



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 07:17 pm GMT

PDB ID : 2D2C  
Title : Crystal Structure Of Cytochrome B6F Complex with DBMIB From M. Laminosus  
Authors : Yan, J.; Kurisu, G.; Cramer, W.A.  
Deposited on : 2005-09-07  
Resolution : 3.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (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

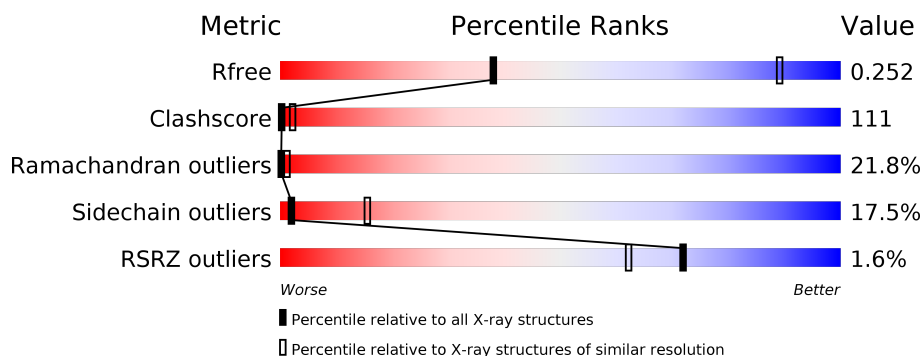
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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.



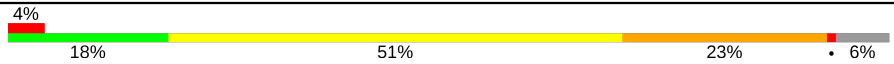

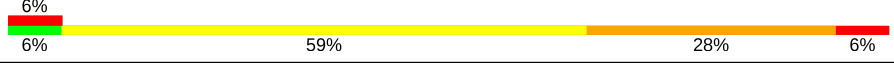
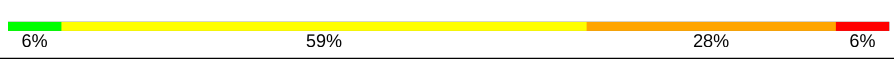
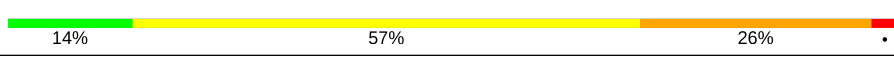
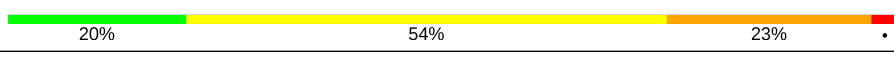


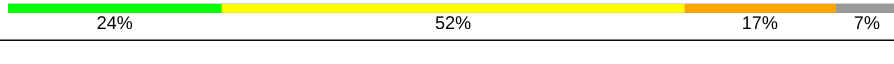
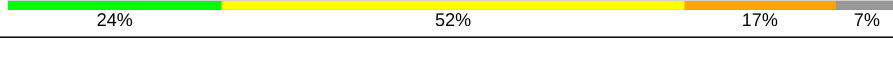
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1028 (4.02-3.58)
Clashscore	122126	1061 (4.00-3.60)
Ramachandran outliers	120053	1025 (4.00-3.60)
Sidechain outliers	120020	1019 (4.00-3.60)
RSRZ outliers	108989	1021 (4.06-3.54)

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	<div> <div>6%</div> <div>58%</div> <div>27%</div> <div>• 6%</div> </div>
1	N	215	<div> <div>9%</div> <div>54%</div> <div>26%</div> <div>5% 6%</div> </div>
2	B	160	<div> <div>12%</div> <div>44%</div> <div>26%</div> <div>• 14%</div> </div>
2	O	160	<div> <div>5%</div> <div>48%</div> <div>25%</div> <div>8% 14%</div> </div>
3	C	289	<div> <div>3%</div> <div>17%</div> <div>56%</div> <div>24%</div> <div>• •</div> </div>
3	P	289	<div> <div>2%</div> <div>14%</div> <div>59%</div> <div>22%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	179	
4	Q	179	
5	E	32	
5	R	32	
6	F	35	
6	S	35	
7	G	37	
7	T	37	
8	H	29	
8	U	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
11	OPC	B	305	-	-	X	-
12	BNT	B	309	-	-	X	-
12	BNT	O	1309	-	-	X	-
13	CLA	B	201	X	-	-	-
13	CLA	O	1201	X	-	-	-
14	FES	D	201	-	-	X	-
14	FES	Q	201	-	-	X	-
15	BCR	R	1101	-	-	-	X

