124.46
12	C	381	HEM	C4B-CHC-C1C	-7.62	113.08	125.82
12	C	382	HEM	C4B-CHC-C1C	-7.28	113.65	125.82
12	D	242	HEM	C3B-CAB-CBB	-7.19	113.44	124.46
12	D	242	HEM	C4B-CHC-C1C	-7.04	114.05	125.82
12	C	381	HEM	C1D-CHD-C4C	-6.86	114.36	125.82
12	D	242	HEM	C1D-CHD-C4C	-6.84	114.39	125.82
12	C	382	HEM	C3B-CAB-CBB	-4.83	117.05	124.46
12	D	242	HEM	CAA-CBA-CGA	-3.48	106.37	112.75
13	C	384	UQ2	C7-C6-C1	-3.09	114.92	118.56
13	C	384	UQ2	CM2-O2-C2	-2.84	106.52	116.61
13	C	383	UQ2	C10-C9-C8	-2.79	118.03	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	383	UQ2	CM5-C5-C6	-2.55	118.66	124.10
12	C	381	HEM	CBA-CAA-C2A	-2.40	108.23	112.53
13	C	384	UQ2	C7-C8-C9	-2.21	122.95	126.70
13	C	383	UQ2	C12-C13-C14	-2.12	119.56	127.73
12	C	382	HEM	CBD-CAD-C3D	-2.12	107.38	113.55
12	C	382	HEM	C2C-C1C-CHC	-2.07	120.53	123.68
13	C	384	UQ2	C5-C6-C1	-2.05	117.78	120.12
13	C	384	UQ2	C8-C7-C6	2.16	118.14	111.64
12	D	242	HEM	CMD-C2D-C3D	2.27	124.38	114.35
12	C	382	HEM	CMD-C2D-C3D	2.41	125.01	114.35
12	C	381	HEM	CMD-C2D-C3D	2.52	125.48	114.35
13	C	384	UQ2	C10-C9-C11	3.07	120.10	115.41
12	C	381	HEM	CMC-C2C-C3C	3.08	124.23	116.53
12	C	381	HEM	CAD-C3D-C4D	3.47	124.70	112.47
12	D	242	HEM	CMC-C2C-C3C	3.64	125.62	116.53
12	C	381	HEM	CMB-C2B-C3B	3.65	125.64	116.53
13	C	383	UQ2	C10-C9-C11	3.73	121.11	115.41
12	D	242	HEM	CAD-C3D-C4D	3.78	125.82	112.47
12	C	382	HEM	CAD-C3D-C2D	3.85	124.29	113.22
12	C	381	HEM	C2D-C3D-C4D	3.90	108.11	101.50
12	C	382	HEM	CAD-C3D-C4D	3.99	126.55	112.47
12	D	242	HEM	CAD-C3D-C2D	4.12	125.07	113.22
13	C	383	UQ2	C7-C6-C1	4.23	123.53	118.56
12	D	242	HEM	C2D-C3D-C4D	4.47	109.07	101.50
12	D	242	HEM	CMB-C2B-C3B	4.48	127.71	116.53
12	C	382	HEM	C2D-C3D-C4D	4.51	109.15	101.50
12	C	382	HEM	CMC-C2C-C3C	4.70	128.26	116.53
12	C	382	HEM	CMB-C2B-C3B	4.75	128.38	116.53
12	C	381	HEM	CAD-C3D-C2D	4.85	127.15	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	381	HEM	3	0
12	C	382	HEM	2	0
13	C	383	UQ2	11	0
13	C	384	UQ2	8	0
12	D	242	HEM	3	0

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.