



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 01:48 pm GMT

PDB ID : 4OGQ  
Title : Internal Lipid Architecture of the Hetero-Oligomeric Cytochrome b6f Complex  
Authors : Hasan, S.S.; Cramer, W.A.  
Deposited on : 2014-01-16  
Resolution : 2.50 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](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:

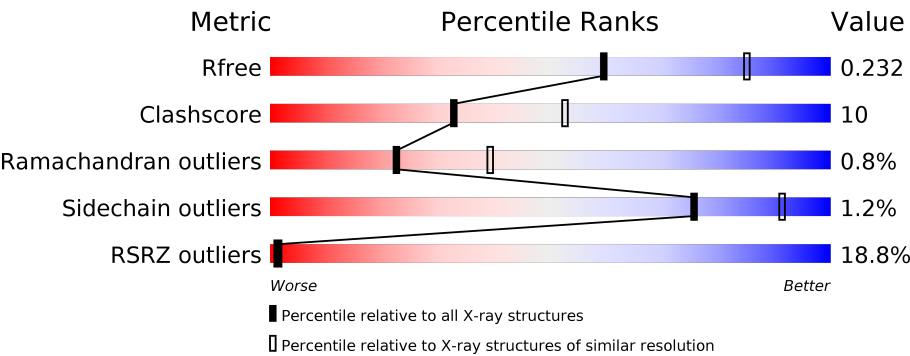
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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>13%</div><div>93%7%</div></div>
2	B	160	<div><div>14%</div><div>89%10%</div></div>
3	C	333	<div><div>14%</div><div>70%14%16%</div></div>
4	D	179	<div><div>36%</div><div>74%18%7%</div></div>
5	E	31	<div><div>16%</div><div>77%16%</div></div>
6	F	34	<div><div>3%</div><div>74%21%6%</div></div>

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Mol	Chain	Length	Quality of chain
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	UMQ	B	203[B]	-	-	-	X
10	UMQ	D	201	-	-	-	X
10	UMQ	G	101	-	-	-	X
11	7PH	B	206	-	-	-	X
11	7PH	C	303	-	-	-	X
11	7PH	F	104	-	-	-	X
12	8K6	A	306	-	-	-	X
12	8K6	A	307	-	-	-	X
12	8K6	A	308	-	-	-	X
12	8K6	B	202[A]	-	-	-	X
14	CLA	B	204	X	-	-	-
15	OPC	B	205	-	-	-	X
17	MYS	D	202	-	-	-	X
20	2WD	D	206	-	-	-	X
22	2WA	F	101	-	-	-	X
24	1O2	F	103	X	-	-	X

## 2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 8396 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	214	Total	C	N	O	S	0	0	0
			1708	1139	271	288	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	159	Total	C	N	O	S	0	0	0
			1232	825	194	208	5			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	281	Total	C	N	O	S	0	0	0
			2137	1361	355	415	6			

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1250	791	213	240	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	31	Total	C	N	O	S	0	0	0
			228	157	35	35	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
			231	156	36	38	1			

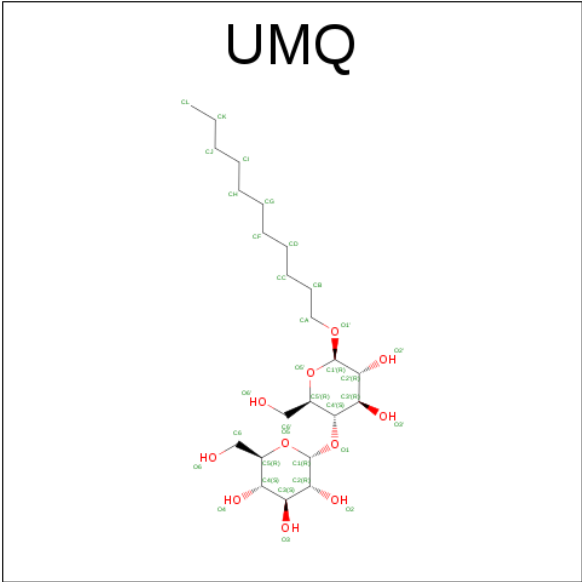
- | Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7   | G     | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 282   | 188 | 44 | 49 | 1 |         |         |       |

- | Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8   | H     | 29       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 228   | 155 | 36 | 35 | 2 |         |         |       |

- # HEM

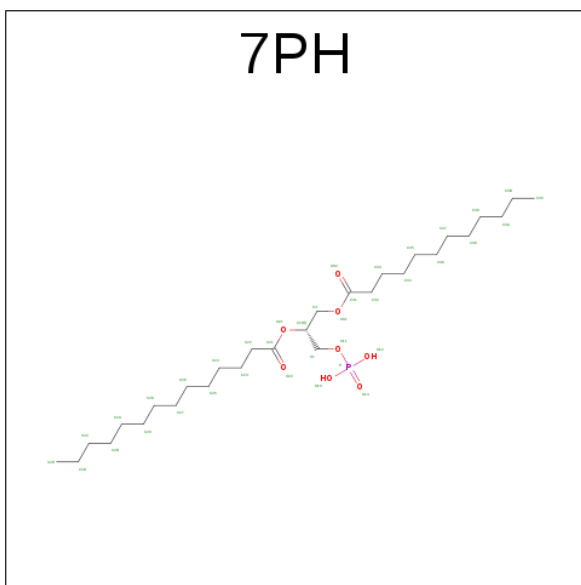
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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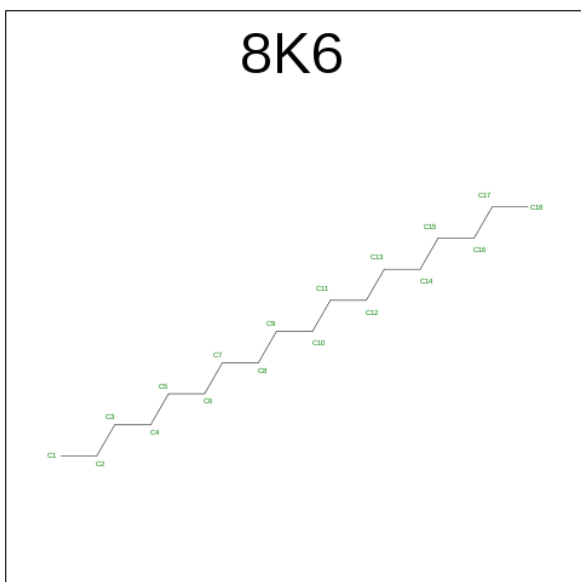
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			34	23	11		
10	B	1	Total	C	O	0	0
			34	23	11		
10	B	1	Total	C	O	0	1
			34	23	11		
10	D	1	Total	C	O	0	0
			34	23	11		
10	G	1	Total	C	O	0	0
			34	23	11		

