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wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 08:53 am BST

PDB ID	:	4I7Z
Title	:	Crystal structure of cytochrome b6f in DOPG, with disordered Rieske Iron-Sulfur Protein soluble domain
Authors	:	Hasan, S.S.; Stofleth, J.T.; Yamashita, E.; Cramer, W.A.
Deposited on	:	2012-12-01
Resolution	:	2.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 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	Percentile Ranks	Value
Rfree		0.274
Clashscore		3
Ramachandran outliers		0.4%
Sidechain outliers		6.6%
RSRZ outliers		11.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
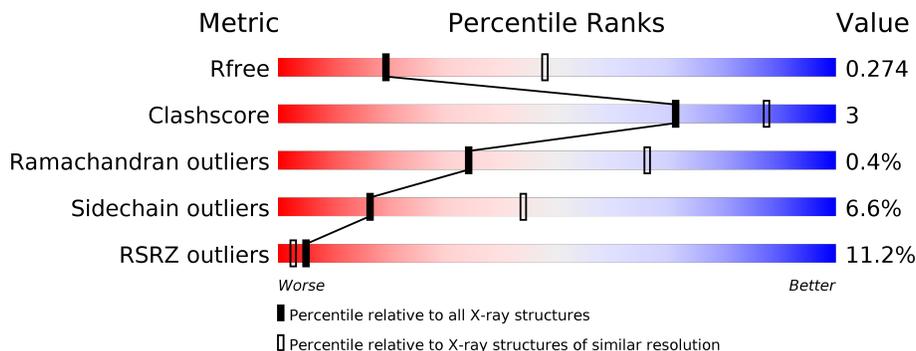
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	89% 10%
2	B	160	5% / 94% 6%
3	C	289	23% / 88% 11%
4	D	179	3% / 21% 79%
5	E	32	9% / 84% 13%
6	F	35	6% / 86% 11%

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Mol	Chain	Length	Quality of chain
7	G	37	19% / 86% / 8% / 5%
8	H	29	69% / 24%

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	8K6	A	305	-	-	-	X
12	UMQ	A	306	X	-	-	-
12	UMQ	A	307	X	-	-	-
12	UMQ	A	308	X	-	-	-
14	CLA	B	201	X	-	-	-
15	OZ2	B	203	X	-	-	-
16	1E2	D	201	X	-	-	-
17	OCT	F	101	-	-	-	X

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 13828 atoms, of which 6869 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
			Total	C	H	N	O	S			
1	A	213	3419	1132	1721	270	286	10	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	159	2538	836	1297	192	208	5	0	0	0

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	288	4450	1415	2234	369	424	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	PRO	GLU	ENGINEERED MUTATION	UNP P83793

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	38	591	194	299	47	49	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	E	28	452	156	237	29	30	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	31	Total	C	H	N	O	S	0	0	0
			482	160	248	34	39	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	35	Total	C	H	N	O	0	0	0
			536	178	268	42	48			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	28	Total	C	H	N	O	S	0	0	0
			449	151	227	35	35	1			

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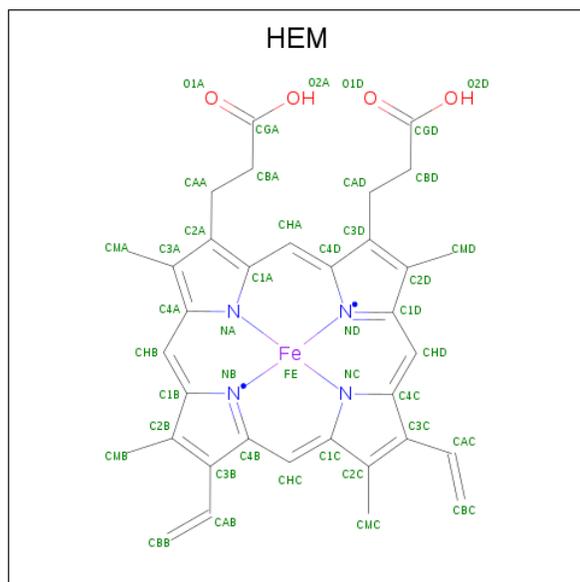