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 14984 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	202	Total	C	N	O	S	0	0	0
			1593	1062	253	268	10			
1	N	202	Total	C	N	O	S	0	0	0
			1593	1062	253	268	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	137	Total	C	N	O	S	0	0	0
			1067	721	164	177	5			
2	O	137	Total	C	N	O	S	0	0	0
			1067	721	164	177	5			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	286	Total	C	N	O	S	0	0	0
			2200	1406	366	421	7			
3	P	286	Total	C	N	O	S	0	0	0
			2200	1406	366	421	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	168	Total	C	N	O	S	0	0	0
			1280	815	223	235	7			
4	Q	168	Total	C	N	O	S	0	0	0
			1280	815	223	235	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	138	ARG	LYS	CONFLICT	UNP P83794
Q	138	ARG	LYS	CONFLICT	UNP P83794

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			270	181	39	48	2			
6	S	35	Total	C	N	O	S	0	0	0
			270	181	39	48	2			

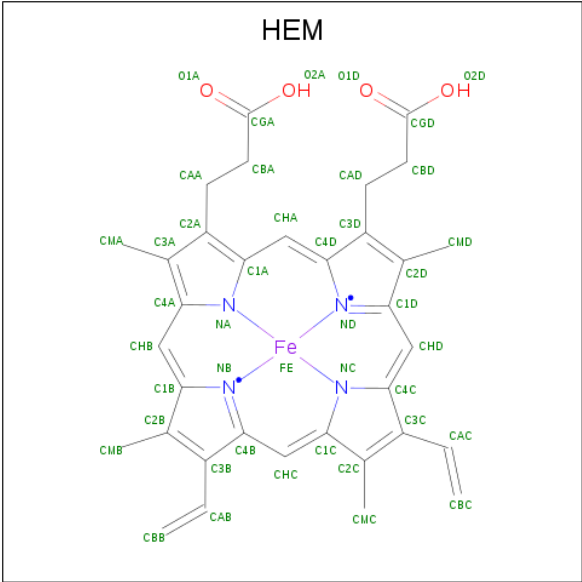
- Molecule 7 is a protein called Cytochrome b6-f complex subunit V.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	27	Total	C	N	O	0	0	0
			216	146	34	36			
7	T	27	Total	C	N	O	0	0	0
			216	146	34	36			

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

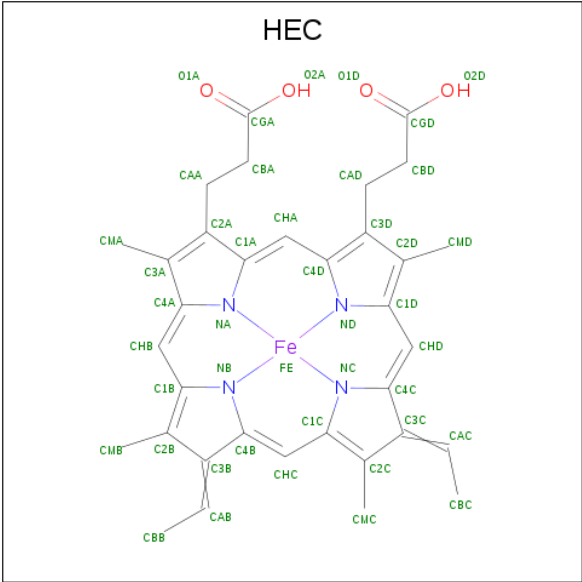
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			
8	U	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



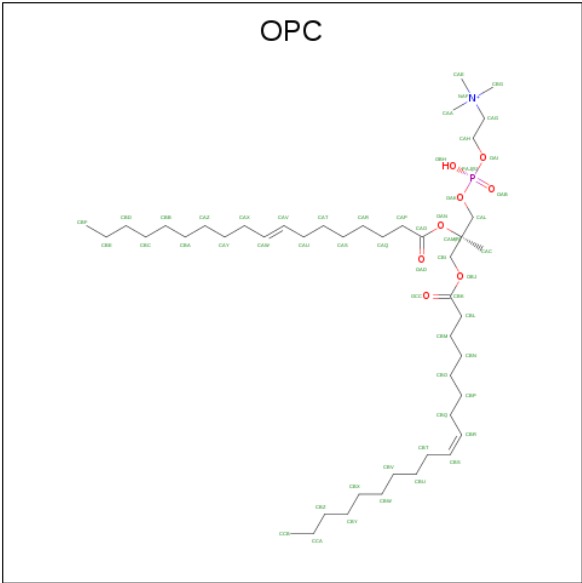
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 10 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- 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<sub>45</sub>H<sub>87</sub>NO<sub>8</sub>P).



