



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 6, 2017 – 11:54 AM EDT

PDB ID : 5NMI
Title : Cytochrome bc1 bound to the inhibitor MJM170
Authors : Capper, N.J.; Antonyuk, S.V.; Hasnain, S.S.
Deposited on : 2017-04-05
Resolution : 3.50 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

<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)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

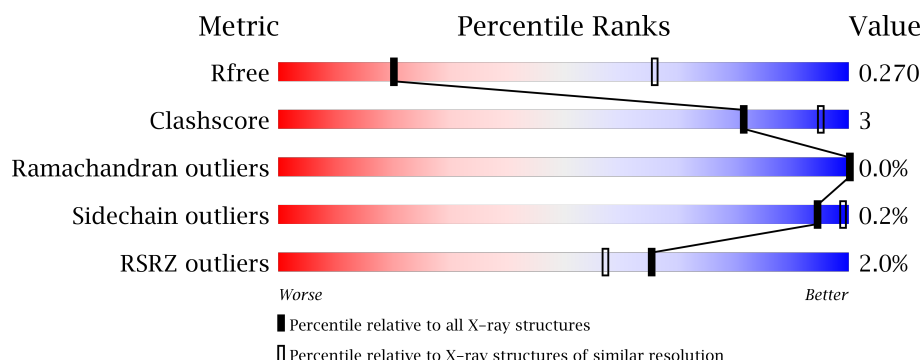
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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	444	<div> <div>96%</div> <div> <div></div> <div>2%</div> <div>97%</div> <div>96%</div> <div>6%</div> <div>96%</div> </div> </div>
1	N	444	<div> <div>2%</div> <div>97%</div> <div>96%</div> <div>6%</div> <div>96%</div> </div>
2	B	423	<div> <div>2%</div> <div>96%</div> <div>96%</div> <div>6%</div> <div>96%</div> </div>
2	O	423	<div> <div>6%</div> <div>94%</div> <div>94%</div> <div>6%</div> <div>94%</div> </div>
3	C	372	<div> <div>96%</div> <div>96%</div> <div>96%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	372	
4	D	240	
4	Q	240	
5	E	274	
5	I	274	
5	R	274	
5	V	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	K	22	
10	X	22	

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
12	MJM	C	503	X	-	-	-
12	MJM	P	404	X	-	-	-
13	PEE	D	502	X	-	-	X
13	PEE	E	502	X	-	-	-
13	PEE	R	201	X	-	-	-
13	PEE	R	202	X	-	-	-
14	CDL	P	401	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 31648 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	48	0	0
			3440	2148	607	665	20			
1	N	444	Total	C	N	O	S	45	0	0
			3440	2148	607	665	20			

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	27	0	0
			3172	1993	562	610	7			
2	O	423	Total	C	N	O	S	8	0	0
			3172	1993	562	610	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	372	Total	C	N	O	S	0	0	0
			2954	1984	460	492	18			
3	P	372	Total	C	N	O	S	0	0	0
			2954	1984	460	492	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
			1913	1222	329	347	15			
4	Q	240	Total	C	N	O	S	5	0	0
			1913	1222	329	347	15			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			
5	I	30	Total	C	N	O	S	9	0	0
			221	137	44	39	1			
5	R	72	Total	C	N	O	S	0	0	0
			540	335	90	113	2			
5	V	30	Total	C	N	O	S	0	0	0
			221	137	44	39	1			

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			870	553	157	158	2			
6	S	99	Total	C	N	O	S	4	0	0
			870	553	157	158	2			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	0	0
			623	407	117	98	1			
7	T	80	Total	C	N	O	S	0	0	0
			677	439	127	110	1			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	3	0	0
			539	327	98	109	5			
8	U	68	Total	C	N	O	S	0	0	0
			557	337	100	115	5			

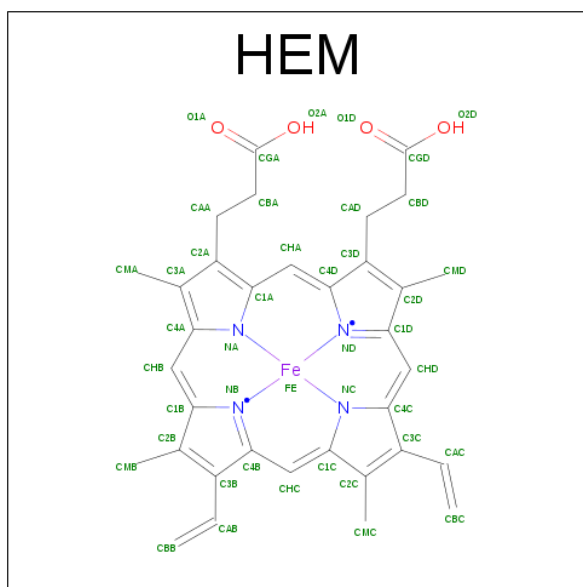
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	59	Total	C	N	O	0	0	0
			492	322	86	84			
9	W	59	Total	C	N	O	0	0	0
			487	320	84	83			

- Molecule 10 is a protein called ARG-ASN-TRP-VAL-PRO-THR-ALA-GLN-LEU-TRP-GLY-ALA-VAL-GLY-ALA-VAL-GLY-LEU-VAL-SER-ALA-THR.