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 10 is PENTADECANE (three-letter code: MYS) (formula: $C_{15}H_{32}$).
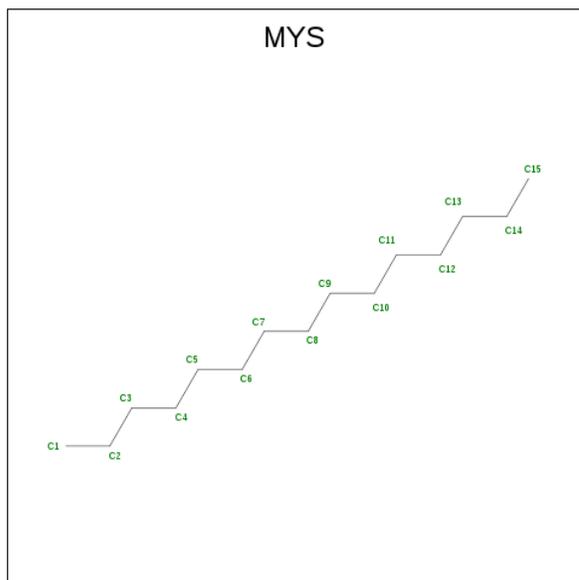
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	H		
10	A	1	47	15	32	0	0

- Molecule 11 is Octadecane (three-letter code: 8K6) (formula: $C_{18}H_{38}$).
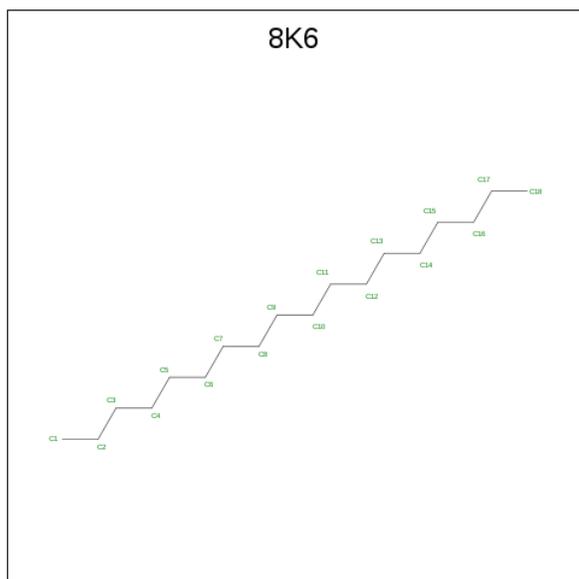
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	H	0	0
			56	18	38		

- Molecule 12 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).
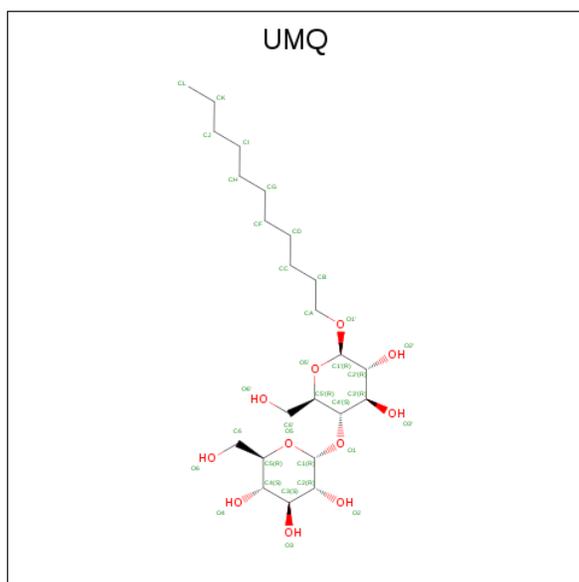
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	A	1	Total	C	H	O	0	0
			78	23	44	11		

