



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:25 am GMT

PDB ID : 2OCC
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

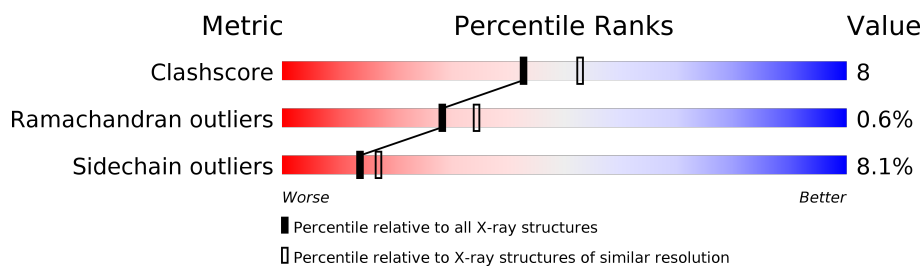
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)















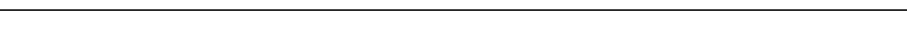




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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 $\leq 5\%$. 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	514	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	
4	D	147	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	84	
7	T	84	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-

2 Entry composition

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			

Continued on next page...

Continued from previous page...

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 (three-letter code: CU) (formula: Cu).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: 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

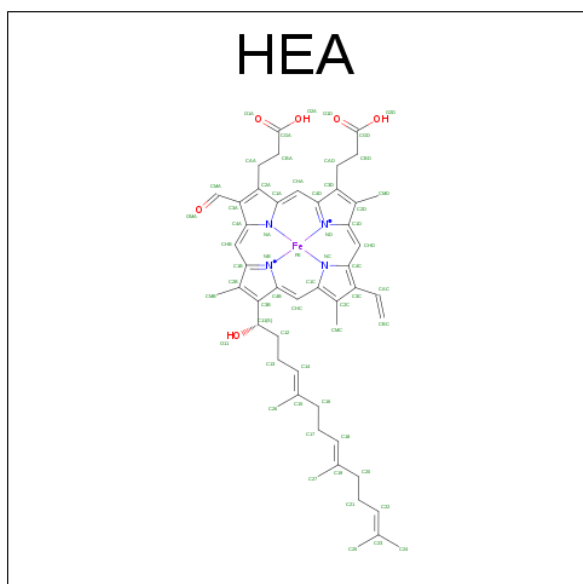
- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



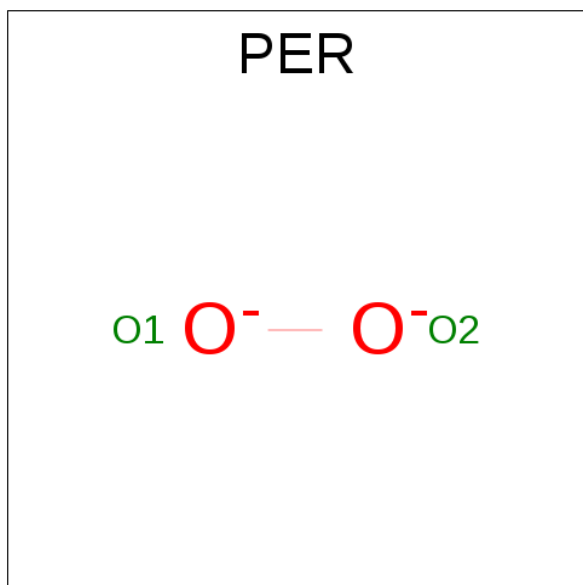
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C Fe N O 60 49 1 4 6	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 19 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



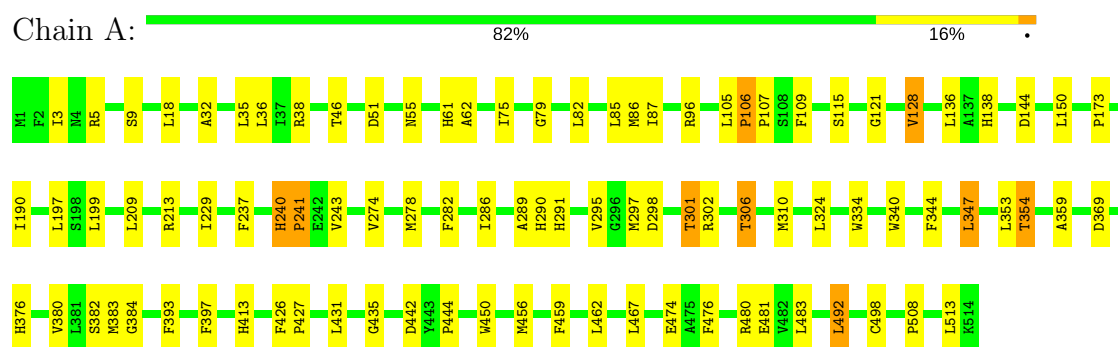
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O		
			2	2	0	0
19	N	1	Total	O		
			2	2	0	0