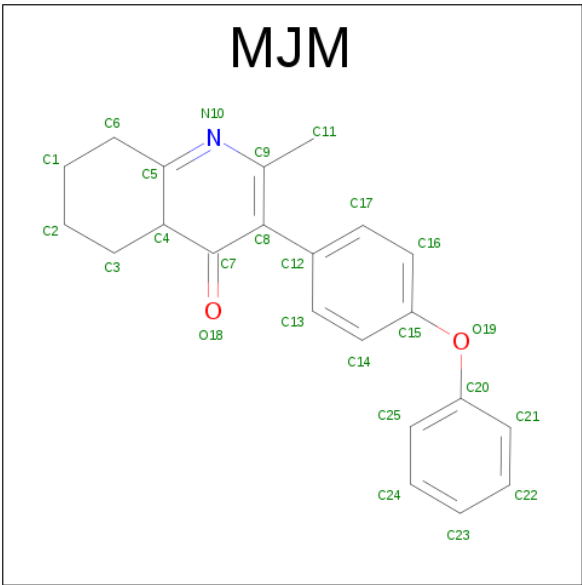
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	22	Total	C	N	O	0	0	0
			159	103	29	27			
10	X	22	Total	C	N	O	12	0	0
			159	103	29	27			

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



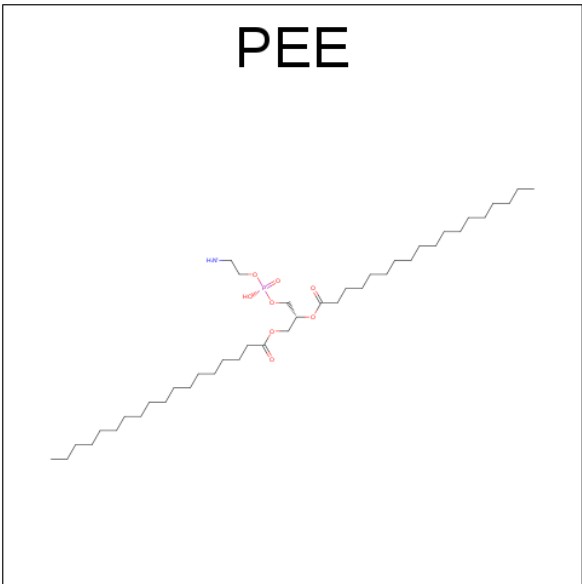
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
11	P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
11	P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0

- Molecule 12 is (4aS)-2-methyl-3-(4-phenoxyphenyl)-5,6,7,8-tetrahydroquinolin-4(4aH)-one (three-letter code: MJM) (formula: $C_{22}H_{21}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	N	O	0	0
			25	22	1	2		
12	P	1	Total	C	N	O	0	0
			25	22	1	2		

- Molecule 13 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₈₃NO₈P).



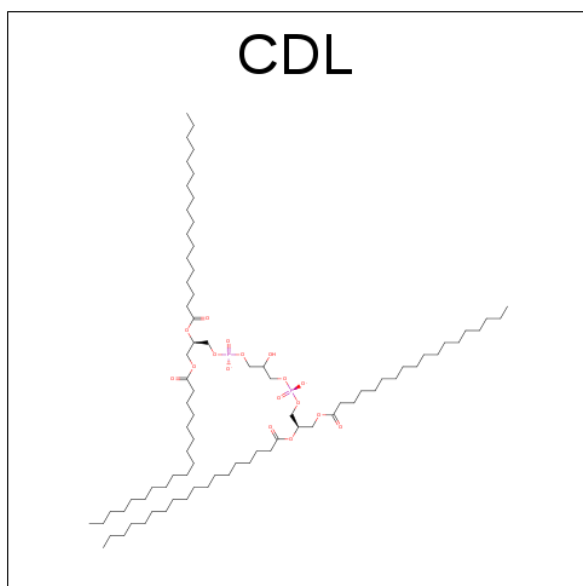
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	N	O	P	0	0
			28	19	1	7	1		

Continued on next page...

Continued from previous page...

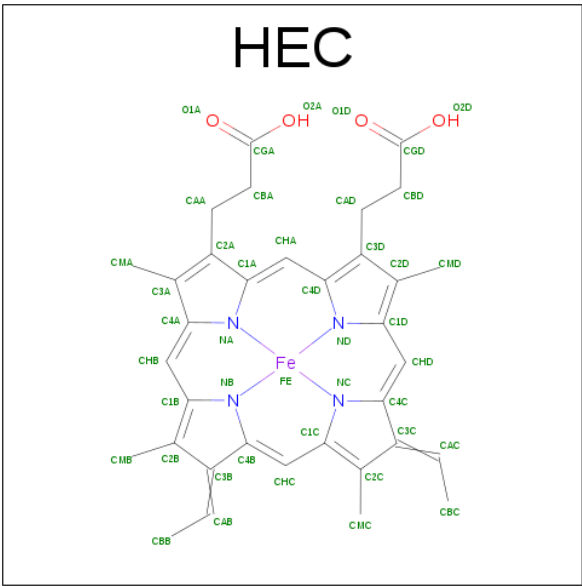
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	D	1	Total	C	N	O	P	0	0
			42	32	1	8	1		
13	E	1	Total	C	N	O	P	0	0
			29	19	1	8	1		
13	P	1	Total	C	N	O	P	0	0
			38	28	1	8	1		
13	R	1	Total	C	N	O	P	0	0
			34	24	1	8	1		
13	R	1	Total	C	N	O	P	0	0
			24	14	1	8	1		

