



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 05:41 AM GMT

PDB ID : 1OCR
Title : BOVINE HEART CYTOCHROME C OXIDASE IN THE FULLY REDUCED STATE
Authors : Tsukihara, T.; Yao, M.
Deposited on : 1998-07-07
Resolution : 2.35 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

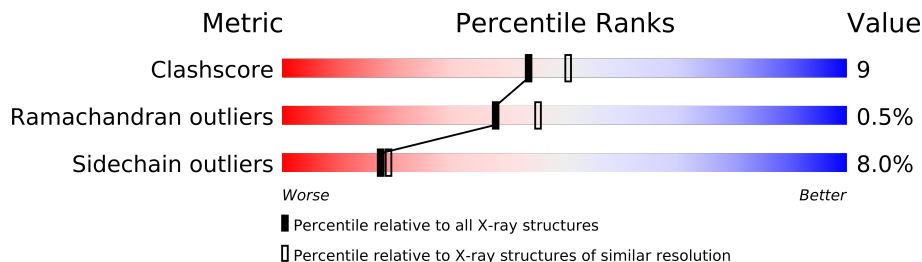
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)







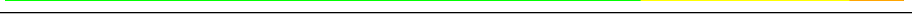

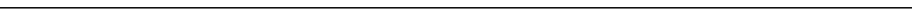
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	
4	D	147	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 28926 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called 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	6	0
			1870	1212	289	351	18			
2	O	227	Total	C	N	O	S	0	6	0
			1870	1212	289	351	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	109	Total	C	N	O	S	0	0	0
			878	558	150	168	2			
5	R	109	Total	C	N	O	S	0	0	0
			878	558	150	168	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	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		

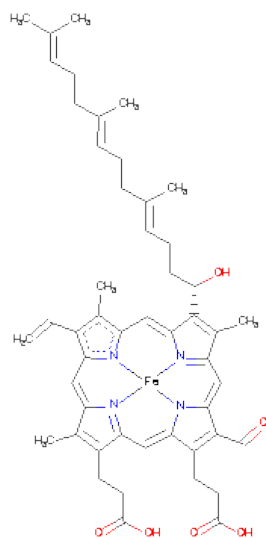
- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- 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	

Continued on next page...

Continued from previous page...

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

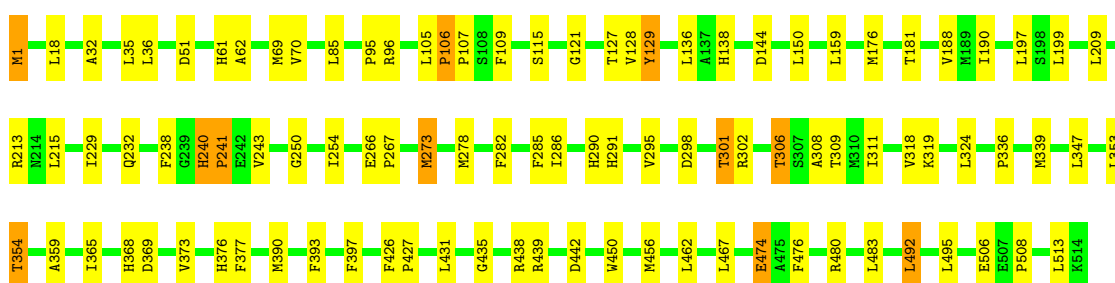
3 Residue-property plots

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

Note EDS was not executed.

