



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 05:46 pm GMT

PDB ID : 4D6T
Title : Cytochrome bc1 bound to the 4(1H)-pyridone GW844520
Authors : Capper, M.J.; O'Neill, P.M.; Fisher, N.; Strange, R.W.; Moss, D.; Ward, S.A.;
Berry, N.G.; Lawrenson, A.S.; Hasnain, S.S.; Biagini, G.A.; Antonyuk, S.V.
Deposited on : 2014-11-14
Resolution : 3.57 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

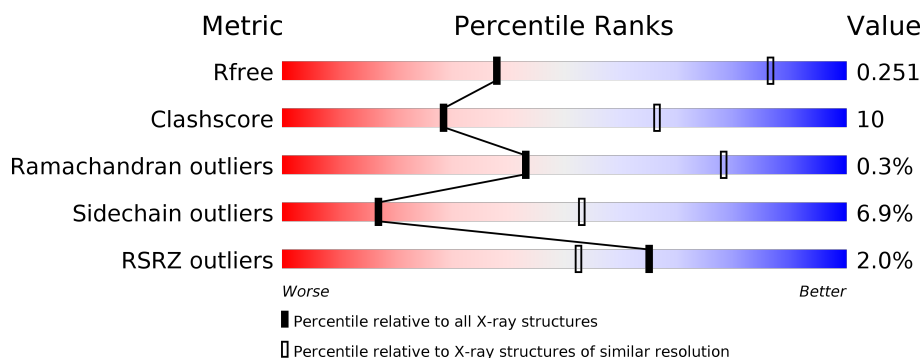
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 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))
R_{free}	111664	1163 (3.70-3.46)
Clashscore	122126	1004 (3.66-3.50)
Ramachandran outliers	120053	1011 (3.68-3.48)
Sidechain outliers	120020	1011 (3.68-3.48)
RSRZ outliers	108989	1072 (3.70-3.46)

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.

Mol	Chain	Length	Quality of chain
1	A	480	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 8%</div> </div> </div>
1	N	480	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>•• 8%</div> </div> </div>
2	B	453	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 7%</div> </div> </div>
3	C	379	<div> <div></div> <div> <div></div> <div>75%</div> <div>19%</div> <div>••</div> </div> </div>
3	P	379	<div> <div></div> <div> <div></div> <div>77%</div> <div>17%</div> <div>••</div> </div> </div>
4	D	265	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>• 9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	Q	265	
5	E	274	
5	I	274	
5	R	274	
6	F	111	
6	S	111	
7	G	82	
7	T	82	
8	H	91	
8	U	91	
9	J	64	
9	W	64	
10	O	453	
11	V	274	

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
14	PO4	F	501	-	-	-	X
14	PO4	N	501	-	-	-	X
14	PO4	S	501	-	-	-	X
15	PEE	C	505	X	-	-	-
15	PEE	D	506	X	-	-	-
15	PEE	P	505	X	-	-	-
15	PEE	Q	506	X	-	-	-
18	FES	R	501	-	-	X	-
19	GOL	R	502	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 31051 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 B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3439	2148	607	664	20			
1	N	444	Total	C	N	O	S	0	0	0
			3432	2142	607	663	20			

- Molecule 2 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	0	0
			3164	1988	561	608	7			

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	374	Total	C	N	O	S	0	0	0
			2968	1993	463	494	18			
3	P	370	Total	C	N	O	S	0	0	0
			2936	1973	456	489	18			

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	240	Total	C	N	O	S	0	0	0
			1912	1222	329	346	15			
4	Q	241	Total	C	N	O	S	0	0	0
			1918	1225	330	348	15			

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	73	Total	C	N	O	S	0	0	0
			549	341	92	114	2			
5	I	21	Total	C	N	O	S	0	0	0
			157	97	31	28	1			
5	R	196	Total	C	N	O	S	0	0	0
			1518	957	263	290	8			

- Molecule 6 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			860	547	154	157	2			
6	S	99	Total	C	N	O	S	0	0	0
			869	553	156	158	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	conflict	UNP P00129
S	56	ASP	ASN	conflict	UNP P00129

- Molecule 7 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	S	0	0	0
			677	439	127	110	1			
7	T	74	Total	C	N	O	S	0	0	0
			624	408	117	98	1			

- Molecule 8 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	65	Total	C	N	O	S	0	0	0
			529	321	96	107	5			
8	U	66	Total	C	N	O	S	0	0	0
			538	327	98	108	5			

- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	58	Total	C	N	O	0	0	0
			482	317	83	82			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	W	59	Total	C	N	O	0	0	0
			487	320	84	83			

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	419	Total	C	N	O	S	0	0	0
			3140	1972	555	606	7			

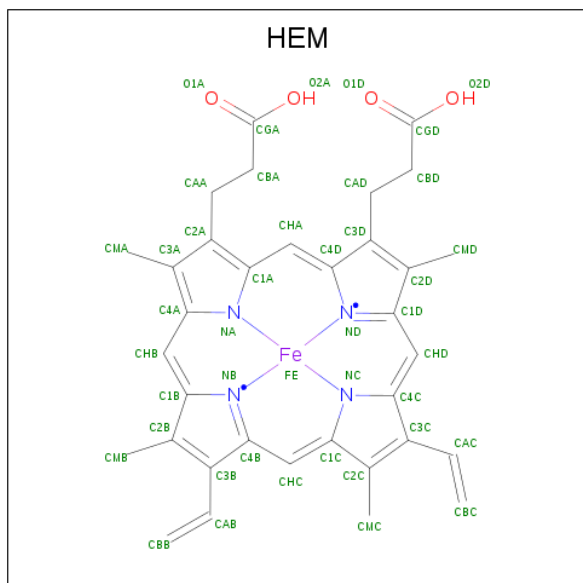
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	305	GLU	GLN	conflict	UNP P23004