- Molecule 11 is (1R)-2-(DODECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL TETRADECANOATE (three-letter code: 7PH) (formula: C<sub>29</sub>H<sub>57</sub>O<sub>8</sub>P).



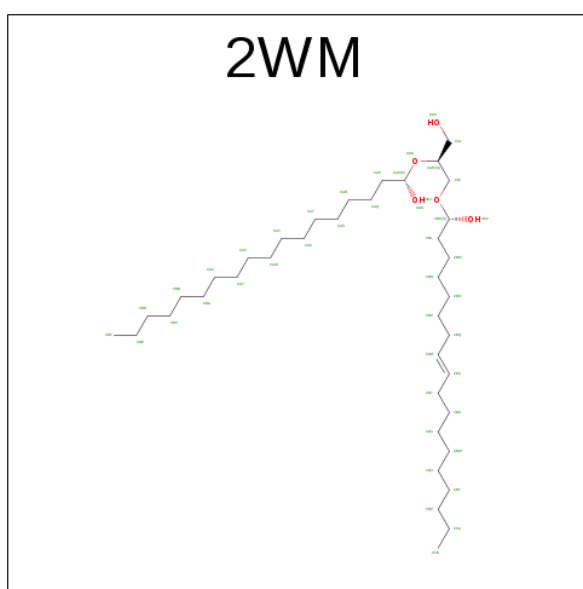
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			32	27	5		
11	B	1	Total	C	O	0	0
			32	27	5		
11	C	1	Total	C	O	0	0
			32	27	5		
11	D	1	Total	C	O	0	0
			32	27	5		
11	F	1	Total	C	O	0	0
			32	27	5		

- Molecule 12 is OCTADECANE (three-letter code: 8K6) (formula: C<sub>18</sub>H<sub>38</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C 18 18	0	0
12	A	1	Total C 18 18	0	0
12	A	1	Total C 14 14	0	0
12	B	1	Total C 18 18	0	1

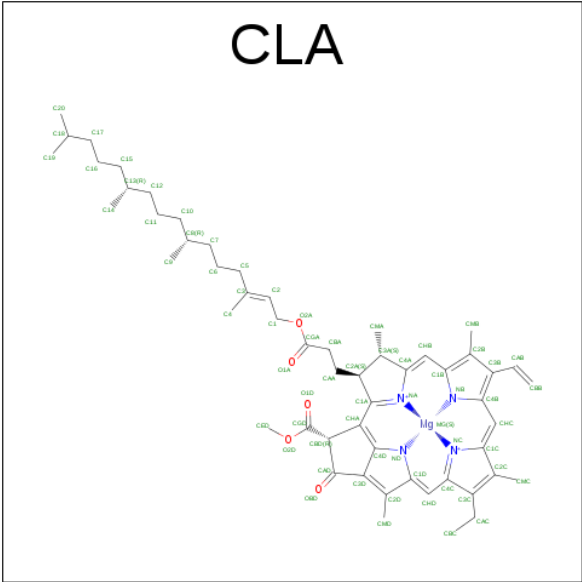
- Molecule 13 is (1S,8E)-1-{[(2S)-3-HYDROXY-2-{[(1S)-1-HYDROXYOCTADECYL]OXY}PROPYL]OXY}OCTADEC-8-EN-1-OL (three-letter code: 2WM) (formula: C<sub>39</sub>H<sub>78</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 44 39 5	0	0

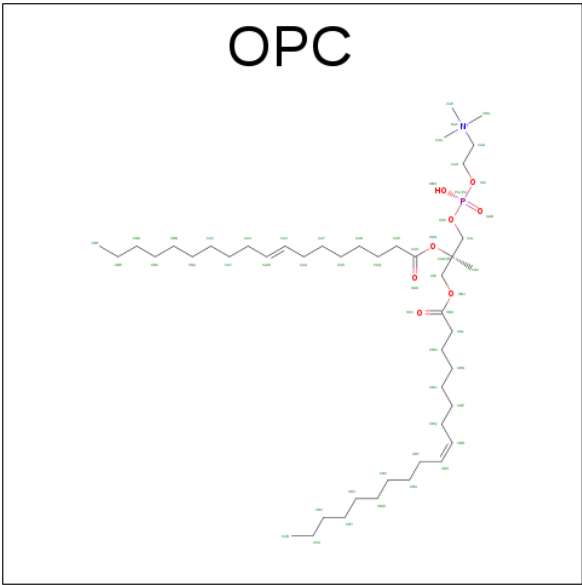
- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).





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

- Molecule 15 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).

