



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:45 AM GMT

PDB ID : 2E75  
Title : Crystal Structure of the Cytochrome b6f Complex with 2-nonyl-4-hydroxyquinoline N-oxide (NQNO) from *M. lamosus*  
Authors : Cramer, W.A.; Yamashita, E.; Zhang, H.  
Deposited on : 2007-01-05  
Resolution : 3.55 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

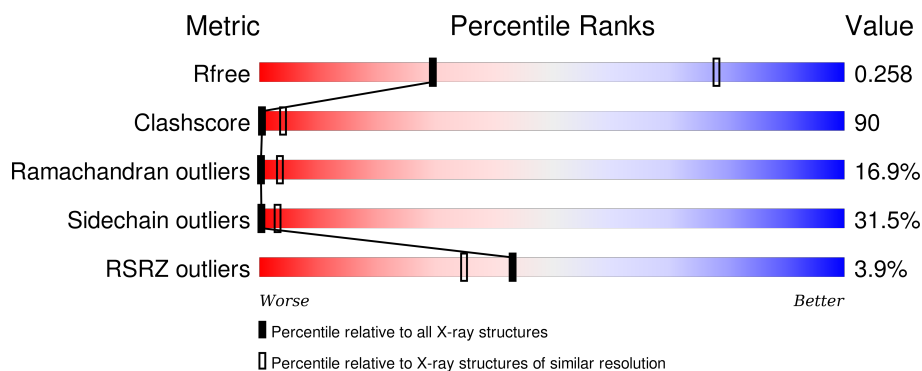
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.55 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.



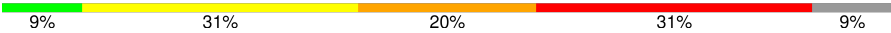


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

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  $\geq 3$ , 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	215	
2	B	160	
3	C	289	
4	D	179	
5	E	32	

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Mol	Chain	Length	Quality of chain
6	F	35	
7	G	37	
8	H	29	

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
10	HEM	A	301	-	-	X	-
10	HEM	A	302	-	-	X	-
10	HEM	C	301	-	-	X	-
11	OPC	A	1002	-	-	X	X
11	OPC	B	1001	-	-	-	X
12	UMQ	A	1102	X	-	-	X
12	UMQ	A	1103	X	-	-	-
12	UMQ	A	1104	X	-	-	-
12	UMQ	C	1101	X	-	-	-
13	QNO	A	501	X	-	-	X
14	CLA	B	201	X	-	-	-
15	FES	D	200	-	-	X	-
16	SQD	D	201	X	-	-	X
17	BCR	G	101	-	-	-	X

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 8046 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 b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1711	1140	272	288	11			

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1249	841	193	209	6			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	288	Total	C	N	O	S	0	0	0
			2216	1415	369	424	8			

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1260	805	218	230	7			

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	32	Total	C	N	O	S	0	0	0
			248	179	34	34	1			

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	32	Total	C	N	O	S	0	0	0
			242	165	35	40	2			

- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	37	Total	C	N	O	S	0	0	0
			283	188	44	50	1			

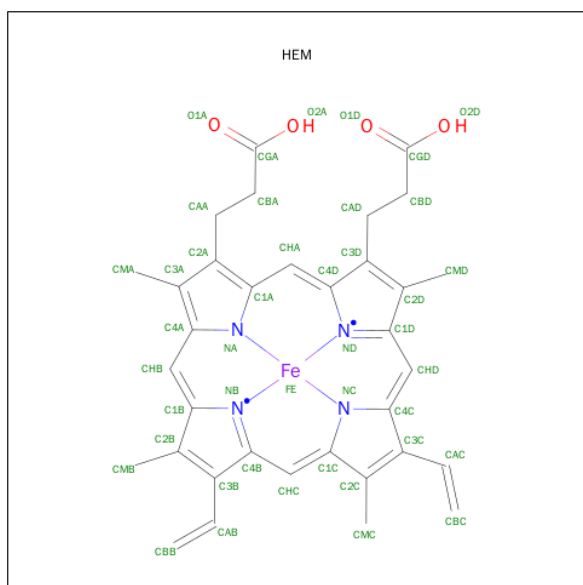
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	29	Total	C	N	O	S	0	0	0
			230	156	36	36	2			

- Molecule 9 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Cd	0	0
			1	1		
9	A	1	Total	Cd	0	0
			1	1		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