- Molecule 11 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

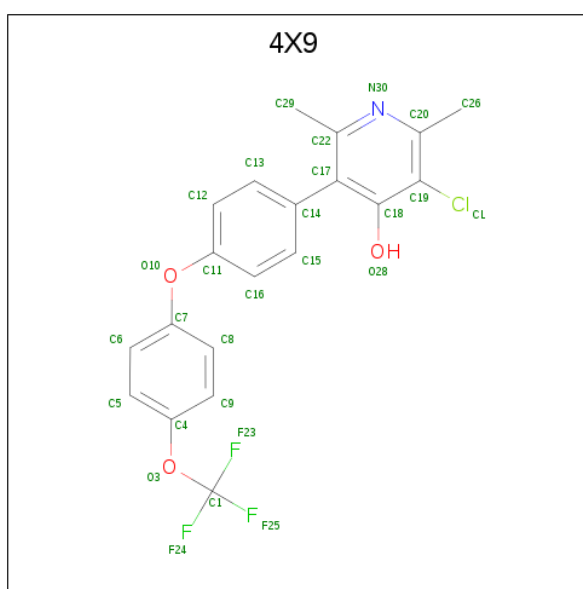
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	V	17	Total	C	N	O	0	0	0
			127	81	24	22			

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



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

- Molecule 13 is 3-chloro-2,6-dimethyl-5-{4-[4-(trifluoromethoxy)phenoxy]phenyl}pyridin-4-ol (three-letter code: 4X9) (formula: $C_{20}H_{15}ClF_3NO_3$).



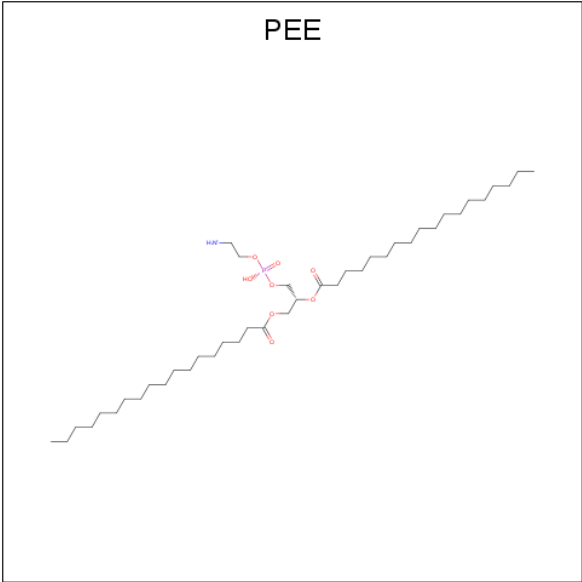
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
13	C	1	Total 28	C 20	Cl 1	F 3	N 1	O 3	0	0
13	P	1	Total 28	C 20	Cl 1	F 3	N 1	O 3	0	0

- Molecule 14 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



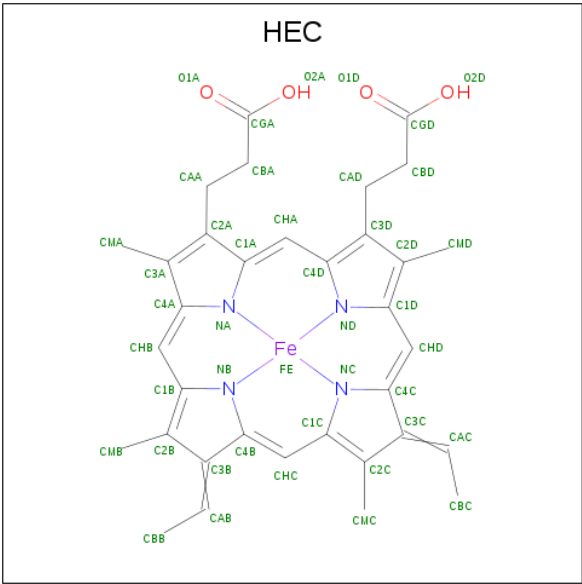
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	O	P	0	0
			5	4	1		
14	D	1	Total	O	P	0	0
			5	4	1		
14	D	1	Total	O	P	0	0
			5	4	1		
14	D	1	Total	O	P	0	0
			5	4	1		
14	E	1	Total	O	P	0	0
			5	4	1		
14	F	1	Total	O	P	0	0
			5	4	1		
14	N	1	Total	O	P	0	0
			5	4	1		
14	N	1	Total	O	P	0	0
			5	4	1		
14	Q	1	Total	O	P	0	0
			5	4	1		
14	Q	1	Total	O	P	0	0
			5	4	1		
14	S	1	Total	O	P	0	0
			5	4	1		

- Molecule 15 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₈₃NO₈P).



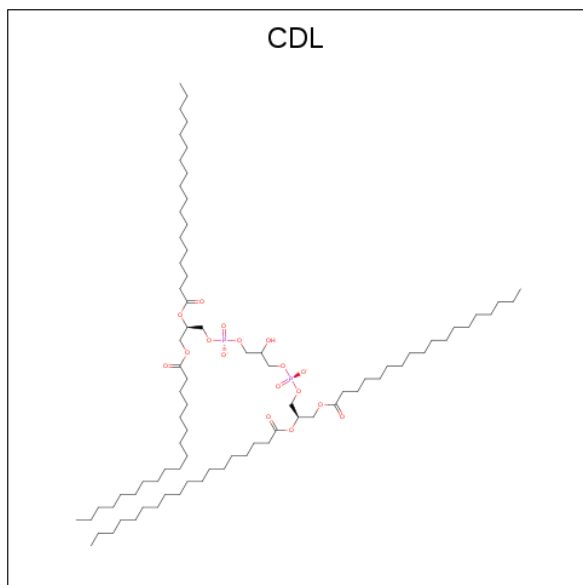
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	D	1	Total	C	N	O	P	0	0
			26	16	1	8	1		
15	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	Q	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 16 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



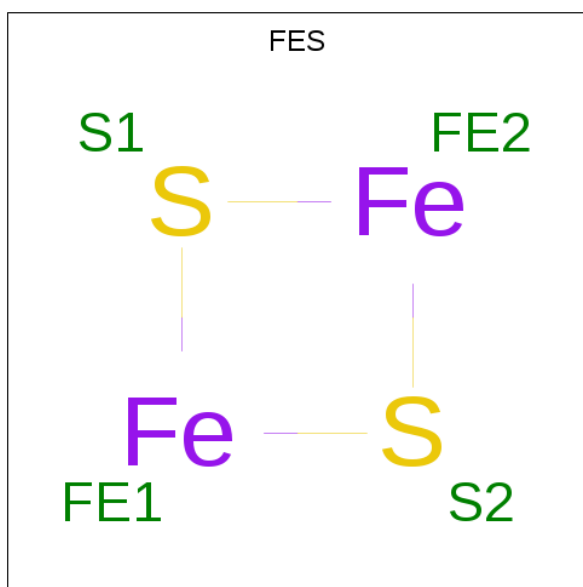
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
16	Q	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 17 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