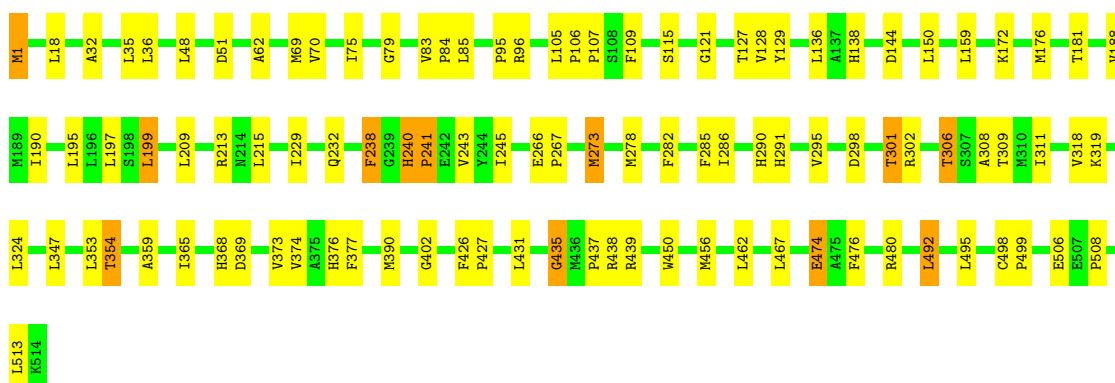
• Molecule 1: CYTOCHROME C OXIDASE

Chain A:



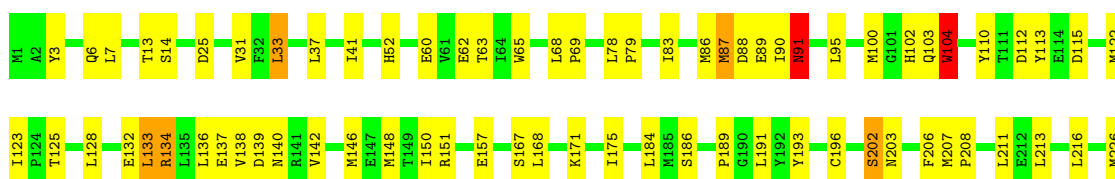
• Molecule 1: CYTOCHROME C OXIDASE

Chain N:



• Molecule 2: CYTOCHROME C OXIDASE

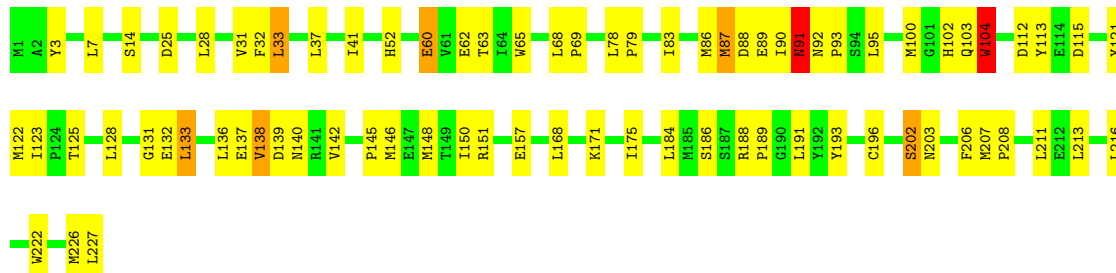
Chain B:



L227

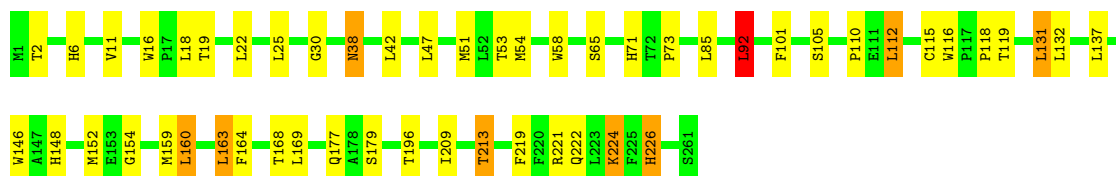
- Molecule 2: CYTOCHROME C OXIDASE

Chain O:



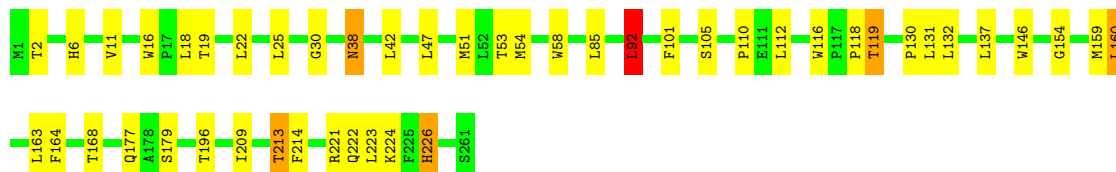
- Molecule 3: CYTOCHROME C OXIDASE

Chain C:



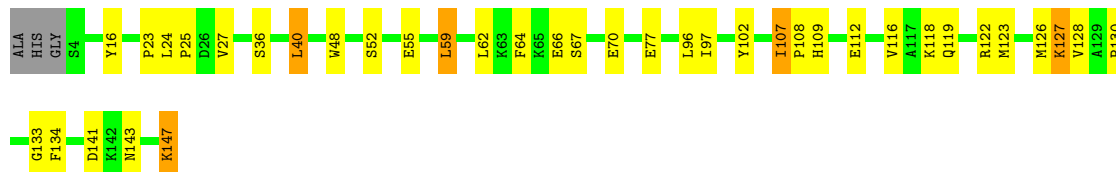
- Molecule 3: CYTOCHROME C OXIDASE

Chain P:



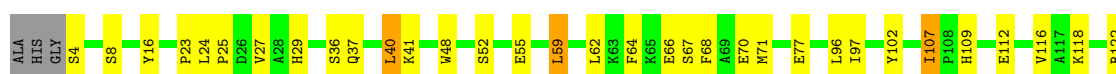
- Molecule 4: CYTOCHROME C OXIDASE

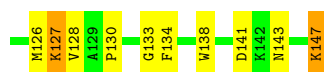
Chain D:



- Molecule 4: CYTOCHROME C OXIDASE

Chain Q:





- Molecule 5: CYTOCHROME C OXIDASE

Chain E:



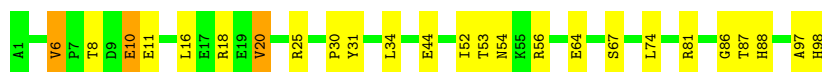
- Molecule 5: CYTOCHROME C OXIDASE

Chain R:



- Molecule 6: CYTOCHROME C OXIDASE

Chain F:



- Molecule 6: CYTOCHROME C OXIDASE

Chain S:



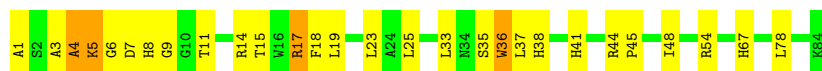
- Molecule 7: CYTOCHROME C OXIDASE

Chain G:



- Molecule 7: CYTOCHROME C OXIDASE

Chain T:



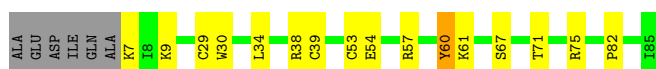
- Molecule 8: CYTOCHROME C OXIDASE

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: A horizontal bar representing the sequence of Chain M. It is divided into three segments: a long green segment (residues 1-28), a long yellow segment (residues 29-41), and a short grey segment (residues 42-47).



● Molecule 13: CYTOCHROME C OXIDASE

Chain Z: A horizontal bar representing the sequence of Chain Z. It is divided into three segments: a long green segment (residues 1-28), a long yellow segment (residues 29-41), and a short grey segment (residues 42-47).



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 – 2.35	Depositor
% Data completeness (in resolution range)	89.8 (15.00-2.35)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, R_{free}	0.203 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28926	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, ZN, CU, HEA