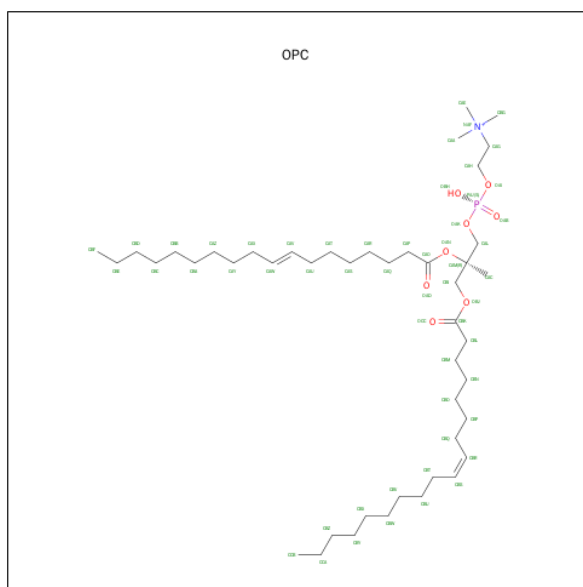
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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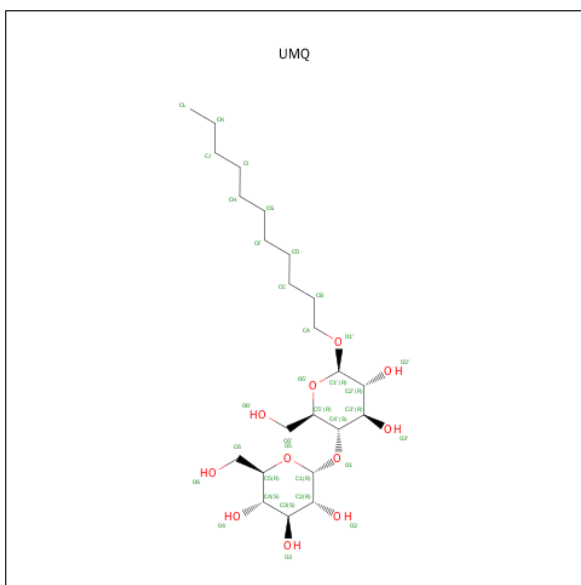
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 11 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (three-letter code: OPC) (formula:  $C_{45}H_{87}NO_8P$ ).



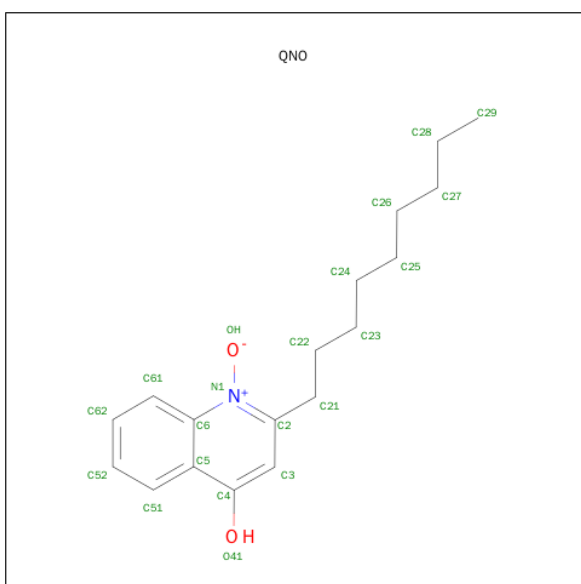
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	
			54	44	1	8	1	
11	B	1	Total	C	N	O	P	
			54	44	1	8	1	

- Molecule 12 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula:  $C_{23}H_{44}O_{11}$ ).



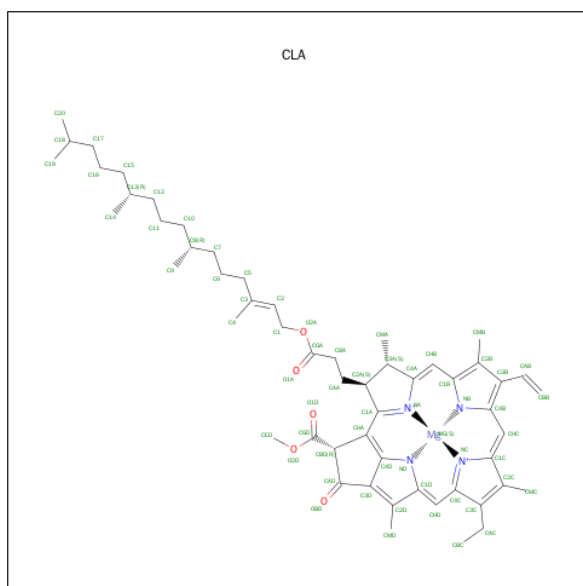
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			34	23	11		
12	A	1	Total	C	O	0	0
			34	23	11		
12	A	1	Total	C	O	0	0
			34	23	11		
12	C	1	Total	C	O	0	0
			34	23	11		