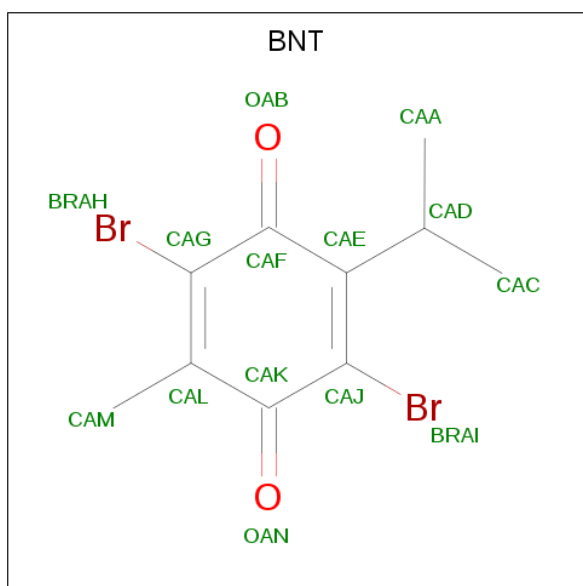
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
11	N	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
11	O	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

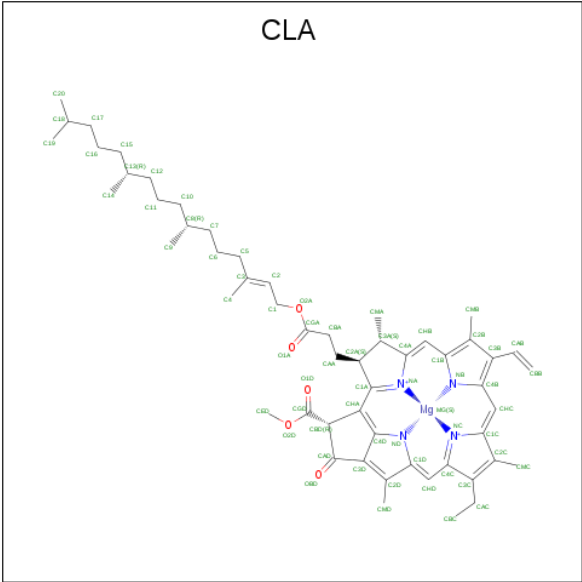
- Molecule 12 is 2,5-DIBROMO-3-ISOPROPYL-6-METHYLBENZO-1,4-QUINONE (three-letter code: BNT) (formula:  $C_{10}H_{10}Br_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	Br	C	O	0	0
			14	2	10	2		
12	O	1	Total	Br	C	O	0	0
			14	2	10	2		

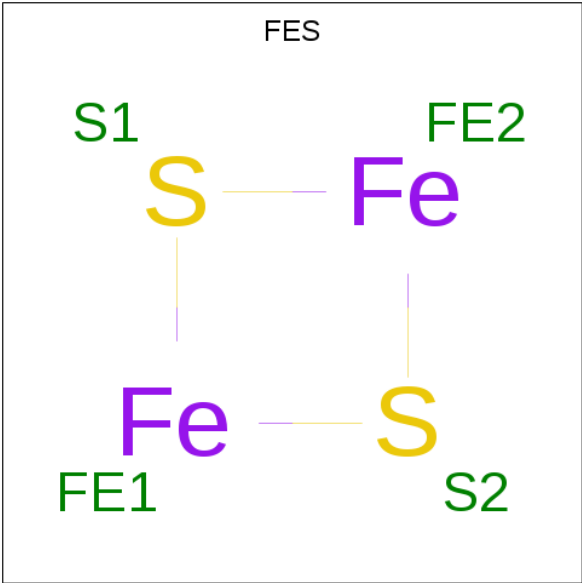
- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).





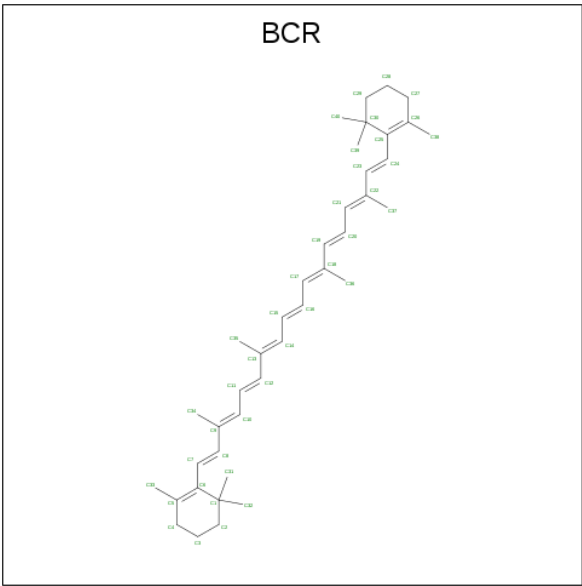
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	O	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	E	1	Total C 40 40	0	0
15	R	1	Total C 40 40	0	0