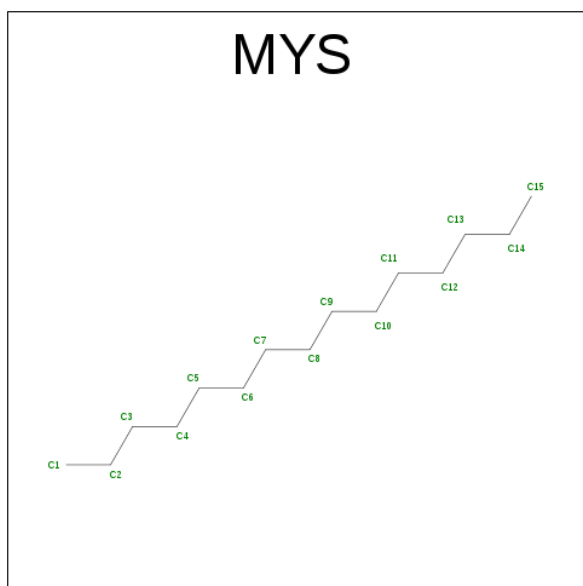


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 16 is CADMIUM ION (three-letter code: CD) (formula: Cd).

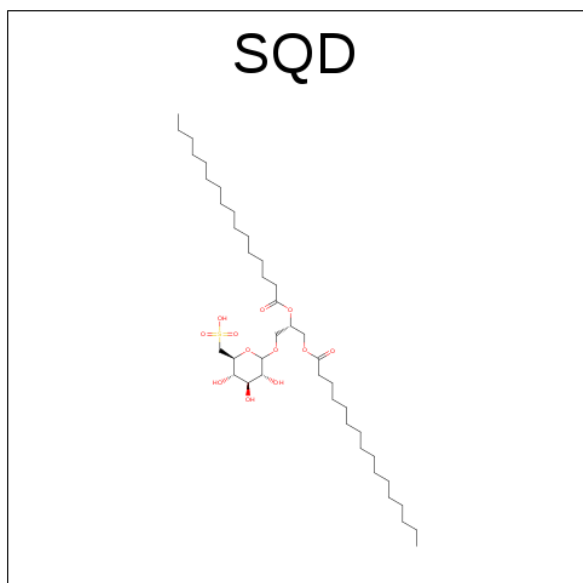
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	C	1	Total	Cd	0	0
			1	1		

- Molecule 17 is PENTADECANE (three-letter code: MYS) (formula:  $C_{15}H_{32}$ ).



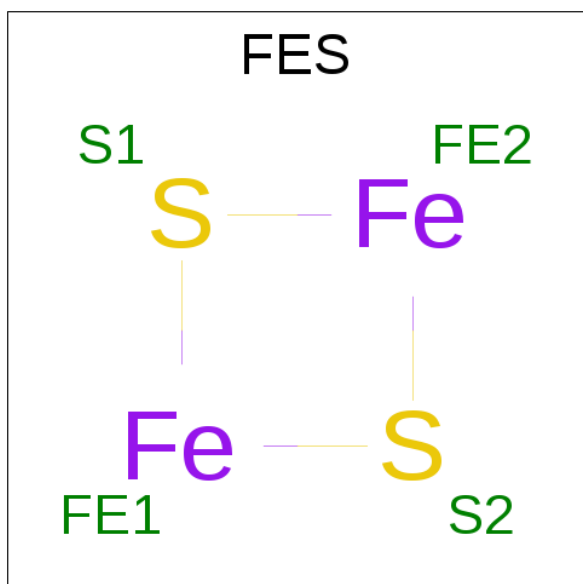
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	D	1	Total	C	0	0
			15	15		

- Molecule 18 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



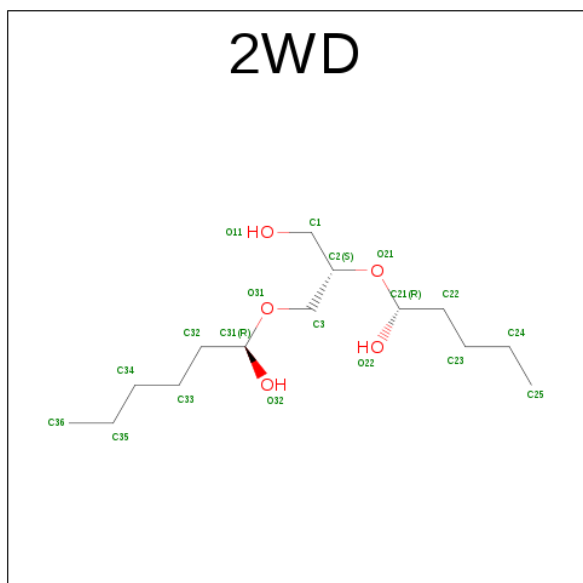
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



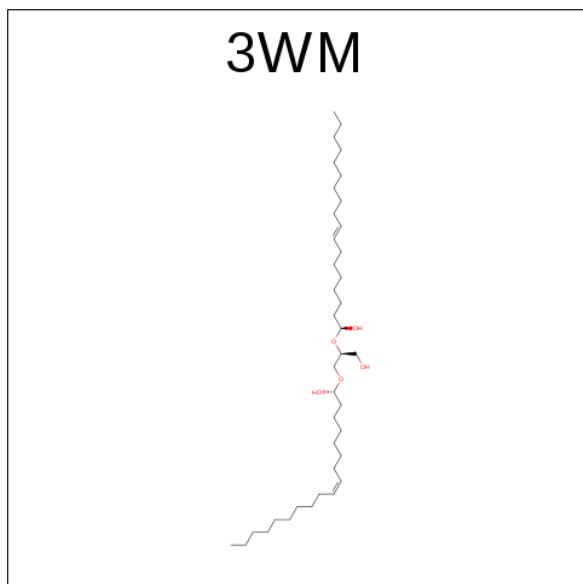
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 20 is (1R)-1-{[(2S)-3-HYDROXY-2-{[(1R)-1-HYDROXYPENTYL]OXY}PROPYL]OXY}HEXAN-1-OL (three-letter code: 2WD) (formula:  $\text{C}_{14}\text{H}_{30}\text{O}_5$ ).