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	0.70	0/4164	0.79	2/5688 (0.0%)
1	N	0.62	0/4164	0.77	1/5688 (0.0%)
2	B	0.71	1/1917 (0.1%)	0.92	4/2612 (0.2%)
2	O	0.66	1/1917 (0.1%)	0.91	3/2612 (0.1%)
3	C	0.67	0/2211	0.70	1/3023 (0.0%)
3	P	0.61	0/2211	0.70	1/3023 (0.0%)
4	D	0.62	0/1229	0.69	1/1658 (0.1%)
4	Q	0.59	0/1229	0.67	1/1658 (0.1%)
5	E	0.63	0/898	0.69	0/1218
5	R	0.57	0/898	0.69	0/1218
6	F	0.65	0/765	0.84	0/1038
6	S	0.63	0/765	0.83	0/1038
7	G	0.65	0/699	0.82	0/950
7	T	0.62	0/699	0.82	0/950
8	H	0.64	0/682	0.73	0/921
8	U	0.59	0/682	0.72	0/921
9	I	0.73	0/611	0.73	0/810
9	V	0.71	0/611	0.72	0/810
10	J	0.65	0/471	0.70	0/636
10	W	0.63	0/471	0.70	0/636
11	K	0.71	0/398	0.73	0/546
11	X	0.60	0/398	0.71	0/546
12	L	0.70	0/399	0.67	0/534
12	Y	0.64	0/399	0.65	0/534
13	M	0.59	0/345	0.69	0/470
13	Z	0.56	0/345	0.71	0/470
All	All	0.65	2/29578 (0.0%)	0.77	14/40208 (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	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	87	MET	C-N	-7.75	1.16	1.34
2	O	87	MET	C-N	-7.37	1.17	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	92	LEU	CA-CB-CG	-7.07	99.05	115.30
4	Q	133	GLY	N-CA-C	6.96	130.50	113.10
4	D	133	GLY	N-CA-C	6.94	130.46	113.10
3	P	92	LEU	CA-CB-CG	-6.72	99.85	115.30
2	B	133	LEU	CA-CB-CG	-5.86	101.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
2	B	110	TYR	Sidechain
1	N	240	HIS	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4025	0	4002	67	0
1	N	4025	0	4002	74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1870	0	1872	52	0
2	O	1870	0	1872	52	0
3	C	2124	0	2044	37	0
3	P	2124	0	2044	33	0
4	D	1195	0	1183	31	0
4	Q	1195	0	1183	35	0
5	E	878	0	868	13	0
5	R	878	0	868	16	0
6	F	748	0	728	17	0
6	S	748	0	728	17	0
7	G	672	0	645	19	0
7	T	672	0	645	23	0
8	H	662	0	623	11	0
8	U	662	0	625	11	0
9	I	598	0	612	8	0
9	V	598	0	612	14	0
10	J	460	0	459	8	0
10	W	460	0	459	8	0
11	K	384	0	366	11	0
11	X	384	0	366	13	0
12	L	386	0	388	8	0
12	Y	386	0	388	10	0
13	M	335	0	352	8	0
13	Z	335	0	352	10	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	12	0
18	N	120	0	108	10	0
All	All	28926	0	28502	500	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 500 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:S:10:GLU:HG2	6:S:25:ARG:HH22	1.30	0.94
6:F:10:GLU:HG2	6:F:25:ARG:HH22	1.30	0.94
3:C:101:PHE:HD1	3:C:196:THR:HG21	1.43	0.84
2:B:78:LEU:HB2	2:B:79:PRO:HD3	1.60	0.83
2:O:78:LEU:HB2	2:O:79:PRO:HD3	1.62	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	491 (96%)	21 (4%)	0	100	100
1	N	512/514 (100%)	492 (96%)	20 (4%)	0	100	100
2	B	231/227 (102%)	208 (90%)	20 (9%)	3 (1%)	18	17
2	O	231/227 (102%)	207 (90%)	21 (9%)	3 (1%)	18	17
3	C	259/261 (99%)	252 (97%)	6 (2%)	1 (0%)	43	52
3	P	259/261 (99%)	252 (97%)	6 (2%)	1 (0%)	43	52
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	135 (95%)	7 (5%)	0	100	100
5	E	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
5	R	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	22	24
6	S	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	22	24
7	G	82/84 (98%)	67 (82%)	11 (13%)	4 (5%)	3	1
7	T	82/84 (98%)	67 (82%)	11 (13%)	4 (5%)	3	1
8	H	77/85 (91%)	73 (95%)	4 (5%)	0	100	100
8	U	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
9	I	71/73 (97%)	65 (92%)	6 (8%)	0	100	100
9	V	71/73 (97%)	65 (92%)	6 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
10	W	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	13	10
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	45/47 (96%)	42 (93%)	3 (7%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	2 (4%)	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	3532/3612 (98%)	3338 (94%)	175 (5%)	19 (0%)	38	45