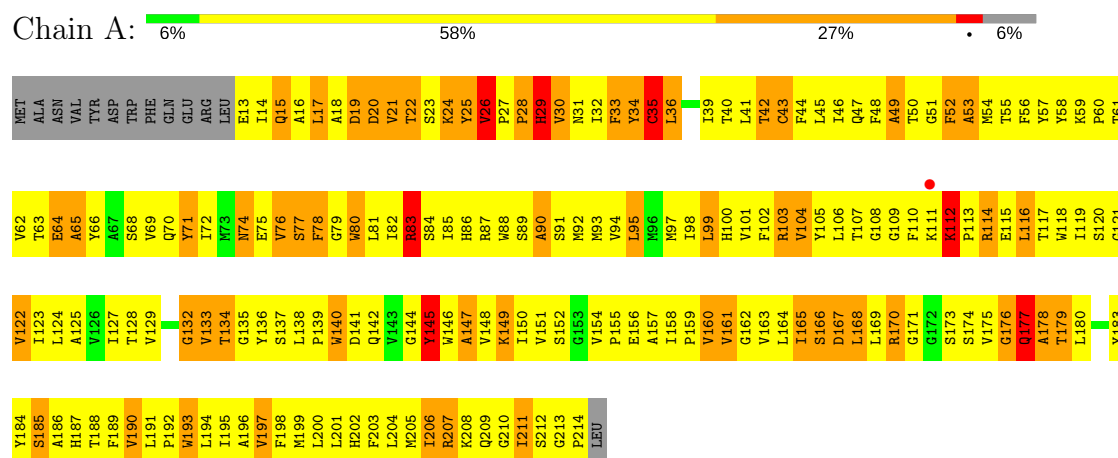
- Molecule 16 is water.

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

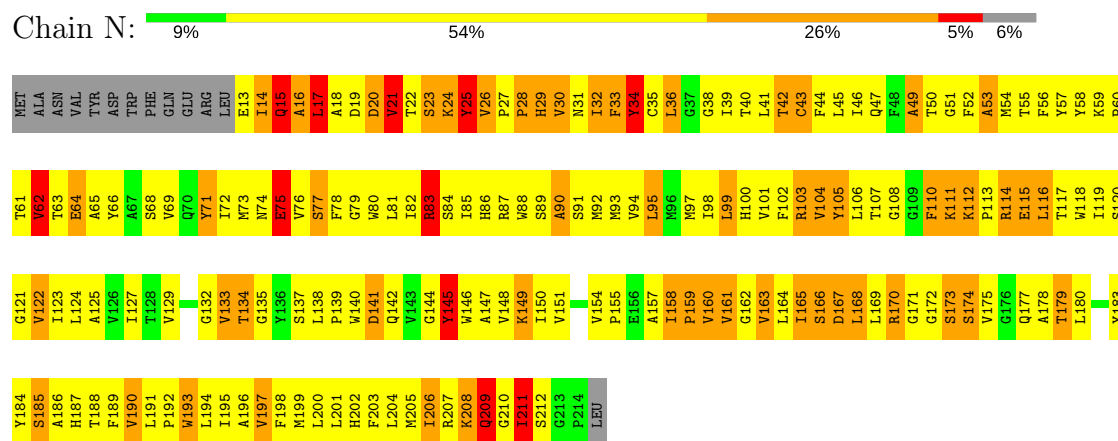
### 3 Residue-property plots

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

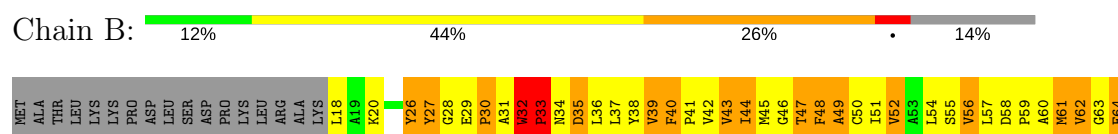
#### • Molecule 1: Cytochrome b6

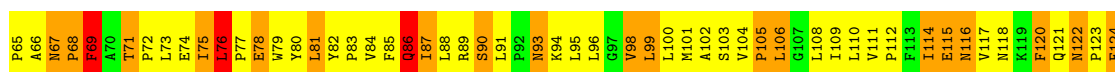


#### • Molecule 1: Cytochrome b6



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

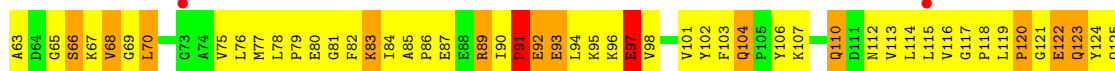
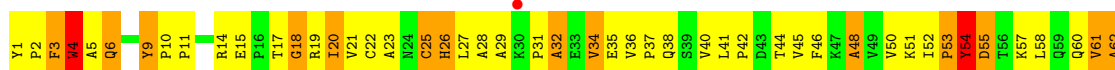
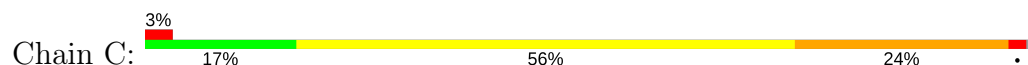




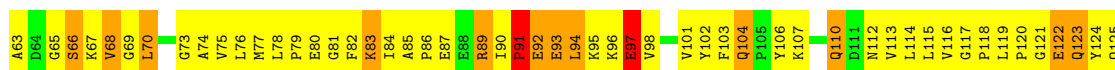
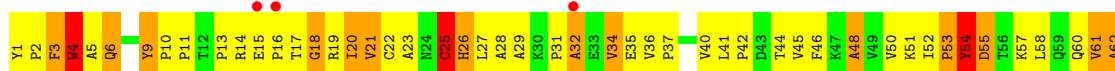
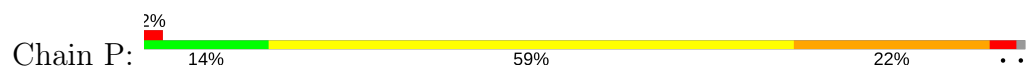
• Molecule 2: Cytochrome b6-f complex subunit 4