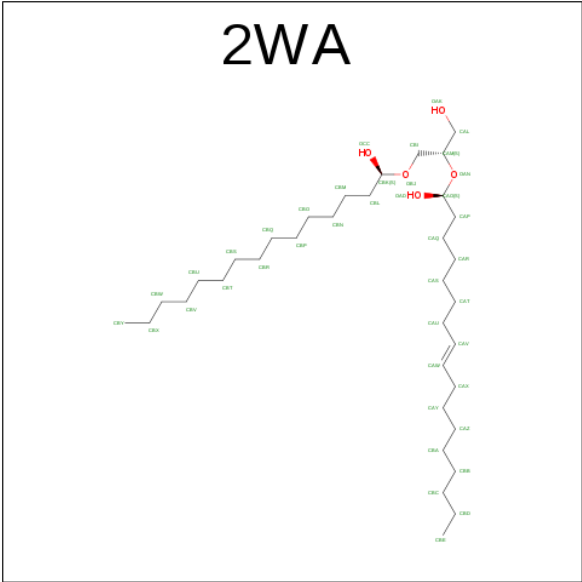
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	D	1	Total	C	O	0	0
			19	14	5		

- Molecule 21 is (1S,8E,1'R,8'Z)-1,1'-{[(2S)-3-HYDROXYPROPANE-1,2-DIYL]BIS(OXY)} BIS(OCTADEC-8-EN-1-OL (three-letter code: 3WM) (formula: C<sub>39</sub>H<sub>76</sub>O<sub>5</sub>).



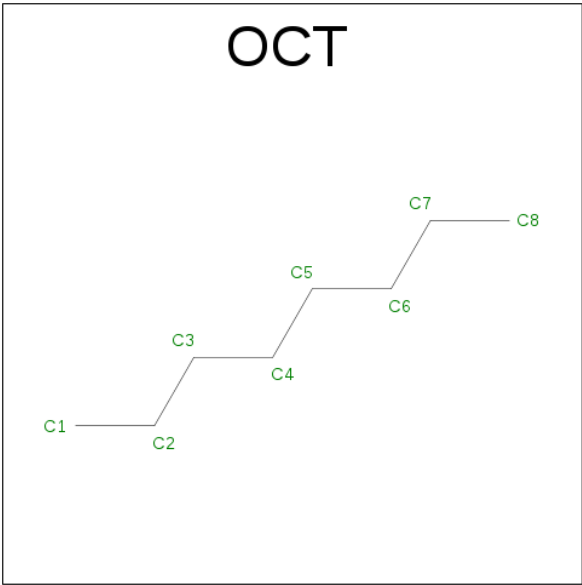
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	E	1	Total	C	O	0	0
			44	39	5		

- Molecule 22 is (1S,8E)-1-{[(2S)-1-HYDROXY-3-{[(1S)-1-HYDROXPENTADECYL]OXY}PROPAN-2-YL]OXY}HEPTADEC-8-EN-1-OL (three-letter code: 2WA) (formula: C<sub>35</sub>H<sub>70</sub>O<sub>5</sub>).



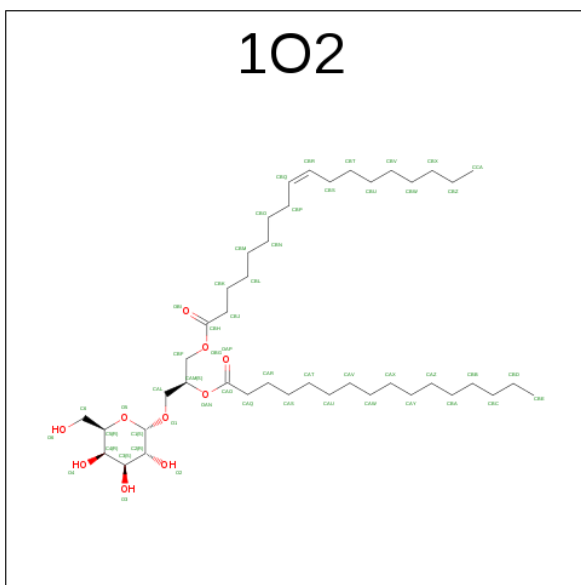
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	F	1	Total	C	O	0
			40	35	5	

- Molecule 23 is N-OCTANE (three-letter code: OCT) (formula: C<sub>8</sub>H<sub>18</sub>).



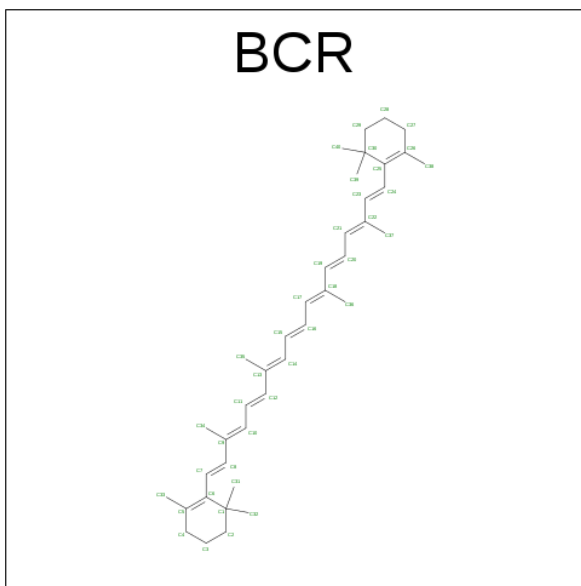
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	F	1	Total	C		0
			8	8		

