Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:21 AM EDT

PDB ID	:	2OCC / pdb_00002occ
Title	:	BOVINE HEART CYTOCHROME C OXIDASE AT THE FULLY OXIDIZED STATE
Authors	:	Tsukihara, T.; Yao, M.
Deposited on	:	1998-05-26
Resolution	:	2.30 Å(reported)

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

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

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

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

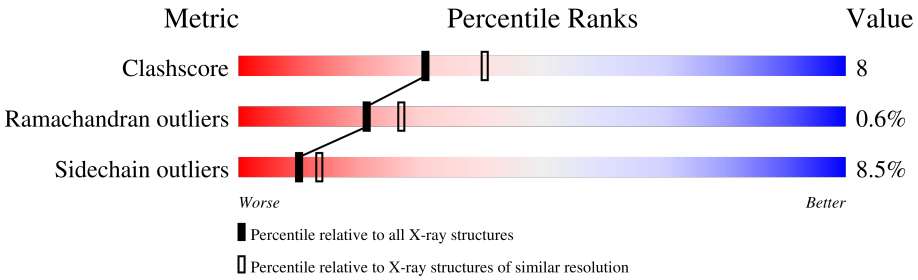
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	73% 23% •
1	N	514	73% 24% •
2	B	227	64% 30% 5% •
2	O	227	63% 31% 6%
3	C	261	79% 18% •
3	P	261	80% 17% •
4	D	147	65% 31% • •
4	Q	147	66% 29% • •

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Mol	Chain	Length	Quality of chain
5	E	109	73% 17% 6%
5	R	109	72% 21%
6	F	98	74% 19% 6%
6	S	98	73% 20% 6%
7	G	84	64% 26% 8%
7	T	84	64% 27% 7%
8	H	85	65% 24% 5% 7%
8	U	85	67% 21% 5% 7%
9	I	73	78% 19%
9	V	73	81% 15%
10	J	59	76% 17% 5%
10	W	59	75% 19% 5%
11	K	56	68% 16% 12%
11	X	56	64% 21% 12%
12	L	47	77% 19%
12	Y	47	77% 19%
13	M	46	72% 13% 9% 7%
13	Z	46	70% 17% 7% 7%

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 28864 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 CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4025	2690	623	677	35			
1	N	514	Total	C	N	O	S	0	0	0
			4025	2690	623	677	35			

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	5	0
			1863	1207	288	350	18			
2	O	227	Total	C	N	O	S	0	5	0
			1863	1207	288	350	18			

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	261	Total	C	N	O	S	0	0	0
			2124	1420	338	353	13			
3	P	261	Total	C	N	O	S	0	0	0
			2124	1420	338	353	13			

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

- Molecule 7 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	S	0	0	0
			672	431	129	111	1			
7	T	84	Total	C	N	O	S	0	0	0
			672	431	129	111	1			

- Molecule 8 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			598	388	107	99	4			
9	V	73	Total	C	N	O	S	0	0	0
			598	388	107	99	4			

- Molecule 10 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

- Molecule 12 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	47	Total	C	N	O	S	0	0	0
			386	257	65	62	2			
12	Y	47	Total	C	N	O	S	0	0	0
			386	257	65	62	2			

- Molecule 13 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Cu	0	0
			1	1		
14	B	2	Total	Cu	0	0
			2	2		
14	N	1	Total	Cu	0	0
			1	1		
14	O	2	Total	Cu	0	0
			2	2		

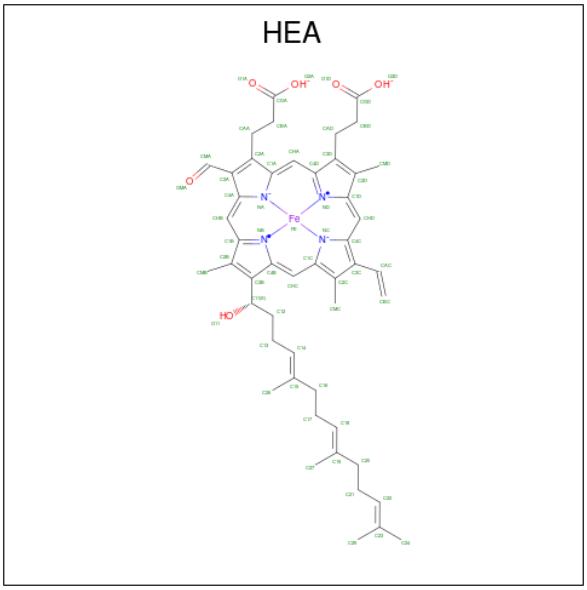
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

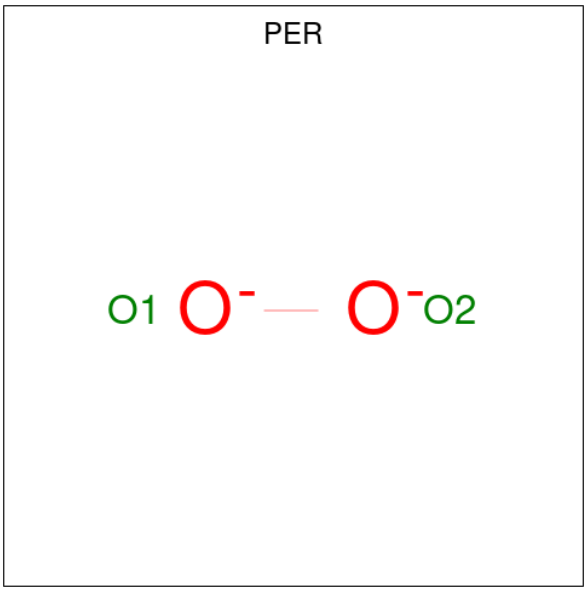
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0

- Molecule 18 is PEROXIDE ION (CCD ID: PER) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 2 2	0	0
18	N	1	Total O 2 2	0	0

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	F	1	Total Zn 1 1	0	0
19	S	1	Total Zn 1 1	0	0

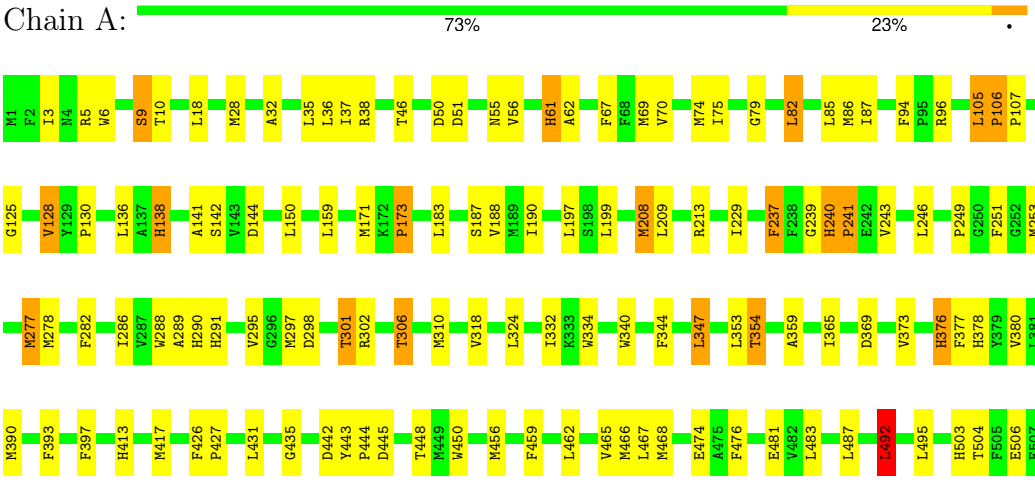
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

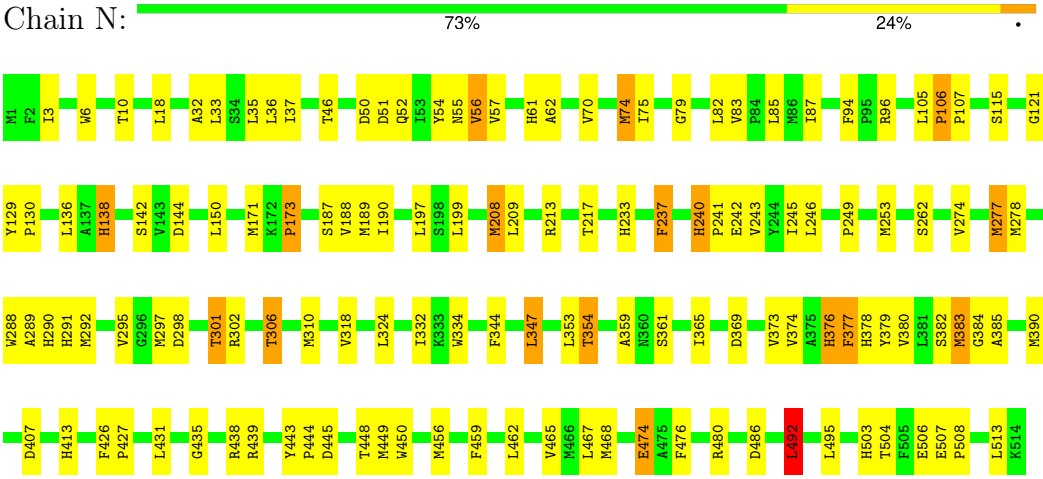
• Molecule 1: CYTOCHROME C OXIDASE

Chain A:



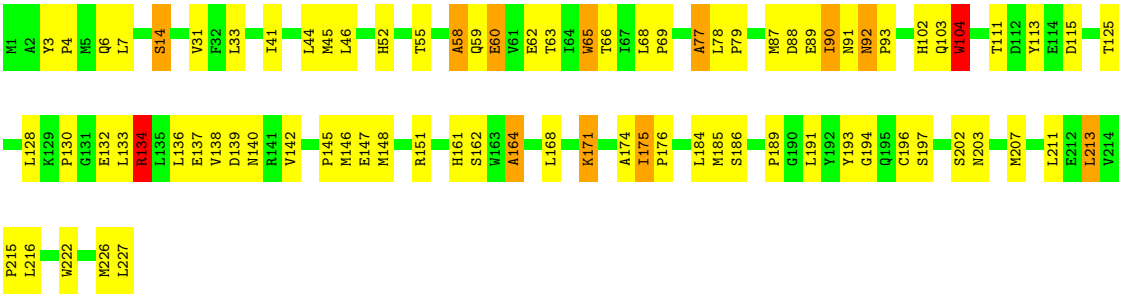
• Molecule 1: CYTOCHROME C OXIDASE

Chain N:



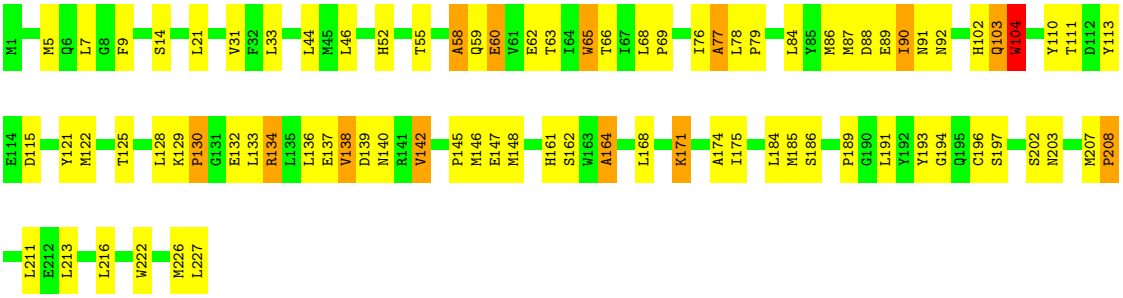
• Molecule 2: CYTOCHROME C OXIDASE

Chain B:



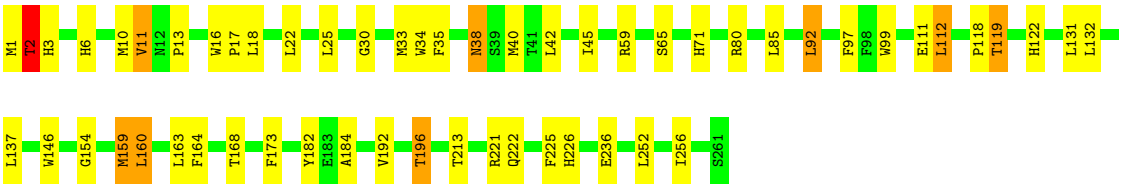
• Molecule 2: CYTOCHROME C OXIDASE

Chain O:



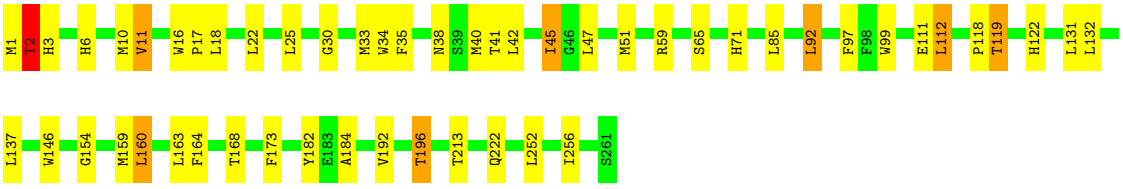
• Molecule 3: CYTOCHROME C OXIDASE

Chain C:



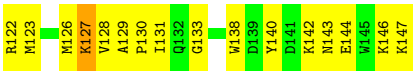
• Molecule 3: CYTOCHROME C OXIDASE

Chain P:



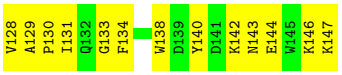
• Molecule 4: CYTOCHROME C OXIDASE

Chain D:



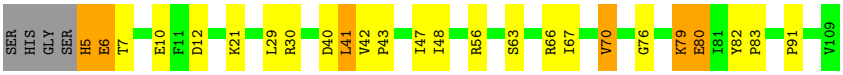
• Molecule 4: CYTOCHROME C OXIDASE

Chain Q:



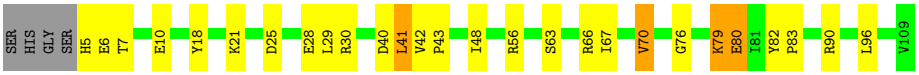
• Molecule 5: CYTOCHROME C OXIDASE

Chain E:



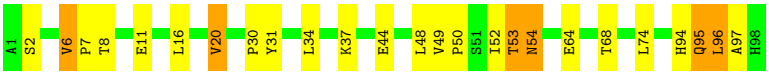
• Molecule 5: CYTOCHROME C OXIDASE

Chain R:



• Molecule 6: CYTOCHROME C OXIDASE

Chain F:



• Molecule 6: CYTOCHROME C OXIDASE

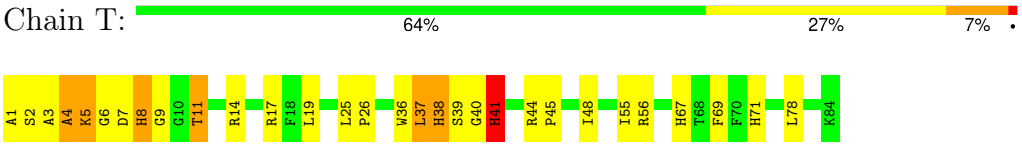
Chain S:

• Molecule 7: CYTOCHROME C OXIDASE

Chain G:

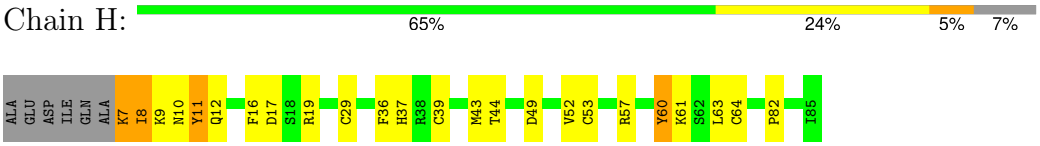
• Molecule 7: CYTOCHROME C OXIDASE

Chain T:



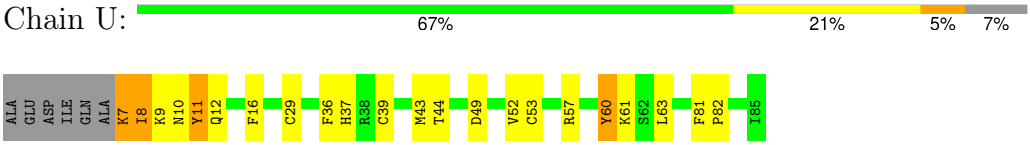
• Molecule 8: CYTOCHROME C OXIDASE

Chain H:



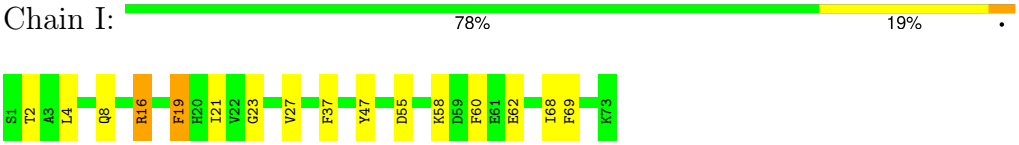
• Molecule 8: CYTOCHROME C OXIDASE

Chain U:



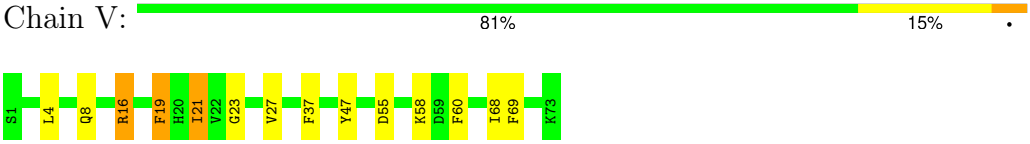
• Molecule 9: CYTOCHROME C OXIDASE

Chain I:



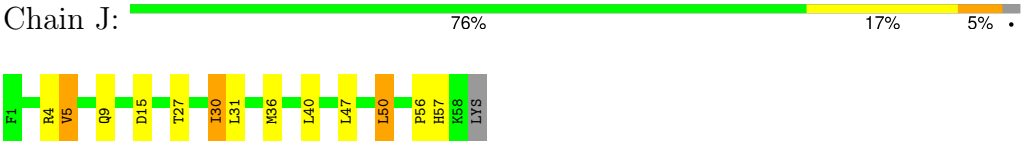
• Molecule 9: CYTOCHROME C OXIDASE

Chain V:



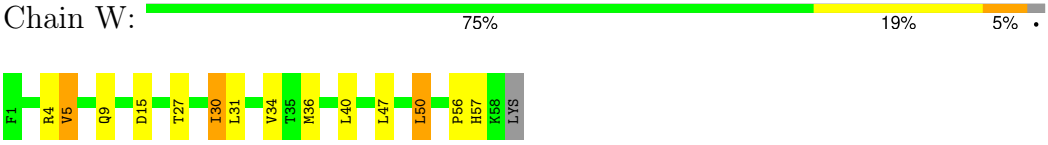
• Molecule 10: CYTOCHROME C OXIDASE

Chain J:



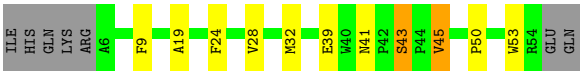
• Molecule 10: CYTOCHROME C OXIDASE

Chain W:



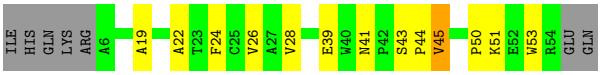
• Molecule 11: CYTOCHROME C OXIDASE

Chain K:



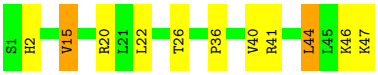
• Molecule 11: CYTOCHROME C OXIDASE

Chain X:



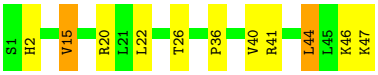
• Molecule 12: CYTOCHROME C OXIDASE

Chain L:



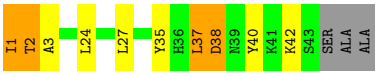
• Molecule 12: CYTOCHROME C OXIDASE

Chain Y:



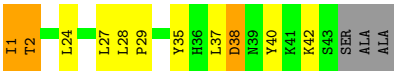
• Molecule 13: CYTOCHROME C OXIDASE

Chain M:



• Molecule 13: CYTOCHROME C OXIDASE

Chain Z:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	189.10Å 210.50Å 178.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	88.9 (15.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.209 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28864	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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: PER, ZN, MG, HEA, NA, CU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.09	15/4164 (0.4%)	1.21	46/5688 (0.8%)
1	N	0.91	15/4164 (0.4%)	1.16	36/5688 (0.6%)
2	B	0.96	2/1909 (0.1%)	1.20	15/2601 (0.6%)
2	O	0.83	2/1909 (0.1%)	1.17	13/2601 (0.5%)
3	C	0.94	0/2211	1.01	12/3023 (0.4%)
3	P	0.80	1/2211 (0.0%)	0.99	9/3023 (0.3%)
4	D	0.79	0/1229	1.11	8/1658 (0.5%)
4	Q	0.69	0/1229	1.07	6/1658 (0.4%)
5	E	0.81	0/871	1.02	6/1182 (0.5%)
5	R	0.73	0/871	1.01	6/1182 (0.5%)
6	F	0.84	0/765	1.13	2/1038 (0.2%)
6	S	0.76	0/765	1.12	4/1038 (0.4%)
7	G	0.96	0/699	1.13	4/950 (0.4%)
7	T	0.89	0/699	1.13	4/950 (0.4%)
8	H	0.82	0/682	1.07	4/921 (0.4%)
8	U	0.71	0/682	1.03	5/921 (0.5%)
9	I	0.86	0/611	0.98	2/810 (0.2%)
9	V	0.74	0/611	0.96	2/810 (0.2%)
10	J	0.80	0/471	1.00	1/636 (0.2%)
10	W	0.71	0/471	0.99	1/636 (0.2%)
11	K	0.96	0/398	1.15	3/546 (0.5%)
11	X	0.72	0/398	1.09	3/546 (0.5%)
12	L	0.94	0/399	0.95	2/534 (0.4%)
12	Y	0.68	0/399	0.97	2/534 (0.4%)
13	M	0.90	0/345	1.05	1/470 (0.2%)
13	Z	0.68	0/345	1.03	1/470 (0.2%)
All	All	0.88	35/29508 (0.1%)	1.10	198/40114 (0.5%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
2	O	0	1
3	C	0	1
3	P	0	1
4	D	0	1
4	Q	0	1
8	H	0	1
8	U	0	1
All	All	0	9

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	MET	SD-CE	-10.36	1.53	1.79
1	N	277	MET	SD-CE	-9.21	1.56	1.79
1	A	61	HIS	CD2-NE2	8.54	1.47	1.37
1	A	61	HIS	ND1-CE1	8.51	1.41	1.32
1	A	376	HIS	CD2-NE2	8.04	1.46	1.37
1	N	61	HIS	CG-CD2	7.83	1.44	1.35
1	N	61	HIS	ND1-CE1	7.79	1.40	1.32
1	A	130	PRO	CA-C	7.79	1.59	1.52
2	B	175	ILE	CA-CB	7.62	1.60	1.54
2	O	175	ILE	CA-CB	7.34	1.60	1.54
1	A	378	HIS	CD2-NE2	7.31	1.45	1.37
1	N	376	HIS	CD2-NE2	7.28	1.45	1.37
1	N	378	HIS	ND1-CE1	7.18	1.39	1.32
1	A	376	HIS	ND1-CE1	7.09	1.39	1.32
1	N	376	HIS	ND1-CE1	7.08	1.39	1.32
1	N	83	VAL	CA-CB	6.68	1.57	1.54
1	A	378	HIS	ND1-CE1	6.45	1.39	1.32
1	N	189	MET	SD-CE	-6.43	1.63	1.79
1	A	69	MET	SD-CE	-6.38	1.63	1.79
1	A	28	MET	SD-CE	-6.24	1.64	1.79
1	N	208	MET	SD-CE	-5.99	1.64	1.79
1	N	130	PRO	CA-C	5.88	1.57	1.52
1	A	61	HIS	CG-CD2	5.88	1.42	1.35
1	N	61	HIS	CD2-NE2	5.75	1.44	1.37
1	A	417	MET	SD-CE	-5.67	1.65	1.79
2	O	142	VAL	CA-CB	5.58	1.60	1.53
2	B	104	TRP	CA-C	-5.52	1.45	1.52
1	A	208	MET	SD-CE	-5.38	1.66	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	378	HIS	CD2-NE2	5.31	1.43	1.37
1	A	383	MET	SD-CE	-5.29	1.66	1.79
1	N	253	MET	SD-CE	-5.19	1.66	1.79
1	N	383	MET	SD-CE	-5.06	1.67	1.79
1	A	253	MET	SD-CE	-5.06	1.67	1.79
3	P	11	VAL	CA-CB	5.04	1.60	1.54
1	N	74	MET	SD-CE	-5.03	1.67	1.79