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



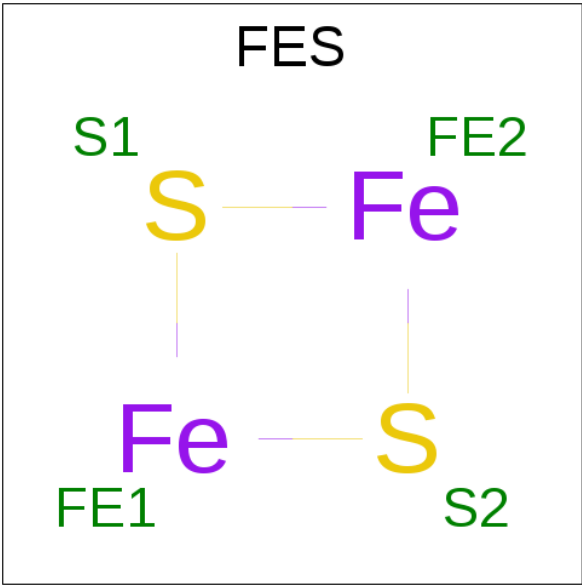
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	O	P	0	0
			42	23	17	2		
14	C	1	Total	C	O	P	0	0
			37	18	17	2		
14	D	1	Total	C	O	P	0	0
			44	27	15	2		
14	P	1	Total	C	O	P	0	0
			42	27	13	2		
14	P	1	Total	C	O	P	0	0
			46	28	16	2		
14	P	1	Total	C	O	P	0	0
			38	19	17	2		

- Molecule 15 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



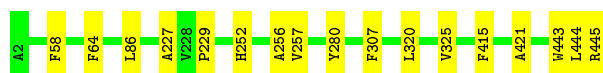
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	E	1	Total	Fe	S	0	0
			4	2	2		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

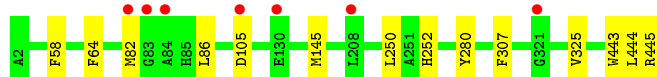
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:  96%



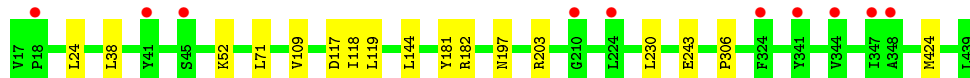
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain N:  97%



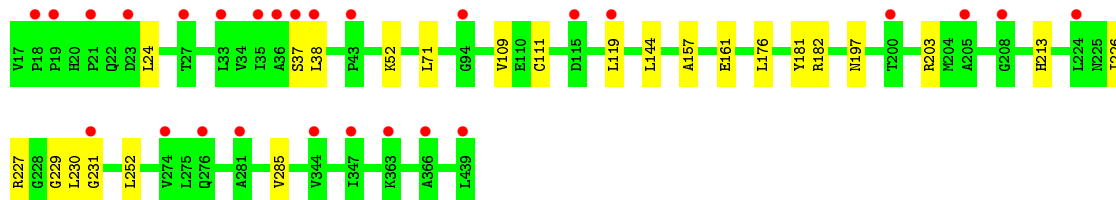
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:  96%



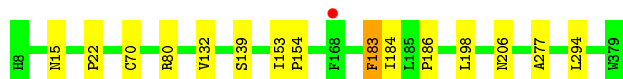
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain O:  94%