- Molecule 24 is (2S)-3-(ALPHA-D-GALACTOPYRANOSYLOXY)-2-(HEXADECANOYLOXY)PROPYL (9Z)-OCTADEC-9-ENOATE (three-letter code: 1O2) (formula: C<sub>43</sub>H<sub>80</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	F	1	Total	C	O	0	0
			49	39	10		

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



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

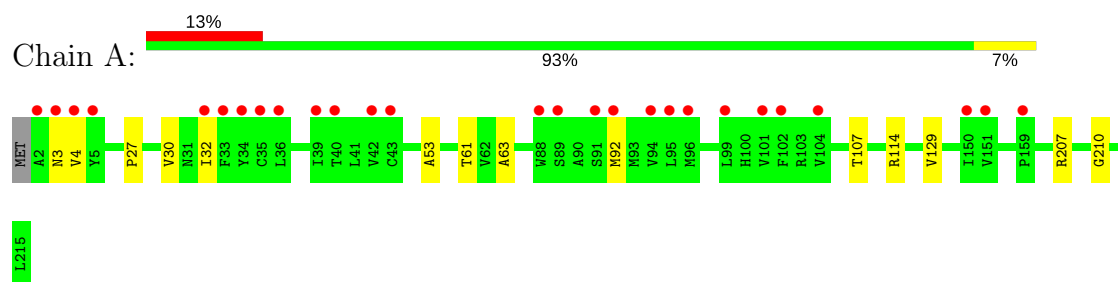
- Molecule 26 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	21	Total 21	O 21	0	0
26	B	25	Total 25	O 25	0	0
26	C	38	Total 38	O 38	0	0
26	D	1	Total 1	O 1	0	0
26	F	1	Total 1	O 1	0	0
26	G	7	Total 7	O 7	0	0

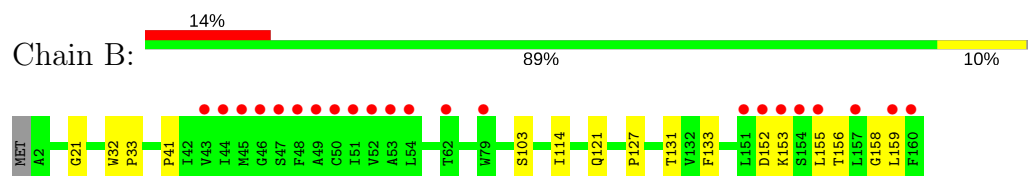
### 3 Residue-property plots [i](#)

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.

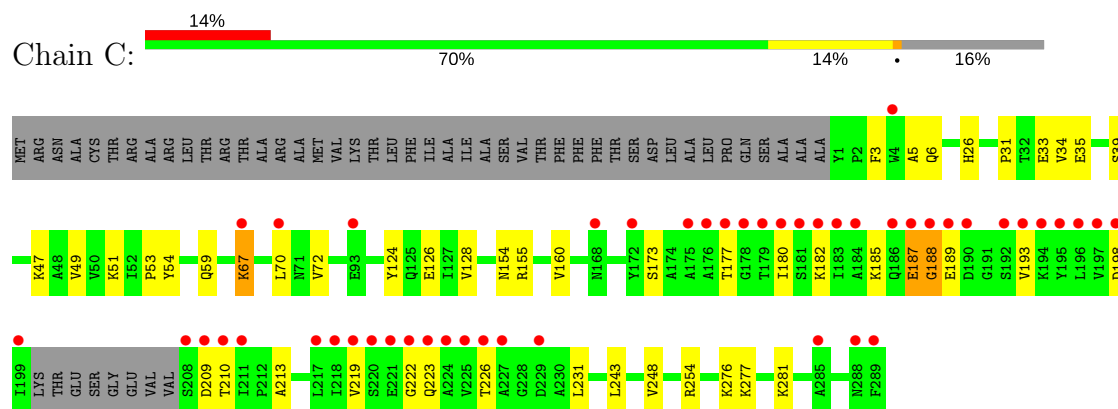
- Molecule 1: Cytochrome b6



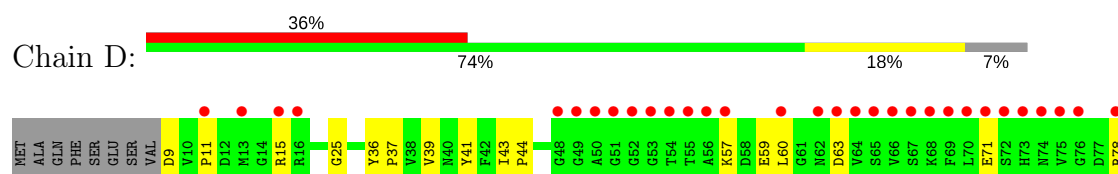
- Molecule 2: Cytochrome b6-f complex subunit 4



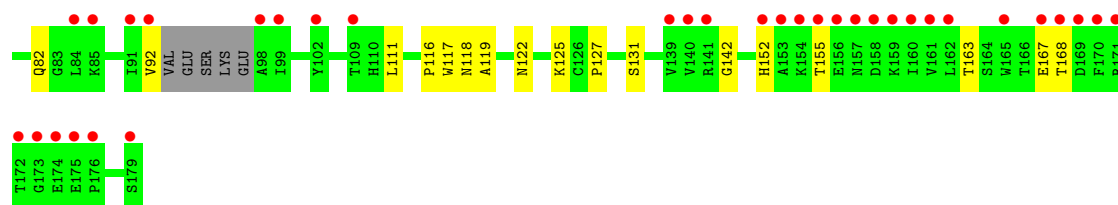
- Molecule 3: Apocytochrome f



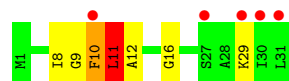
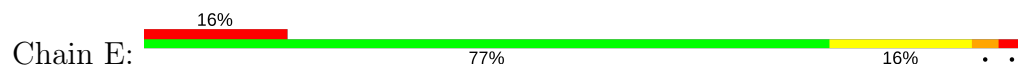
- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 1