- Molecule 13 is 2-NONYL-4-HYDROXYQUINOLINE N-OXIDE (three-letter code: QNO) (formula:  $C_{18}H_{25}NO_2$ ).



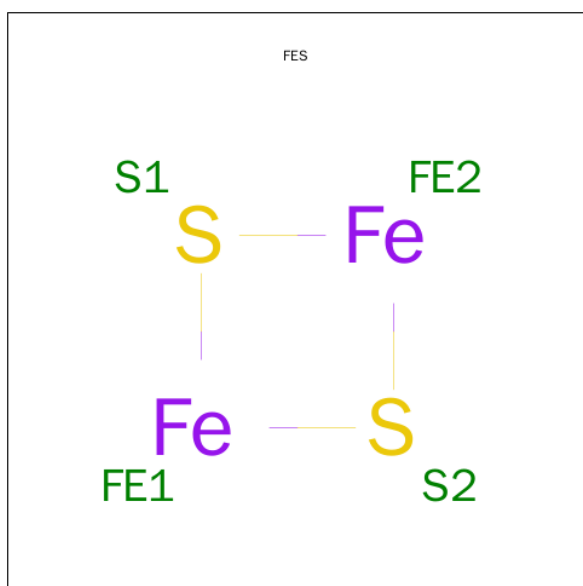
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	O	0	0
			21	18	1	2		

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

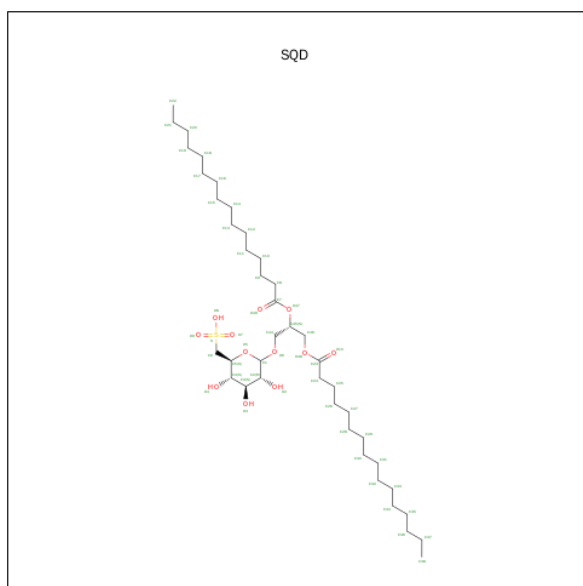
- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).





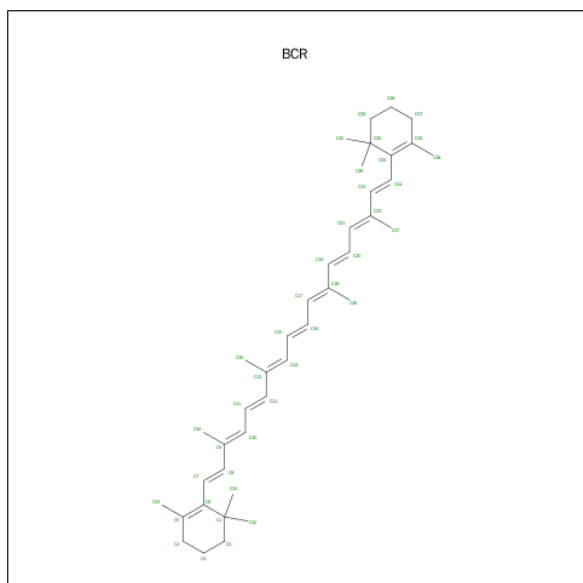
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	D	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	1	Total C 40 40	0	0