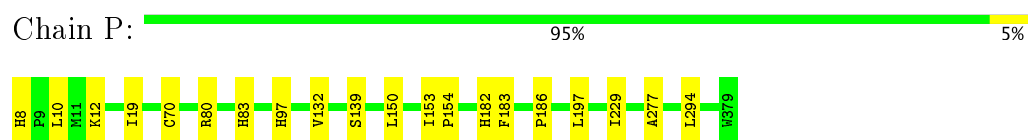


- Molecule 3: Cytochrome b

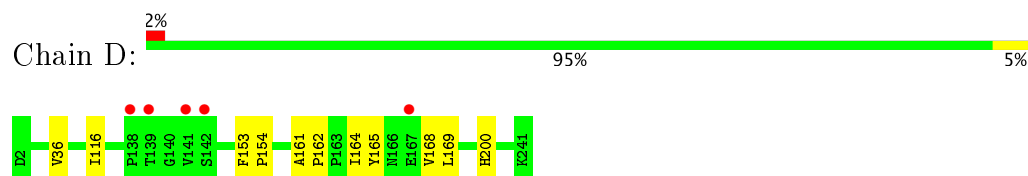
Chain C:  96%



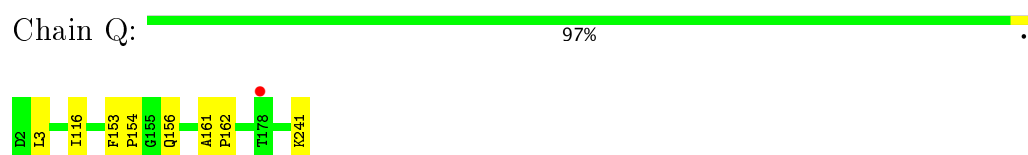
- Molecule 3: Cytochrome b



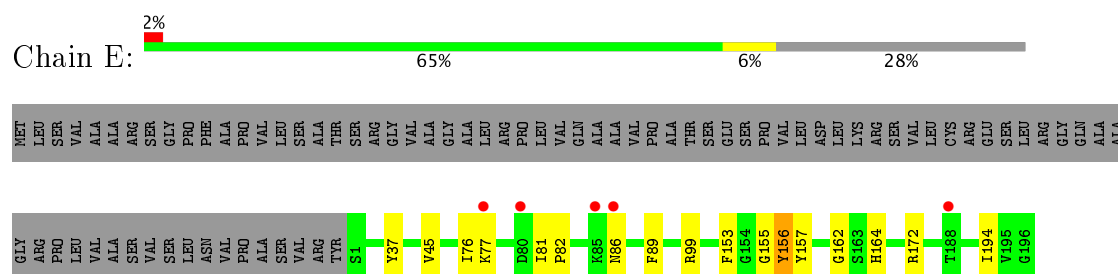
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



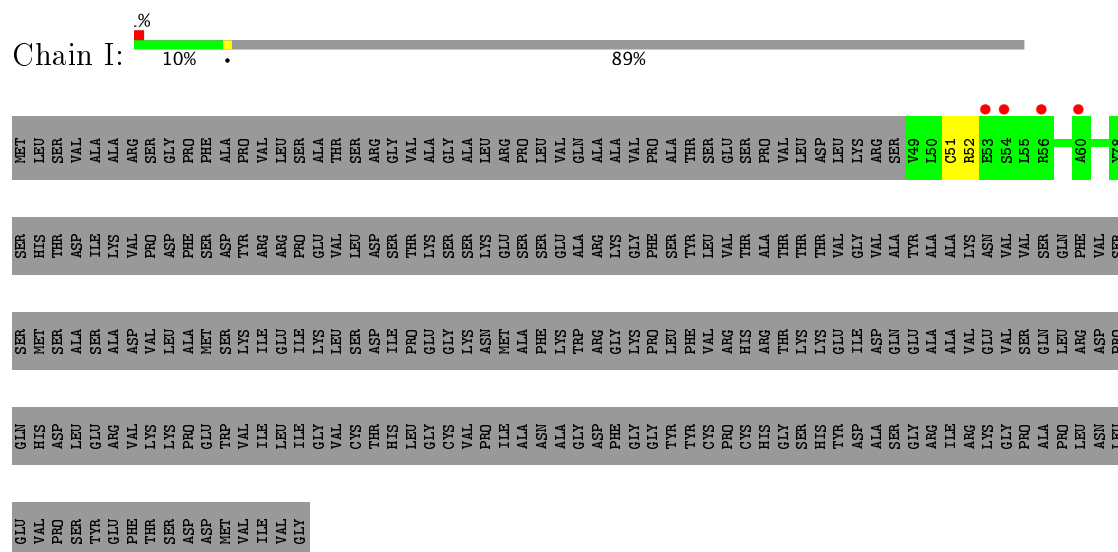
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