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	Q	133	GLY	N-CA-C	15.22	130.91	112.49
4	D	133	GLY	N-CA-C	15.09	130.74	112.49
1	A	61	HIS	ND1-CE1-NE2	9.96	118.36	108.40
1	A	61	HIS	CE1-NE2-CD2	-9.26	99.74	109.00
1	N	82	LEU	N-CA-C	9.03	122.80	111.69
1	N	378	HIS	CA-CB-CG	-8.89	104.91	113.80
1	N	61	HIS	ND1-CE1-NE2	8.72	117.12	108.40
1	A	376	HIS	ND1-CE1-NE2	8.48	116.88	108.40
2	O	59	GLN	N-CA-C	8.46	121.26	111.11
1	A	435	GLY	N-CA-C	8.22	127.02	115.43
7	G	44	ARG	N-CA-C	8.15	118.97	109.60
2	B	59	GLN	N-CA-C	8.14	120.88	111.11
7	T	44	ARG	N-CA-C	8.04	118.84	109.60
1	A	376	HIS	CE1-NE2-CD2	-8.01	100.99	109.00
1	A	378	HIS	ND1-CE1-NE2	7.99	116.39	108.40
1	N	56	VAL	N-CA-C	-7.87	102.77	110.72
1	N	376	HIS	ND1-CE1-NE2	7.86	116.26	108.40
8	H	8	ILE	N-CA-C	7.80	119.37	107.99
8	U	8	ILE	N-CA-C	7.75	119.31	107.99
2	O	58	ALA	N-CA-C	7.69	119.57	111.03
1	N	332	ILE	N-CA-C	7.65	118.86	109.30
1	N	125	GLY	N-CA-C	-7.56	103.16	112.68
1	A	332	ILE	N-CA-C	7.55	118.74	109.30
2	B	58	ALA	N-CA-C	7.55	119.42	111.03
1	A	378	HIS	CA-CB-CG	-7.51	106.29	113.80
1	N	130	PRO	N-CA-C	-7.42	101.65	110.70
5	R	42	VAL	N-CA-C	-7.39	99.50	107.77
4	Q	129	ALA	CA-C-N	7.32	127.95	120.04
4	Q	129	ALA	C-N-CA	7.32	127.95	120.04
3	C	184	ALA	CA-C-N	7.28	127.44	119.87
3	C	184	ALA	C-N-CA	7.28	127.44	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	104	TRP	N-CA-C	7.28	126.30	110.80
4	D	129	ALA	CA-C-N	7.26	127.89	120.04
4	D	129	ALA	C-N-CA	7.26	127.89	120.04
1	A	130	PRO	N-CA-C	-7.23	101.88	110.70
1	A	82	LEU	N-CA-C	7.22	122.35	112.90
1	N	288	TRP	N-CA-C	7.19	120.03	111.33
7	G	11	THR	N-CA-C	7.12	125.96	110.80
1	A	288	TRP	N-CA-C	7.10	119.92	111.33
3	P	184	ALA	CA-C-N	7.10	127.25	119.87
3	P	184	ALA	C-N-CA	7.10	127.25	119.87
5	E	42	VAL	N-CA-C	-7.10	99.82	107.77
7	T	11	THR	N-CA-C	7.05	125.82	110.80
2	O	104	TRP	N-CA-C	7.04	125.80	110.80
13	Z	27	LEU	N-CA-C	7.02	120.33	111.69
1	A	125	GLY	N-CA-C	-7.01	103.84	112.68
1	N	435	GLY	N-CA-C	7.00	125.86	115.64
1	A	378	HIS	CE1-NE2-CD2	-6.94	102.06	109.00
8	U	63	LEU	N-CA-C	6.90	120.17	111.69
1	A	56	VAL	N-CA-C	-6.86	103.80	110.72
1	N	443	TYR	N-CA-C	6.82	116.16	108.25
5	E	21	LYS	CA-C-N	6.79	127.06	119.32
5	E	21	LYS	C-N-CA	6.79	127.06	119.32
2	B	66	THR	N-CA-C	-6.73	104.10	112.72
7	T	69	PHE	N-CA-C	6.70	119.16	111.11
12	Y	2	HIS	N-CA-C	-6.65	104.99	113.23
1	A	142	SER	N-CA-C	6.59	119.06	111.02
1	N	142	SER	N-CA-C	6.58	119.04	111.02
1	N	171	MET	N-CA-C	6.57	120.93	112.26
8	H	63	LEU	N-CA-C	6.55	119.75	111.69
3	C	256	ILE	N-CA-C	6.54	117.16	110.82
1	N	376	HIS	CE1-NE2-CD2	-6.49	102.51	109.00
2	O	66	THR	N-CA-C	-6.49	104.41	112.72
1	A	445	ASP	N-CA-C	6.49	119.18	111.33
1	A	10	THR	N-CA-C	-6.46	103.06	111.71
3	P	256	ILE	N-CA-C	6.43	117.06	110.82
5	R	79	LYS	N-CA-C	6.24	120.36	112.87
1	N	10	THR	N-CA-C	-6.22	103.37	111.71
1	A	61	HIS	CA-CB-CG	6.22	120.02	113.80
1	N	262	SER	N-CA-C	-6.22	105.33	113.17
1	N	378	HIS	ND1-CE1-NE2	6.22	114.62	108.40
5	R	21	LYS	CA-C-N	6.21	126.67	119.47
5	R	21	LYS	C-N-CA	6.21	126.67	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	U	9	LYS	N-CA-C	-6.20	105.66	112.72
7	G	69	PHE	N-CA-C	6.20	118.54	111.11
1	A	94	PHE	CA-C-N	6.17	126.07	119.28
1	A	94	PHE	C-N-CA	6.17	126.07	119.28
1	N	445	ASP	N-CA-C	6.17	118.79	111.33
2	O	77	ALA	N-CA-C	6.15	117.99	111.28
1	N	94	PHE	CA-C-N	6.12	126.01	119.28
1	N	94	PHE	C-N-CA	6.12	126.01	119.28
13	M	27	LEU	N-CA-C	6.11	119.21	111.69
5	E	79	LYS	N-CA-C	6.10	120.19	112.87
1	N	495	LEU	N-CA-C	6.09	120.17	112.87
8	H	9	LYS	N-CA-C	-6.08	105.79	112.72
1	A	105	LEU	CA-C-N	-6.07	114.12	120.38
1	A	105	LEU	C-N-CA	-6.07	114.12	120.38
2	B	77	ALA	N-CA-C	6.06	117.88	111.28
5	E	76	GLY	CA-C-N	6.03	125.73	119.64
5	E	76	GLY	C-N-CA	6.03	125.73	119.64
1	N	61	HIS	CE1-NE2-CD2	-6.01	102.98	109.00
1	N	50	ASP	N-CA-C	5.97	117.75	110.41
10	W	57	HIS	N-CA-C	5.93	118.49	107.99
1	A	448	THR	N-CA-C	5.92	117.53	111.14
2	B	103	GLN	CA-C-N	5.89	132.80	121.54
2	B	103	GLN	C-N-CA	5.89	132.80	121.54
12	L	2	HIS	N-CA-C	-5.89	105.92	113.23
1	A	377	PHE	N-CA-C	5.86	119.53	112.38
1	A	50	ASP	N-CA-C	5.82	117.57	110.41
3	P	159	MET	N-CA-C	-5.82	104.84	111.07
4	Q	32	ASN	N-CA-C	5.80	119.04	107.62
7	T	48	ILE	N-CA-C	-5.79	100.71	107.61
10	J	57	HIS	N-CA-C	5.77	118.21	107.99
1	A	237	PHE	N-CA-C	-5.76	105.14	111.82
3	C	2	THR	N-CA-C	5.75	123.05	110.80
1	N	448	THR	N-CA-C	5.75	117.63	111.36
4	D	89	ILE	N-CA-C	-5.74	104.92	110.72
1	A	171	MET	N-CA-C	5.74	119.84	112.26
2	O	65	TRP	N-CA-C	5.74	119.81	113.21
6	S	2	SER	N-CA-C	5.73	119.25	110.20
1	A	9	SER	N-CA-C	5.72	117.67	110.24
6	F	2	SER	N-CA-C	5.72	119.24	110.20
12	Y	20	ARG	N-CA-C	-5.71	105.14	111.36
9	V	4	LEU	N-CA-C	-5.70	101.85	110.28
2	B	65	TRP	N-CA-C	5.68	119.75	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	2	THR	N-CA-C	5.68	122.90	110.80
9	I	4	LEU	N-CA-C	-5.68	102.08	110.48
1	N	377	PHE	N-CA-C	5.67	119.30	112.38
1	A	443	TYR	N-CA-C	5.67	114.82	108.25
3	C	11	VAL	N-CA-C	5.66	116.91	109.21
1	N	70	VAL	N-CA-C	5.66	115.85	110.42
5	R	76	GLY	CA-C-N	5.62	125.31	119.64
5	R	76	GLY	C-N-CA	5.62	125.31	119.64
2	O	103	GLN	CA-C-N	5.61	132.26	121.54
2	O	103	GLN	C-N-CA	5.61	132.26	121.54
9	I	37	PHE	N-CA-C	5.59	118.56	111.69
1	A	466	MET	N-CA-C	-5.58	105.28	111.36
11	K	41	ASN	CA-C-N	5.57	125.56	120.21
11	K	41	ASN	C-N-CA	5.57	125.56	120.21
11	X	19	ALA	N-CA-C	5.53	117.11	111.14
1	A	239	GLY	N-CA-C	5.53	119.58	112.83
1	A	70	VAL	N-CA-C	5.53	115.73	110.42
1	A	506	GLU	N-CA-C	-5.51	105.38	111.71
3	C	159	MET	N-CA-C	-5.51	105.18	111.07
1	A	141	ALA	N-CA-C	5.50	119.25	112.54
1	A	376	HIS	CB-CG-CD2	-5.49	124.06	131.20
6	S	62	CYS	N-CA-C	5.46	117.67	111.11
1	N	492	LEU	N-CA-C	5.46	118.73	111.75
2	B	164	ALA	N-CA-C	5.43	117.65	109.23
3	C	45	ILE	N-CA-C	-5.43	105.21	110.42
12	L	20	ARG	N-CA-C	-5.42	105.53	111.82
1	A	251	PHE	N-CA-C	-5.42	105.37	111.28
1	N	237	PHE	N-CA-C	-5.41	105.54	111.82
1	N	6	TRP	N-CA-C	5.37	119.89	113.23
3	P	59	ARG	N-CA-C	-5.37	105.34	111.14
3	P	35	PHE	N-CA-C	5.34	117.10	111.28
1	A	262	SER	N-CA-C	-5.34	106.44	113.17
1	A	183	LEU	N-CA-C	5.33	117.09	111.28
11	K	19	ALA	N-CA-C	5.29	116.91	111.03
2	B	55	THR	N-CA-C	5.28	117.89	110.23
3	C	35	PHE	N-CA-C	5.28	117.03	111.28
1	A	173	PRO	N-CA-C	-5.25	104.29	110.70
4	D	101	HIS	N-CA-C	5.25	118.15	111.69
4	D	76	ASN	N-CA-C	-5.24	106.75	112.72
1	A	487	LEU	N-CA-C	5.22	118.64	111.54
1	N	217	THR	N-CA-C	-5.22	103.02	110.59
2	B	147	GLU	N-CA-C	5.20	118.76	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	208	PRO	N-CA-C	5.19	118.49	111.22
3	P	45	ILE	N-CA-C	-5.18	105.45	110.42
3	C	99	TRP	N-CA-C	-5.17	105.53	111.07
1	N	61	HIS	CB-CG-CD2	-5.17	124.47	131.20
4	D	32	ASN	N-CA-C	5.17	117.04	108.20
2	B	14	SER	CA-C-N	5.16	124.78	119.05
2	B	14	SER	C-N-CA	5.16	124.78	119.05
1	N	506	GLU	N-CA-C	-5.15	105.79	111.71
2	O	55	THR	N-CA-C	5.15	117.69	110.23
3	C	38	ASN	N-CA-C	5.15	121.76	110.80
8	U	81	PHE	CA-C-N	5.14	124.81	119.56
8	U	81	PHE	C-N-CA	5.14	124.81	119.56
1	A	37	ILE	CB-CA-C	-5.13	105.40	111.97
3	P	99	TRP	N-CA-C	-5.13	105.58	111.07
1	A	274	VAL	N-CA-C	-5.12	105.72	110.53
3	C	59	ARG	N-CA-C	-5.11	105.60	111.07
2	O	164	ALA	N-CA-C	5.11	117.15	109.23
1	A	492	LEU	N-CA-C	5.11	118.29	111.75
11	X	41	ASN	CA-C-N	5.11	125.11	120.21
11	X	41	ASN	C-N-CA	5.11	125.11	120.21
4	Q	113	GLU	N-CA-C	5.11	117.51	111.33
3	C	225	PHE	N-CA-C	5.09	118.75	112.24
6	F	49	VAL	N-CA-C	5.08	112.58	107.55
9	V	37	PHE	N-CA-C	5.08	117.94	111.69
1	A	67	PHE	N-CA-C	5.08	118.63	112.23
6	S	47	ASN	N-CA-C	-5.08	101.69	109.76
2	B	60	GLU	N-CA-C	5.07	121.59	110.80
1	N	129	TYR	CB-CA-C	-5.06	101.47	109.42
1	N	407	ASP	N-CA-C	5.06	118.23	111.75
2	O	147	GLU	N-CA-C	5.06	118.58	111.90
1	A	6	TRP	N-CA-C	5.06	119.50	113.23
4	D	113	GLU	N-CA-C	5.05	117.17	111.11
8	H	64	CYS	N-CA-C	5.05	116.02	109.65
7	G	75	VAL	CB-CA-C	-5.04	105.18	110.62
6	S	39	THR	N-CA-C	-5.04	102.02	109.94
1	N	376	HIS	CB-CG-CD2	-5.04	124.66	131.20
2	B	134	ARG	N-CA-C	5.03	121.52	110.80
4	Q	101	HIS	N-CA-C	5.02	117.86	111.69
1	A	495	LEU	N-CA-C	5.01	118.89	112.87
2	O	60	GLU	N-CA-C	5.01	121.47	110.80
1	N	507	GLU	N-CA-C	-5.00	99.44	108.85

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
3	C	182	TYR	Sidechain
4	D	140	TYR	Sidechain
8	H	11	TYR	Sidechain
1	N	240	HIS	Sidechain
2	O	103	GLN	Mainchain
3	P	182	TYR	Sidechain
4	Q	140	TYR	Sidechain
8	U	11	TYR	Sidechain

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	4025	0	4002	72	0
1	N	4025	0	4002	79	0
2	B	1863	0	1867	51	0
2	O	1863	0	1867	49	0
3	C	2124	0	2044	31	0
3	P	2124	0	2044	29	0
4	D	1195	0	1183	35	0
4	Q	1195	0	1183	38	0
5	E	852	0	845	17	0
5	R	852	0	845	19	0
6	F	748	0	728	16	0
6	S	748	0	728	13	0
7	G	672	0	645	18	0
7	T	672	0	645	17	0
8	H	662	0	623	13	0
8	U	662	0	623	13	0
9	I	598	0	612	11	0
9	V	598	0	612	9	0
10	J	460	0	459	5	0
10	W	460	0	459	7	0
11	K	384	0	366	10	0
11	X	384	0	366	10	0
12	L	386	0	388	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Y	386	0	388	8	0
13	M	335	0	352	8	0
13	Z	335	0	352	9	0
14	A	1	0	0	0	0
14	B	2	0	0	0	0
14	N	1	0	0	0	0
14	O	2	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	6	0
17	N	120	0	108	3	0
18	A	2	0	0	1	0
18	N	2	0	0	1	0
19	F	1	0	0	0	0
19	S	1	0	0	0	0
All	All	28864	0	28444	475	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 8.