3 Residue-property plots

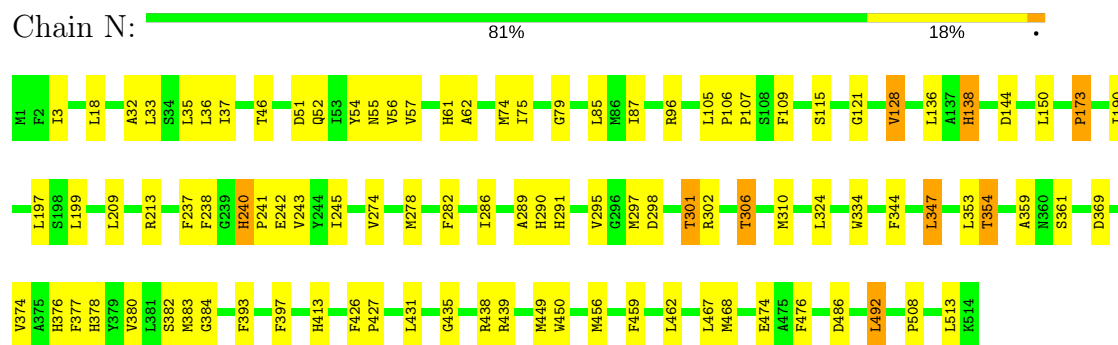
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