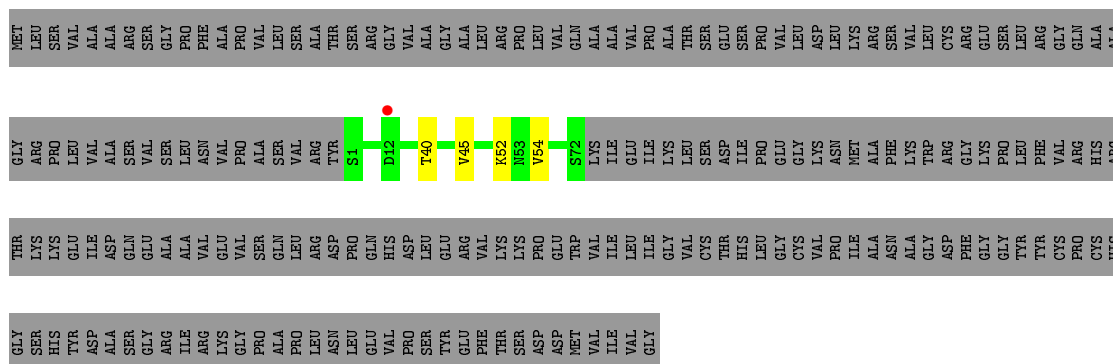


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



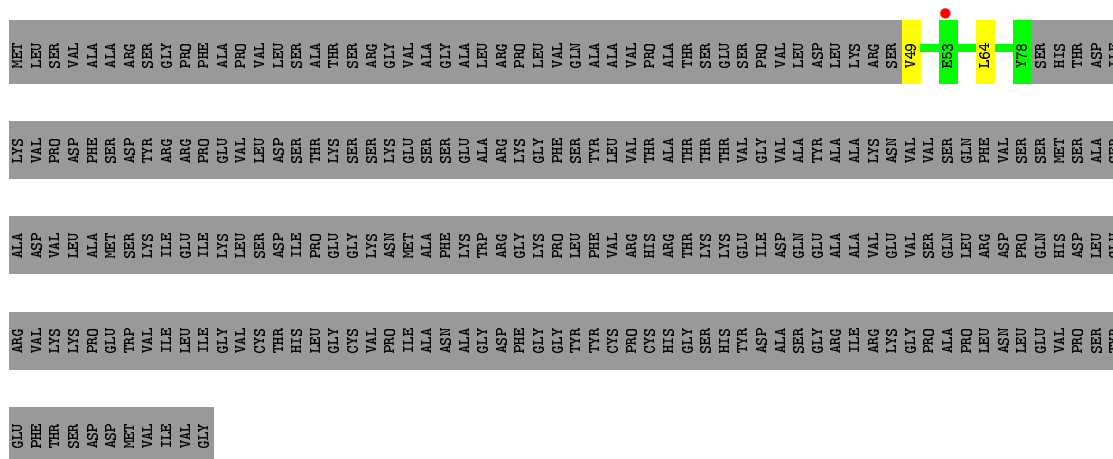
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain R:  25% 74%




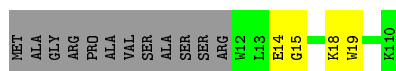
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain V:  10% 89%




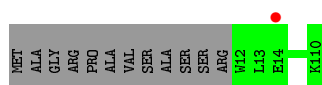
- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain F:  86% 11%




- Molecule 6: Cytochrome b-c1 complex subunit 7

Chain S:  89% 11%



- Molecule 7: Cytochrome b-c1 complex subunit 8

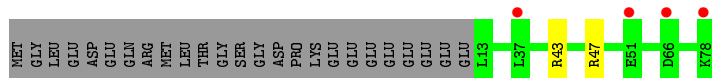
Chain G:  85% 5% 10%



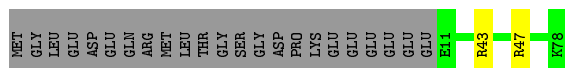
- Molecule 7: Cytochrome b-c1 complex subunit 8



- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



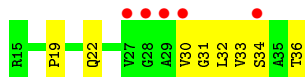
- Molecule 9: Cytochrome b-c1 complex subunit 9



- Molecule 9: Cytochrome b-c1 complex subunit 9

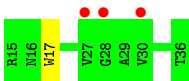


- Molecule 10: ARG-ASN-TRP-VAL-PRO-THR-ALA-GLN-LEU-TRP-GLY-ALA-VAL-GLY-ALA-VAL-GLY-LEU-VAL-SER-ALA-THR



- Molecule 10: ARG-ASN-TRP-VAL-PRO-THR-ALA-GLN-LEU-TRP-GLY-ALA-VAL-GLY-ALA-VAL-GLY-LEU-VAL-SER-ALA-THR





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	129.48Å 129.48Å 720.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.74 – 3.50 64.74 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (64.74-3.50) 99.6 (64.74-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.248 , 0.268 0.250 , 0.270	Depositor DCC
R_{free} test set	4341 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	78.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.096 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	31648	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, MJM, HEC, FES, 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	0.35	0/3512	0.60	0/4766
1	N	0.37	0/3512	0.60	0/4766
2	B	0.36	0/3232	0.56	0/4386
2	O	0.36	0/3232	0.56	0/4386
3	C	0.37	1/3051 (0.0%)	0.53	0/4177
3	P	0.37	0/3051	0.53	0/4177
4	D	0.36	0/1972	0.58	0/2676
4	Q	0.41	1/1972 (0.1%)	0.59	1/2676 (0.0%)
5	E	0.37	0/1553	0.61	0/2100
5	I	0.49	0/223	0.82	0/302
5	R	0.35	0/548	0.53	0/741
5	V	0.41	0/223	0.73	0/302
6	F	0.36	0/889	0.58	0/1191
6	S	0.36	0/889	0.57	0/1191
7	G	0.40	0/644	0.62	0/871
7	T	0.40	0/699	0.61	0/946
8	H	0.34	0/544	0.59	0/729
8	U	0.34	0/562	0.61	0/753
9	J	0.37	0/504	0.55	0/678
9	W	0.37	0/500	0.56	0/675
10	K	0.46	0/163	0.56	0/225
10	X	0.69	1/163 (0.6%)	0.56	0/225
All	All	0.37	3/31638 (0.0%)	0.58	1/42939 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	241	LYS	CA-CB	-8.75	1.34	1.53
10	X	17	TRP	CB-CG	7.05	1.62	1.50
3	C	183	PHE	CG-CD2	-5.48	1.30	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	241	LYS	CB-CA-C	-5.13	100.14	110.40

There are no chirality outliers.

There are no planarity outliers.