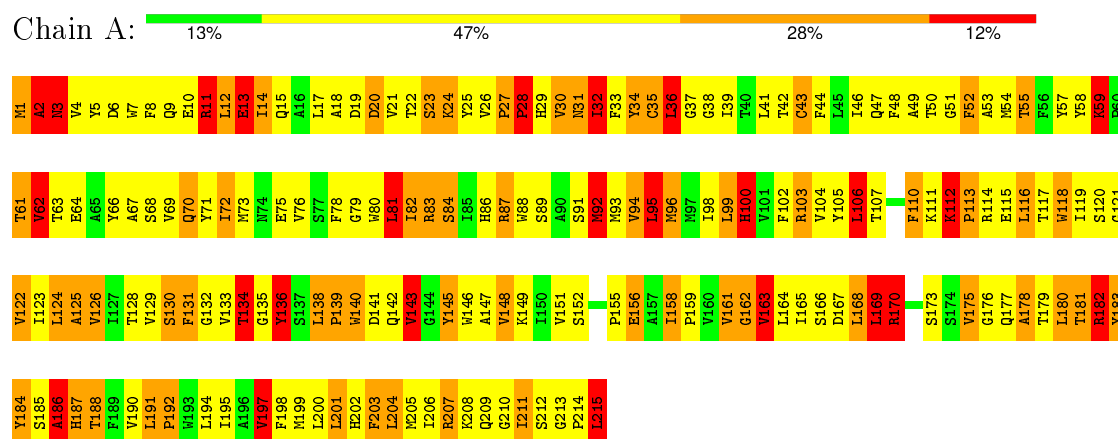
- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	3	Total O 3 3	0	0
18	B	2	Total O 2 2	0	0