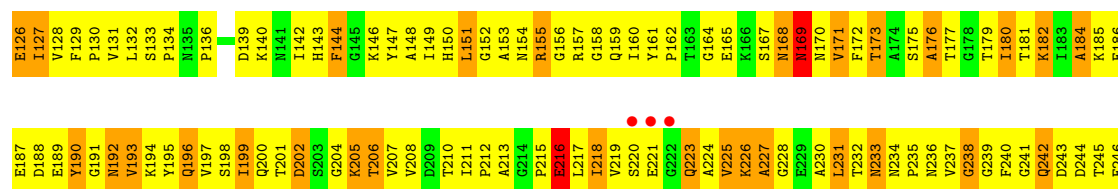


• Molecule 3: Apocytochrome f

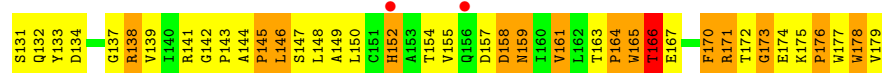
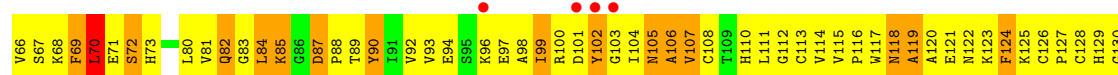
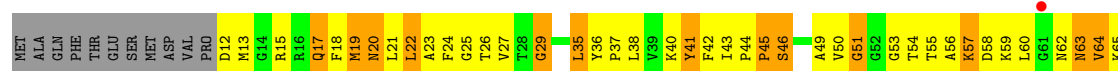
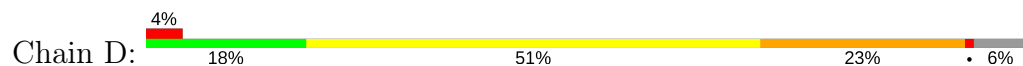


• Molecule 3: Apocytochrome f

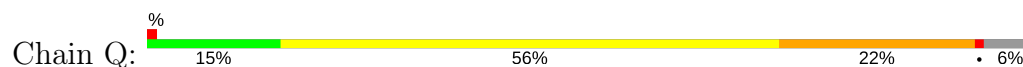




• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



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




• Molecule 5: Cytochrome b6-f complex subunit VI

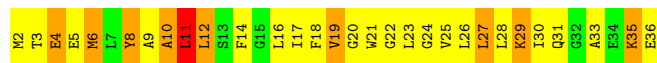


• Molecule 5: Cytochrome b6-f complex subunit VI



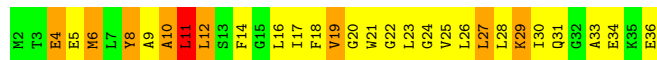
- Molecule 6: Cytochrome b6-f complex subunit VII

Chain F: 



- Molecule 6: Cytochrome b6-f complex subunit VII

Chain S: 



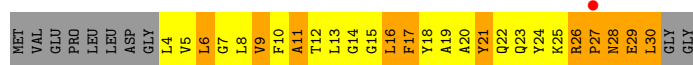
- Molecule 7: Cytochrome b6-f complex subunit V

Chain G: 



- Molecule 7: Cytochrome b6-f complex subunit V

Chain T: 



- Molecule 8: Cytochrome b6-f complex subunit VIII

Chain H: 



- Molecule 8: Cytochrome b6-f complex subunit VIII

Chain U: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.59Å 156.59Å 361.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.76 – 3.80 49.31 – 3.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.76-3.80) 92.5 (49.31-3.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.04 (at 3.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.276 , 0.378 0.263 , 0.252	Depositor DCC
$R_{free}$ test set	1490 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 89.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	14984	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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, 0.333 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: OPC, CLA, BNT, FES, HEC, HEM, BCR

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	0.58	0/1641	0.80	1/2239 (0.0%)
1	N	0.56	0/1641	0.80	1/2239 (0.0%)
2	B	0.61	0/1102	0.97	3/1515 (0.2%)
2	O	0.65	0/1102	1.04	5/1515 (0.3%)
3	C	0.54	0/2248	0.76	0/3061
3	P	0.57	0/2248	0.75	0/3061
4	D	0.63	0/1312	0.80	0/1786
4	Q	0.59	0/1312	0.81	0/1786
5	E	0.68	0/253	0.88	0/340
5	R	0.71	0/253	0.87	0/340
6	F	0.64	0/274	0.77	0/366
6	S	0.61	0/274	0.77	0/366
7	G	0.71	0/221	0.97	1/299 (0.3%)
7	T	0.73	0/221	0.87	0/299
8	H	0.62	0/220	0.83	0/301
8	U	0.61	0/220	0.83	0/301
All	All	0.60	0/14542	0.83	11/19814 (0.1%)