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	3440	0	3337	20	0
1	N	3440	0	3337	13	0
2	B	3172	0	3152	9	0
2	O	3172	0	3152	20	0
3	C	2954	0	3010	29	0
3	P	2954	0	3010	32	0
4	D	1913	0	1860	10	0
4	Q	1913	0	1860	5	0
5	E	1519	0	1503	21	0
5	I	221	0	234	2	0
5	R	540	0	534	5	0
5	V	221	0	234	5	0
6	F	870	0	864	3	0
6	S	870	0	864	0	0
7	G	623	0	631	7	0
7	T	677	0	673	2	0
8	H	539	0	524	1	0
8	U	557	0	536	2	0
9	J	492	0	494	1	0
9	W	487	0	487	2	0
10	K	159	0	159	11	0
10	X	159	0	159	0	0
11	C	86	0	60	15	0
11	P	86	0	60	14	0
12	C	25	0	0	0	0
12	P	25	0	0	1	0
13	C	28	0	32	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D	42	0	57	5	0
13	E	29	0	32	1	0
13	P	38	0	50	0	0
13	R	58	0	64	3	0
14	C	79	0	46	1	0
14	D	44	0	40	0	0
14	P	126	0	101	3	0
15	D	43	0	31	1	0
15	Q	43	0	31	1	0
16	E	4	0	0	0	0
All	All	31648	0	31218	190	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 3.

The worst 5 of 190 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)
13:D:502:PEE:C1	13:D:502:PEE:C2	2.00	1.39
3:C:183:PHE:CE1	11:C:501:HEM:HBC1	1.89	1.08
3:C:183:PHE:CD2	3:P:183:PHE:CD1	2.44	1.06
2:O:197:ASN:O	2:O:230:LEU:HD12	1.62	0.98
3:C:183:PHE:CE2	3:P:183:PHE:CD1	2.55	0.94

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	442/444 (100%)	422 (96%)	20 (4%)	0	100	100
1	N	442/444 (100%)	417 (94%)	25 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	421/423 (100%)	396 (94%)	25 (6%)	0	100	100
2	O	421/423 (100%)	393 (93%)	27 (6%)	1 (0%)	51	85
3	C	370/372 (100%)	356 (96%)	14 (4%)	0	100	100
3	P	370/372 (100%)	356 (96%)	14 (4%)	0	100	100
4	D	238/240 (99%)	227 (95%)	11 (5%)	0	100	100
4	Q	238/240 (99%)	228 (96%)	10 (4%)	0	100	100
5	E	194/274 (71%)	182 (94%)	12 (6%)	0	100	100
5	I	28/274 (10%)	24 (86%)	4 (14%)	0	100	100
5	R	70/274 (26%)	70 (100%)	0	0	100	100
5	V	28/274 (10%)	26 (93%)	2 (7%)	0	100	100
6	F	97/111 (87%)	95 (98%)	2 (2%)	0	100	100
6	S	97/111 (87%)	96 (99%)	1 (1%)	0	100	100
7	G	72/82 (88%)	66 (92%)	6 (8%)	0	100	100
7	T	78/82 (95%)	71 (91%)	7 (9%)	0	100	100
8	H	64/91 (70%)	63 (98%)	1 (2%)	0	100	100
8	U	66/91 (72%)	66 (100%)	0	0	100	100
9	J	57/64 (89%)	54 (95%)	3 (5%)	0	100	100
9	W	57/64 (89%)	54 (95%)	3 (5%)	0	100	100
10	K	20/22 (91%)	19 (95%)	1 (5%)	0	100	100
10	X	20/22 (91%)	20 (100%)	0	0	100	100
All	All	3890/4794 (81%)	3701 (95%)	188 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	231	GLY

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	368/368 (100%)	366 (100%)	2 (0%)	91	96
1	N	368/368 (100%)	366 (100%)	2 (0%)	91	96
2	B	332/332 (100%)	332 (100%)	0	100	100
2	O	332/332 (100%)	332 (100%)	0	100	100
3	C	320/320 (100%)	320 (100%)	0	100	100
3	P	320/320 (100%)	320 (100%)	0	100	100
4	D	205/205 (100%)	205 (100%)	0	100	100
4	Q	205/205 (100%)	205 (100%)	0	100	100
5	E	168/228 (74%)	167 (99%)	1 (1%)	89	96
5	I	24/228 (10%)	24 (100%)	0	100	100
5	R	62/228 (27%)	62 (100%)	0	100	100
5	V	24/228 (10%)	24 (100%)	0	100	100
6	F	91/99 (92%)	91 (100%)	0	100	100
6	S	91/99 (92%)	91 (100%)	0	100	100
7	G	66/72 (92%)	66 (100%)	0	100	100
7	T	71/72 (99%)	71 (100%)	0	100	100
8	H	63/85 (74%)	63 (100%)	0	100	100
8	U	65/85 (76%)	65 (100%)	0	100	100
9	J	50/54 (93%)	50 (100%)	0	100	100
9	W	49/54 (91%)	49 (100%)	0	100	100
10	K	15/15 (100%)	15 (100%)	0	100	100
10	X	15/15 (100%)	15 (100%)	0	100	100
All	All	3304/4012 (82%)	3299 (100%)	5 (0%)	94	99