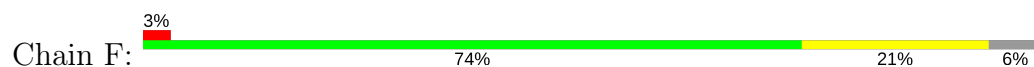




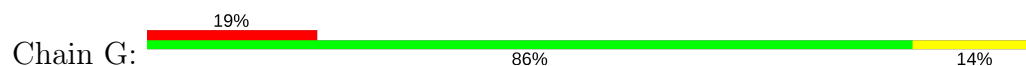
• Molecule 5: Cytochrome b6-f complex subunit 6



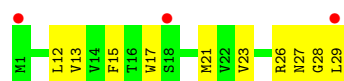
• Molecule 6: Cytochrome b6-f complex subunit 7



• 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, $\alpha$ , $\beta$ , $\gamma$	159.23Å 159.23Å 365.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.57 – 2.50 39.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.57-2.50) 89.3 (39.57-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.201 , 0.232 0.200 , 0.232	Depositor DCC
$R_{free}$ test set	4696 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.4	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 80.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8396	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2WA, 2WD, 1O2, 3WM, MYS, CLA, 2WM, BCR, 7PH, FES, OPC, UMQ, CD, 8K6, OCT, HEM, 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	0.26	0/1761	0.41	0/2401
2	B	0.23	0/1271	0.38	0/1742
3	C	0.22	0/2182	0.38	0/2972
4	D	0.22	0/1281	0.40	0/1745
5	E	0.25	0/231	0.65	0/309
6	F	0.22	0/234	0.33	0/315
7	G	0.23	0/287	0.34	0/387
8	H	0.26	0/234	0.39	0/319
All	All	0.23	0/7481	0.40	0/10190

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
5	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	10	PHE	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	1708	0	1721	13	0
2	B	1232	0	1278	14	0
3	C	2137	0	2122	28	0
4	D	1250	0	1208	20	0
5	E	228	0	257	9	0
6	F	231	0	252	8	0
7	G	282	0	303	4	0
8	H	228	0	243	9	0
9	A	129	0	90	9	0
9	C	43	0	30	3	0
10	A	34	0	44	9	0
10	B	68	0	87	17	0
10	D	34	0	44	4	0
10	G	34	0	44	4	0
11	A	32	0	45	1	0
11	B	32	0	45	5	0
11	C	32	0	45	4	0
11	D	32	0	45	1	0
11	F	32	0	45	6	0
12	A	50	0	103	8	0
12	B	18	0	38	2	0
13	A	44	0	78	0	0
14	B	65	0	72	4	0
15	B	54	0	83	5	0
16	C	1	0	0	0	0
17	D	15	0	32	1	0
18	D	54	0	77	2	0
19	D	4	0	0	0	0
20	D	19	0	30	2	0
21	E	44	0	76	9	0
22	F	40	0	70	7	0
23	F	8	0	18	0	0
24	F	49	0	69	11	0
25	G	40	0	56	2	0
26	A	21	0	0	0	0
26	B	25	0	0	1	0
26	C	38	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	D	1	0	0	0	0
26	F	1	0	0	0	0
26	G	7	0	0	0	0
All	All	8396	0	8750	168	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 10.

The worst 5 of 168 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)
10:G:101:UMQ:C5'	10:G:101:UMQ:O5'	1.63	1.46
10:A:304:UMQ:C5'	10:A:304:UMQ:O5'	1.63	1.45
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C5'	1.63	1.44
10:B:201:UMQ:C1'	10:B:201:UMQ:O5'	1.69	1.41
10:B:203[B]:UMQ:O5'	10:B:203[B]:UMQ:C1'	1.69	1.38

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	212/215 (99%)	202 (95%)	9 (4%)	1 (0%)	32	53
2	B	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
3	C	277/333 (83%)	249 (90%)	23 (8%)	5 (2%)	10	17
4	D	162/179 (90%)	147 (91%)	15 (9%)	0	100	100
5	E	29/31 (94%)	26 (90%)	2 (7%)	1 (3%)	4	5
6	F	30/34 (88%)	30 (100%)	0	0	100	100
7	G	35/37 (95%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
All	All	929/1018 (91%)	865 (93%)	57 (6%)	7 (1%)	22	39

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	173	SER
1	A	3	ASN
3	C	185	LYS
5	E	11	LEU
3	C	189	GLU

### 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	183/184 (100%)	183 (100%)	0	100	100
2	B	133/134 (99%)	131 (98%)	2 (2%)	70	89
3	C	231/272 (85%)	228 (99%)	3 (1%)	73	90
4	D	133/145 (92%)	130 (98%)	3 (2%)	56	81
5	E	21/21 (100%)	20 (95%)	1 (5%)	30	53
6	F	22/24 (92%)	22 (100%)	0	100	100
7	G	29/29 (100%)	29 (100%)	0	100	100
8	H	24/24 (100%)	24 (100%)	0	100	100
All	All	776/833 (93%)	767 (99%)	9 (1%)	75	91

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	231	LEU
5	E	11	LEU
4	D	111	LEU
3	C	67	LYS