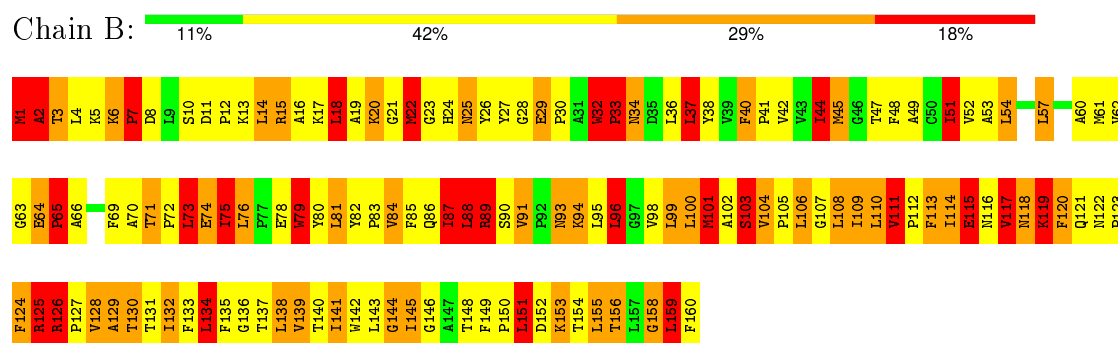
### 3 Residue-property plots

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

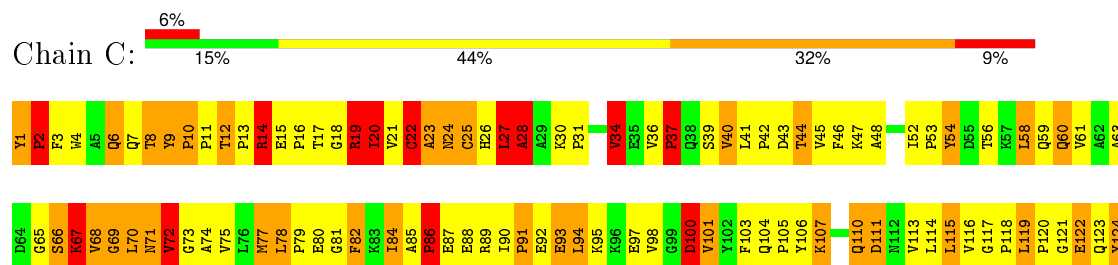
#### • Molecule 1: Cytochrome b6

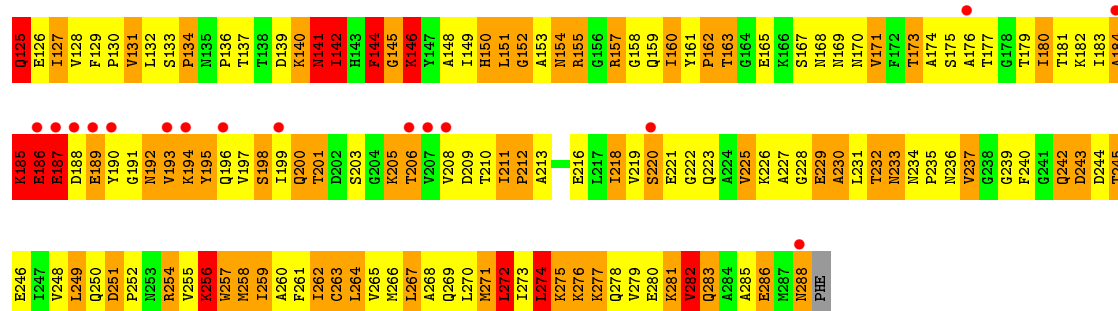


#### • Molecule 2: Cytochrome b6-f complex subunit 4

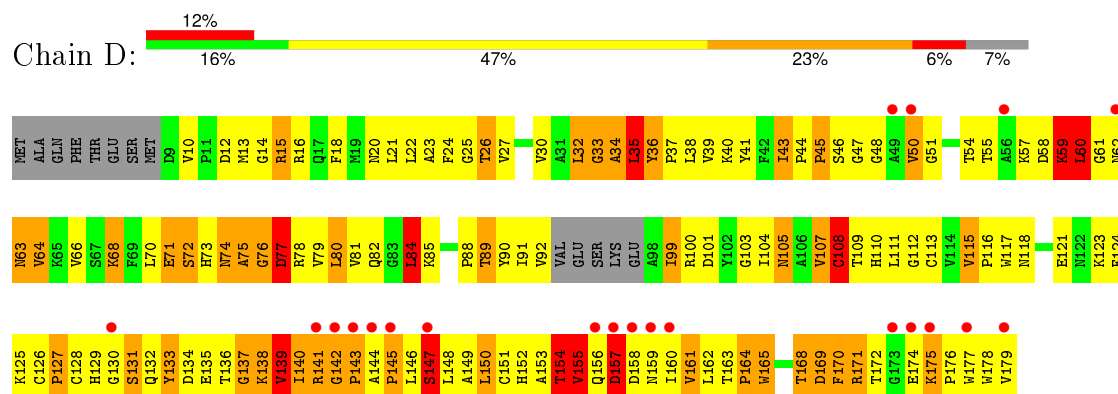


#### • Molecule 3: Apocytochrome f

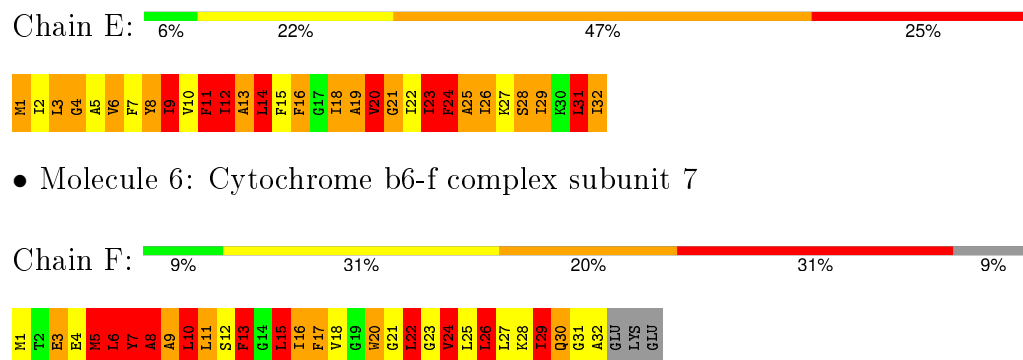




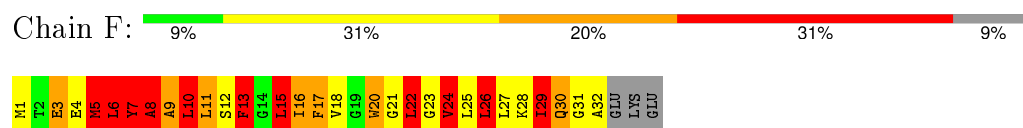
- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



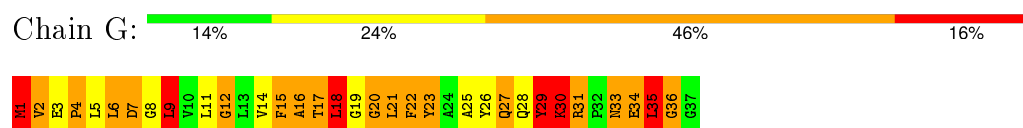
- Molecule 5: Cytochrome b6-f complex subunit 6