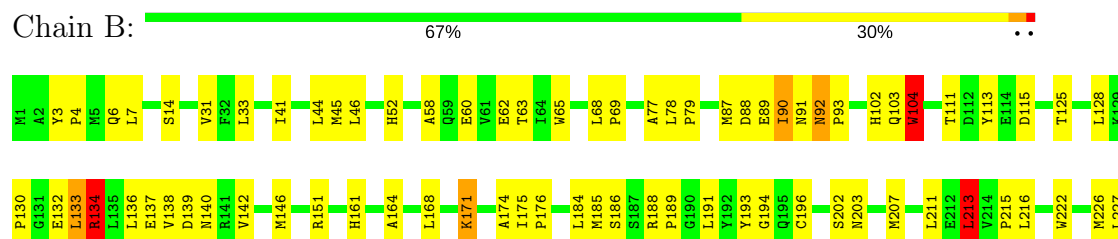
• Molecule 1: CYTOCHROME C OXIDASE



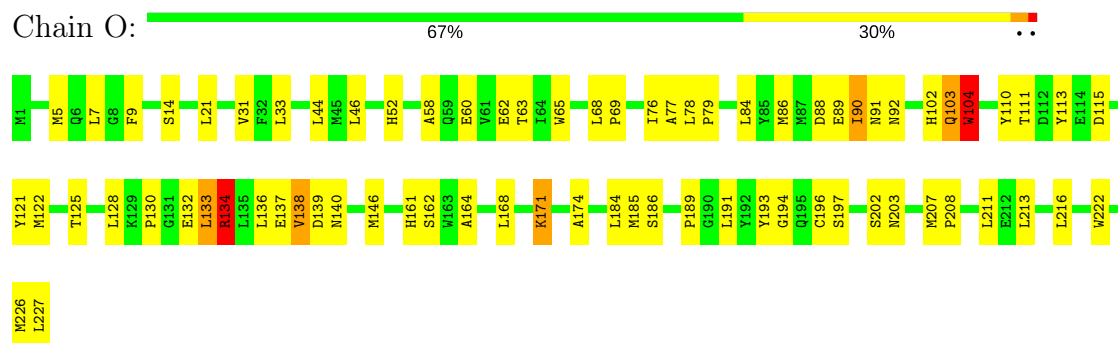
• Molecule 1: CYTOCHROME C OXIDASE



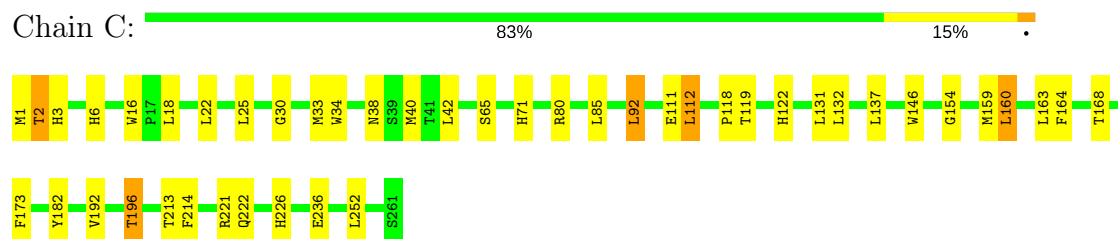
• Molecule 2: CYTOCHROME C OXIDASE



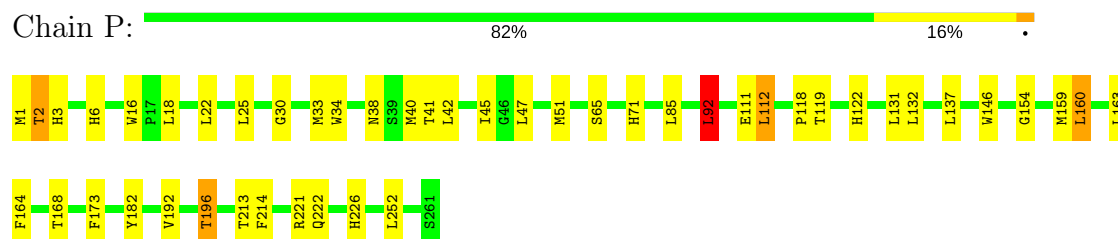
• Molecule 2: CYTOCHROME C OXIDASE



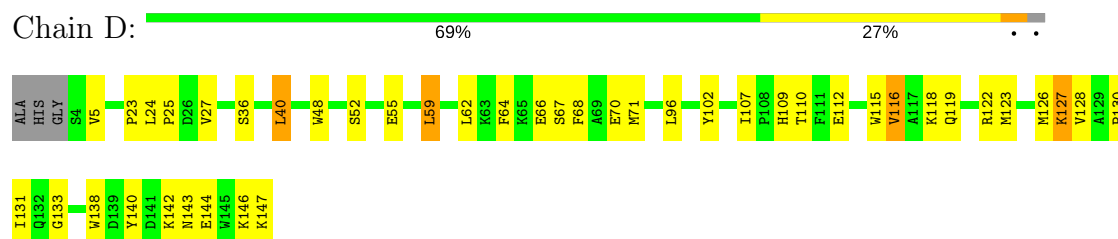
- Molecule 3: CYTOCHROME C OXIDASE



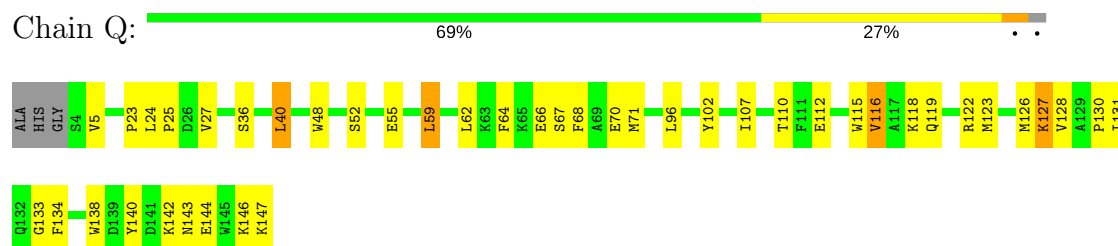
- Molecule 3: CYTOCHROME C OXIDASE




- Molecule 4: CYTOCHROME C OXIDASE



- Molecule 4: CYTOCHROME C OXIDASE



- Molecule 5: CYTOCHROME C OXIDASE

Chain E:  77% 15% . . .



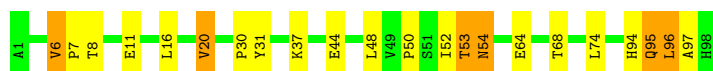
- Molecule 5: CYTOCHROME C OXIDASE

Chain R:  75% 18% . . .




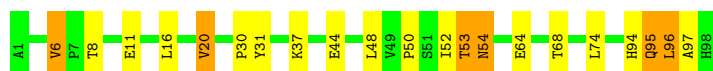
- Molecule 6: CYTOCHROME C OXIDASE

Chain F:  78% 16% 6%



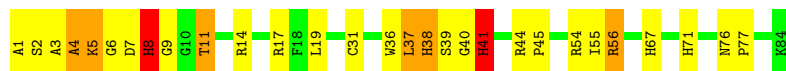
- Molecule 6: CYTOCHROME C OXIDASE

Chain S:  79% 15% 6%



- Molecule 7: CYTOCHROME C OXIDASE

Chain G:  65% 25% 7% .



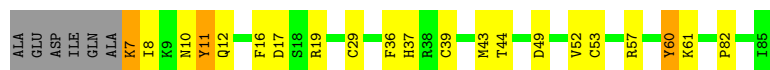
- Molecule 7: CYTOCHROME C OXIDASE

Chain T:  69% 21% 8% .



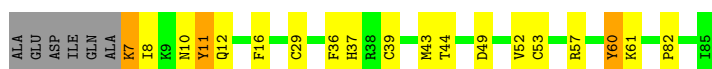
- Molecule 8: CYTOCHROME C OXIDASE

Chain H:  68% 21% . 7%



- Molecule 8: CYTOCHROME C OXIDASE

Chain U:  71% 19% . 7%



• Molecule 9: CYTOCHROME C OXIDASE

Chain I: 81% 16% .



• Molecule 9: CYTOCHROME C OXIDASE

Chain V: 84% 14% .



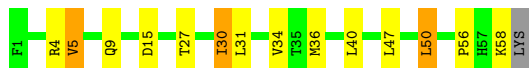
• Molecule 10: CYTOCHROME C OXIDASE

Chain J: 76% 17% 5% .



• Molecule 10: CYTOCHROME C OXIDASE

Chain W: 75% 19% 5% .



• Molecule 11: CYTOCHROME C OXIDASE

Chain K: 75% 9% 13% .



• Molecule 11: CYTOCHROME C OXIDASE

Chain X: 68% 16% 13% .



• Molecule 12: CYTOCHROME C OXIDASE

Chain L: 79% 17% .



• Molecule 12: CYTOCHROME C OXIDASE

Chain Y:

79%

17%



• Molecule 13: CYTOCHROME C OXIDASE

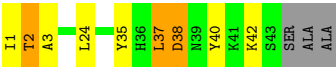
Chain M:

74%

13%

7%

7%



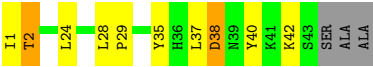
• Molecule 13: CYTOCHROME C OXIDASE

Chain Z:

72%

17%

7%



4 Data and refinement statistics

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: MG, NA, ZN, PER, HEA, 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	0.72	1/4164 (0.0%)	0.80	2/5688 (0.0%)
1	N	0.62	1/4164 (0.0%)	0.77	2/5688 (0.0%)
2	B	0.70	0/1909	0.91	5/2601 (0.2%)
2	O	0.64	0/1909	0.89	3/2601 (0.1%)
3	C	0.68	0/2211	0.71	1/3023 (0.0%)
3	P	0.61	0/2211	0.70	1/3023 (0.0%)
4	D	0.63	0/1229	0.72	1/1658 (0.1%)
4	Q	0.60	0/1229	0.70	1/1658 (0.1%)
5	E	0.62	0/871	0.71	1/1182 (0.1%)
5	R	0.55	0/871	0.70	1/1182 (0.1%)
6	F	0.63	0/765	0.79	0/1038
6	S	0.60	0/765	0.79	0/1038
7	G	0.80	1/699 (0.1%)	0.84	1/950 (0.1%)
7	T	0.74	0/699	0.84	1/950 (0.1%)
8	H	0.63	0/682	0.69	0/921
8	U	0.60	0/682	0.67	0/921
9	I	0.70	0/611	0.69	0/810
9	V	0.65	0/611	0.67	0/810
10	J	0.66	0/471	0.69	0/636
10	W	0.65	0/471	0.69	0/636
11	K	0.70	0/398	0.75	0/546
11	X	0.60	0/398	0.72	0/546
12	L	0.75	0/399	0.64	0/534
12	Y	0.65	0/399	0.63	0/534
13	M	0.63	0/345	0.70	0/470
13	Z	0.59	0/345	0.70	0/470
All	All	0.66	3/29508 (0.0%)	0.76	20/40114 (0.0%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	31	CYS	CB-SG	-5.89	1.72	1.81
1	N	61	HIS	CG-CD2	5.13	1.44	1.35
1	A	498	CYS	CB-SG	-5.00	1.73	1.81

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	133	GLY	N-CA-C	7.12	130.91	113.10
4	D	133	GLY	N-CA-C	7.06	130.74	113.10
5	E	41	LEU	CA-CB-CG	6.75	130.83	115.30
1	A	480	ARG	NE-CZ-NH2	-6.70	116.95	120.30
2	O	103	GLN	CA-C-N	-6.54	102.80	117.20
5	R	41	LEU	CA-CB-CG	6.50	130.25	115.30
3	C	92	LEU	CA-CB-CG	-6.36	100.68	115.30
2	B	103	GLN	CA-C-N	-6.20	103.55	117.20
3	P	92	LEU	CA-CB-CG	-5.95	101.61	115.30
2	B	104	TRP	N-CA-C	5.67	126.30	111.00
2	B	213	LEU	CA-CB-CG	-5.57	102.48	115.30
1	A	435	GLY	N-CA-C	5.57	127.02	113.10
7	G	11	THR	N-CA-C	5.54	125.96	111.00
7	T	11	THR	N-CA-C	5.49	125.82	111.00
2	O	104	TRP	N-CA-C	5.48	125.80	111.00
2	B	133	LEU	CA-CB-CG	-5.45	102.76	115.30
2	O	133	LEU	CA-CB-CG	-5.17	103.41	115.30
1	N	378	HIS	CA-CB-CG	-5.11	104.91	113.60
1	N	435	GLY	N-CA-C	5.11	125.86	113.10
2	B	188	ARG	NE-CZ-NH2	-5.07	117.77	120.30