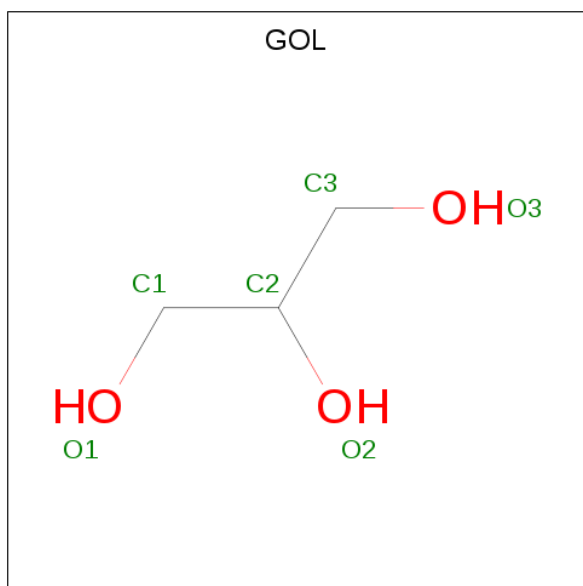
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	O	P		
			39	24	13	2	0	0
17	G	1	Total	C	O	P		
			44	25	17	2	0	0
17	Q	1	Total	C	O	P		
			39	24	13	2	0	0
17	T	1	Total	C	O	P		
			49	30	17	2	0	0

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 19 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

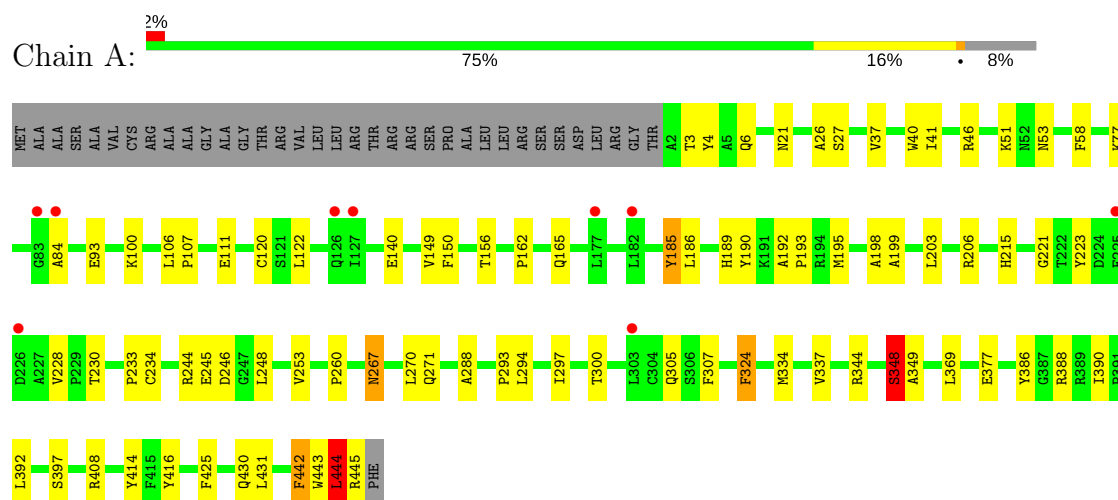


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	R	1	Total	C	O	0	0
			6	3	3		

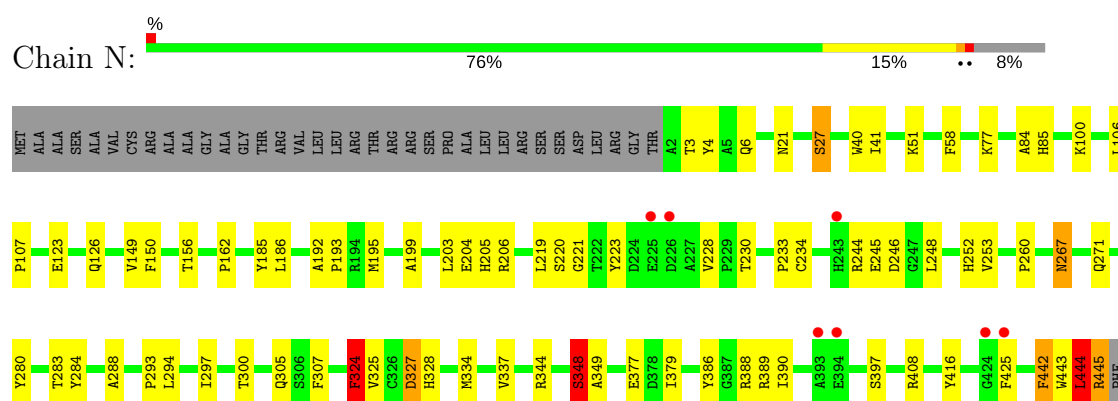
3 Residue-property plots

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.

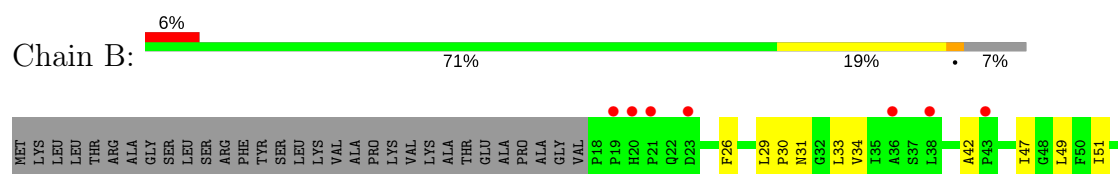
• Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