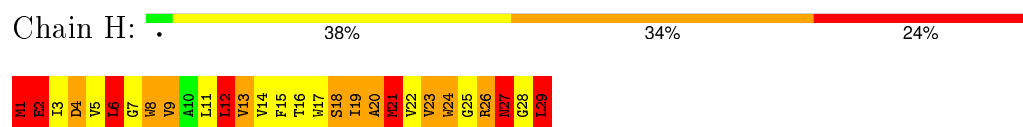
- Molecule 6: Cytochrome b6-f complex subunit 7



- Molecule 7: Cytochrome b6-f complex subunit 5



- Molecule 8: Cytochrome b6-f complex subunit 8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	159.16Å 159.16Å 362.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.94 – 3.55 49.94 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.94-3.55) 99.7 (49.94-3.55)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.89 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.201 , 0.267 0.198 , 0.258	Depositor DCC
$R_{free}$ test set	1702 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	94.2	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 85.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 33625 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8046	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: UMQ, CLA, CD, FES, OPC, HEM, QNO, BCR, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.99	39/1763 (2.2%)	2.01	64/2405 (2.7%)
2	B	1.88	24/1288 (1.9%)	2.04	46/1765 (2.6%)
3	C	1.53	29/2264 (1.3%)	1.52	25/3082 (0.8%)
4	D	1.26	3/1292 (0.2%)	1.37	14/1760 (0.8%)
5	E	1.79	3/253 (1.2%)	1.95	8/340 (2.4%)
6	F	2.27	10/246 (4.1%)	2.19	12/331 (3.6%)
7	G	1.78	3/289 (1.0%)	1.87	7/391 (1.8%)
8	H	1.97	6/236 (2.5%)	2.11	12/323 (3.7%)
All	All	1.73	117/7631 (1.5%)	1.78	188/10397 (1.8%)

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	6
2	B	0	7
3	C	0	8
5	E	0	4
6	F	0	1
7	G	0	4
8	H	0	2
All	All	0	32

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	15	ARG	CZ-NH1	11.16	1.47	1.33
2	B	115	GLU	CG-CD	11.14	1.68	1.51
1	A	122	VAL	CA-CB	-10.27	1.33	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	87	GLU	CG-CD	9.96	1.66	1.51
3	C	72	VAL	CB-CG1	-9.56	1.32	1.52

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	15	ARG	NE-CZ-NH2	-24.30	108.15	120.30
1	A	106	LEU	CB-CG-CD1	-12.98	88.93	111.00
1	A	83	ARG	NE-CZ-NH1	-12.94	113.83	120.30
2	B	125	ARG	NE-CZ-NH1	-12.28	114.16	120.30
2	B	15	ARG	NE-CZ-NH1	10.86	125.73	120.30

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	PRO	Peptide
1	A	135	GLY	Peptide
1	A	158	ILE	Peptide
1	A	2	ALA	Peptide
1	A	27	PRO	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	1711	0	1736	339	0
2	B	1249	0	1308	324	0
3	C	2216	0	2232	414	0
4	D	1260	0	1243	185	0
5	E	248	0	284	77	0
6	F	242	0	260	69	0
7	G	283	0	289	61	0
8	H	230	0	239	82	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	129	0	90	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	43	0	30	22	0
11	A	54	0	79	27	0
11	B	54	0	83	11	0
12	A	102	0	123	11	0
12	C	34	0	42	10	0
13	A	21	0	24	7	0
14	B	65	0	72	16	0
15	D	4	0	0	3	0
16	D	54	0	53	11	0
17	G	40	0	52	12	0
18	A	3	0	0	0	0
18	B	2	0	0	0	0
All	All	8046	0	8239	1456	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 90.