- Molecule 13 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

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

CLA
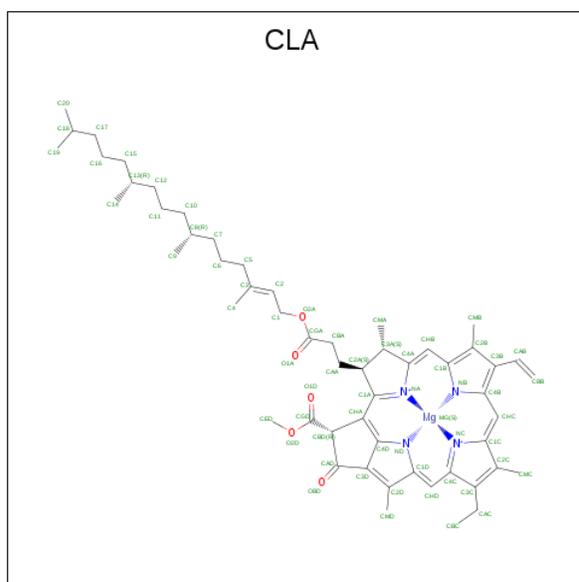
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	Mg	N	O		
14	B	1	129	55	64	1	4	5	0	0

- Molecule 15 is (2R)-3-{[(R)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-2-[(6Z)-tridec-6-enoyloxy]propyl (9Z)-octadec-9-enoate (three-letter code: OZ2) (formula: $C_{37}H_{69}O_{10}P$).


OZ2
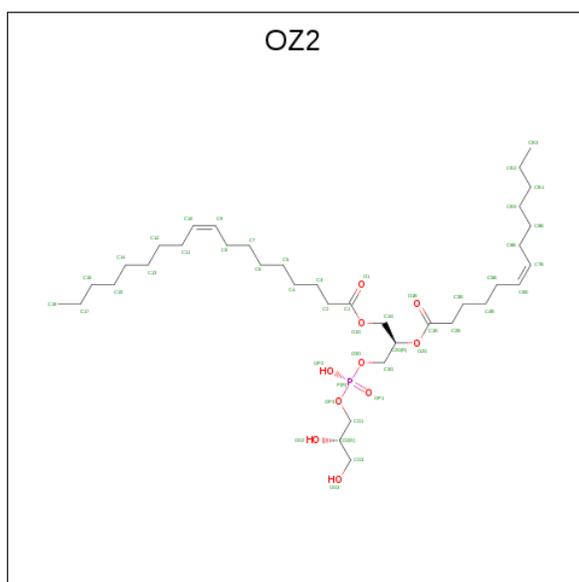
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
15	B	1	32	21	10	1	0	0
15	C	1	38	27	10	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
15	G	1	44	33	10	1	0	0

- Molecule 16 is (2S)-3-(acetyloxy)-2-hydroxypropyl 6-deoxy-6-sulfo-beta-D-glucopyranoside (three-letter code: 1E2) (formula: $C_{11}H_{20}O_{11}S$).
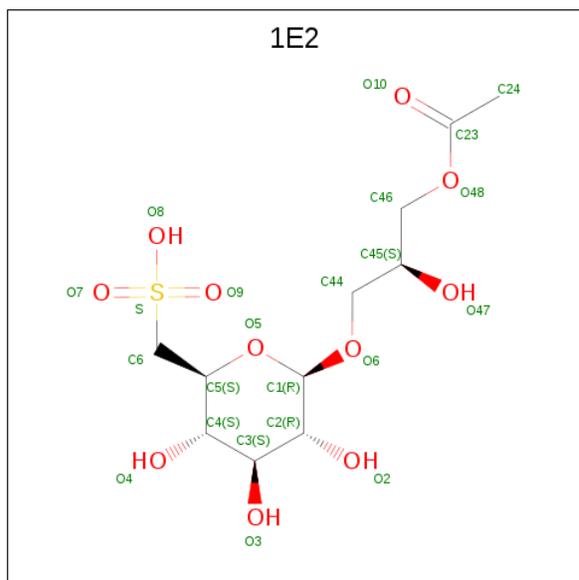
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
16	D	1	23	11	11	1	0	0