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

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	62	0
1	N	4025	0	4002	66	0
2	B	1863	0	1867	48	0
2	O	1863	0	1867	45	0
3	C	2124	0	2044	28	0
3	P	2124	0	2044	28	0
4	D	1195	0	1183	35	0
4	Q	1195	0	1183	39	0
5	E	852	0	845	17	0
5	R	852	0	845	18	0
6	F	748	0	728	15	0
6	S	748	0	728	13	0
7	G	672	0	645	18	0
7	T	672	0	645	16	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	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	X	384	0	366	10	0
12	L	386	0	388	7	0
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	F	1	0	0	0	0
17	S	1	0	0	0	0
18	A	120	0	108	5	0
18	N	120	0	108	4	0
19	A	2	0	0	1	0
19	N	2	0	0	1	0
All	All	28864	0	28444	443	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 (443) 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)
19:A:520:PER:O1	19:A:520:PER:O2	1.69	1.11
19:N:520:PER:O2	19:N:520:PER:O1	1.63	1.11
3:P:2:THR:HG23	6:S:96:LEU:HD12	1.58	0.85
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:85:LEU:O	1:N:492:LEU:HD13	1.86	0.75
1:A:197:LEU:HD12	7:T:4:ALA:HB2	1.69	0.72
1:A:190:ILE:HG12	7:T:6:GLY:HA3	1.71	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
1:A:508:PRO:HG3	3:C:6:HIS:HB3	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:O:111:THR:O	2:O:111:THR:HG22	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
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
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
7:G:1:ALA:HB1	1:N:286:ILE:HG22	1.81	0.63
18:A:515:HEA:HMC1	18:A:515:HEA:HBC1	1.80	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
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	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
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: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:HA	8:H:7:LYS:HE3	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:164:PHE:O	3:P:168:THR:HG23	2.01	0.60
3:P:221:ARG:HE	3:P:226:HIS:HD1	1.48	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
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
1:N:347:LEU:HG	1:N:383:MET:HE2	1.85	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: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
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
5:E:43:PRO:HB2	5:E:48:ILE:HD11	1.86	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
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
3:C:221:ARG:HE	3:C:226:HIS:HD1	1.53	0.55
1:A:36:LEU:HD13	12:L:40:VAL:HG21	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:GLY:HA2	6:F:6:VAL:HG22	1.89	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
9:V:19:PHE:CD1	9:V:19:PHE:C	2.80	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
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:196:CYS:HB2	2:O:207:MET:HG3	1.89	0.54
2:O:58:ALA:O	2:O:62:GLU:HG3	2.07	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:B:193:TYR:HE1	4:D:126:MET:HE1	1.72	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:O	1:A:128:VAL:HG22	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
8:H:60:TYR:C	8:H:60:TYR:CD1	2.81	0.54
2:O:161:HIS:HB2	2:O:174:ALA:HB3	1.90	0.54
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
9:I:19:PHE:C	9:I:19:PHE:CD1	2.82	0.53
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.90	0.53
1:A:310:MET:HE1	2:B:77:ALA:HB2	1.89	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
3:P:1:MET:HB3	6:S:96:LEU:HD11	1.89	0.53
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.90	0.53
1:A:347:LEU:HG	1:A:383:MET:HE2	1.90	0.53
2:O:191:LEU:HB2	4:Q:126:MET:HE1	1.91	0.53
4:D:110:THR:HG22	4:D:115:TRP:CE2	2.44	0.53
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.09	0.53
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.09	0.53
3:P:154:GLY:HA2	6:S:6:VAL:HG22	1.91	0.53
7:T:67:HIS:HD2	7:T:71:HIS:CD2	2.27	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:290:HIS:HD2	1:A:291:HIS:CD2	2.27	0.52
1:A:35:LEU:HD11	1:A:462:LEU:HB2	1.91	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:N:456:MET:HG2	4:Q:96:LEU:HD13	1.91	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
1:A:347:LEU:HG	1:A:383:MET:CE	2.40	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
2:B:226:MET:O	2:B:227:LEU:HB2	2.10	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
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
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
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
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
9:V:19:PHE:HD1	9:V:19:PHE:C	2.15	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
2:B:164:ALA:O	2:B:194:GLY:HA3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:106:PRO:HB2	1:N:107:PRO:HD3	1.94	0.49
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.95	0.49
4:D:24:LEU:HD12	5:E:30:ARG:HA	1.93	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
8:U:60:TYR:CD1	8:U:60:TYR:C	2.86	0.49
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
8:H:52:VAL:HG21	8:U:43:MET:HE1	1.94	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
8:U:49:ASP:O	8:U:52:VAL:HG22	2.13	0.48
9:I:19:PHE:HD1	9:I:19:PHE:C	2.17	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:O	9:I:2:THR:HG23	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
5:R:80:GLU:CD	5:R:80:GLU:H	2.17	0.47
4:D:64:PHE:CE1	5:E:66:ARG:HD2	2.49	0.47
3:C:1:MET:HB3	6:F:96:LEU:HD11	1.96	0.47
8:H:43:MET:HE1	8:U:52:VAL:HG21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:112:GLU:O	4:Q:116:VAL:HG13	2.15	0.47
2:O:191:LEU:HB2	4:Q:126:MET:CE	2.44	0.47
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.96	0.47
1:N:310:MET:CE	2:O:77:ALA:HB2	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