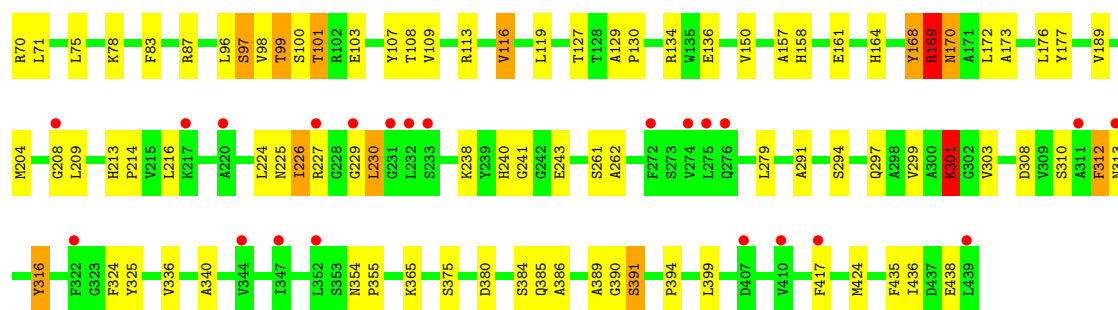


• Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

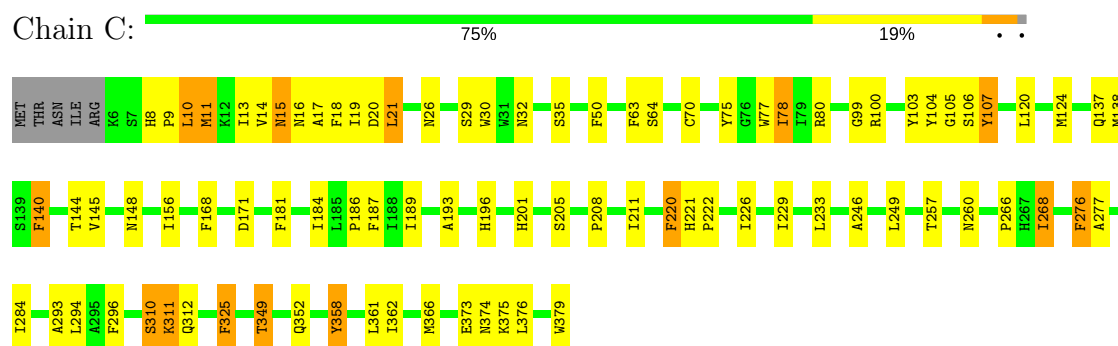


• Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

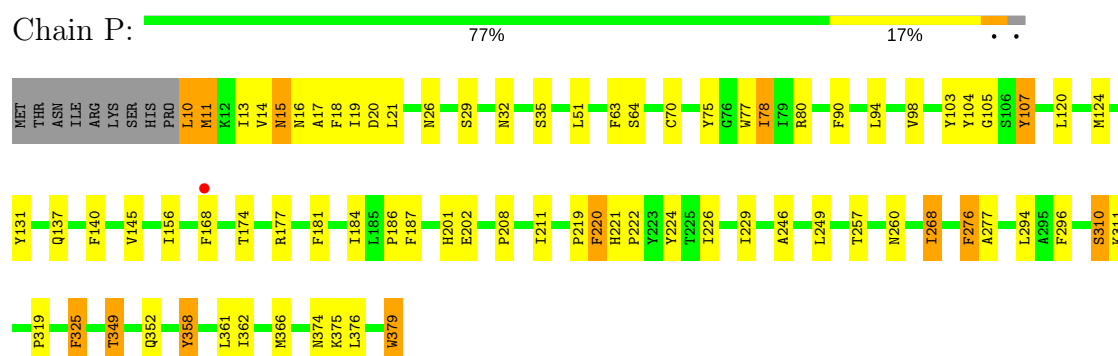




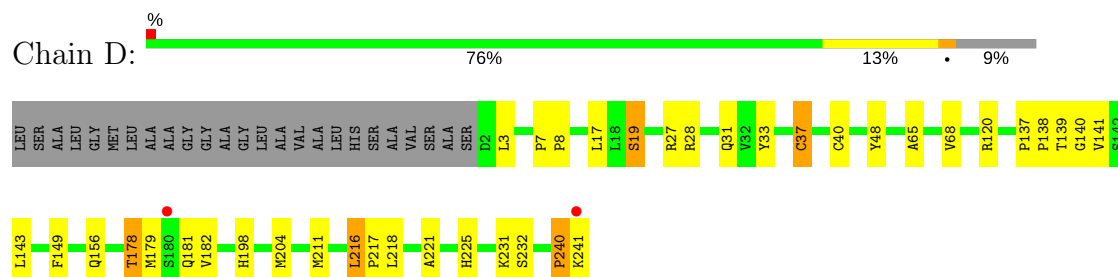
• Molecule 3: CYTOCHROME B



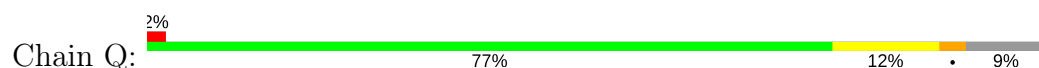
• Molecule 3: CYTOCHROME B

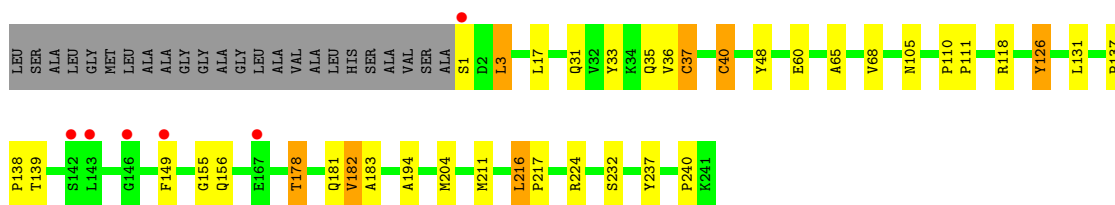


• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

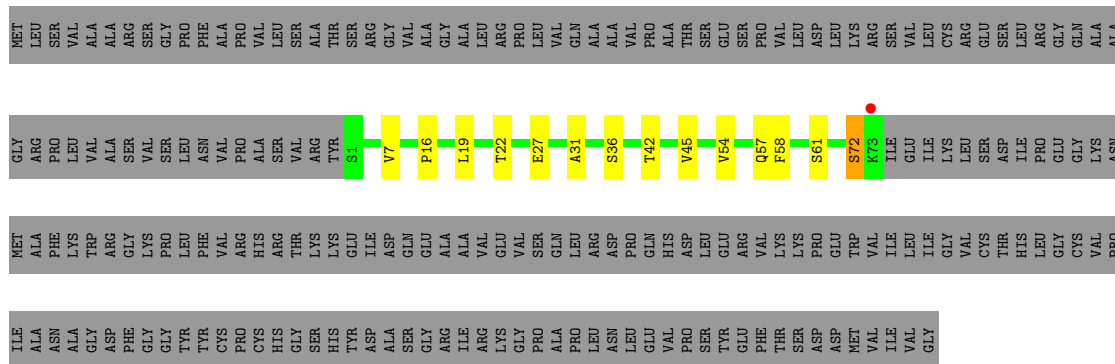


• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

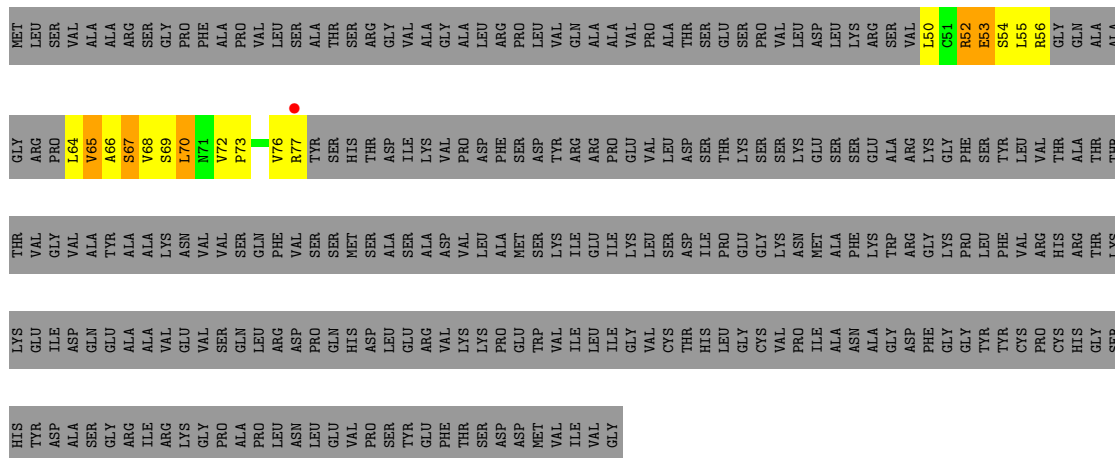




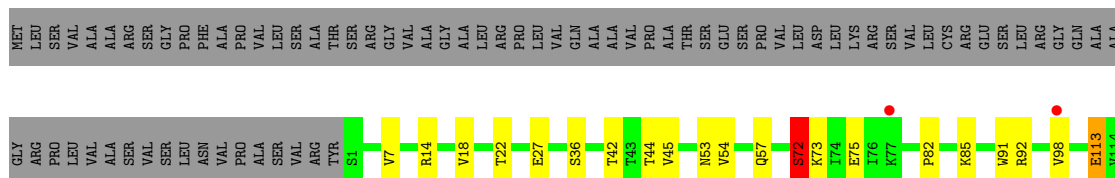
- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

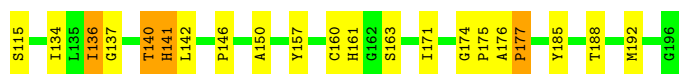


- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

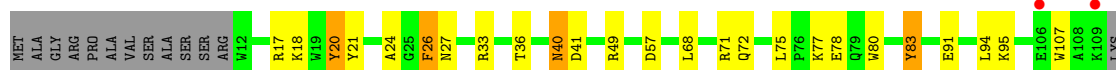


- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL





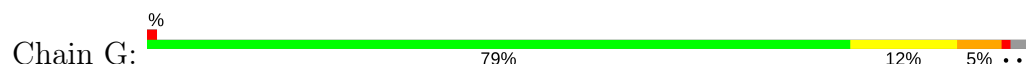
• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7



• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7



• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8



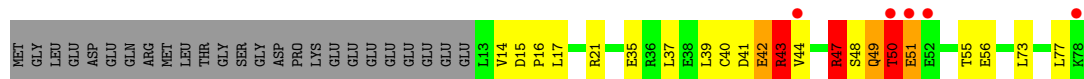
• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8



• Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL



• Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL



• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9



MET	VAL
A2	
P3	
T4	
L5	
L13	
F20	
I24	
A28	
F35	
D36	
Q37	