- Molecule 17 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).
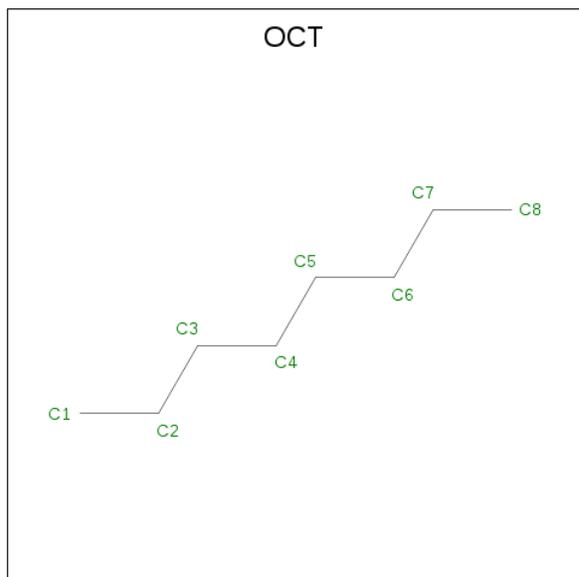
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	F	1	Total 26	C 8	H 18	0	0

- Molecule 18 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

BCR
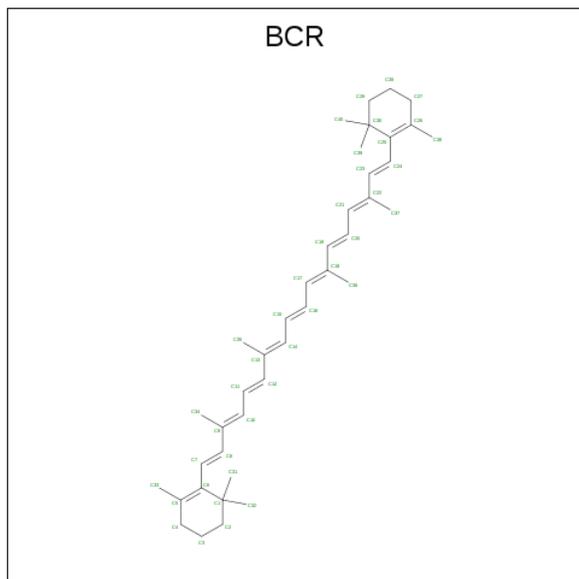
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	G	1	Total 96	C 40	H 56	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	8	Total 8	O 8	0	0
19	B	4	Total 4	O 4	0	0
19	C	1	Total 1	O 1	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

Chain A:

- Molecule 2: Cytochrome b6-f complex subunit 4

Chain B:

- Molecule 3: Apocytochrome f

Chain C:

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

Chain D:

- Molecule 5: Cytochrome b6-f complex subunit 6

Chain E:

9%

84%

13%

• Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:

6%

86%

11%
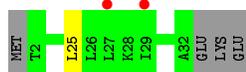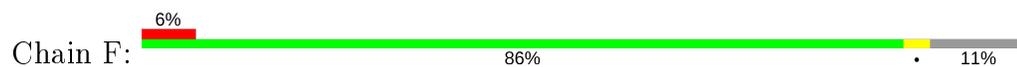
• Molecule 7: Cytochrome b6-f complex subunit 5

Chain G:

19%

86%

8%

5%
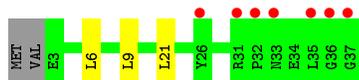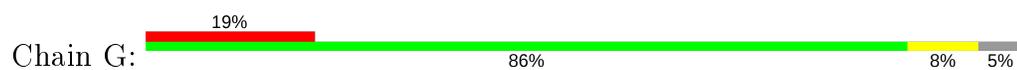
• Molecule 8: Cytochrome b6-f complex subunit 8

Chain H:

69%

24%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	159.45Å 159.45Å 362.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.52 – 2.80 48.52 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.52-2.80) 99.2 (48.52-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309, REFMAC	Depositor
R, R_{free}	0.248 , 0.272 0.251 , 0.274	Depositor DCC
R_{free} test set	3406 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 66.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13828	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ 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: UMQ, MYS, CLA, CD, 1E2, OZ2, HEM, 8K6, OCT, 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	0.30	0/1750	0.45	0/2388
2	B	0.26	0/1280	0.41	0/1755
3	C	0.26	0/2264	0.44	0/3082
4	D	0.28	0/300	0.40	0/408
5	E	0.28	0/220	0.42	0/297
6	F	0.28	0/238	0.40	0/321
7	G	0.29	0/274	0.39	0/371
8	H	0.29	0/228	0.47	0/313
All	All	0.28	0/6554	0.43	0/8935

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1698	1721	1720	9	0
2	B	1241	1297	1296	3	0
3	C	2216	2234	2233	9	0
4	D	292	299	299	0	0
5	E	215	237	237	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	234	248	248	0	0
7	G	268	268	268	0	0
8	H	222	227	227	4	0
9	A	129	0	90	23	0
9	C	43	0	30	6	0
10	A	15	32	32	0	0
11	A	18	38	38	0	0
12	A	102	130	126	2	0
13	A	1	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
14	B	65	64	71	1	0
15	B	32	0	32	0	0
15	C	38	0	43	0	0
15	G	44	0	54	1	0
16	D	23	0	18	2	0
17	F	8	18	18	0	0
18	G	40	56	56	0	0
19	A	8	0	0	1	0
19	B	4	0	0	0	0
19	C	1	0	0	0	0
All	All	6959	6869	7136	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 49 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)
9:A:303:HEM:HHA	9:A:303:HEM:HBD1	1.52	0.90
9:A:302:HEM:HBC2	9:A:302:HEM:HMC2	1.58	0.83
9:A:303:HEM:HMC1	9:A:303:HEM:HBC2	1.60	0.83
9:A:303:HEM:HBB2	9:A:303:HEM:HMB1	1.65	0.79
9:C:301:HEM:HMC1	9:C:301:HEM:HBC2	1.65	0.77

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	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
2	B	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
3	C	286/289 (99%)	244 (85%)	39 (14%)	3 (1%)	15	44
4	D	36/179 (20%)	35 (97%)	1 (3%)	0	100	100
5	E	26/32 (81%)	25 (96%)	1 (4%)	0	100	100
6	F	29/35 (83%)	28 (97%)	1 (3%)	0	100	100
7	G	33/37 (89%)	30 (91%)	3 (9%)	0	100	100
8	H	26/29 (90%)	26 (100%)	0	0	100	100
All	All	804/976 (82%)	745 (93%)	56 (7%)	3 (0%)	34	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	186	GLU
3	C	205	LYS
3	C	20	ILE

5.3.2 Protein sidechains (i)

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%)	171 (93%)	12 (7%)	16	44
2	B	136/137 (99%)	132 (97%)	4 (3%)	42	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	242/243 (100%)	224 (93%)	18 (7%)	13	37
4	D	31/146 (21%)	30 (97%)	1 (3%)	39	73
5	E	21/25 (84%)	20 (95%)	1 (5%)	25	58
6	F	23/27 (85%)	22 (96%)	1 (4%)	29	62
7	G	26/28 (93%)	23 (88%)	3 (12%)	5	17
8	H	23/24 (96%)	18 (78%)	5 (22%)	1	3
All	All	685/814 (84%)	640 (93%)	45 (7%)	16	44