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Mol	Chain	Res	Type
4	D	71	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	154	ASN

### 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 ⓘ

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	$\# Z  > 2$
9	HEM	A	301	1	28,50,50	2.17	7 (25%)	17,82,82	1.53	5 (29%)
9	HEM	A	302	1	28,50,50	2.14	6 (21%)	17,82,82	1.49	4 (23%)
9	HEM	A	303	1,26	28,50,50	2.27	6 (21%)	17,82,82	1.47	2 (11%)
10	UMQ	A	304	-	35,35,35	3.77	17 (48%)	46,46,46	2.19	8 (17%)
11	7PH	A	305	-	31,31,37	1.25	2 (6%)	33,33,42	1.22	2 (6%)
12	8K6	A	306	-	17,17,17	0.09	0	16,16,16	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	8K6	A	307	-	17,17,17	0.08	0	16,16,16	0.87	0
12	8K6	A	308	-	13,13,17	0.10	0	12,12,16	0.78	0
13	2WM	A	309	-	43,43,43	0.65	2 (4%)	43,45,45	0.50	0
10	UMQ	B	201	-	35,35,35	3.76	17 (48%)	46,46,46	2.21	7 (15%)
12	8K6	B	202[A]	-	17,17,17	0.09	0	16,16,16	0.85	0
10	UMQ	B	203[B]	-	35,35,35	3.77	17 (48%)	46,46,46	2.21	9 (19%)
14	CLA	B	204	26	56,73,73	1.10	4 (7%)	65,113,113	1.22	7 (10%)
15	OPC	B	205	-	53,53,54	1.03	2 (3%)	58,61,64	1.03	2 (3%)
11	7PH	B	206	-	31,31,37	1.26	2 (6%)	33,33,42	1.18	2 (6%)
9	HEM	C	301	3	28,50,50	2.14	6 (21%)	17,82,82	1.49	3 (17%)
11	7PH	C	303	-	31,31,37	1.26	2 (6%)	33,33,42	1.23	2 (6%)
10	UMQ	D	201	-	35,35,35	3.78	17 (48%)	46,46,46	2.25	9 (19%)
17	MYS	D	202	-	14,14,14	0.09	0	13,13,13	0.83	0
11	7PH	D	203	-	31,31,37	1.26	2 (6%)	33,33,42	1.15	2 (6%)
18	SQD	D	204	-	53,54,54	0.96	5 (9%)	63,65,65	1.70	10 (15%)
19	FES	D	205	4	0,4,4	0.00	-	0,4,4	0.00	-
20	2WD	D	206	-	18,18,18	1.14	1 (5%)	18,20,20	0.55	0
21	3WM	E	101	-	43,43,43	0.76	1 (2%)	43,45,45	0.53	0
22	2WA	F	101	-	39,39,39	0.89	1 (2%)	39,41,41	0.53	0
23	OCT	F	102	-	7,7,7	0.13	0	6,6,6	0.70	0
24	1O2	F	103	-	49,49,53	1.46	5 (10%)	57,57,61	1.15	6 (10%)
11	7PH	F	104	-	31,31,37	1.26	2 (6%)	33,33,42	1.21	2 (6%)
10	UMQ	G	101	-	35,35,35	3.77	17 (48%)	46,46,46	2.23	8 (17%)
25	BCR	G	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	4 (7%)

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
9	HEM	A	303	1,26	-	0/6/54/54	0/0/8/8
10	UMQ	A	304	-	-	0/20/60/60	0/2/2/2
11	7PH	A	305	-	-	0/33/33/39	0/0/0/0
12	8K6	A	306	-	-	0/15/15/15	0/0/0/0
12	8K6	A	307	-	-	0/15/15/15	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	8K6	A	308	-	-	0/11/11/15	0/0/0/0
13	2WM	A	309	-	-	0/44/45/45	0/0/0/0
10	UMQ	B	201	-	-	0/20/60/60	0/2/2/2
12	8K6	B	202[A]	-	-	0/15/15/15	0/0/0/0
10	UMQ	B	203[B]	-	-	1/20/60/60	0/2/2/2
14	CLA	B	204	26	3/3/20/25	0/37/135/135	0/0/9/9
15	OPC	B	205	-	-	0/57/57/60	0/0/0/0
11	7PH	B	206	-	-	0/33/33/39	0/0/0/0
9	HEM	C	301	3	-	0/6/54/54	0/0/8/8
11	7PH	C	303	-	-	0/33/33/39	0/0/0/0
10	UMQ	D	201	-	-	0/20/60/60	0/2/2/2
17	MYS	D	202	-	-	0/12/12/12	0/0/0/0
11	7PH	D	203	-	-	0/33/33/39	0/0/0/0
18	SQD	D	204	-	-	0/49/69/69	0/1/1/1
19	FES	D	205	4	-	0/0/4/4	0/1/1/1
20	2WD	D	206	-	-	0/19/20/20	0/0/0/0
21	3WM	E	101	-	-	0/44/45/45	0/0/0/0
22	2WA	F	101	-	-	0/40/41/41	0/0/0/0
23	OCT	F	102	-	-	0/5/5/5	0/0/0/0
24	1O2	F	103	-	1/1/8/10	0/44/64/68	0/1/1/1
11	7PH	F	104	-	-	0/33/33/39	0/0/0/0
10	UMQ	G	101	-	-	0/20/60/60	0/2/2/2
25	BCR	G	102	-	-	0/29/63/63	0/2/2/2

The worst 5 of 143 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	203[B]	UMQ	C6-C5	-5.78	1.32	1.51
10	B	201	UMQ	C6-C5	-5.75	1.32	1.51
10	D	201	UMQ	C6-C5	-5.74	1.32	1.51
10	A	304	UMQ	C6-C5	-5.73	1.32	1.51
10	G	101	UMQ	C6-C5	-5.70	1.32	1.51

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	201	UMQ	C1'-O5'-C5'	-9.70	95.44	113.72
10	G	101	UMQ	C1'-O5'-C5'	-9.35	96.10	113.72
10	B	203[B]	UMQ	C1'-O5'-C5'	-9.19	96.41	113.72
10	A	304	UMQ	C1'-O5'-C5'	-9.14	96.50	113.72
10	B	201	UMQ	C1'-O5'-C5'	-9.10	96.57	113.72

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	F	103	1O2	C1
14	B	204	CLA	NC
14	B	204	CLA	ND
14	B	204	CLA	NA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	203[B]	UMQ	CA-O1'-C1'-O5'

There are no ring outliers.