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	PHE
1	A	443	TRP
5	E	156	TYR
1	N	58	PHE
1	N	443	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

21 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$
11	HEM	C	501	3	28,50,50	0.80	1 (3%)	17,82,82	1.39	3 (17%)
11	HEM	C	502	3	28,50,50	0.84	1 (3%)	17,82,82	1.18	1 (5%)
12	MJM	C	503	-	25,28,28	1.43	1 (4%)	30,39,39	1.06	2 (6%)
13	PEE	C	504	-	27,27,50	1.23	4 (14%)	28,31,55	0.72	0
14	CDL	C	505	-	41,41,99	1.46	4 (9%)	43,53,111	1.60	6 (13%)
14	CDL	C	506	-	36,36,99	1.33	4 (11%)	38,48,111	1.46	4 (10%)
15	HEC	D	501	4	28,50,50	2.45	12 (42%)	16,82,82	2.14	5 (31%)
13	PEE	D	502	-	41,41,50	4.13	5 (12%)	43,46,55	3.32	7 (16%)
14	CDL	D	503	-	42,42,99	1.00	2 (4%)	40,51,111	1.07	2 (5%)
16	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
13	PEE	E	502	-	28,28,50	1.14	2 (7%)	30,33,55	1.19	2 (6%)
14	CDL	P	401	-	41,41,99	0.99	2 (4%)	42,50,111	1.28	3 (7%)
11	HEM	P	402	3	28,50,50	1.03	2 (7%)	17,82,82	1.29	2 (11%)
11	HEM	P	403	3	28,50,50	0.93	2 (7%)	17,82,82	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MJM	P	404	-	25,28,28	1.40	1 (4%)	30,39,39	1.32	4 (13%)
13	PEE	P	405	-	37,37,50	1.28	5 (13%)	39,42,55	0.85	2 (5%)
14	CDL	P	406	-	45,45,99	1.12	3 (6%)	46,56,111	1.59	8 (17%)
14	CDL	P	407	-	37,37,99	1.33	4 (10%)	39,49,111	1.28	2 (5%)
15	HEC	Q	501	4	28,50,50	2.53	14 (50%)	16,82,82	2.21	4 (25%)
13	PEE	R	201	-	33,33,50	1.15	2 (6%)	35,38,55	1.26	4 (11%)
13	PEE	R	202	-	23,23,50	1.22	2 (8%)	25,28,55	1.12	3 (12%)

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
11	HEM	C	501	3	-	0/6/54/54	0/0/8/8
11	HEM	C	502	3	-	0/6/54/54	0/0/8/8
12	MJM	C	503	-	1/1/5/5	0/8/35/35	0/3/4/4
13	PEE	C	504	-	-	0/30/30/54	0/0/0/0
14	CDL	C	505	-	-	0/49/49/110	0/0/0/0
14	CDL	C	506	-	-	1/44/44/110	0/0/0/0
15	HEC	D	501	4	-	0/6/54/54	0/0/8/8
13	PEE	D	502	-	1/1/4/4	0/45/45/54	0/0/0/0
14	CDL	D	503	-	-	0/48/48/110	0/0/0/0
16	FES	E	501	5	-	0/0/4/4	0/1/1/1
13	PEE	E	502	-	1/1/4/4	0/32/32/54	0/0/0/0
14	CDL	P	401	-	-	2/48/48/110	0/0/0/0
11	HEM	P	402	3	-	0/6/54/54	0/0/8/8
11	HEM	P	403	3	-	0/6/54/54	0/0/8/8
12	MJM	P	404	-	1/1/5/5	0/8/35/35	0/3/4/4
13	PEE	P	405	-	-	0/41/41/54	0/0/0/0
14	CDL	P	406	-	-	0/55/55/110	0/0/0/0
14	CDL	P	407	-	-	0/45/45/110	0/0/0/0
15	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
13	PEE	R	201	-	1/1/4/4	0/37/37/54	0/0/0/0
13	PEE	R	202	-	1/1/4/4	0/27/27/54	0/0/0/0

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	502	PEE	O2-C2	-18.69	0.97	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	501	HEC	C4B-NB	-3.73	1.32	1.36
15	Q	501	HEC	C4B-NB	-3.59	1.32	1.36
15	Q	501	HEC	C4A-NA	-3.50	1.32	1.36
11	P	402	HEM	C1B-NB	-3.44	1.32	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	502	PEE	O3-C3-C2	-9.96	83.62	108.66
13	D	502	PEE	C3-C2-C1	-8.70	92.24	111.86
14	C	505	CDL	CB4-OB6-CB5	-5.42	107.47	117.94
14	P	406	CDL	CB4-OB6-CB5	-4.83	106.46	117.88
15	Q	501	HEC	C1D-C2D-C3D	-4.80	103.66	107.00

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	E	502	PEE	C2
13	R	202	PEE	C2
13	D	502	PEE	C2
13	R	201	PEE	C2
12	C	503	MJM	C4

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	506	CDL	CA4-OA6-CA5-C11
14	P	401	CDL	CB4-OB6-CB5-OB7
14	P	401	CDL	CB4-OB6-CB5-C51

There are no ring outliers.