All (475) 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)
18:A:520:PER:O2	18:A:520:PER:O1	1.69	1.11
18:N:520:PER:O1	18:N:520:PER:O2	1.63	1.11
1:N:365:ILE:HG13	2:O:87:MET:HE1	1.58	0.86
3:P:2:THR:HG23	6:S:96:LEU:HD12	1.58	0.85
1:A:365:ILE:HG13	2:B:87:MET:HE1	1.60	0.83
3:C:2:THR:HG23	6:F:96:LEU:HD12	1.61	0.82
1:N:306:THR:HB	1:N:359:ALA:O	1.82	0.79
1:N:347:LEU:HG	1:N:383:MET:HE2	1.65	0.78
1:N:85:LEU:O	1:N:492:LEU:HD13	1.86	0.75
1:A:190:ILE:HG12	7:T:6:GLY:HA3	1.71	0.72
1:A:197:LEU:HD12	7:T:4:ALA:HB2	1.69	0.72
1:N:508:PRO:HG3	3:P:6:HIS:HB3	1.71	0.72
7:G:6:GLY:HA3	1:N:190:ILE:HG12	1.72	0.71
2:B:78:LEU:HB2	2:B:79:PRO:HD3	1.72	0.71
1:A:306:THR:HB	1:A:359:ALA:O	1.90	0.71
3:C:192:VAL:O	3:C:196:THR:HB	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:MET:HE1	2:B:77:ALA:HB2	1.72	0.69
1:A:508:PRO:HG3	3:C:6:HIS:HB3	1.74	0.69
1:A:347:LEU:HG	1:A:383:MET:HE2	1.73	0.69
7:G:4:ALA:HB2	1:N:197:LEU:HD12	1.73	0.69
4:Q:52:SER:OG	4:Q:55:GLU:HG3	1.92	0.69
6:F:8:THR:OG1	6:F:11:GLU:HG2	1.92	0.69
1:N:310:MET:HE1	2:O:77:ALA:HB2	1.75	0.68
2:O:111:THR:HG22	2:O:111:THR:O	1.93	0.68
1:A:85:LEU:O	1:A:492:LEU:HD13	1.94	0.68
1:A:286:ILE:HG22	7:T:1:ALA:HB1	1.74	0.67
8:H:52:VAL:HG21	8:U:43:MET:HE1	1.76	0.67
1:A:282:PHE:HB2	7:T:5:LYS:HB3	1.75	0.67
2:B:111:THR:HG22	2:B:111:THR:O	1.94	0.67
8:H:43:MET:HE1	8:U:52:VAL:HG21	1.76	0.67
1:A:197:LEU:HD12	7:T:4:ALA:CB	2.26	0.66
6:S:8:THR:OG1	6:S:11:GLU:HG2	1.94	0.66
4:D:52:SER:OG	4:D:55:GLU:HG3	1.95	0.66
2:B:89[A]:GLU:HB2	2:B:91[A]:ASN:ND2	2.12	0.65
3:C:2:THR:HG22	6:F:52:ILE:HG12	1.79	0.65
3:P:192:VAL:O	3:P:196:THR:HB	1.96	0.65
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.78	0.65
7:G:4:ALA:HB2	1:N:197:LEU:CD1	2.27	0.65
2:O:89[A]:GLU:HB2	2:O:91[A]:ASN:ND2	2.12	0.64
7:G:5:LYS:HB3	1:N:282:PHE:HB2	1.78	0.64
2:B:14:SER:HB3	2:B:168:LEU:HD23	1.80	0.64
1:A:197:LEU:CD1	7:T:4:ALA:HB2	2.28	0.64
2:O:78:LEU:HB2	2:O:79:PRO:HD3	1.78	0.64
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.32	0.64
3:P:119:THR:HG21	8:U:82:PRO:O	1.98	0.63
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.80	0.63
2:O:14:SER:HB3	2:O:168:LEU:HD23	1.79	0.63
2:O:145:PRO:HG3	2:O:148:MET:HE2	1.80	0.63
1:A:187:SER:CB	1:A:277:MET:HE1	2.28	0.63
7:G:1:ALA:HB1	1:N:286:ILE:HG22	1.81	0.63
4:Q:23:PRO:O	5:R:66:ARG:HD3	1.99	0.63
4:D:23:PRO:O	5:E:66:ARG:HD3	1.99	0.62
1:A:354:THR:CG2	1:A:376:HIS:HB2	2.29	0.62
2:O:52:HIS:CD2	5:R:40:ASP:HB2	2.34	0.62
2:O:186:SER:HB3	2:O:213:LEU:HD22	1.81	0.62
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.80	0.62
1:N:347:LEU:HG	1:N:383:MET:CE	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.82	0.61
7:G:4:ALA:CB	1:N:197:LEU:HD12	2.29	0.61
1:N:187:SER:CB	1:N:277:MET:HE1	2.30	0.61
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.88	0.61
8:U:7:LYS:HA	8:U:7:LYS:HE3	1.81	0.61
8:U:39:CYS:CB	8:U:53:CYS:SG	2.88	0.61
8:H:7:LYS:HE3	8:H:7:LYS:HA	1.81	0.61
3:C:119:THR:HG21	8:H:82:PRO:O	2.01	0.61
3:P:2:THR:HG22	6:S:52:ILE:HG12	1.82	0.60
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.89	0.60
2:B:145:PRO:HG3	2:B:148:MET:HE2	1.83	0.60
3:P:164:PHE:O	3:P:168:THR:HG23	2.01	0.60
2:B:193:TYR:HE1	4:D:126:MET:HE1	1.67	0.60
2:B:186:SER:HB3	2:B:213:LEU:HD22	1.84	0.59
4:Q:67:SER:OG	4:Q:70:GLU:HG3	2.03	0.59
7:G:67:HIS:HD2	7:G:71:HIS:CD2	2.20	0.59
2:O:136:LEU:HB3	2:O:193:TYR:CD2	2.37	0.59
3:P:34:TRP:CD1	3:P:40:MET:HG2	2.38	0.59
9:V:19:PHE:CD1	9:V:19:PHE:C	2.80	0.59
2:B:52:HIS:CD2	5:E:40:ASP:HB2	2.37	0.59
1:N:209:LEU:O	1:N:213:ARG:HG3	2.03	0.59
7:G:40:GLY:O	7:G:41:HIS:HB2	2.02	0.59
8:H:60:TYR:CD1	8:H:60:TYR:C	2.81	0.58
13:Z:38:ASP:O	13:Z:42:LYS:HG2	2.03	0.58
4:Q:102:TYR:CD1	13:Z:35:TYR:HE1	2.22	0.58
2:B:164:ALA:HB2	2:B:171:LYS:HD3	1.85	0.58
1:N:289:ALA:HB1	1:N:297:MET:HE1	1.85	0.58
1:N:431:LEU:HD21	1:N:450:TRP:HB2	1.85	0.58
1:A:209:LEU:O	1:A:213:ARG:HG3	2.04	0.58
6:F:8:THR:HG1	6:F:11:GLU:HG2	1.67	0.58
2:O:68:LEU:HB3	2:O:69:PRO:HD3	1.85	0.58
4:Q:107:ILE:CD1	11:X:39:GLU:HG3	2.34	0.58
10:W:56:PRO:HD3	12:Y:46:LYS:HE3	1.85	0.58
4:Q:66:GLU:O	5:R:66:ARG:NH2	2.37	0.58
1:N:354:THR:CG2	1:N:376:HIS:HB2	2.34	0.57
2:O:164:ALA:HB2	2:O:171:LYS:HD3	1.84	0.57
2:O:146:MET:SD	2:O:189:PRO:HB3	2.45	0.57
4:D:66:GLU:O	5:E:66:ARG:NH2	2.37	0.57
1:N:354:THR:HG21	1:N:376:HIS:HA	1.87	0.57
2:O:132:GLU:HA	4:Q:122:ARG:NH1	2.19	0.57
4:D:138:TRP:CH2	11:K:50:PRO:HG2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:43:PRO:HB2	5:E:48:ILE:HD11	1.86	0.57
2:O:193:TYR:HE1	4:Q:126:MET:HE1	1.70	0.57
13:M:38:ASP:O	13:M:42:LYS:HG2	2.04	0.57
1:N:36:LEU:HD13	12:Y:40:VAL:HG21	1.87	0.56
1:N:115:SER:O	1:N:121:GLY:HA2	2.05	0.56
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.87	0.56
1:N:138:HIS:O	1:N:213:ARG:NH2	2.39	0.56
9:I:19:PHE:CD1	9:I:19:PHE:C	2.82	0.56
1:N:390:MET:HE2	1:N:390:MET:HA	1.87	0.56
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.41	0.56
6:F:16:LEU:O	6:F:20:VAL:HG13	2.06	0.56
3:P:160:LEU:HD13	3:P:222:GLN:HG2	1.88	0.56
1:A:354:THR:HG21	1:A:376:HIS:HA	1.88	0.55
1:A:289:ALA:HB1	1:A:297:MET:HE1	1.89	0.55
1:A:36:LEU:HD13	12:L:40:VAL:HG21	1.88	0.55
3:C:221:ARG:HE	3:C:226:HIS:HD1	1.53	0.55
9:V:19:PHE:C	9:V:19:PHE:HD1	2.15	0.55
3:C:154:GLY:HA2	6:F:6:VAL:HG22	1.89	0.55
1:A:74:MET:HE3	1:A:249:PRO:HB2	1.88	0.55
2:B:58:ALA:O	2:B:62:GLU:HG3	2.07	0.55
3:C:160:LEU:HD13	3:C:222:GLN:HG2	1.89	0.55
13:M:1:ILE:HG13	13:M:2:THR:H	1.72	0.54
1:N:87:ILE:O	1:N:173:PRO:HD3	2.07	0.54
1:N:503:HIS:CD2	3:P:10:MET:HE2	2.42	0.54
7:T:40:GLY:O	7:T:41:HIS:HB2	2.08	0.54
2:B:132:GLU:HA	4:D:122:ARG:NH1	2.22	0.54
2:O:58:ALA:O	2:O:62:GLU:HG3	2.07	0.54
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.89	0.54
2:B:136:LEU:HB3	2:B:193:TYR:CD2	2.42	0.54
4:D:102:TYR:CD1	13:M:35:TYR:HE1	2.26	0.54
2:O:191:LEU:HB2	4:Q:126:MET:HE3	1.89	0.54
4:D:127:LYS:O	4:D:130:PRO:HD3	2.08	0.54
4:Q:68:PHE:HA	4:Q:71:MET:HG2	1.88	0.54
1:A:128:VAL:HG22	1:A:128:VAL:O	2.07	0.54
6:F:53:THR:HG22	6:F:54:ASN:ND2	2.22	0.54
10:J:56:PRO:HD3	12:L:46:LYS:HE3	1.88	0.54
3:C:34:TRP:CD1	3:C:40:MET:HG2	2.43	0.54
4:D:67:SER:OG	4:D:70:GLU:HG3	2.08	0.54
2:B:68:LEU:HB3	2:B:69:PRO:HD3	1.90	0.54
2:O:161:HIS:HB2	2:O:174:ALA:HB3	1.90	0.54
8:U:60:TYR:CD1	8:U:60:TYR:C	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.88	0.54
3:C:164:PHE:O	3:C:168:THR:HG23	2.08	0.54
4:D:40:LEU:HD13	4:D:59:LEU:HD13	1.88	0.54
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.90	0.53
9:V:55:ASP:HB3	9:V:58:LYS:HB3	1.90	0.53
10:W:36:MET:O	10:W:40:LEU:HG	2.07	0.53
4:D:107:ILE:CD1	11:K:39:GLU:HG3	2.37	0.53
9:I:19:PHE:C	9:I:19:PHE:HD1	2.17	0.53
3:P:1:MET:HB3	6:S:96:LEU:HD11	1.89	0.53
1:A:503:HIS:CD2	3:C:10:MET:HE2	2.43	0.53
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.90	0.53
2:B:191:LEU:HB2	4:D:126:MET:HE3	1.91	0.53
4:D:110:THR:HG22	4:D:115:TRP:CE2	2.44	0.53
3:P:154:GLY:HA2	6:S:6:VAL:HG22	1.91	0.53
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.09	0.53
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.09	0.53
7:T:67:HIS:HD2	7:T:71:HIS:CD2	2.27	0.53
1:A:138:HIS:O	1:A:213:ARG:NH2	2.42	0.53
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.44	0.53
1:A:35:LEU:HD11	1:A:462:LEU:HB2	1.91	0.52
1:A:290:HIS:HD2	1:A:291:HIS:CD2	2.27	0.52
2:B:90[B]:ILE:HD12	8:H:16:PHE:CZ	2.44	0.52
1:N:128:VAL:HG22	1:N:128:VAL:O	2.08	0.52
13:Z:1:ILE:HG13	13:Z:2:THR:H	1.74	0.52
1:A:187:SER:HB2	1:A:277:MET:HE1	1.90	0.52
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.45	0.52