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
2	O	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	144	GLY	N-CA-C	-7.42	94.56	113.10
2	O	144	GLY	N-CA-C	-6.42	97.05	113.10
2	O	149	LEU	CA-CB-CG	5.70	128.41	115.30
2	O	21	GLY	N-CA-C	5.70	127.35	113.10
2	B	69	PHE	N-CA-C	5.60	126.13	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	TYR	Sidechain
2	O	80	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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	1593	0	1623	444	0
1	N	1593	0	1623	469	0
2	B	1067	0	1106	356	0
2	O	1067	0	1106	382	0
3	C	2200	0	2216	423	0
3	P	2200	0	2216	470	0
4	D	1280	0	1265	223	0
4	Q	1280	0	1265	218	0
5	E	248	0	284	135	0
5	R	248	0	284	120	0
6	F	270	0	282	93	0
6	S	270	0	282	75	0
7	G	216	0	220	89	0
7	T	216	0	220	99	0
8	H	214	0	224	37	0
8	U	214	0	224	35	0
9	A	86	0	60	12	0
9	C	43	0	30	4	0
9	N	86	0	60	11	0
9	P	43	0	30	5	0
10	A	43	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	N	43	0	31	10	0
11	B	54	0	83	34	0
11	C	54	0	83	20	0
11	N	54	0	83	14	0
11	O	54	0	83	17	0
12	B	14	0	10	9	0
12	O	14	0	10	7	0
13	B	65	0	70	6	0
13	O	65	0	70	8	0
14	D	4	0	0	3	0
14	Q	4	0	0	2	0
15	E	40	0	56	11	0
15	R	40	0	56	8	0
16	A	1	0	0	1	0
16	N	1	0	0	2	0
All	All	14984	0	15286	3367	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 111.

The worst 5 of 3367 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:34:TYR:HA	1:A:103:ARG:HH11	1.06	1.18
1:N:162:GLY:O	1:N:165:ILE:HG22	1.45	1.16
1:A:106:LEU:HG	5:E:18:ILE:HD12	1.22	1.16
3:C:171:VAL:HG13	3:C:234:ASN:HB2	1.22	1.14
3:P:271:MET:HB3	4:Q:23:ALA:HA	1.15	1.14

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	200/215 (93%)	90 (45%)	64 (32%)	46 (23%)	0	1
1	N	200/215 (93%)	92 (46%)	58 (29%)	50 (25%)	0	1
2	B	135/160 (84%)	56 (42%)	45 (33%)	34 (25%)	0	1
2	O	135/160 (84%)	52 (38%)	39 (29%)	44 (33%)	0	0
3	C	284/289 (98%)	153 (54%)	83 (29%)	48 (17%)	0	4
3	P	284/289 (98%)	153 (54%)	81 (28%)	50 (18%)	0	3
4	D	166/179 (93%)	85 (51%)	50 (30%)	31 (19%)	0	2
4	Q	166/179 (93%)	86 (52%)	49 (30%)	31 (19%)	0	2
5	E	30/32 (94%)	13 (43%)	6 (20%)	11 (37%)	0	0
5	R	30/32 (94%)	13 (43%)	6 (20%)	11 (37%)	0	0
6	F	33/35 (94%)	15 (46%)	11 (33%)	7 (21%)	0	2
6	S	33/35 (94%)	15 (46%)	12 (36%)	6 (18%)	0	3
7	G	25/37 (68%)	11 (44%)	10 (40%)	4 (16%)	0	4
7	T	25/37 (68%)	11 (44%)	10 (40%)	4 (16%)	0	4
8	H	25/29 (86%)	12 (48%)	6 (24%)	7 (28%)	0	0
8	U	25/29 (86%)	12 (48%)	6 (24%)	7 (28%)	0	0
All	All	1796/1952 (92%)	869 (48%)	536 (30%)	391 (22%)	0	1

5 of 391 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	20	ASP
1	A	21	VAL
1	A	22	THR
1	A	26	VAL

### 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	172/184 (94%)	145 (84%)	27 (16%)	3	20
1	N	172/184 (94%)	141 (82%)	31 (18%)	2	14
2	B	116/136 (85%)	99 (85%)	17 (15%)	3	22
2	O	116/136 (85%)	92 (79%)	24 (21%)	1	9
3	C	240/243 (99%)	198 (82%)	42 (18%)	2	15
3	P	240/243 (99%)	199 (83%)	41 (17%)	2	16
4	D	136/146 (93%)	110 (81%)	26 (19%)	1	12
4	Q	136/146 (93%)	110 (81%)	26 (19%)	1	12
5	E	25/25 (100%)	22 (88%)	3 (12%)	5	29
5	R	25/25 (100%)	22 (88%)	3 (12%)	5	29
6	F	27/27 (100%)	23 (85%)	4 (15%)	3	22
6	S	27/27 (100%)	22 (82%)	5 (18%)	2	13
7	G	21/28 (75%)	15 (71%)	6 (29%)	0	3
7	T	21/28 (75%)	14 (67%)	7 (33%)	0	2
8	H	22/24 (92%)	20 (91%)	2 (9%)	10	42
8	U	22/24 (92%)	20 (91%)	2 (9%)	10	42
All	All	1518/1626 (93%)	1252 (82%)	266 (18%)	2	15