The worst 5 of 1456 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)
1:A:59:LYS:CE	1:A:59:LYS:CD	1.75	1.60
2:B:88:LEU:CG	2:B:88:LEU:CD1	1.75	1.59
6:F:6:LEU:CG	6:F:6:LEU:CD2	1.75	1.59
8:H:29:LEU:CD2	8:H:29:LEU:CG	1.78	1.58
5:E:12:ILE:CD1	5:E:12:ILE:CG1	1.79	1.58

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	213/215 (99%)	142 (67%)	53 (25%)	18 (8%)	1	14
2	B	158/160 (99%)	91 (58%)	36 (23%)	31 (20%)	0	2
3	C	286/289 (99%)	195 (68%)	50 (18%)	41 (14%)	0	5
4	D	162/179 (90%)	93 (57%)	39 (24%)	30 (18%)	0	2
5	E	30/32 (94%)	9 (30%)	10 (33%)	11 (37%)	0	0
6	F	30/35 (86%)	14 (47%)	8 (27%)	8 (27%)	0	0
7	G	35/37 (95%)	13 (37%)	9 (26%)	13 (37%)	0	0
8	H	27/29 (93%)	14 (52%)	6 (22%)	7 (26%)	0	1
All	All	941/976 (96%)	571 (61%)	211 (22%)	159 (17%)	0	3

5 of 159 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	23	SER
1	A	28	PRO
1	A	112	LYS
1	A	136	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	184/184 (100%)	138 (75%)	46 (25%)	1	6
2	B	137/137 (100%)	98 (72%)	39 (28%)	0	4
3	C	242/243 (100%)	151 (62%)	91 (38%)	0	1
4	D	134/146 (92%)	96 (72%)	38 (28%)	0	4
5	E	25/25 (100%)	17 (68%)	8 (32%)	0	2
6	F	24/27 (89%)	11 (46%)	13 (54%)	0	0
7	G	28/28 (100%)	20 (71%)	8 (29%)	0	4
8	H	24/24 (100%)	16 (67%)	8 (33%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	798/814 (98%)	547 (68%)	251 (32%)	<b>0</b> <b>3</b>

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	94	LEU
3	C	182	LYS
6	F	22	LEU
3	C	111	ASP
3	C	142	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	168	ASN
3	C	233	ASN
4	D	132	GLN
3	C	170	ASN
3	C	234	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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
11	OPC	A	1002	-	53,53,54	2.11	14 (26%)	57,61,64	2.89	26 (45%)
12	UMQ	A	1102	1	35,35,35	1.97	7 (20%)	46,46,46	3.22	20 (43%)
12	UMQ	A	1103	-	35,35,35	1.68	5 (14%)	46,46,46	3.05	16 (34%)
12	UMQ	A	1104	-	35,35,35	1.55	3 (8%)	46,46,46	3.12	12 (26%)
10	HEM	A	301	1	30,50,50	2.85	12 (40%)	24,82,82	3.79	12 (50%)
10	HEM	A	302	1	30,50,50	2.84	11 (36%)	24,82,82	3.77	13 (54%)
10	HEM	A	303	1,18,13	30,50,50	2.80	10 (33%)	24,82,82	3.20	9 (37%)
13	QNO	A	501	10	22,22,22	3.36	6 (27%)	23,28,28	4.24	7 (30%)
11	OPC	B	1001	-	53,53,54	2.10	16 (30%)	57,61,64	2.53	25 (43%)
14	CLA	B	201	18	55,73,73	1.91	11 (20%)	61,113,113	3.51	35 (57%)
12	UMQ	C	1101	-	35,35,35	1.80	7 (20%)	46,46,46	3.61	21 (45%)
10	HEM	C	301	3	30,50,50	2.00	10 (33%)	24,82,82	4.19	14 (58%)
15	FES	D	200	4	0,4,4	0.00	-	0,4,4	0.00	-
16	SQD	D	201	-	53,54,54	2.92	23 (43%)	61,65,65	5.18	33 (54%)
17	BCR	G	101	-	41,41,41	3.62	22 (53%)	56,56,56	6.68	34 (60%)

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	OPC	A	1002	-	-	0/57/57/60	0/0/0/0
12	UMQ	A	1102	1	2/2/10/10	0/20/60/60	0/2/2/2
12	UMQ	A	1103	-	2/2/10/10	0/20/60/60	0/2/2/2
12	UMQ	A	1104	-	2/2/10/10	0/20/60/60	0/2/2/2
10	HEM	A	301	1	-	0/10/54/54	0/0/8/8
10	HEM	A	302	1	-	0/10/54/54	0/0/8/8
10	HEM	A	303	1,18,13	-	0/10/54/54	0/0/8/8
13	QNO	A	501	10	1/1/0/0	0/9/9/9	0/2/2/2
11	OPC	B	1001	-	-	0/57/57/60	0/0/0/0
14	CLA	B	201	18	4/4/20/25	0/37/135/135	0/0/9/9
12	UMQ	C	1101	-	2/2/10/10	0/20/60/60	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEM	C	301	3	-	0/10/54/54	0/0/8/8
15	FES	D	200	4	-	0/0/4/4	0/1/1/1
16	SQD	D	201	-	3/3/9/9	0/49/69/69	0/1/1/1
17	BCR	G	101	-	-	0/29/63/63	0/2/2/2