1:N:456:MET:HG2	4:Q:96:LEU:HD13	1.91	0.52
5:R:80:GLU:H	5:R:80:GLU:CD	2.17	0.52
6:S:16:LEU:O	6:S:20:VAL:HG13	2.09	0.52
1:N:144:ASP:OD1	1:N:213:ARG:HD3	2.10	0.52
3:P:112:LEU:HG	3:P:118:PRO:HG3	1.92	0.52
4:Q:24:LEU:HD12	5:R:30:ARG:HA	1.91	0.52
7:T:9:GLY:HA2	7:T:19:LEU:HD11	1.91	0.52
6:S:53:THR:HG22	6:S:54:ASN:ND2	2.24	0.52
2:B:161:HIS:HB2	2:B:174:ALA:HB3	1.91	0.52
8:H:49:ASP:O	8:H:52:VAL:HG22	2.10	0.52
1:N:74:MET:HE1	1:N:246:LEU:O	2.10	0.52
2:O:162:SER:HB3	2:O:197:SER:C	2.35	0.52
1:A:344:PHE:CD1	1:A:344:PHE:C	2.88	0.52
4:Q:64:PHE:CE1	5:R:66:ARG:HD2	2.45	0.52
5:R:63:SER:O	5:R:67:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.92	0.51
12:L:46:LYS:O	12:L:47:LYS:HB2	2.10	0.51
1:N:354:THR:HG23	1:N:376:HIS:HB2	1.93	0.51
1:A:237:PHE:HZ	7:T:2:SER:HB2	1.75	0.51
1:N:344:PHE:CD1	1:N:344:PHE:C	2.88	0.51
8:U:39:CYS:C	8:U:53:CYS:SG	2.93	0.51
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.11	0.51
1:A:354:THR:HG23	1:A:376:HIS:HB2	1.91	0.51
1:A:298:ASP:HB2	1:A:301:THR:HG23	1.92	0.51
8:H:39:CYS:C	8:H:53:CYS:SG	2.94	0.51
2:O:184:LEU:HD11	2:O:211:LEU:HD21	1.93	0.51
1:A:51:ASP:O	1:A:55:ASN:ND2	2.44	0.50
4:D:5:VAL:O	4:D:5:VAL:HG13	2.11	0.50
1:A:87:ILE:O	1:A:173:PRO:HD3	2.11	0.50
11:X:24:PHE:O	11:X:28:VAL:HG23	2.11	0.50
1:N:74:MET:HE3	1:N:249:PRO:HB2	1.92	0.50
4:D:23:PRO:O	4:D:25:PRO:HD3	2.11	0.50
1:N:290:HIS:CD2	1:N:291:HIS:NE2	2.79	0.50
2:O:226:MET:O	2:O:227:LEU:HB2	2.11	0.50
4:Q:40:LEU:HD13	4:Q:59:LEU:HD13	1.94	0.50
2:B:226:MET:O	2:B:227:LEU:HB2	2.10	0.50
10:J:36:MET:O	10:J:40:LEU:HG	2.12	0.50
2:O:86:MET:O	2:O:89[A]:GLU:HG2	2.11	0.50
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.46	0.50
1:A:347:LEU:HG	1:A:383:MET:CE	2.40	0.50
2:B:164:ALA:O	2:B:194:GLY:HA3	2.12	0.50
3:C:112:LEU:HG	3:C:118:PRO:HG3	1.94	0.50
7:G:55:ILE:O	7:G:56:ARG:HD3	2.12	0.50
4:Q:110:THR:HG22	4:Q:115:TRP:CE2	2.47	0.50
4:Q:118:LYS:HD2	11:X:53:TRP:HA	1.94	0.50
1:A:115:SER:O	1:A:121:GLY:HA2	2.12	0.49
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.95	0.49
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.94	0.49
4:D:24:LEU:HD12	5:E:30:ARG:HA	1.93	0.49
1:N:187:SER:HB2	1:N:277:MET:HE1	1.94	0.49
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.94	0.49
1:N:380:VAL:O	1:N:384:GLY:HA3	2.12	0.49
2:O:90[B]:ILE:HD12	8:U:16:PHE:CZ	2.47	0.49
4:Q:146:LYS:O	4:Q:147:LYS:HG3	2.11	0.49
12:L:41:ARG:HD2	13:M:40:TYR:CZ	2.48	0.49
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:30:ILE:HG13	10:W:31:LEU:N	2.27	0.49
2:B:139:ASP:OD1	2:B:140:ASN:N	2.46	0.49
2:O:89[A]:GLU:HB2	2:O:91[A]:ASN:HD22	1.78	0.49
2:O:164:ALA:O	2:O:194:GLY:HA3	2.13	0.49
4:Q:142:LYS:HB2	4:Q:144:GLU:HG2	1.95	0.49
1:N:290:HIS:HD2	1:N:291:HIS:CD2	2.31	0.48
2:O:139:ASP:OD1	2:O:140:ASN:N	2.45	0.48
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.48	0.48
5:E:80:GLU:CD	5:E:80:GLU:H	2.22	0.48
8:U:49:ASP:O	8:U:52:VAL:HG22	2.13	0.48
4:D:119:GLN:O	4:D:123:MET:HG3	2.14	0.48
1:N:361:SER:OG	2:O:84:LEU:HD13	2.14	0.48
1:A:302:ARG:O	1:A:306:THR:CG2	2.62	0.48
4:D:68:PHE:HA	4:D:71:MET:HG2	1.96	0.48
4:Q:68:PHE:CZ	5:R:70:VAL:HG23	2.49	0.48
1:A:393:PHE:O	1:A:397:PHE:HB2	2.14	0.48
10:J:50:LEU:HD22	10:J:50:LEU:O	2.14	0.48
3:P:41:THR:O	3:P:45:ILE:HG12	2.14	0.48
9:I:2:THR:HG23	9:I:2:THR:O	2.13	0.47
9:I:55:ASP:HB3	9:I:58:LYS:HB3	1.95	0.47
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.13	0.47
3:C:1:MET:HB3	6:F:96:LEU:HD11	1.96	0.47
4:D:64:PHE:CE1	5:E:66:ARG:HD2	2.49	0.47
2:O:191:LEU:HB2	4:Q:126:MET:CE	2.44	0.47
4:Q:112:GLU:O	4:Q:116:VAL:HG13	2.15	0.47
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.96	0.47
2:B:145:PRO:CG	2:B:148:MET:HE2	2.44	0.47
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.50	0.47
2:O:222:TRP:CZ2	2:O:226:MET:HG3	2.49	0.47
8:U:36:PHE:HD2	8:U:37:HIS:CE1	2.32	0.47
5:E:63:SER:O	5:E:67:ILE:HG13	2.14	0.47
3:P:2:THR:HG23	6:S:96:LEU:CD1	2.40	0.47
5:R:18:TYR:OH	5:R:28:GLU:O	2.30	0.47
7:T:55:ILE:O	7:T:56:ARG:HD3	2.15	0.47
5:E:5:HIS:HB3	5:E:6:GLU:H	1.59	0.47
7:G:7:ASP:CG	7:G:8:HIS:H	2.23	0.47
1:N:75:ILE:O	1:N:79:GLY:HA3	2.15	0.47
1:A:128:VAL:O	1:A:128:VAL:CG2	2.63	0.47
1:A:240:HIS:O	1:A:243:VAL:HG22	2.15	0.47
1:N:51:ASP:O	1:N:55:ASN:ND2	2.47	0.47
2:B:89[A]:GLU:HB2	2:B:91[A]:ASN:HD22	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:40:ASP:O	5:E:41:LEU:HB3	2.15	0.46
10:J:5:VAL:O	10:J:9:GLN:HG3	2.15	0.46
1:N:459:PHE:O	1:N:462:LEU:HB3	2.14	0.46
1:A:456:MET:HG2	4:D:96:LEU:HD13	1.96	0.46
3:C:146:TRP:CZ2	7:G:17:ARG:HD3	2.50	0.46
4:D:23:PRO:HG3	5:E:70:VAL:HG21	1.97	0.46
1:N:128:VAL:O	1:N:128:VAL:CG2	2.63	0.46
3:C:2:THR:HG22	6:F:52:ILE:CG1	2.44	0.46
3:C:80:ARG:NH2	3:C:236:GLU:OE2	2.49	0.46
5:E:7:THR:HG23	5:E:10:GLU:H	1.81	0.46
10:W:50:LEU:O	10:W:50:LEU:HD22	2.15	0.46
1:A:75:ILE:O	1:A:79:GLY:HA3	2.15	0.46
1:N:438:ARG:O	1:N:439:ARG:HB2	2.16	0.46
8:U:8:ILE:HB	8:U:10:ASN:OD1	2.15	0.46
5:R:7:THR:HG23	5:R:10:GLU:H	1.81	0.46
7:G:2:SER:HB2	1:N:237:PHE:HZ	1.81	0.46
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.97	0.46
1:N:187:SER:HB3	1:N:277:MET:HE1	1.97	0.46
7:G:9:GLY:HA2	7:G:19:LEU:HD11	1.97	0.46
1:N:476:PHE:HB3	12:Y:15:VAL:CG2	2.46	0.46
4:Q:107:ILE:HD11	11:X:39:GLU:HG3	1.97	0.46
1:A:82:LEU:O	1:A:86:MET:HG3	2.16	0.46
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.50	0.46
1:N:62:ALA:HB2	17:N:515:HEA:HBD1	1.97	0.46
11:X:43:SER:OG	11:X:45:VAL:HG13	2.16	0.46
11:K:43:SER:OG	11:K:45:VAL:HG13	2.16	0.46
3:C:173:PHE:CD1	3:C:173:PHE:C	2.94	0.46
4:D:146:LYS:O	4:D:147:LYS:HG3	2.16	0.46
1:N:3:ILE:N	1:N:3:ILE:HD12	2.31	0.46
3:P:160:LEU:HD13	3:P:222:GLN:CG	2.46	0.46
4:D:107:ILE:HD11	11:K:39:GLU:HG3	1.99	0.45
1:N:240:HIS:O	1:N:243:VAL:HG22	2.16	0.45
6:F:30:PRO:HG2	6:F:31:TYR:CD2	2.51	0.45
13:M:1:ILE:HG13	13:M:2:THR:N	2.31	0.45
13:M:37:LEU:HA	13:M:37:LEU:HD23	1.76	0.45
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.97	0.45
7:T:37:LEU:O	7:T:38:HIS:ND1	2.50	0.45
9:V:68:ILE:HG13	9:V:69:PHE:N	2.30	0.45
1:A:302:ARG:O	1:A:306:THR:HG23	2.17	0.45
4:D:109:HIS:O	4:D:112:GLU:HG2	2.16	0.45
9:I:23:GLY:O	9:I:27:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:173:PHE:CD1	3:P:173:PHE:C	2.94	0.45
4:D:112:GLU:O	4:D:116:VAL:HG13	2.16	0.45
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.98	0.45
2:B:222:TRP:CZ2	2:B:226:MET:HG3	2.51	0.45
4:D:142:LYS:HB2	4:D:144:GLU:HG2	1.99	0.45
1:N:413:HIS:CE1	1:N:468:MET:HB2	2.52	0.45
3:P:146:TRP:CZ2	7:T:17:ARG:HD3	2.51	0.45
4:Q:138:TRP:CZ3	11:X:50:PRO:HG2	2.52	0.45
11:K:24:PHE:O	11:K:28:VAL:HG23	2.16	0.45
3:P:16:TRP:HA	3:P:16:TRP:CE3	2.52	0.45
3:C:160:LEU:HD13	3:C:222:GLN:CG	2.47	0.45
10:J:30:ILE:HG13	10:J:31:LEU:N	2.32	0.45
1:A:5:ARG:O	1:A:9:SER:HB2	2.16	0.45
17:A:515:HEA:HBC1	17:A:515:HEA:HMC1	1.98	0.45
17:A:515:HEA:HMB3	17:A:515:HEA:H11	1.85	0.45
1:N:298:ASP:HB2	1:N:301:THR:HG23	1.98	0.45
2:B:184:LEU:HD11	2:B:211:LEU:HD21	1.99	0.44
3:P:30:GLY:HA2	3:P:42:LEU:HB3	1.99	0.44
7:T:3:ALA:O	7:T:4:ALA:HB2	2.16	0.44
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	1.99	0.44
2:O:121:TYR:O	2:O:138:VAL:HA	2.17	0.44
9:V:60:PHE:CE1	9:V:69:PHE:CE2	3.05	0.44
13:Z:1:ILE:HG13	13:Z:2:THR:N	2.32	0.44
2:B:133:LEU:HD23	2:B:133:LEU:HA	1.79	0.44
3:C:154:GLY:O	6:F:6:VAL:HG13	2.17	0.44
3:P:47:LEU:O	3:P:51:MET:HG2	2.17	0.44
9:V:21:ILE:HD12	9:V:21:ILE:HA	1.76	0.44
1:A:144:ASP:OD1	1:A:213:ARG:HD3	2.17	0.44
7:G:37:LEU:O	7:G:38:HIS:ND1	2.50	0.44
2:O:62:GLU:HA	2:O:65:TRP:CD1	2.52	0.44
5:R:90:ARG:HD3	5:R:90:ARG:HA	1.76	0.44