5 of 266 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	16	LEU
1	N	149	LYS
4	Q	170	PHE
7	G	26	ARG
1	N	71	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	118	ASN
1	N	15	GLN
4	Q	122	ASN
4	D	159	ASN
1	N	47	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 ⓘ

20 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$
9	HEM	A	301	1	27,50,50	1.96	7 (25%)	17,82,82	2.86	6 (35%)
9	HEM	A	302	1	27,50,50	1.90	8 (29%)	17,82,82	4.38	7 (41%)
10	HEC	A	303	1,16	26,50,50	2.24	10 (38%)	18,82,82	2.55	9 (50%)
13	CLA	B	201	-	58,73,73	2.42	13 (22%)	66,113,113	2.00	18 (27%)
11	OPC	B	305	-	53,53,54	1.36	10 (18%)	59,61,64	1.11	3 (5%)
12	BNT	B	309	-	12,14,14	3.21	4 (33%)	13,21,21	1.51	2 (15%)
9	HEM	C	301	3	27,50,50	1.79	4 (14%)	17,82,82	2.72	5 (29%)
11	OPC	C	306	-	53,53,54	1.36	10 (18%)	59,61,64	1.23	5 (8%)
14	FES	D	201	4	0,4,4	0.00	-	0,4,4	0.00	-
15	BCR	E	101	-	41,41,41	2.53	15 (36%)	56,56,56	2.39	21 (37%)
11	OPC	N	1305	-	53,53,54	1.37	10 (18%)	59,61,64	1.20	5 (8%)
9	HEM	N	301	1	27,50,50	1.82	7 (25%)	17,82,82	3.10	8 (47%)
9	HEM	N	302	1	27,50,50	2.00	8 (29%)	17,82,82	4.71	8 (47%)
10	HEC	N	303	1,16	26,50,50	2.13	9 (34%)	18,82,82	3.32	9 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	CLA	O	1201	-	58,73,73	2.14	16 (27%)	66,113,113	1.99	16 (24%)
11	OPC	O	1306	-	53,53,54	1.37	10 (18%)	59,61,64	1.14	4 (6%)
12	BNT	O	1309	-	12,14,14	3.37	4 (33%)	13,21,21	1.46	2 (15%)
9	HEM	P	301	3	27,50,50	1.78	6 (22%)	17,82,82	2.78	7 (41%)
14	FES	Q	201	4	0,4,4	0.00	-	0,4,4	0.00	-
15	BCR	R	1101	-	41,41,41	2.59	16 (39%)	56,56,56	2.38	22 (39%)

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
9	HEM	A	301	1	-	0/6/54/54	0/0/8/8
9	HEM	A	302	1	-	0/6/54/54	0/0/8/8
10	HEC	A	303	1,16	-	0/6/54/54	0/0/8/8
13	CLA	B	201	-	6/6/20/25	0/37/135/135	0/0/9/9
11	OPC	B	305	-	-	2/57/57/60	0/0/0/0
12	BNT	B	309	-	-	0/4/28/28	0/1/1/1
9	HEM	C	301	3	-	0/6/54/54	0/0/8/8
11	OPC	C	306	-	-	2/57/57/60	0/0/0/0
14	FES	D	201	4	-	0/0/4/4	0/1/1/1
15	BCR	E	101	-	-	0/29/63/63	0/2/2/2
11	OPC	N	1305	-	-	2/57/57/60	0/0/0/0
9	HEM	N	301	1	-	0/6/54/54	0/0/8/8
9	HEM	N	302	1	-	0/6/54/54	0/0/8/8
10	HEC	N	303	1,16	-	0/6/54/54	0/0/8/8
13	CLA	O	1201	-	6/6/20/25	0/37/135/135	0/0/9/9
11	OPC	O	1306	-	-	2/57/57/60	0/0/0/0
12	BNT	O	1309	-	-	0/4/28/28	0/1/1/1
9	HEM	P	301	3	-	0/6/54/54	0/0/8/8
14	FES	Q	201	4	-	0/0/4/4	0/1/1/1
15	BCR	R	1101	-	-	0/29/63/63	0/2/2/2

The worst 5 of 167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	1309	BNT	CAD-CAE	-9.51	1.39	1.52
12	B	309	BNT	CAD-CAE	-8.77	1.40	1.52
13	O	1201	CLA	C3A-C2A	-6.88	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	201	CLA	C3A-C2A	-6.45	1.36	1.54
10	A	303	HEC	C3B-C2B	-6.16	1.34	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	302	HEM	CBA-CAA-C2A	-12.32	88.92	112.48
9	A	302	HEM	CBA-CAA-C2A	-11.59	90.33	112.48
9	A	301	HEM	CMA-C3A-C4A	-7.93	116.28	128.46
9	A	302	HEM	CMA-C3A-C4A	-7.62	116.75	128.46
9	P	301	HEM	CMA-C3A-C4A	-7.58	116.82	128.46