2:O:193:TYR:HE1	4:Q:126:MET:HE1	1.78	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
2:O:162:SER:HB3	2:O:197:SER:C	2.35	0.47
3:P:2:THR:HG23	6:S:96:LEU:CD1	2.40	0.47
1:A:344:PHE:C	1:A:344:PHE:CD1	2.88	0.47
7:T:55:ILE:O	7:T:56:ARG:HD3	2.15	0.47
5:E:40:ASP:O	5:E:41:LEU:HB3	2.15	0.47
5:E:5:HIS:HB3	5:E:6:GLU:H	1.59	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
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
1:N:344:PHE:C	1:N:344:PHE:CD1	2.88	0.46
10:W:50:LEU:HD22	10:W:50:LEU:O	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
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.97	0.46
7:G:2:SER:HB2	1:N:237:PHE:HZ	1.81	0.46
7:G:9:GLY:HA2	7:G:19:LEU:HD11	1.97	0.46
4:Q:107:ILE:HD11	11:X:39:GLU:HG3	1.97	0.46
8:U:39:CYS:C	8:U:53:CYS:SG	2.93	0.46
1:N:476:PHE:HB3	12:Y:15:VAL:CG2	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	18: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
4:D:146:LYS:O	4:D:147:LYS:HG3	2.16	0.46
8:H:39:CYS:C	8:H:53:CYS:SG	2.94	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
1:A:310:MET:CE	2:B:77:ALA:HB2	2.45	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
1:N:347:LEU:HG	1:N:383:MET:HE3	1.98	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
1:N:74:MET:HE3	1:N:74:MET:HB3	1.84	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
4:Q:123:MET:HE2	4:Q:134:PHE:CE2	2.52	0.45
1:A:5:ARG:O	1:A:9:SER:HB2	2.16	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	18:A:515:HEA:HBD1	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	9:V:21:ILE:HD12	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
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:CA	8:H:7:LYS:HE3	2.48	0.44
18:N:515:HEA:HMB1	18:N:515:HEA:H11	1.75	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
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
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
2:B:44:LEU:O	9:I:16:ARG:NH2	2.51	0.43
4:Q:131:ILE:HD12	9:V:47:TYR:CE2	2.52	0.43
4:Q:24:LEU:HB3	5:R:30:ARG:HG2	1.99	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	18: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
7:T:25:LEU:HD23	7:T:25:LEU:HA	1.86	0.43
4:D:126:MET:HG3	4:D:128:VAL:HG23	2.00	0.43
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.54	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
2:B:111:THR:CG2	2:B:111:THR:O	2.63	0.43
1:N:289:ALA:HB1	1:N:297:MET:HE1	2.01	0.43
6:S:30:PRO:HG2	6:S:31:TYR:CD2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HA	10:W:31:LEU:HD23	1.89	0.42
1:A:334:TRP:HH2	2:B:46:LEU:HD13	1.84	0.42
3:C:252:LEU:HA	3:C:252:LEU:HD23	1.86	0.42
8:H:57:ARG:O	8:H:61:LYS:HB2	2.19	0.42
4:Q:5:VAL:O	4:Q:5:VAL:HG13	2.18	0.42
10:W:5:VAL:O	10:W:9:GLN:HG3	2.19	0.42
1:A:289:ALA:HB1	1:A:297:MET:HE1	2.02	0.42
2:O:111:THR:CG2	2:O:111:THR:O	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
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
7:G:7:ASP:CG	7:G:8:HIS:H	2.23	0.42
3:P:252:LEU:HD23	3:P:252:LEU:HA	1.79	0.42
1:N:508:PRO:CG	3:P:6:HIS:HB3	2.47	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
2:B:87:MET:HB3	2:B:87:MET:HE2	1.78	0.42
5:E:80:GLU:H	5:E:80:GLU:CD	2.22	0.42
9:I:21:ILE:HD12	9:I:21:ILE:HA	1.71	0.42
4:Q:118:LYS:HA	11:X:51:LYS:O	2.20	0.42
4:Q:23:PRO:HG3	5:R:70:VAL:HG21	2.00	0.42
3:P:154:GLY:HA2	6:S:6:VAL:CG2	2.49	0.42
3:P:122:HIS:NE2	7:T:45:PRO:HB3	2.35	0.42
12:Y:44:LEU:HA	12:Y:44:LEU:HD12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:102:TYR:CD1	13:Z:35:TYR:CE1	3.05	0.41
1:A:3:ILE:N	1:A:3:ILE:HD12	2.34	0.41
2:B:146:MET:SD	2:B:189:PRO:HB3	2.60	0.41
2:B:191:LEU:HB2	4:D:126:MET:CE	2.50	0.41
18:N:516:HEA:H11	18:N:516:HEA:HMB1	1.90	0.41
18:A:515:HEA:H212	18: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:N	2:O:110:TYR:CD1	2.88	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
3:C:16:TRP:HA	3:C:16:TRP:CE3	2.55	0.41
5:E:12:ASP:HA	5:E:47:ILE:HD11	2.03	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:133:LEU:HD23	2:O:133:LEU:HA	1.81	0.41
2:O:76:ILE:O	2:O:79:PRO:HD2	2.20	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
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.56	0.41
1:A:340:TRP:HZ2	1:A:413:HIS:CD2	2.39	0.41
1:A:61:HIS:HE1	18:A:515:HEA:C4B	2.34	0.41
3:C:173:PHE:CD1	3:C:173:PHE:C	2.94	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
7:G:44:ARG:HA	7:G:45:PRO:HD3	1.81	0.41
4:D:138:TRP:CZ3	11:K:50:PRO:HG2	2.56	0.41
1:N:52:GLN:O	1:N:56:VAL:HG23	2.21	0.41
1:N:310:MET:HE1	2:O:77:ALA:HB2	2.02	0.41
6:F:6:VAL:HA	6:F:7:PRO:HD3	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:175:ILE:HA	2:B:176:PRO:HD3	1.98	0.40
2:B:4:PRO:HB2	11:K:43:SER:HA	2.03	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:N	6:S:54:ASN:ND2	2.69	0.40
3:P:16:TRP:HE3	3:P:16:TRP:HA	1.85	0.40
3:P:173:PHE:CD1	3:P:173:PHE:C	2.94	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
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:274:VAL:O	1:N:278:MET:HG3	2.22	0.40
1:N:54:TYR:O	1:N:57:VAL:HB	2.22	0.40
1:N:449:MET:SD	2:O:5:MET:HG2	2.61	0.40
3:C:2:THR:HG23	6:F:96:LEU:CD1	2.42	0.40
2:B:191:LEU:HB2	4:D:126:MET:HE1	2.03	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%)	20	23
2	O	230/227 (101%)	208 (90%)	20 (9%)	2 (1%)	20	23
3	C	259/261 (99%)	252 (97%)	6 (2%)	1 (0%)	38	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	259/261 (99%)	252 (97%)	6 (2%)	1 (0%)	38	47
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%)	8	6
6	S	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	8	6
7	G	82/84 (98%)	65 (79%)	12 (15%)	5 (6%)	2	0
7	T	82/84 (98%)	66 (80%)	11 (13%)	5 (6%)	2	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%)	10	9
10	W	56/59 (95%)	55 (98%)	0	1 (2%)	10	9
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%)	28	34