11:K:32:MET:HE2	11:K:32:MET:HB3	1.81	0.44
1:N:197:LEU:O	3:P:92:LEU:HD22	2.17	0.44
2:B:62:GLU:HA	2:B:65:TRP:CD1	2.52	0.44
7:G:3:ALA:O	7:G:4:ALA:HB2	2.18	0.44
8:H:7:LYS:HE3	8:H:7:LYS:CA	2.48	0.44
4:Q:128:VAL:O	4:Q:134:PHE:HB3	2.18	0.44
2:B:215:PRO:HD3	9:I:60:PHE:CD1	2.53	0.44
1:N:310:MET:CE	2:O:77:ALA:HB2	2.44	0.44
2:O:44:LEU:O	9:V:16:ARG:NH2	2.50	0.44
1:A:426:PHE:N	1:A:427:PRO:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:302:ARG:O	1:N:306:THR:CG2	2.66	0.44
2:O:122:MET:HB2	2:O:208:PRO:HD2	2.00	0.44
1:A:74:MET:HE1	1:A:246:LEU:O	2.18	0.43
2:B:44:LEU:O	9:I:16:ARG:NH2	2.51	0.43
4:Q:24:LEU:HB3	5:R:30:ARG:HG2	1.99	0.43
4:Q:131:ILE:HD12	9:V:47:TYR:CE2	2.52	0.43
1:A:197:LEU:O	3:C:92:LEU:HD22	2.19	0.43
12:Y:41:ARG:HG3	13:Z:40:TYR:CE2	2.53	0.43
1:A:38:ARG:HD2	17:A:515:HEA:OMA	2.18	0.43
4:D:68:PHE:CZ	5:E:70:VAL:HG23	2.53	0.43
1:A:380:VAL:O	1:A:384:GLY:HA3	2.18	0.43
1:A:390:MET:HE2	1:A:390:MET:HA	2.01	0.43
1:N:144:ASP:CG	1:N:213:ARG:HH11	2.26	0.43
7:T:25:LEU:HD23	7:T:25:LEU:HA	1.86	0.43
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.54	0.43
4:D:126:MET:HG3	4:D:128:VAL:HG23	2.00	0.43
8:H:36:PHE:HD2	8:H:37:HIS:CE1	2.37	0.43
1:N:51:ASP:HB3	1:N:55:ASN:ND2	2.34	0.43
4:D:118:LYS:HD2	11:K:53:TRP:HA	2.01	0.43
9:V:23:GLY:O	9:V:27:VAL:HG23	2.18	0.43
1:A:32:ALA:HB3	12:L:36:PRO:HG2	2.01	0.43
1:A:468:MET:HE2	1:A:468:MET:HB3	1.70	0.43
2:B:111:THR:O	2:B:111:THR:CG2	2.63	0.43
2:B:162:SER:HB3	2:B:197:SER:C	2.43	0.43
6:S:30:PRO:HG2	6:S:31:TYR:CD2	2.54	0.43
11:X:22:ALA:O	11:X:26:VAL:HG23	2.18	0.43
1:A:481:GLU:O	13:M:3:ALA:HB1	2.19	0.43
11:K:9:PHE:CD1	11:K:9:PHE:C	2.97	0.43
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.54	0.43
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	2.00	0.43
1:N:426:PHE:N	1:N:427:PRO:HD2	2.34	0.42
10:W:31:LEU:HD23	10:W:31:LEU:HA	1.89	0.42
1:A:334:TRP:HH2	2:B:46:LEU:HD13	1.84	0.42
3:C:252:LEU:HD23	3:C:252:LEU:HA	1.86	0.42
8:H:57:ARG:O	8:H:61:LYS:HB2	2.19	0.42
4:Q:5:VAL:HG13	4:Q:5:VAL:O	2.18	0.42
10:W:5:VAL:O	10:W:9:GLN:HG3	2.19	0.42
2:O:111:THR:O	2:O:111:THR:CG2	2.63	0.42
5:R:40:ASP:O	5:R:41:LEU:HB3	2.19	0.42
1:A:442:ASP:OD2	2:B:134:ARG:NH2	2.53	0.42
2:B:90[A]:ILE:CD1	2:B:151:ARG:HH21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:379:TYR:CE2	1:N:383:MET:HE1	2.55	0.42
8:U:57:ARG:O	8:U:61:LYS:HB2	2.19	0.42
6:F:94:HIS:CD2	6:F:95:GLN:HG3	2.54	0.42
1:N:233:HIS:CE1	1:N:292:MET:HE1	2.54	0.42
1:N:468:MET:HE2	1:N:468:MET:HB3	1.77	0.42
1:N:508:PRO:CG	3:P:6:HIS:HB3	2.47	0.42
3:P:252:LEU:HD23	3:P:252:LEU:HA	1.79	0.42
1:A:310:MET:CE	2:B:77:ALA:HB2	2.45	0.42
2:B:102:HIS:O	2:B:104:TRP:N	2.52	0.42
3:C:154:GLY:HA2	6:F:6:VAL:CG2	2.49	0.42
7:G:76:ASN:HA	7:G:77:PRO:HD2	1.94	0.42
1:N:384:GLY:O	1:N:385:ALA:C	2.63	0.42
1:N:474:GLU:CD	1:N:480:ARG:HH22	2.27	0.42
9:I:21:ILE:HA	9:I:21:ILE:HD12	1.71	0.42
3:P:122:HIS:NE2	7:T:45:PRO:HB3	2.35	0.42
3:P:154:GLY:HA2	6:S:6:VAL:CG2	2.49	0.42
4:Q:23:PRO:HG3	5:R:70:VAL:HG21	2.00	0.42
4:Q:118:LYS:HA	11:X:51:LYS:O	2.20	0.42
12:Y:44:LEU:HD12	12:Y:44:LEU:HA	1.86	0.42
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	2.02	0.42
1:N:374:VAL:HA	1:N:377:PHE:CE2	2.55	0.42
1:N:393:PHE:O	1:N:397:PHE:HB2	2.20	0.42
6:S:48:LEU:O	6:S:50:PRO:HD3	2.19	0.42
1:A:459:PHE:O	1:A:462:LEU:HB3	2.20	0.42
2:B:90[A]:ILE:HD11	2:B:151:ARG:NH2	2.35	0.42
3:P:65:SER:HB3	3:P:71:HIS:CE1	2.55	0.42
10:W:30:ILE:O	10:W:34:VAL:HG23	2.20	0.42
1:N:302:ARG:O	1:N:306:THR:HG23	2.20	0.41
4:Q:102:TYR:CD1	13:Z:35:TYR:CE1	3.05	0.41
1:A:3:ILE:HD12	1:A:3:ILE:N	2.34	0.41
1:A:187:SER:HB3	1:A:277:MET:HE1	1.99	0.41
2:B:146:MET:SD	2:B:189:PRO:HB3	2.60	0.41
17:A:515:HEA:H212	17:A:515:HEA:H271	1.88	0.41
2:B:92[A]:ASN:HA	2:B:93:PRO:HD2	1.57	0.41
2:O:110:TYR:CD1	2:O:110:TYR:N	2.88	0.41
2:O:145:PRO:CG	2:O:148:MET:HE2	2.48	0.41
4:Q:134:PHE:CE1	11:X:44:PRO:HG2	2.56	0.41
3:C:122:HIS:NE2	7:G:45:PRO:HB3	2.35	0.41
4:D:131:ILE:HD12	9:I:47:TYR:CE2	2.55	0.41
1:N:33:LEU:O	1:N:37:ILE:HG13	2.20	0.41
4:Q:119:GLN:O	4:Q:123:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:TRP:CE3	3:C:16:TRP:HA	2.55	0.41
5:E:12:ASP:HA	5:E:47:ILE:HD11	2.03	0.41
17:N:515:HEA:HMB3	17:N:515:HEA:H11	1.90	0.41
1:A:274:VAL:O	1:A:278:MET:HG3	2.21	0.41
2:B:3:TYR:CZ	2:B:6:GLN:HG3	2.56	0.41
8:H:17:ASP:OD1	8:H:19:ARG:HG3	2.21	0.41
12:L:44:LEU:HA	12:L:44:LEU:HD12	1.88	0.41
2:O:76:ILE:O	2:O:79:PRO:HD2	2.20	0.41
2:O:133:LEU:HD23	2:O:133:LEU:HA	1.81	0.41
3:C:30:GLY:HA2	3:C:42:LEU:HB3	2.02	0.41
6:F:48:LEU:O	6:F:50:PRO:HD3	2.20	0.41
6:S:94:HIS:CD2	6:S:95:GLN:HG3	2.55	0.41
7:T:7:ASP:CG	7:T:8:HIS:H	2.28	0.41
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.56	0.41
1:A:61:HIS:HE1	17:A:515:HEA:C4B	2.34	0.41
1:A:340:TRP:HZ2	1:A:413:HIS:CD2	2.39	0.41
9:I:58:LYS:O	9:I:62:GLU:HG3	2.20	0.41
9:I:68:ILE:HG13	9:I:69:PHE:N	2.34	0.41
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.55	0.41
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.20	0.41
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.93	0.41
2:B:41:ILE:O	2:B:45:MET:HG2	2.21	0.41
3:C:42:LEU:HD12	3:C:42:LEU:HA	1.76	0.41
4:D:24:LEU:HB3	5:E:30:ARG:HG2	2.02	0.41
4:D:138:TRP:CZ3	11:K:50:PRO:HG2	2.56	0.41
7:G:44:ARG:HA	7:G:45:PRO:HD3	1.81	0.41
1:N:52:GLN:O	1:N:56:VAL:HG23	2.21	0.41
17:N:515:HEA:HBC1	17:N:515:HEA:HMC3	2.01	0.41
3:C:159:MET:SD	3:C:159:MET:C	3.04	0.41
6:F:6:VAL:HA	6:F:7:PRO:HD3	1.90	0.41
8:H:8:ILE:HB	8:H:10:ASN:OD1	2.21	0.41
2:O:102:HIS:O	2:O:104:TRP:N	2.54	0.41
2:B:4:PRO:HB2	11:K:43:SER:HA	2.03	0.40
2:B:175:ILE:HA	2:B:176:PRO:HD3	1.98	0.40
2:B:191:LEU:HB2	4:D:126:MET:CE	2.50	0.40
4:D:102:TYR:CD1	13:M:35:TYR:CE1	3.08	0.40
2:O:9:PHE:HB2	2:O:21:LEU:HD21	2.02	0.40
6:S:54:ASN:ND2	6:S:54:ASN:N	2.69	0.40
3:P:16:TRP:HA	3:P:16:TRP:HE3	1.85	0.40
1:A:240:HIS:HB3	1:A:241:PRO:HD3	2.02	0.40
1:A:476:PHE:HB3	12:L:15:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.91	0.40
1:N:486:ASP:OD1	13:Z:1:ILE:HD11	2.21	0.40
2:O:89[A]:GLU:HG3	2:O:89[A]:GLU:O	2.21	0.40
1:N:54:TYR:O	1:N:57:VAL:HB	2.22	0.40
1:N:274:VAL:O	1:N:278:MET:HG3	2.22	0.40
1:N:449:MET:SD	2:O:5:MET:HG2	2.61	0.40
2:O:129:LYS:O	2:O:130:PRO:C	2.65	0.40
3:C:2:THR:HG23	6:F:96:LEU:CD1	2.42	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	512/514 (100%)	494 (96%)	18 (4%)	0	100	100
1	N	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
2	B	230/227 (101%)	208 (90%)	20 (9%)	2 (1%)	14	17
2	O	230/227 (101%)	208 (90%)	20 (9%)	2 (1%)	14	17
3	C	259/261 (99%)	252 (97%)	6 (2%)	1 (0%)	30	38
3	P	259/261 (99%)	252 (97%)	6 (2%)	1 (0%)	30	38
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	5	4
6	S	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	5	4
7	G	82/84 (98%)	65 (79%)	12 (15%)	5 (6%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	T	82/84 (98%)	66 (80%)	11 (13%)	5 (6%)	1 0
8	H	77/85 (91%)	72 (94%)	5 (6%)	0	100 100
8	U	77/85 (91%)	72 (94%)	5 (6%)	0	100 100
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100 100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100 100
10	J	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	6 6
10	W	56/59 (95%)	55 (98%)	0	1 (2%)	6 6
11	K	47/56 (84%)	43 (92%)	4 (8%)	0	100 100
11	X	47/56 (84%)	42 (89%)	5 (11%)	0	100 100
12	L	45/47 (96%)	44 (98%)	1 (2%)	0	100 100
12	Y	45/47 (96%)	44 (98%)	1 (2%)	0	100 100
13	M	41/46 (89%)	41 (100%)	0	0	100 100
13	Z	41/46 (89%)	41 (100%)	0	0	100 100
All	All	3522/3612 (98%)	3343 (95%)	157 (4%)	22 (1%)	21 27