K58	
Y59	
E60	
ASN	
LYS	
GLU	

G352	A185	R70	NET
V303	A166	L71	LYS
H304	A167		LEU
E305	Y168	S74	LEU
	R169	L75	THR
V309	R170		ARG
S310	A171	K78	ALA
A311	L172		GLY
N312	A173	F83	SER
N313		K84	LEU
Y316	L176	R85	SER
		T86	ARG
F324	I183	R87	PHE
Y325	V189	G88	TYR
T326		R89	SER
	F199	E90	LEU
V336			LYS
	G208	K95	VAL
A340	L209	L96	ALA
		S97	PRO
N354	H213	V98	LYS
P355	P214	T99	VAL
	Y215	S100	LYS
S375	L216	T101	ALA
			THR
Q385	L224	Y107	GLU
A386	N225	T108	ALA
	T226	V109	PRO
A389	R227		ALA
G390	G228	R113	GLY
S391	G229	V116	VAL
	L230		PRO
D407	G231	L119	PRO
	L232		HIS
F417	S233	F122	P21
	G234	L123	
M424		L124	F26
F435	K238	M125	L29
I436	V239	V126	P30
D437	H240	T127	N31
A438	G241	T128	G32
L439	G242	A129	L33
	E243	P130	V34
	T244		
		R134	S37
	S261	M135	
	A262	E136	Y41
			A42
	L279	L144	
	A291	V150	I47
		A151	G48
	S294		L49
		A157	F50
	Q297	H158	I51
	V299	E161	E58
	A300		
A303		H164	L63

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	129.90Å 129.90Å 722.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.57 49.81 – 3.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.57) 99.9 (49.81-3.57)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.206 , 0.252 0.207 , 0.251	Depositor DCC
R_{free} test set	3953 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	122.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 79.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31051	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CDL, PO4, FES, 4X9, HEC, HEM, PEE