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	91[A]	ASN
2	B	91[B]	ASN
7	G	4	ALA
2	O	91[A]	ASN
2	O	91[B]	ASN

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%)	397 (93%)	30 (7%)	21	23
1	N	427/427 (100%)	398 (93%)	29 (7%)	22	25
2	B	217/211 (103%)	202 (93%)	15 (7%)	22	24
2	O	217/211 (103%)	202 (93%)	15 (7%)	22	24
3	C	226/226 (100%)	208 (92%)	18 (8%)	17	19
3	P	226/226 (100%)	207 (92%)	19 (8%)	16	17
4	D	128/129 (99%)	116 (91%)	12 (9%)	13	12
4	Q	128/129 (99%)	117 (91%)	11 (9%)	15	16
5	E	95/95 (100%)	92 (97%)	3 (3%)	51	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	95/95 (100%)	92 (97%)	3 (3%)	51	67
6	F	81/81 (100%)	73 (90%)	8 (10%)	11	11
6	S	81/81 (100%)	72 (89%)	9 (11%)	9	9
7	G	68/68 (100%)	57 (84%)	11 (16%)	3	2
7	T	68/68 (100%)	57 (84%)	11 (16%)	3	2
8	H	71/75 (95%)	66 (93%)	5 (7%)	21	23
8	U	71/75 (95%)	66 (93%)	5 (7%)	21	23
9	I	58/58 (100%)	55 (95%)	3 (5%)	32	40
9	V	58/58 (100%)	55 (95%)	3 (5%)	32	40
10	J	49/50 (98%)	43 (88%)	6 (12%)	7	6
10	W	49/50 (98%)	43 (88%)	6 (12%)	7	6
11	K	39/46 (85%)	35 (90%)	4 (10%)	10	10
11	X	39/46 (85%)	35 (90%)	4 (10%)	10	10
12	L	40/40 (100%)	33 (82%)	7 (18%)	3	2
12	Y	40/40 (100%)	33 (82%)	7 (18%)	3	2
13	M	37/38 (97%)	35 (95%)	2 (5%)	31	38
13	Z	37/38 (97%)	35 (95%)	2 (5%)	31	38
All	All	3072/3088 (100%)	2824 (92%)	248 (8%)	17	18

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	45	VAL
1	N	273	MET
10	W	4	ARG
12	L	9	LYS
1	N	18	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	36	HIS
2	O	203	ASN
7	T	51	HIS
7	G	51	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	71	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	67,67,67	1.79	11 (16%)	80,103,103	2.09	25 (31%)
18	HEA	A	516	1	67,67,67	1.81	13 (19%)	80,103,103	1.72	19 (23%)
18	HEA	N	515	1	67,67,67	1.76	11 (16%)	80,103,103	2.05	23 (28%)
18	HEA	N	516	1	67,67,67	1.57	7 (10%)	80,103,103	1.64	21 (26%)

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	-	0/30/76/76	0/0/8/8
18	HEA	A	516	1	-	0/30/76/76	0/0/8/8
18	HEA	N	515	1	-	0/30/76/76	0/0/8/8
18	HEA	N	516	1	-	0/30/76/76	0/0/8/8

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	515	HEA	C1B-C2B	8.24	1.50	1.40
18	N	515	HEA	C1B-C2B	6.62	1.48	1.40
18	N	515	HEA	C3B-C11	-5.86	1.46	1.52
18	A	515	HEA	C3B-C11	-5.49	1.47	1.52
18	A	516	HEA	C3C-C4C	4.98	1.48	1.40

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	C4B-C3B-C11	5.69	134.94	124.67
18	A	515	HEA	C13-C14-C15	-5.64	115.63	127.80
18	N	515	HEA	C13-C14-C15	-5.47	115.99	127.80
18	N	515	HEA	C4B-C3B-C11	5.34	134.30	124.67
18	A	516	HEA	C2D-C1D-ND	4.76	113.00	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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