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
2	O	134	ARG
7	T	4	ALA
2	B	104	TRP
2	B	134	ARG
3	C	2	THR
7	G	11	THR
2	O	104	TRP
3	P	2	THR
7	T	11	THR
7	G	38	HIS
7	G	41	HIS
6	S	97	ALA
7	T	38	HIS
7	T	41	HIS
6	F	97	ALA
7	T	8	HIS
10	W	15	ASP
6	F	64	GLU

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Mol	Chain	Res	Type
7	G	8	HIS
10	J	15	ASP
6	S	64	GLU

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	427/427 (100%)	396 (93%)	31 (7%)	13	18
1	N	427/427 (100%)	396 (93%)	31 (7%)	13	18
2	B	216/211 (102%)	193 (89%)	23 (11%)	6	8
2	O	216/211 (102%)	195 (90%)	21 (10%)	8	10
3	C	226/226 (100%)	206 (91%)	20 (9%)	9	12
3	P	226/226 (100%)	206 (91%)	20 (9%)	9	12
4	D	128/129 (99%)	120 (94%)	8 (6%)	16	23
4	Q	128/129 (99%)	120 (94%)	8 (6%)	16	23
5	E	92/95 (97%)	84 (91%)	8 (9%)	9	12
5	R	92/95 (97%)	85 (92%)	7 (8%)	12	16
6	F	81/81 (100%)	70 (86%)	11 (14%)	3	4
6	S	81/81 (100%)	70 (86%)	11 (14%)	3	4
7	G	68/68 (100%)	61 (90%)	7 (10%)	7	8
7	T	68/68 (100%)	60 (88%)	8 (12%)	5	6
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	13
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	13
9	I	58/58 (100%)	55 (95%)	3 (5%)	21	31
9	V	58/58 (100%)	54 (93%)	4 (7%)	14	20
10	J	49/50 (98%)	43 (88%)	6 (12%)	5	5
10	W	49/50 (98%)	43 (88%)	6 (12%)	5	5
11	K	39/46 (85%)	37 (95%)	2 (5%)	21	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	X	39/46 (85%)	38 (97%)	1 (3%)	40 59
12	L	40/40 (100%)	36 (90%)	4 (10%)	7 9
12	Y	40/40 (100%)	36 (90%)	4 (10%)	7 9
13	M	37/38 (97%)	32 (86%)	5 (14%)	4 4
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4 4
All	All	3064/3088 (99%)	2798 (91%)	266 (9%)	10 12

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	46	THR
1	A	96	ARG
1	A	105	LEU
1	A	106	PRO
1	A	128	VAL
1	A	136	LEU
1	A	138	HIS
1	A	150	LEU
1	A	159	LEU
1	A	188	VAL
1	A	199	LEU
1	A	241	PRO
1	A	295	VAL
1	A	301	THR
1	A	306	THR
1	A	318	VAL
1	A	324	LEU
1	A	347	LEU
1	A	353	LEU
1	A	354	THR
1	A	369	ASP
1	A	373	VAL
1	A	382	SER
1	A	444	PRO
1	A	465	VAL
1	A	467	LEU
1	A	474	GLU
1	A	492	LEU
1	A	504	THR

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Mol	Chain	Res	Type
1	A	513	LEU
2	B	7	LEU
2	B	31	VAL
2	B	33	LEU
2	B	60	GLU
2	B	63	THR
2	B	88[A]	ASP
2	B	88[B]	ASP
2	B	90[A]	ILE
2	B	90[B]	ILE
2	B	92[A]	ASN
2	B	92[B]	ASN
2	B	113	TYR
2	B	115	ASP
2	B	125	THR
2	B	130	PRO
2	B	134	ARG
2	B	138	VAL
2	B	142	VAL
2	B	171	LYS
2	B	185	MET
2	B	202	SER
2	B	213	LEU
2	B	216	LEU
3	C	3	HIS
3	C	11	VAL
3	C	13	PRO
3	C	17	PRO
3	C	18	LEU
3	C	22	LEU
3	C	33	MET
3	C	38	ASN
3	C	85	LEU
3	C	92	LEU
3	C	111	GLU
3	C	112	LEU
3	C	119	THR
3	C	131	LEU
3	C	132	LEU
3	C	137	LEU
3	C	160	LEU
3	C	163	LEU

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Mol	Chain	Res	Type
3	C	196	THR
3	C	213	THR
4	D	27	VAL
4	D	36	SER
4	D	40	LEU
4	D	59	LEU
4	D	62	LEU
4	D	116	VAL
4	D	127	LYS
4	D	143	ASN
5	E	5	HIS
5	E	6	GLU
5	E	29	LEU
5	E	41	LEU
5	E	70	VAL
5	E	79	LYS
5	E	80	GLU
5	E	91	PRO
6	F	6	VAL
6	F	20	VAL
6	F	34	LEU
6	F	37	LYS
6	F	44	GLU
6	F	53	THR
6	F	54	ASN
6	F	68	THR
6	F	74	LEU
6	F	95	GLN
6	F	96	LEU
7	G	5	LYS
7	G	14	ARG
7	G	36	TRP
7	G	37	LEU
7	G	39	SER
7	G	41	HIS
7	G	78	LEU
8	H	7	LYS
8	H	11	TYR
8	H	12	GLN
8	H	29	CYS
8	H	44	THR
8	H	60	TYR

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Mol	Chain	Res	Type
9	I	8	GLN
9	I	16	ARG
9	I	19	PHE
10	J	4	ARG
10	J	5	VAL
10	J	27	THR
10	J	30	ILE
10	J	47	LEU
10	J	50	LEU
11	K	43	SER
11	K	45	VAL
12	L	15	VAL
12	L	22	LEU
12	L	26	THR
12	L	44	LEU
13	M	1	ILE
13	M	2	THR
13	M	24	LEU
13	M	37	LEU
13	M	38	ASP
1	N	18	LEU
1	N	46	THR
1	N	96	ARG
1	N	105	LEU
1	N	106	PRO
1	N	128	VAL
1	N	136	LEU
1	N	138	HIS
1	N	150	LEU
1	N	173	PRO
1	N	188	VAL
1	N	199	LEU
1	N	241	PRO
1	N	295	VAL
1	N	301	THR
1	N	306	THR
1	N	318	VAL
1	N	324	LEU
1	N	347	LEU
1	N	353	LEU
1	N	354	THR
1	N	369	ASP

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Mol	Chain	Res	Type
1	N	373	VAL
1	N	382	SER
1	N	444	PRO
1	N	465	VAL
1	N	467	LEU
1	N	474	GLU
1	N	492	LEU
1	N	504	THR
1	N	513	LEU
2	O	7	LEU
2	O	31	VAL
2	O	33	LEU
2	O	60	GLU
2	O	63	THR
2	O	88[A]	ASP
2	O	88[B]	ASP
2	O	90[A]	ILE
2	O	90[B]	ILE
2	O	92[A]	ASN
2	O	92[B]	ASN
2	O	113	TYR
2	O	115	ASP
2	O	125	THR
2	O	130	PRO
2	O	138	VAL
2	O	142	VAL
2	O	171	LYS
2	O	185	MET
2	O	202	SER
2	O	216	LEU
3	P	2	THR
3	P	3	HIS
3	P	11	VAL
3	P	17	PRO
3	P	18	LEU
3	P	22	LEU
3	P	33	MET
3	P	38	ASN
3	P	85	LEU
3	P	92	LEU
3	P	111	GLU
3	P	112	LEU

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Mol	Chain	Res	Type
3	P	119	THR
3	P	131	LEU
3	P	132	LEU
3	P	137	LEU
3	P	160	LEU
3	P	163	LEU
3	P	196	THR
3	P	213	THR
4	Q	27	VAL
4	Q	36	SER
4	Q	40	LEU
4	Q	59	LEU
4	Q	62	LEU
4	Q	116	VAL
4	Q	127	LYS
4	Q	143	ASN
5	R	5	HIS
5	R	6	GLU
5	R	29	LEU
5	R	41	LEU
5	R	70	VAL
5	R	79	LYS
5	R	80	GLU
6	S	6	VAL
6	S	20	VAL
6	S	34	LEU
6	S	37	LYS
6	S	44	GLU
6	S	53	THR
6	S	54	ASN
6	S	68	THR
6	S	74	LEU
6	S	95	GLN
6	S	96	LEU
7	T	5	LYS
7	T	14	ARG
7	T	26	PRO
7	T	36	TRP
7	T	37	LEU
7	T	39	SER
7	T	41	HIS
7	T	78	LEU

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Mol	Chain	Res	Type
8	U	7	LYS
8	U	11	TYR
8	U	12	GLN
8	U	29	CYS
8	U	44	THR
8	U	60	TYR
9	V	8	GLN
9	V	16	ARG
9	V	19	PHE
9	V	21	ILE
10	W	4	ARG
10	W	5	VAL
10	W	27	THR
10	W	30	ILE
10	W	47	LEU
10	W	50	LEU
11	X	45	VAL
12	Y	15	VAL
12	Y	22	LEU
12	Y	26	THR
12	Y	44	LEU
13	Z	1	ILE
13	Z	2	THR
13	Z	24	LEU
13	Z	37	LEU
13	Z	38	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	43	GLN
1	A	55	ASN
1	A	413	HIS
1	A	503	HIS
1	A	512	ASN
2	B	22	HIS
2	B	52	HIS
2	B	195	GLN
2	B	203	ASN
3	C	38	ASN
3	C	68	GLN

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Mol	Chain	Res	Type
3	C	70	HIS
3	C	222	GLN
4	D	109	HIS
4	D	119	GLN
6	F	54	ASN
7	G	38	HIS
7	G	41	HIS
7	G	71	HIS
8	H	32	ASN
12	L	42	HIS
1	N	4	ASN
1	N	43	GLN
1	N	55	ASN
1	N	413	HIS
1	N	503	HIS
2	O	22	HIS
2	O	52	HIS
3	P	38	ASN
3	P	68	GLN
3	P	70	HIS
3	P	222	GLN
4	Q	109	HIS
4	Q	119	GLN
6	S	54	ASN
6	S	98	HIS
7	T	38	HIS
7	T	41	HIS
7	T	71	HIS
8	U	28	ASN
8	U	32	ASN
12	Y	42	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
17	HEA	A	515	1	67,67,67	1.46	6 (8%)	81,103,103	1.30	8 (9%)
17	HEA	N	515	1	67,67,67	1.34	6 (8%)	81,103,103	1.31	5 (6%)
18	PER	N	520	14,17	1,1,1	1.45	0	-		
17	HEA	A	516	1,18	67,67,67	1.41	12 (17%)	81,103,103	1.65	15 (18%)
17	HEA	N	516	1,18	67,67,67	1.16	6 (8%)	81,103,103	1.58	17 (20%)
18	PER	A	520	14,17	1,1,1	1.87	0	-		

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
17	HEA	N	515	1	-	7/36/76/76	-
17	HEA	N	516	1,18	-	4/36/76/76	-
17	HEA	A	516	1,18	-	2/36/76/76	-
17	HEA	A	515	1	-	9/36/76/76	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	515	HEA	C11-C3B	-6.54	1.43	1.51
17	N	515	HEA	C11-C3B	-6.51	1.43	1.51
17	A	515	HEA	FE-NC	4.11	2.08	1.95
17	A	516	HEA	CMA-C3A	-3.98	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	516	HEA	C4B-NB	3.71	1.46	1.40
17	A	515	HEA	CMA-C3A	-3.31	1.38	1.45
17	N	516	HEA	CMD-C2D	3.30	1.57	1.50
17	N	516	HEA	CMA-C3A	-3.24	1.38	1.45
17	A	516	HEA	CMD-C2D	3.06	1.57	1.50
17	A	516	HEA	C1D-C2D	2.88	1.50	1.44
17	A	516	HEA	FE-ND	-2.86	1.86	1.94
17	A	516	HEA	FE-NA	2.82	2.04	1.95
17	N	516	HEA	C11-C3B	2.73	1.54	1.51
17	A	515	HEA	CHD-C1D	2.71	1.43	1.38
17	N	515	HEA	CMA-C3A	-2.67	1.39	1.45
17	N	515	HEA	C20-C19	-2.66	1.45	1.51
17	A	516	HEA	FE-NB	-2.54	1.87	1.94
17	A	515	HEA	C4B-NB	2.50	1.44	1.40
17	A	516	HEA	C1C-C2C	2.46	1.48	1.43
17	N	515	HEA	C1C-C2C	2.36	1.48	1.43
17	N	516	HEA	C1D-C2D	2.28	1.49	1.44
17	N	516	HEA	CAA-C2A	2.27	1.57	1.51
17	N	515	HEA	FE-NA	2.26	2.02	1.95
17	N	515	HEA	C1B-NB	2.17	1.43	1.38
17	A	516	HEA	FE-NC	2.13	2.02	1.95
17	N	516	HEA	C4B-C3B	2.09	1.48	1.44
17	A	515	HEA	C4D-ND	2.08	1.42	1.38
17	A	516	HEA	C4D-ND	2.06	1.42	1.38
17	A	516	HEA	C3C-C2C	-2.04	1.34	1.41
17	A	516	HEA	C3C-C4C	2.03	1.48	1.42