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	0.46	1/3511 (0.0%)	0.69	5/4766 (0.1%)
1	N	0.42	0/3503	0.70	7/4755 (0.1%)
2	B	0.69	3/3224 (0.1%)	0.80	10/4375 (0.2%)
3	C	0.50	0/3065	0.68	0/4196
3	P	0.48	1/3031 (0.0%)	0.67	0/4150
4	D	0.42	0/1971	0.62	0/2676
4	Q	0.42	0/1977	0.61	0/2684
5	E	0.41	0/557	0.62	0/752
5	I	0.57	0/156	1.24	2/209 (1.0%)
5	R	0.43	0/1552	0.78	7/2100 (0.3%)
6	F	0.46	0/879	0.68	0/1180
6	S	0.47	0/888	0.65	0/1191
7	G	0.52	1/699 (0.1%)	1.26	6/946 (0.6%)
7	T	0.49	0/645	0.74	0/873
8	H	2.11	7/534 (1.3%)	1.96	8/718 (1.1%)
8	U	1.48	6/543 (1.1%)	2.09	10/729 (1.4%)
9	J	0.42	0/495	0.59	0/667
9	W	0.43	0/500	0.60	0/675
10	O	0.50	2/3197 (0.1%)	0.95	12/4336 (0.3%)
11	V	0.58	0/129	0.86	0/177
All	All	0.59	21/31056 (0.1%)	0.82	67/42155 (0.2%)

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	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	H	0	1
8	U	0	3
10	O	0	2
All	All	0	11

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	169	ARG	CZ-NH2	28.39	1.70	1.33
8	H	43	ARG	CZ-NH1	26.86	1.68	1.33
8	H	47	ARG	CZ-NH2	25.79	1.66	1.33
8	U	47	ARG	CZ-NH2	25.71	1.66	1.33
8	H	43	ARG	NE-CZ	23.73	1.64	1.33

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	47	ARG	NE-CZ-NH2	-37.30	101.65	120.30
8	H	47	ARG	NE-CZ-NH2	33.38	136.99	120.30
7	G	75	ALA	N-CA-CB	-19.29	83.10	110.10
8	U	43	ARG	NH1-CZ-NH2	-18.82	98.69	119.40
10	O	169	ARG	NH1-CZ-NH2	-17.91	99.70	119.40

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	444	LEU	Peptide
2	B	169	ARG	Sidechain
2	B	301	LYS	Peptide
7	G	77	TYR	Peptide
8	H	50	THR	Peptide

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	3439	0	3337	45	0
1	N	3432	0	3330	42	0
2	B	3164	0	3144	80	0
3	C	2968	0	3028	82	0
3	P	2936	0	2996	71	0
4	D	1912	0	1861	42	0
4	Q	1918	0	1870	38	0
5	E	549	0	547	9	0
5	I	157	0	171	27	0
5	R	1518	0	1504	27	0
6	F	860	0	849	24	1
6	S	869	0	862	24	0
7	G	677	0	672	9	0
7	T	624	0	630	8	0
8	H	529	0	512	45	0
8	U	538	0	522	23	1
9	J	482	0	483	8	0
9	W	487	0	487	9	0
10	O	3140	0	3121	104	0
11	V	127	0	135	40	0
12	C	86	0	60	10	0
12	P	86	0	60	10	0
13	C	28	0	14	6	0
13	P	28	0	14	5	0
14	C	5	0	0	0	0
14	D	15	0	0	0	0
14	E	5	0	0	0	0
14	F	5	0	0	0	0
14	N	10	0	0	0	0
14	Q	10	0	0	0	0
14	S	5	0	0	0	0
15	C	49	0	72	1	0
15	D	26	0	26	0	0
15	P	49	0	72	1	0
15	Q	51	0	82	3	0
16	D	43	0	32	12	0
16	Q	43	0	32	10	0
17	D	39	0	39	0	0
17	G	44	0	32	0	0
17	Q	39	0	39	1	0
17	T	49	0	42	1	0
18	R	4	0	0	3	0
19	R	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31051	0	30685	645	1

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 10.

The worst 5 of 645 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)
8:H:43:ARG:NH1	8:H:43:ARG:CZ	1.68	1.56
2:B:169:ARG:NH2	2:B:169:ARG:CZ	1.70	1.49
8:H:47:ARG:CD	8:H:50:THR:HG21	1.35	1.44
8:H:47:ARG:CD	8:H:50:THR:CG2	2.07	1.32
8:H:47:ARG:HD2	8:H:50:THR:CG2	1.62	1.28

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:57:ASP:OD2	8:U:42:GLU:OE2[1_655]	1.73	0.47

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	442/480 (92%)	405 (92%)	35 (8%)	2 (0%)	31	71
1	N	442/480 (92%)	407 (92%)	33 (8%)	2 (0%)	31	71
2	B	420/453 (93%)	375 (89%)	44 (10%)	1 (0%)	49	83
3	C	372/379 (98%)	347 (93%)	23 (6%)	2 (0%)	31	71
3	P	368/379 (97%)	337 (92%)	30 (8%)	1 (0%)	43	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	238/265 (90%)	216 (91%)	21 (9%)	1 (0%)	36	75
4	Q	239/265 (90%)	218 (91%)	20 (8%)	1 (0%)	36	75
5	E	71/274 (26%)	64 (90%)	7 (10%)	0	100	100
5	I	17/274 (6%)	12 (71%)	5 (29%)	0	100	100
5	R	194/274 (71%)	174 (90%)	19 (10%)	1 (0%)	31	71
6	F	96/111 (86%)	87 (91%)	9 (9%)	0	100	100
6	S	97/111 (87%)	89 (92%)	8 (8%)	0	100	100
7	G	78/82 (95%)	67 (86%)	10 (13%)	1 (1%)	13	54
7	T	72/82 (88%)	62 (86%)	10 (14%)	0	100	100
8	H	63/91 (69%)	59 (94%)	4 (6%)	0	100	100
8	U	64/91 (70%)	61 (95%)	3 (5%)	0	100	100
9	J	56/64 (88%)	51 (91%)	5 (9%)	0	100	100
9	W	57/64 (89%)	51 (90%)	6 (10%)	0	100	100
10	O	417/453 (92%)	376 (90%)	41 (10%)	0	100	100
11	V	15/274 (6%)	12 (80%)	3 (20%)	0	100	100
All	All	3818/4946 (77%)	3470 (91%)	336 (9%)	12 (0%)	43	78

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	N	267	ASN
3	P	107	TYR
5	R	177	PRO
3	C	107	TYR