13 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	501	HEM	13	0
11	C	502	HEM	2	0
14	C	505	CDL	1	0
15	D	501	HEC	1	0
13	D	502	PEE	5	0
13	E	502	PEE	1	0
11	P	402	HEM	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	P	403	HEM	8	0
12	P	404	MJM	1	0
14	P	406	CDL	3	0
15	Q	501	HEC	1	0
13	R	201	PEE	2	0
13	R	202	PEE	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 ⓘ

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	438/444 (98%)	-0.18	0 100 100	47, 92, 130, 166	0
1	N	439/444 (98%)	0.01	7 (1%) 72 64	57, 109, 153, 181	2 (0%)
2	B	418/423 (98%)	0.08	10 (2%) 59 50	64, 106, 143, 196	0
2	O	422/423 (99%)	0.26	27 (6%) 20 17	71, 115, 151, 203	0
3	C	372/372 (100%)	-0.32	1 (0%) 93 90	46, 73, 105, 141	0
3	P	372/372 (100%)	-0.33	0 100 100	33, 62, 92, 127	0
4	D	240/240 (100%)	-0.03	5 (2%) 64 55	56, 96, 132, 181	0
4	Q	240/240 (100%)	-0.18	1 (0%) 92 89	52, 82, 120, 138	1 (0%)
5	E	196/274 (71%)	-0.07	5 (2%) 56 47	48, 107, 143, 166	0
5	I	29/274 (10%)	0.58	4 (13%) 3 4	84, 130, 157, 166	0
5	R	72/274 (26%)	-0.20	1 (1%) 75 67	55, 84, 118, 130	0
5	V	30/274 (10%)	0.53	1 (3%) 47 39	89, 132, 168, 208	0
6	F	99/111 (89%)	-0.19	0 100 100	50, 78, 127, 141	0
6	S	99/111 (89%)	-0.39	1 (1%) 82 75	53, 82, 115, 128	1 (1%)
7	G	74/82 (90%)	-0.21	0 100 100	54, 85, 127, 147	0
7	T	80/82 (97%)	-0.07	1 (1%) 77 69	57, 82, 129, 161	0
8	H	66/91 (72%)	0.48	4 (6%) 22 18	85, 135, 156, 182	1 (1%)
8	U	68/91 (74%)	-0.05	0 100 100	64, 95, 126, 141	0
9	J	59/64 (92%)	-0.08	2 (3%) 46 38	57, 83, 123, 138	0
9	W	59/64 (92%)	-0.21	0 100 100	60, 95, 126, 141	0
10	K	22/22 (100%)	0.95	5 (22%) 1 1	123, 151, 173, 200	0
10	X	22/22 (100%)	1.33	3 (13%) 3 4	92, 131, 143, 167	2 (9%)
All	All	3916/4794 (81%)	-0.06	78 (1%) 65 57	33, 93, 143, 208	7 (0%)

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	139	THR	3.9
8	H	51	GLU	3.9
5	I	56	ARG	3.7
2	O	18	PRO	3.7
2	O	37	SER	3.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
14	CDL	P	401	42/100	0.88	0.36	2.12	53,90,135,159	0
13	PEE	D	502	42/51	0.93	0.31	2.06	60,79,102,111	0
13	PEE	C	504	28/51	0.91	0.36	1.65	35,45,57,59	0
13	PEE	P	405	38/51	0.93	0.34	1.12	41,56,81,81	0
13	PEE	R	202	24/51	0.93	0.32	1.09	26,37,52,55	0
14	CDL	D	503	44/100	0.88	0.30	1.04	42,86,112,116	0
14	CDL	P	407	38/100	0.93	0.26	0.94	53,71,87,90	0
11	HEM	P	403	43/43	0.97	0.27	0.90	52,55,60,61	0
14	CDL	C	505	42/100	0.84	0.27	0.37	45,88,122,130	0
14	CDL	C	506	37/100	0.94	0.28	0.26	59,73,108,108	0
13	PEE	E	502	29/51	0.90	0.29	0.23	47,83,98,103	0
11	HEM	P	402	43/43	0.97	0.27	0.21	43,55,60,74	0
15	HEC	D	501	43/43	0.95	0.29	0.18	66,84,109,147	0
11	HEM	C	501	43/43	0.97	0.27	0.15	51,59,77,90	0
13	PEE	R	201	34/51	0.95	0.22	0.08	57,78,91,101	0
12	MJM	C	503	25/25	0.95	0.22	0.02	49,56,68,69	0
15	HEC	Q	501	43/43	0.96	0.28	-0.01	59,79,111,145	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
11	HEM	C	502	43/43	0.97	0.23	-0.07	45,53,71,76	0
14	CDL	P	406	46/100	0.89	0.22	-0.32	70,106,125,128	0
12	MJM	P	404	25/25	0.94	0.20	-1.37	49,56,64,69	0
16	FES	E	501	4/4	0.96	0.12	-1.42	104,106,122,144	0

6.5 Other polymers [i](#)

There are no such residues in this entry.