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	515	HEA	C13-C14-C15	-5.77	114.41	127.62
17	A	515	HEA	C13-C14-C15	-5.31	115.47	127.62
17	A	516	HEA	C4B-NB-C1B	-4.97	99.32	105.21
17	A	516	HEA	C2D-C1D-ND	4.35	114.84	109.84
17	N	516	HEA	C1D-C2D-C3D	-4.26	102.50	106.98
17	A	516	HEA	C1D-C2D-C3D	-4.13	102.63	106.98
17	N	516	HEA	C3C-C4C-NC	4.04	113.20	109.80
17	A	516	HEA	C3B-C4B-NB	3.77	114.18	109.84
17	A	516	HEA	CMB-C2B-C3B	-3.49	123.53	130.28
17	A	516	HEA	CMD-C2D-C1D	3.46	130.44	125.03
17	N	516	HEA	C3B-C4B-NB	3.41	113.76	109.84
17	A	516	HEA	C3C-C4C-NC	3.40	112.67	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	516	HEA	CMB-C2B-C3B	-3.34	123.81	130.28
17	N	515	HEA	C3C-C4C-NC	3.25	112.54	109.80
17	N	516	HEA	C4B-NB-C1B	-3.18	101.44	105.21
17	N	516	HEA	CMD-C2D-C1D	3.17	129.99	125.03
17	N	516	HEA	C2D-C1D-ND	3.12	113.42	109.84
17	A	516	HEA	C1D-ND-C4D	-3.04	101.60	105.21
17	A	515	HEA	C17-C18-C19	-3.03	120.69	127.62
17	A	516	HEA	C2B-C1B-NB	2.96	113.32	109.90
17	A	516	HEA	C27-C19-C20	2.94	120.32	115.23
17	N	515	HEA	C17-C18-C19	-2.83	121.15	127.62
17	N	516	HEA	CHB-C4A-NA	-2.46	121.78	124.45
17	N	516	HEA	C2A-C1A-NA	2.45	112.69	110.32
17	N	516	HEA	C2B-C1B-NB	2.43	112.71	109.90
17	N	516	HEA	C4B-C3B-C2B	-2.42	103.37	107.44
17	N	515	HEA	CHC-C4B-NB	-2.37	121.43	124.37
17	A	516	HEA	CHB-C1B-C2B	-2.35	121.32	125.03
17	N	516	HEA	CHB-C1B-C2B	-2.34	121.34	125.03
17	A	516	HEA	CHC-C4B-C3B	-2.24	120.14	125.80
17	A	515	HEA	C4B-NB-C1B	-2.18	102.62	105.21
17	N	516	HEA	C12-C13-C14	-2.16	106.49	112.16
17	A	515	HEA	CHB-C1B-NB	2.15	126.74	124.42
17	N	516	HEA	C20-C19-C18	-2.15	116.34	121.17
17	A	516	HEA	C4B-C3B-C2B	-2.12	103.87	107.44
17	A	515	HEA	C3C-C4C-NC	2.11	111.57	109.80
17	N	516	HEA	CHC-C4B-C3B	-2.08	120.54	125.80
17	A	515	HEA	C2D-C1D-ND	2.08	112.23	109.84
17	A	516	HEA	C1B-C2B-C3B	2.07	109.19	106.80
17	A	515	HEA	CMB-C2B-C3B	-2.05	126.31	130.28
17	N	516	HEA	C4A-NA-C1A	-2.05	102.48	105.82
17	A	516	HEA	C12-C13-C14	-2.05	106.78	112.16
17	N	516	HEA	C1D-ND-C4D	-2.04	102.79	105.21
17	A	515	HEA	CHB-C1B-C2B	-2.02	121.84	125.03
17	N	515	HEA	C1B-C2B-C3B	2.00	109.11	106.80

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	515	HEA	C15-C16-C17-C18
17	N	515	HEA	C15-C16-C17-C18
17	A	515	HEA	C26-C15-C16-C17
17	N	515	HEA	C26-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
17	N	515	HEA	C14-C15-C16-C17
17	A	515	HEA	C14-C15-C16-C17
17	A	516	HEA	CAD-CBD-CGD-O1D
17	N	516	HEA	CAD-CBD-CGD-O1D
17	N	516	HEA	CAD-CBD-CGD-O2D
17	A	516	HEA	CAD-CBD-CGD-O2D
17	A	515	HEA	C27-C19-C20-C21
17	A	515	HEA	CAD-CBD-CGD-O1D
17	A	515	HEA	C2C-C3C-CAC-CBC
17	N	515	HEA	CAD-CBD-CGD-O1D
17	N	515	HEA	CAA-CBA-CGA-O1A
17	A	515	HEA	CAA-CBA-CGA-O1A
17	N	515	HEA	CAD-CBD-CGD-O2D
17	A	515	HEA	CAA-CBA-CGA-O2A
17	A	515	HEA	CAD-CBD-CGD-O2D
17	N	516	HEA	CAA-CBA-CGA-O1A
17	N	515	HEA	CAA-CBA-CGA-O2A
17	N	516	HEA	CAA-CBA-CGA-O2A

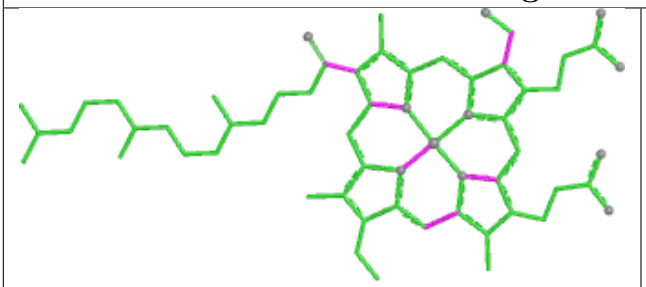
There are no ring outliers.

4 monomers are involved in 11 short contacts:

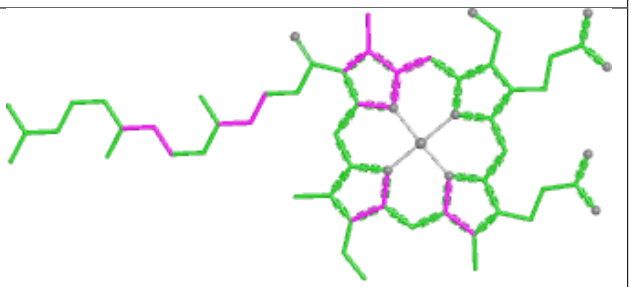
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	515	HEA	6	0
17	N	515	HEA	3	0
18	N	520	PER	1	0
18	A	520	PER	1	0

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

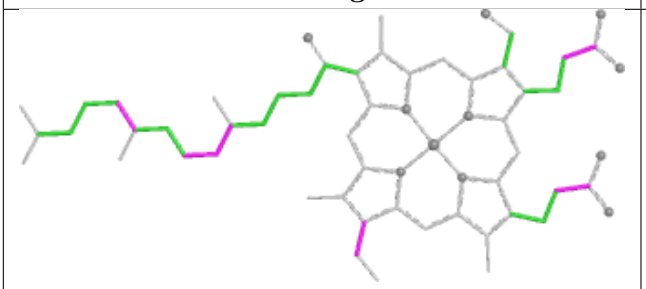
Ligand HEA A 515



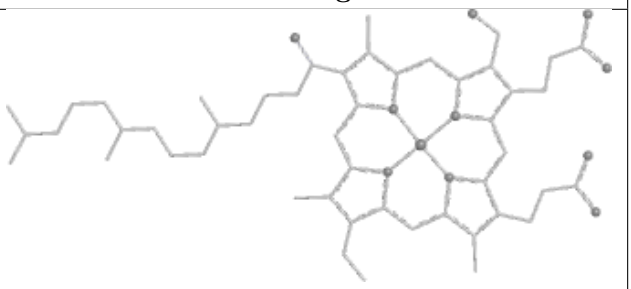
Bond lengths



Bond angles

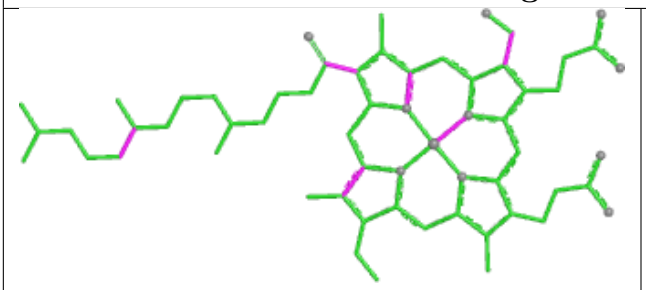


Torsions

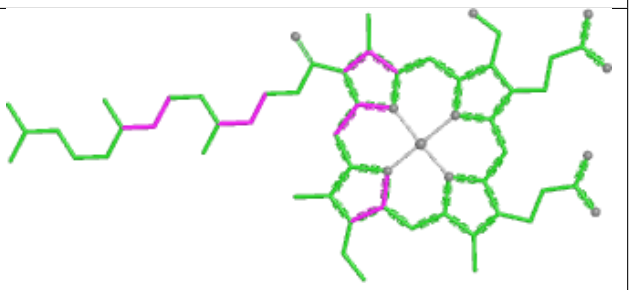


Rings

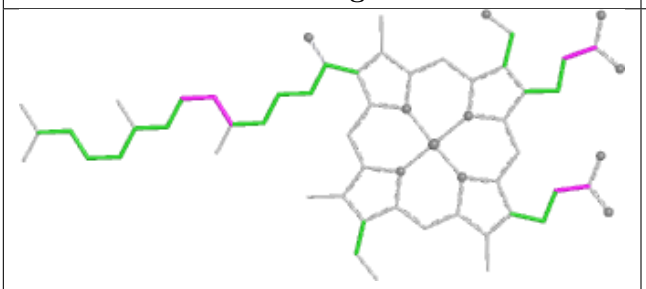
Ligand HEA N 515



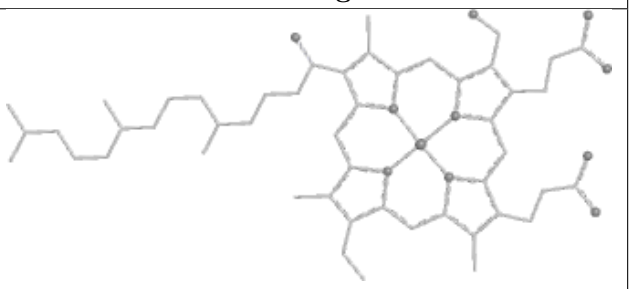
Bond lengths



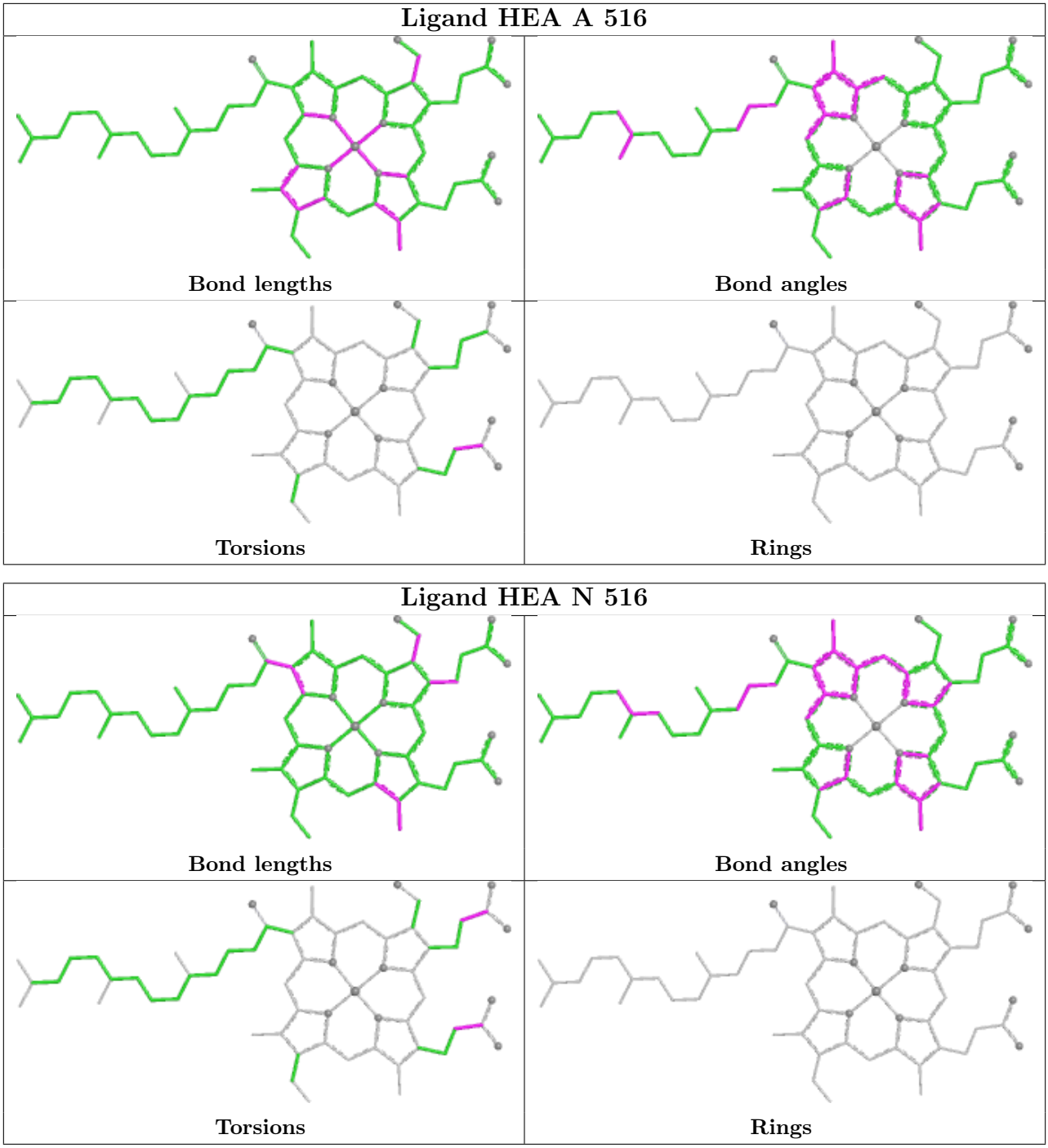
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.