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	368/394 (93%)	350 (95%)	18 (5%)	27	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	367/394 (93%)	347 (95%)	20 (5%)	24	61
2	B	331/355 (93%)	309 (93%)	22 (7%)	18	55
3	C	322/327 (98%)	301 (94%)	21 (6%)	19	55
3	P	318/327 (97%)	297 (93%)	21 (7%)	18	55
4	D	205/218 (94%)	196 (96%)	9 (4%)	31	68
4	Q	206/218 (94%)	196 (95%)	10 (5%)	27	64
5	E	63/228 (28%)	57 (90%)	6 (10%)	9	41
5	I	19/228 (8%)	13 (68%)	6 (32%)	0	3
5	R	168/228 (74%)	158 (94%)	10 (6%)	21	58
6	F	90/99 (91%)	82 (91%)	8 (9%)	11	43
6	S	91/99 (92%)	84 (92%)	7 (8%)	14	48
7	G	71/72 (99%)	64 (90%)	7 (10%)	8	39
7	T	66/72 (92%)	59 (89%)	7 (11%)	7	36
8	H	62/85 (73%)	54 (87%)	8 (13%)	5	27
8	U	63/85 (74%)	56 (89%)	7 (11%)	7	35
9	J	49/54 (91%)	45 (92%)	4 (8%)	12	46
9	W	49/54 (91%)	44 (90%)	5 (10%)	8	37
10	O	328/355 (92%)	304 (93%)	24 (7%)	15	51
11	V	15/228 (7%)	12 (80%)	3 (20%)	1	10
All	All	3251/4120 (79%)	3028 (93%)	223 (7%)	17	53

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	54	SER
1	N	397	SER
7	T	59	TYR
5	I	67	SER
1	N	156	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	8	HIS

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Mol	Chain	Res	Type
7	G	73	ASN
3	P	16	ASN
3	C	16	ASN
1	A	271	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

29 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	HEM	C	501	3	27,50,50	1.16	2 (7%)	17,82,82	1.57	1 (5%)
12	HEM	C	502	3	27,50,50	0.99	2 (7%)	17,82,82	1.17	1 (5%)
13	4X9	C	503	-	30,30,30	3.01	7 (23%)	41,44,44	1.21	2 (4%)
14	PO4	C	504	-	4,4,4	0.88	0	6,6,6	0.37	0
15	PEE	C	505	-	48,48,50	0.99	2 (4%)	51,53,55	0.97	4 (7%)
16	HEC	D	501	4	26,50,50	2.43	11 (42%)	18,82,82	3.12	9 (50%)
14	PO4	D	502	-	4,4,4	0.63	0	6,6,6	0.55	0
14	PO4	D	503	-	4,4,4	0.76	0	6,6,6	0.58	0
14	PO4	D	504	-	4,4,4	0.72	0	6,6,6	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CDL	D	505	-	38,38,99	1.27	3 (7%)	43,47,111	1.20	4 (9%)
15	PEE	D	506	-	25,25,50	1.49	2 (8%)	28,30,55	1.50	4 (14%)
14	PO4	E	501	-	4,4,4	0.58	0	6,6,6	0.71	0
14	PO4	F	501	-	4,4,4	0.72	0	6,6,6	0.55	0
17	CDL	G	501	-	43,43,99	1.54	4 (9%)	49,55,111	1.59	8 (16%)
14	PO4	N	1001	-	4,4,4	0.67	0	6,6,6	0.69	0
14	PO4	N	501	-	4,4,4	0.69	0	6,6,6	0.86	0
12	HEM	P	501	3	27,50,50	0.88	2 (7%)	17,82,82	1.68	5 (29%)
12	HEM	P	502	3	27,50,50	1.04	2 (7%)	17,82,82	1.53	4 (23%)
13	4X9	P	503	-	30,30,30	2.85	6 (20%)	41,44,44	1.45	6 (14%)
15	PEE	P	505	-	48,48,50	1.08	2 (4%)	51,53,55	0.85	3 (5%)
14	PO4	Q	1001	-	4,4,4	0.74	0	6,6,6	0.42	0
14	PO4	Q	1002	-	4,4,4	0.74	0	6,6,6	0.43	0
16	HEC	Q	501	4	26,50,50	2.44	12 (46%)	18,82,82	2.61	6 (33%)
17	CDL	Q	505	-	38,38,99	1.25	3 (7%)	43,47,111	1.23	5 (11%)
15	PEE	Q	506	-	50,50,50	1.05	2 (4%)	53,55,55	1.27	5 (9%)
18	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
19	GOL	R	502	-	5,5,5	0.31	0	5,5,5	0.45	0
14	PO4	S	501	-	4,4,4	0.72	0	6,6,6	0.42	0
17	CDL	T	501	-	48,48,99	1.39	4 (8%)	54,60,111	1.19	5 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HEM	C	501	3	-	0/6/54/54	0/0/8/8
12	HEM	C	502	3	-	0/6/54/54	0/0/8/8
13	4X9	C	503	-	-	0/13/13/13	0/3/3/3
14	PO4	C	504	-	-	0/0/0/0	0/0/0/0
15	PEE	C	505	-	1/1/4/4	0/52/52/54	0/0/0/0
16	HEC	D	501	4	-	0/6/54/54	0/0/8/8
14	PO4	D	502	-	-	0/0/0/0	0/0/0/0
14	PO4	D	503	-	-	0/0/0/0	0/0/0/0
14	PO4	D	504	-	-	0/0/0/0	0/0/0/0
17	CDL	D	505	-	-	0/43/43/110	0/0/0/0
15	PEE	D	506	-	1/1/4/4	0/29/29/54	0/0/0/0
14	PO4	E	501	-	-	0/0/0/0	0/0/0/0
14	PO4	F	501	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CDL	G	501	-	-	0/52/52/110	0/0/0/0
14	PO4	N	1001	-	-	0/0/0/0	0/0/0/0
14	PO4	N	501	-	-	0/0/0/0	0/0/0/0
12	HEM	P	501	3	-	0/6/54/54	0/0/8/8
12	HEM	P	502	3	-	0/6/54/54	0/0/8/8
13	4X9	P	503	-	-	0/13/13/13	0/3/3/3
15	PEE	P	505	-	1/1/4/4	0/52/52/54	0/0/0/0
14	PO4	Q	1001	-	-	0/0/0/0	0/0/0/0
14	PO4	Q	1002	-	-	0/0/0/0	0/0/0/0
16	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
17	CDL	Q	505	-	-	0/43/43/110	0/0/0/0
15	PEE	Q	506	-	1/1/4/4	0/54/54/54	0/0/0/0
18	FES	R	501	5	-	0/0/4/4	0/1/1/1
19	GOL	R	502	-	-	0/4/4/4	0/0/0/0
14	PO4	S	501	-	-	0/0/0/0	0/0/0/0
17	CDL	T	501	-	-	0/57/57/110	0/0/0/0