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	O	1201	CLA	C8
13	O	1201	CLA	C2A
13	O	1201	CLA	NA
13	O	1201	CLA	NC
13	O	1201	CLA	C3A

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	N	1305	OPC	CAM-OAN-CAO-OAD
11	O	1306	OPC	CAM-OAN-CAO-OAD
11	C	306	OPC	CAM-OAN-CAO-OAD
11	B	305	OPC	CAM-OAN-CAO-OAD
11	N	1305	OPC	CAM-OAN-CAO-CAP

There are no ring outliers.

20 monomers are involved in 171 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	301	HEM	4	0
9	A	302	HEM	8	0
10	A	303	HEC	4	0
13	B	201	CLA	6	0
11	B	305	OPC	34	0
12	B	309	BNT	9	0
9	C	301	HEM	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	306	OPC	20	0
14	D	201	FES	3	0
15	E	101	BCR	11	0
11	N	1305	OPC	14	0
9	N	301	HEM	8	0
9	N	302	HEM	3	0
10	N	303	HEC	10	0
13	O	1201	CLA	8	0
11	O	1306	OPC	17	0
12	O	1309	BNT	7	0
9	P	301	HEM	5	0
14	Q	201	FES	2	0
15	R	1101	BCR	8	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	202/215 (93%)	-0.41	1 (0%) 90 86	12, 58, 120, 164	0
1	N	202/215 (93%)	-0.46	0 100 100	11, 53, 104, 158	0
2	B	137/160 (85%)	-0.54	0 100 100	16, 67, 137, 177	0
2	O	137/160 (85%)	-0.43	1 (0%) 87 82	13, 63, 130, 183	0
3	C	286/289 (98%)	-0.26	10 (3%) 44 34	9, 85, 150, 200	1 (0%)
3	P	286/289 (98%)	-0.18	6 (2%) 63 53	1, 85, 160, 200	1 (0%)
4	D	168/179 (93%)	-0.20	7 (4%) 36 28	18, 93, 169, 200	0
4	Q	168/179 (93%)	-0.37	2 (1%) 79 71	26, 94, 158, 195	0
5	E	32/32 (100%)	-0.08	2 (6%) 20 15	20, 67, 163, 195	0
5	R	32/32 (100%)	-0.55	0 100 100	21, 59, 111, 162	0
6	F	35/35 (100%)	-0.43	0 100 100	8, 69, 133, 144	0
6	S	35/35 (100%)	-0.48	0 100 100	16, 71, 113, 153	0
7	G	27/37 (72%)	-0.33	0 100 100	34, 66, 133, 147	0
7	T	27/37 (72%)	-0.33	1 (3%) 41 32	30, 76, 136, 178	0
8	H	27/29 (93%)	-0.58	0 100 100	25, 68, 119, 156	0
8	U	27/29 (93%)	-0.46	0 100 100	29, 69, 128, 180	0
All	All	1828/1952 (93%)	-0.34	30 (1%) 72 62	1, 73, 149, 200	2 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	156	GLN	5.5
4	D	152	HIS	4.9
4	D	103	GLY	4.5
4	D	61	GLY	4.4
3	P	221	GLU	4.4

## 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
15	BCR	R	1101	40/40	0.77	0.99	181,181,181,181	0
11	OPC	N	1305	54/55	0.84	0.44	107,107,107,107	0
15	BCR	E	101	40/40	0.85	0.54	84,84,84,84	0
11	OPC	C	306	54/55	0.86	0.36	84,84,84,84	0
11	OPC	O	1306	54/55	0.86	0.38	73,73,73,73	0
12	BNT	O	1309	14/14	0.92	0.29	64,64,64,64	0
11	OPC	B	305	54/55	0.92	0.23	66,66,66,66	0
13	CLA	O	1201	65/65	0.93	0.39	29,72,72,72	0
12	BNT	B	309	14/14	0.93	0.30	64,64,64,64	0
13	CLA	B	201	65/65	0.93	0.48	20,112,112,112	0
10	HEC	A	303	43/43	0.94	0.27	57,104,104,104	0
10	HEC	N	303	43/43	0.95	0.25	67,74,74,74	0
9	HEM	C	301	43/43	0.96	0.26	36,59,59,59	0
9	HEM	A	302	43/43	0.97	0.29	41,58,58,58	0
9	HEM	P	301	43/43	0.97	0.24	54,76,76,76	0
9	HEM	A	301	43/43	0.97	0.33	31,48,48,48	0
9	HEM	N	301	43/43	0.98	0.36	26,64,64,64	0
9	HEM	N	302	43/43	0.98	0.29	30,61,61,61	0
14	FES	Q	201	4/4	0.99	0.13	28,28,53,53	0
14	FES	D	201	4/4	0.99	0.13	70,70,97,97	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.