27 monomers are involved in 106 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	301	HEM	2	0
9	A	302	HEM	2	0
9	A	303	HEM	5	0
10	A	304	UMQ	9	0
11	A	305	7PH	1	0
12	A	306	8K6	2	0
12	A	307	8K6	2	0
12	A	308	8K6	5	0
10	B	201	UMQ	7	0
12	B	202[A]	8K6	2	0
10	B	203[B]	UMQ	10	0
14	B	204	CLA	4	0
15	B	205	OPC	5	0
11	B	206	7PH	5	0
9	C	301	HEM	3	0
11	C	303	7PH	4	0
10	D	201	UMQ	4	0
17	D	202	MYS	1	0
11	D	203	7PH	1	0
18	D	204	SQD	2	0
20	D	206	2WD	2	0
21	E	101	3WM	9	0
22	F	101	2WA	7	0
24	F	103	1O2	11	0
11	F	104	7PH	6	0
10	G	101	UMQ	4	0
25	G	102	BCR	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	214/215 (99%)	0.47	27 (12%) 4 3	43, 59, 97, 186	0
2	B	159/160 (99%)	0.54	22 (13%) 3 3	52, 77, 124, 195	0
3	C	281/333 (84%)	0.89	48 (17%) 2 1	57, 85, 191, 249	0
4	D	166/179 (92%)	2.12	65 (39%) 0 0	50, 145, 205, 239	0
5	E	31/31 (100%)	0.43	5 (16%) 2 2	81, 98, 123, 153	0
6	F	32/34 (94%)	0.13	1 (3%) 49 52	69, 87, 131, 169	0
7	G	37/37 (100%)	1.08	7 (18%) 1 1	57, 74, 144, 155	0
8	H	29/29 (100%)	1.10	3 (10%) 7 6	59, 71, 100, 144	0
All	All	949/1018 (93%)	0.93	178 (18%) 1 1	43, 81, 185, 249	0

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	199	ILE	12.1
2	B	160	PHE	11.6
4	D	69	PHE	9.7
3	C	183	ILE	9.2
3	C	196	LEU	9.2

### 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 ⓘ

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
11	7PH	B	206	32/38	0.56	0.71	18.50	77,132,182,184	0
20	2WD	D	206	19/19	0.63	0.67	18.26	75,123,142,145	0
24	1O2	F	103	49/53	0.65	0.63	10.23	80,127,216,220	0
17	MYS	D	202	15/15	0.56	0.39	8.09	93,107,121,126	0
12	8K6	A	307	18/18	0.67	0.36	7.01	76,108,124,127	0
10	UMQ	G	101	34/34	0.51	0.69	6.08	81,173,199,284	0
10	UMQ	D	201	34/34	0.59	0.66	5.78	102,210,248,264	0
12	8K6	A	306	18/18	0.63	0.30	5.47	93,113,147,148	0
11	7PH	C	303	32/38	0.67	0.40	4.28	73,117,149,150	0
12	8K6	B	202[A]	18/18	0.64	0.46	3.60	47,102,122,122	18
10	UMQ	B	203[B]	34/34	0.77	0.41	3.54	80,103,132,144	34
12	8K6	A	308	14/18	0.77	0.30	3.45	62,82,95,99	0
11	7PH	F	104	32/38	0.81	0.28	3.27	81,101,172,175	0
22	2WA	F	101	40/40	0.63	0.38	2.80	70,111,169,182	0
15	OPC	B	205	54/55	0.95	0.23	2.40	55,92,121,137	0
13	2WM	A	309	44/44	0.77	0.29	1.68	70,96,152,158	0
11	7PH	D	203	32/38	0.65	0.25	1.57	54,81,153,157	0
11	7PH	A	305	32/38	0.71	0.37	1.41	93,126,189,190	0
18	SQD	D	204	54/54	0.92	0.27	1.30	73,116,159,177	0
21	3WM	E	101	44/44	0.62	0.35	1.28	60,97,122,125	0
10	UMQ	B	201	34/34	0.86	0.30	0.86	64,114,151,224	0
25	BCR	G	102	40/40	0.66	0.35	0.85	49,74,116,122	0
14	CLA	B	204	65/65	0.93	0.21	0.53	59,79,107,117	0
9	HEM	A	302	43/43	0.99	0.23	0.24	34,57,71,76	0
9	HEM	A	301	43/43	0.98	0.18	-0.10	31,50,65,78	0
9	HEM	C	301	43/43	0.98	0.17	-0.19	46,69,96,113	0
9	HEM	A	303	43/43	0.97	0.21	-0.21	47,66,85,95	0
19	FES	D	205	4/4	0.99	0.06	-1.84	96,97,100,102	0
23	OCT	F	102	8/8	0.75	0.48	-	101,106,110,116	0
10	UMQ	A	304	34/34	0.67	0.46	-	127,146,201,254	0
16	CD	C	302	1/1	0.67	0.11	-	136,136,136,136	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.