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	503	4X9	O28-C18	-4.80	1.25	1.37
13	C	503	4X9	O28-C18	-4.58	1.26	1.37
12	C	501	HEM	C3B-C2B	-4.51	1.34	1.40
12	P	502	HEM	C3B-C2B	-2.77	1.36	1.40
12	C	502	HEM	C3B-C2B	-2.18	1.37	1.40

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	501	HEC	C1D-C2D-C3D	-6.86	102.23	107.00
16	D	501	HEC	C1D-C2D-C3D	-6.10	102.75	107.00
16	D	501	HEC	CAA-CBA-CGA	-4.75	104.54	112.66
13	P	503	4X9	C18-C19-CL	-4.46	113.39	118.09
12	C	501	HEM	CBA-CAA-C2A	-4.07	104.71	112.48

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	Q	506	PEE	C2
15	C	505	PEE	C2
15	D	506	PEE	C2
15	P	505	PEE	C2

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	501	HEM	4	0
12	C	502	HEM	6	0
13	C	503	4X9	6	0
15	C	505	PEE	1	0
16	D	501	HEC	12	0
12	P	501	HEM	7	0
12	P	502	HEM	3	0
13	P	503	4X9	5	0
15	P	505	PEE	1	0
16	Q	501	HEC	10	0
17	Q	505	CDL	1	0
15	Q	506	PEE	3	0
18	R	501	FES	3	0
17	T	501	CDL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/480 (92%)	-0.14	9 (2%) 65 52	92, 150, 191, 255	0
1	N	444/480 (92%)	-0.33	7 (1%) 72 60	87, 132, 176, 243	0
2	B	422/453 (93%)	0.14	29 (6%) 17 12	108, 157, 200, 247	0
3	C	374/379 (98%)	-0.50	0 100 100	77, 103, 137, 225	0
3	P	370/379 (97%)	-0.44	1 (0%) 93 89	79, 112, 148, 183	0
4	D	240/265 (90%)	-0.31	2 (0%) 86 76	92, 121, 153, 178	0
4	Q	241/265 (90%)	-0.10	6 (2%) 57 44	86, 131, 168, 211	0
5	E	73/274 (26%)	-0.36	1 (1%) 75 63	93, 130, 158, 170	0
5	I	21/274 (7%)	0.63	1 (4%) 30 22	146, 192, 220, 228	0
5	R	196/274 (71%)	-0.15	2 (1%) 82 71	91, 150, 193, 230	0
6	F	98/111 (88%)	-0.44	2 (2%) 65 52	91, 124, 157, 171	0
6	S	99/111 (89%)	-0.44	0 100 100	85, 122, 168, 182	0
7	G	80/82 (97%)	-0.29	1 (1%) 77 65	88, 119, 189, 293	0
7	T	74/82 (90%)	-0.40	2 (2%) 54 42	83, 124, 181, 201	0
8	H	65/91 (71%)	-0.47	0 100 100	103, 136, 171, 223	0
8	U	66/91 (72%)	0.09	5 (7%) 14 10	132, 163, 213, 245	0
9	J	58/64 (90%)	-0.06	0 100 100	103, 137, 165, 175	0
9	W	59/64 (92%)	-0.19	1 (1%) 70 58	102, 121, 153, 162	0
10	O	419/453 (92%)	-0.21	7 (1%) 70 58	97, 146, 193, 250	0
11	V	17/274 (6%)	1.19	3 (17%) 1 1	176, 209, 228, 268	0
All	All	3860/4946 (78%)	-0.23	79 (2%) 65 52	77, 133, 189, 293	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	ASP	5.9
11	V	62	ARG	4.8
2	B	232	LEU	4.7
1	N	225	GLU	4.2
2	B	21	PRO	4.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	PO4	S	501	5/5	0.39	0.52	225,226,243,252	0
14	PO4	F	501	5/5	0.51	0.58	242,243,245,246	0
14	PO4	D	504	5/5	0.57	0.23	179,190,194,195	0
14	PO4	Q	1001	5/5	0.66	0.20	194,205,216,232	0
14	PO4	N	501	5/5	0.67	0.45	112,126,127,137	0
14	PO4	D	502	5/5	0.71	0.27	176,192,199,203	0
19	GOL	R	502	6/6	0.72	1.89	169,181,193,193	0
14	PO4	Q	1002	5/5	0.72	0.20	210,211,220,230	0
14	PO4	E	501	5/5	0.74	0.32	124,134,144,145	0
14	PO4	D	503	5/5	0.82	0.61	168,169,177,181	0
14	PO4	C	504	5/5	0.82	0.39	121,121,134,149	0
13	4X9	P	503	28/28	0.88	0.32	109,147,226,261	0
15	PEE	Q	506	51/51	0.90	0.40	100,134,171,187	0
13	4X9	C	503	28/28	0.90	0.39	116,143,206,215	0
15	PEE	C	505	49/51	0.91	0.49	94,116,135,137	0
17	CDL	D	505	39/100	0.91	0.27	85,124,146,148	0
17	CDL	G	501	44/100	0.92	0.28	95,115,153,168	0
17	CDL	T	501	49/100	0.92	0.31	93,129,160,167	0
15	PEE	P	505	49/51	0.93	0.33	100,122,154,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	PO4	N	1001	5/5	0.93	0.42	120,127,135,137	0
17	CDL	Q	505	39/100	0.93	0.28	100,126,146,148	0
15	PEE	D	506	26/51	0.93	0.26	107,127,169,176	0
18	FES	R	501	4/4	0.97	0.14	125,158,164,170	0
12	HEM	C	502	43/43	0.98	0.26	71,85,99,106	0
12	HEM	P	502	43/43	0.98	0.23	74,89,104,106	0
12	HEM	P	501	43/43	0.98	0.30	86,101,116,124	0
12	HEM	C	501	43/43	0.98	0.27	89,99,107,115	0
16	HEC	D	501	43/43	0.98	0.24	80,111,127,138	0
16	HEC	Q	501	43/43	0.98	0.28	106,117,136,143	0

6.5 Other polymers [i](#)

There are no such residues in this entry.