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

Continued on next page...

Continued from previous page...

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/427 (100%)	402 (94%)	25 (6%)	23	30
1	N	427/427 (100%)	401 (94%)	26 (6%)	22	29
2	B	216/211 (102%)	193 (89%)	23 (11%)	8	9
2	O	216/211 (102%)	195 (90%)	21 (10%)	9	11
3	C	226/226 (100%)	209 (92%)	17 (8%)	16	19
3	P	226/226 (100%)	208 (92%)	18 (8%)	14	17
4	D	128/129 (99%)	120 (94%)	8 (6%)	21	28
4	Q	128/129 (99%)	120 (94%)	8 (6%)	21	28
5	E	92/95 (97%)	85 (92%)	7 (8%)	15	19
5	R	92/95 (97%)	85 (92%)	7 (8%)	15	19
6	F	81/81 (100%)	71 (88%)	10 (12%)	5	6
6	S	81/81 (100%)	71 (88%)	10 (12%)	5	6
7	G	68/68 (100%)	59 (87%)	9 (13%)	5	5
7	T	68/68 (100%)	58 (85%)	10 (15%)	3	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	71/75 (95%)	65 (92%)	6 (8%)	12	15
8	U	71/75 (95%)	65 (92%)	6 (8%)	12	15
9	I	58/58 (100%)	55 (95%)	3 (5%)	27	36
9	V	58/58 (100%)	55 (95%)	3 (5%)	27	36
10	J	49/50 (98%)	42 (86%)	7 (14%)	4	3
10	W	49/50 (98%)	42 (86%)	7 (14%)	4	3
11	K	39/46 (85%)	37 (95%)	2 (5%)	28	37
11	X	39/46 (85%)	37 (95%)	2 (5%)	28	37
12	L	40/40 (100%)	35 (88%)	5 (12%)	5	5
12	Y	40/40 (100%)	35 (88%)	5 (12%)	5	5
13	M	37/38 (97%)	33 (89%)	4 (11%)	7	8
13	Z	37/38 (97%)	33 (89%)	4 (11%)	7	8
All	All	3064/3088 (99%)	2811 (92%)	253 (8%)	14	16

All (253) 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	109	PHE
1	A	128	VAL
1	A	136	LEU
1	A	150	LEU
1	A	199	LEU
1	A	241	PRO
1	A	295	VAL
1	A	301	THR
1	A	306	THR
1	A	324	LEU
1	A	347	LEU
1	A	353	LEU
1	A	354	THR
1	A	369	ASP
1	A	382	SER
1	A	444	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	467	LEU
1	A	474	GLU
1	A	492	LEU
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	18	LEU
3	C	22	LEU
3	C	33	MET
3	C	38	ASN
3	C	85	LEU
3	C	111	GLU
3	C	112	LEU
3	C	131	LEU
3	C	132	LEU
3	C	137	LEU
3	C	159	MET
3	C	160	LEU
3	C	163	LEU
3	C	196	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	213	THR
3	C	214	PHE
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
6	F	6	VAL
6	F	20	VAL
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	8	HIS
7	G	14	ARG
7	G	36	TRP
7	G	37	LEU
7	G	39	SER
7	G	41	HIS
7	G	54	ARG
7	G	56	ARG
8	H	7	LYS
8	H	11	TYR
8	H	12	GLN
8	H	29	CYS
8	H	44	THR
8	H	60	TYR

Continued on next page...

Continued from previous page...