The worst 5 of 157 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	201	SQD	C6-S	-12.70	1.59	1.77
10	A	302	HEM	C3B-C4B	-10.99	1.42	1.51
17	G	101	BCR	C8-C9	-10.84	1.21	1.45
10	A	303	HEM	C3B-C4B	-10.09	1.42	1.51
10	A	301	HEM	C3D-C4D	-8.54	1.40	1.51

The worst 5 of 277 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	301	HEM	C3B-CAB-CBB	-13.90	103.13	124.46
16	D	201	SQD	O3-C3-C4	-12.73	81.67	110.34
10	A	301	HEM	C3B-CAB-CBB	-12.25	105.67	124.46
17	G	101	BCR	C33-C5-C6	-11.24	113.57	124.61
13	A	501	QNO	OH-N1-C6	-9.80	105.27	118.80

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	1104	UMQ	C2'
12	A	1104	UMQ	C1'
16	D	201	SQD	C3
16	D	201	SQD	C5
16	D	201	SQD	C4

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 184 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1002	OPC	27	0
12	A	1102	UMQ	7	0
12	A	1103	UMQ	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1104	UMQ	2	0
10	A	301	HEM	22	0
10	A	302	HEM	25	0
10	A	303	HEM	9	0
13	A	501	QNO	7	0
11	B	1001	OPC	11	0
14	B	201	CLA	16	0
12	C	1101	UMQ	10	0
10	C	301	HEM	22	0
15	D	200	FES	3	0
16	D	201	SQD	11	0
17	G	101	BCR	12	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	215/215 (100%)	-0.85	0	100	100	4, 22, 60, 162	0
2	B	160/160 (100%)	-0.81	0	100	100	9, 41, 93, 133	0
3	C	288/289 (99%)	-0.10	16 (5%)	28	22	5, 47, 145, 170	1 (0%)
4	D	166/179 (92%)	0.23	21 (12%)	5	5	8, 101, 150, 182	0
5	E	32/32 (100%)	-0.68	0	100	100	22, 52, 98, 119	0
6	F	32/35 (91%)	-0.61	0	100	100	10, 41, 112, 123	0
7	G	37/37 (100%)	-0.76	0	100	100	13, 33, 115, 123	0
8	H	29/29 (100%)	-0.81	0	100	100	15, 28, 51, 97	0
All	All	959/976 (98%)	-0.41	37 (3%)	43	35	4, 42, 139, 182	1 (0%)

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	179	VAL	6.9
4	D	144	ALA	4.2
4	D	49	ALA	4.1
4	D	145	PRO	4.0
3	C	189	GLU	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
12	UMQ	A	1102	34/34	0.83	0.32	4.44	31,112,145,149	0
11	OPC	A	1002	54/55	0.90	0.40	4.00	2,64,206,220	0
11	OPC	B	1001	54/55	0.94	0.38	3.76	8,70,138,157	0
17	BCR	G	101	40/40	0.93	0.36	3.51	2,49,145,149	0
13	QNO	A	501	21/21	0.95	0.20	2.21	45,63,95,120	0
16	SQD	D	201	54/54	0.87	0.41	2.13	39,165,201,204	0
12	UMQ	C	1101	34/34	0.86	0.23	1.54	4,86,151,160	0
14	CLA	B	201	65/65	0.97	0.20	0.85	12,42,72,111	0
12	UMQ	A	1103	34/34	0.93	0.30	0.55	40,101,144,155	0
12	UMQ	A	1104	34/34	0.85	0.28	0.31	23,131,208,216	0
10	HEM	A	303	43/43	0.99	0.15	0.27	2,35,56,61	0
10	HEM	A	301	43/43	0.99	0.16	0.19	2,13,37,60	0
10	HEM	A	302	43/43	0.99	0.15	0.11	2,8,43,49	0
10	HEM	C	301	43/43	0.98	0.21	-0.23	2,33,74,95	0
15	FES	D	200	4/4	0.98	0.11	-1.18	89,90,95,104	0
9	CD	B	161	1/1	0.98	0.08	-2.44	161,161,161,161	0
9	CD	A	216	1/1	1.00	0.12	-	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.