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
10	J	58	LYS
11	K	43	SER
11	K	45	VAL
12	L	2	HIS
12	L	15	VAL
12	L	22	LEU
12	L	26	THR
12	L	44	LEU
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	109	PHE
1	N	128	VAL
1	N	136	LEU
1	N	138	HIS
1	N	150	LEU
1	N	173	PRO
1	N	199	LEU
1	N	238	PHE
1	N	241	PRO
1	N	295	VAL
1	N	301	THR
1	N	306	THR
1	N	324	LEU
1	N	347	LEU
1	N	353	LEU
1	N	354	THR
1	N	369	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	382	SER
1	N	467	LEU
1	N	474	GLU
1	N	492	LEU
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	134	ARG
2	O	138	VAL
2	O	171	LYS
2	O	185	MET
2	O	202	SER
2	O	216	LEU
3	P	3	HIS
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
3	P	131	LEU
3	P	132	LEU
3	P	137	LEU
3	P	159	MET
3	P	160	LEU
3	P	163	LEU
3	P	196	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	213	THR
3	P	214	PHE
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	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	8	HIS
7	T	14	ARG
7	T	36	TRP
7	T	37	LEU
7	T	39	SER
7	T	41	HIS
7	T	54	ARG
7	T	56	ARG
7	T	78	LEU
8	U	7	LYS
8	U	11	TYR
8	U	12	GLN
8	U	29	CYS
8	U	44	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	U	60	TYR
9	V	8	GLN
9	V	16	ARG
9	V	19	PHE
10	W	4	ARG
10	W	5	VAL
10	W	27	THR
10	W	30	ILE
10	W	47	LEU
10	W	50	LEU
10	W	58	LYS
11	X	43	SER
11	X	45	VAL
12	Y	2	HIS
12	Y	15	VAL
12	Y	22	LEU
12	Y	26	THR
12	Y	44	LEU
13	Z	2	THR
13	Z	24	LEU
13	Z	37	LEU
13	Z	38	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	413	HIS
1	A	503	HIS
3	C	38	ASN
3	C	222	GLN
3	C	230	ASN
6	F	54	ASN
7	G	71	HIS
1	N	55	ASN
1	N	413	HIS
1	N	503	HIS
3	P	38	ASN
3	P	222	GLN
3	P	230	ASN
4	Q	109	HIS
6	S	54	ASN
6	S	98	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	T	71	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 carbohydrates 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	$\# Z > 2$
18	HEA	A	515	1	44,67,67	1.86	10 (22%)	37,103,103	1.51	6 (16%)
18	HEA	A	516	1,19	44,67,67	2.02	9 (20%)	37,103,103	1.43	6 (16%)
19	PER	A	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
18	HEA	N	515	1	44,67,67	1.65	8 (18%)	37,103,103	1.68	7 (18%)
18	HEA	N	516	1,19	44,67,67	1.64	8 (18%)	37,103,103	1.41	5 (13%)
19	PER	N	520	18,14	0,1,1	0.00	-	0,0,0	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
18	HEA	A	515	1	2/2/7/16	0/24/76/76	0/0/8/8
18	HEA	A	516	1,19	2/2/7/16	0/24/76/76	0/0/8/8
19	PER	A	520	18,14	-	0/0/0/0	0/0/0/0
18	HEA	N	515	1	2/2/7/16	0/24/76/76	0/0/8/8
18	HEA	N	516	1,19	2/2/7/16	0/24/76/76	0/0/8/8
19	PER	N	520	18,14	-	0/0/0/0	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C3C-C2C	-4.61	1.34	1.40
18	A	516	HEA	C3A-CMA	-4.23	1.36	1.46
18	A	516	HEA	C3A-C2A	-3.86	1.35	1.40
18	A	515	HEA	C3A-CMA	-3.59	1.38	1.46
18	N	516	HEA	C3A-CMA	-3.53	1.38	1.46
18	A	515	HEA	C3A-C2A	-3.52	1.35	1.40
18	N	515	HEA	C3A-CMA	-2.99	1.39	1.46
18	N	516	HEA	C3C-C2C	-2.80	1.36	1.40
18	N	515	HEA	C3A-C2A	-2.75	1.36	1.40
18	A	515	HEA	C3B-C2B	-2.60	1.32	1.41
18	N	515	HEA	C3C-C2C	-2.56	1.37	1.40
18	N	515	HEA	C20-C19	-2.50	1.45	1.51
18	A	515	HEA	C3C-C2C	-2.09	1.37	1.40
18	A	515	HEA	C1C-NC	2.06	1.40	1.36
18	A	516	HEA	C1B-NB	2.08	1.40	1.36
18	A	516	HEA	C4A-NA	2.11	1.39	1.36
18	A	515	HEA	C4C-NC	2.14	1.40	1.36
18	N	516	HEA	C4A-NA	2.28	1.39	1.36
18	N	516	HEA	C1D-ND	2.33	1.39	1.36
18	A	516	HEA	CMD-C2D	2.56	1.57	1.51
18	N	516	HEA	CAA-C2A	2.58	1.57	1.52
18	A	516	HEA	C1D-ND	2.66	1.39	1.36
18	N	516	HEA	CMD-C2D	2.79	1.57	1.51
18	A	516	HEA	C4D-ND	3.15	1.42	1.36
18	A	515	HEA	C4D-ND	3.17	1.42	1.36
18	N	515	HEA	C1B-NB	3.25	1.43	1.36
18	A	515	HEA	C1D-ND	3.26	1.40	1.36
18	N	515	HEA	C1A-NA	3.76	1.41	1.36
18	N	516	HEA	C1A-NA	3.93	1.41	1.36
18	N	515	HEA	C4A-NA	4.19	1.41	1.36
18	N	515	HEA	C4B-NB	4.73	1.42	1.36
18	A	515	HEA	C1A-NA	4.87	1.42	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	516	HEA	C4B-NB	5.59	1.43	1.36
18	A	515	HEA	C4B-NB	6.56	1.44	1.36
18	A	516	HEA	C4B-NB	8.34	1.46	1.36

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	515	HEA	C13-C14-C15	-5.28	114.41	127.68
18	N	516	HEA	C4B-C3B-C2B	-5.01	103.37	106.87
18	A	515	HEA	C13-C14-C15	-4.86	115.47	127.68
18	A	516	HEA	C4B-C3B-C2B	-4.29	103.87	106.87
18	N	515	HEA	CMB-C2B-C1B	-2.85	124.08	128.46
18	A	515	HEA	C17-C18-C19	-2.78	120.69	127.68
18	N	515	HEA	C17-C18-C19	-2.60	121.15	127.68
18	N	515	HEA	C20-C21-C22	-2.38	103.79	111.97
18	A	516	HEA	CMC-C2C-C1C	-2.38	124.81	128.46
18	N	516	HEA	C20-C19-C18	-2.32	116.34	121.10
18	A	515	HEA	C20-C21-C22	-2.31	104.05	111.97
18	N	516	HEA	C12-C13-C14	-2.22	106.49	112.33
18	A	515	HEA	CMB-C2B-C1B	-2.20	125.08	128.46
18	A	516	HEA	C12-C13-C14	-2.11	106.78	112.33
18	A	515	HEA	C16-C17-C18	-2.10	104.78	111.97
18	N	515	HEA	C16-C15-C14	2.07	125.34	121.10
18	A	515	HEA	C1B-C2B-C3B	2.11	108.46	107.00
18	N	516	HEA	C1B-C2B-C3B	2.40	108.67	107.00
18	N	515	HEA	C3C-C4C-NC	2.57	112.54	109.21
18	A	516	HEA	C3C-C4C-NC	2.67	112.67	109.21
18	A	516	HEA	C27-C19-C20	2.90	120.32	115.29
18	N	515	HEA	C1B-C2B-C3B	3.04	109.11	107.00
18	N	516	HEA	C3C-C4C-NC	3.09	113.20	109.21
18	A	516	HEA	C1B-C2B-C3B	3.16	109.19	107.00

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	N	516	HEA	ND
18	N	516	HEA	NB
18	A	516	HEA	ND
18	A	516	HEA	NB
18	A	515	HEA	ND
18	A	515	HEA	NB
18	N	515	HEA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
18	N	515	HEA	NB

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	5	0
19	A	520	PER	1	0
18	N	515	HEA	3	0
18	N	516	HEA	1	0
19	N	520	PER	1	0

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.