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	190	TYR
3	C	218	ILE
8	H	6	LEU
3	C	200	GLN
3	C	226	LYS

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

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 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	#$|Z| > 2$
15	OZ2	B	203	-	31,31,47	1.23	3 (9%)	34,37,53	1.49	4 (11%)
9	HEM	C	301	3	27,50,50	2.15	5 (18%)	17,82,82	1.59	3 (17%)
10	MYS	A	304	-	14,14,14	0.32	0	13,13,13	0.79	0
15	OZ2	C	303	-	37,37,47	1.24	4 (10%)	40,43,53	1.22	3 (7%)
12	UMQ	A	306	-	35,35,35	1.25	5 (14%)	46,46,46	2.31	12 (26%)
11	8K6	A	305	-	17,17,17	0.20	0	16,16,16	0.53	0
14	CLA	B	201	19	59,73,73	1.47	5 (8%)	67,113,113	1.52	11 (16%)
17	OCT	F	101	-	7,7,7	0.25	0	6,6,6	0.65	0
9	HEM	A	303	19	27,50,50	2.15	6 (22%)	17,82,82	1.30	1 (5%)
12	UMQ	A	307	-	35,35,35	1.31	5 (14%)	46,46,46	2.43	11 (23%)
16	1E2	D	201	-	22,23,23	1.77	2 (9%)	30,33,33	3.14	9 (30%)
9	HEM	A	301	1	27,50,50	2.11	6 (22%)	17,82,82	1.43	3 (17%)
12	UMQ	A	308	-	35,35,35	1.31	6 (17%)	46,46,46	2.01	9 (19%)
18	BCR	G	101	-	41,41,41	2.19	21 (51%)	56,56,56	2.27	21 (37%)
15	OZ2	G	102	-	43,43,47	1.16	4 (9%)	46,49,53	1.15	2 (4%)
9	HEM	A	302	1	27,50,50	2.15	5 (18%)	17,82,82	1.39	1 (5%)

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
15	OZ2	B	203	-	1/1/5/9	13/35/35/52	-
9	HEM	C	301	3	-	2/6/54/54	-
10	MYS	A	304	-	-	2/12/12/12	-
15	OZ2	C	303	-	-	16/42/42/52	-
12	UMQ	A	306	-	3/3/10/10	9/20/60/60	0/2/2/2
11	8K6	A	305	-	-	4/15/15/15	-
14	CLA	B	201	19	3/3/22/25	17/37/135/135	-
17	OCT	F	101	-	-	0/5/5/5	-
9	HEM	A	303	19	-	4/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	UMQ	A	307	-	3/3/10/10	8/20/60/60	0/2/2/2
16	1E2	D	201	-	1/1/8/8	6/15/35/35	0/1/1/1
9	HEM	A	301	1	-	3/6/54/54	-
12	UMQ	A	308	-	2/2/10/10	5/20/60/60	0/2/2/2
18	BCR	G	101	-	-	18/29/63/63	0/2/2/2
15	OZ2	G	102	-	-	13/48/48/52	-
9	HEM	A	302	1	-	2/6/54/54	-

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	201	CLA	C4B-NB	8.09	1.42	1.35
16	D	201	1E2	O47-C45	-6.44	1.24	1.43
9	C	301	HEM	C3D-C2D	5.38	1.53	1.37
9	A	301	HEM	C3D-C2D	5.35	1.53	1.37
9	A	302	HEM	C3D-C2D	5.34	1.53	1.37

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	D	201	1E2	O7-S-C6	8.91	117.53	106.94
12	A	306	UMQ	O5-C5-C4	7.92	124.07	109.69
16	D	201	1E2	O9-S-C6	-7.36	98.19	106.94
12	A	307	UMQ	O1'-C1'-C2'	7.10	119.39	108.30
12	A	307	UMQ	O5'-C5'-C4'	7.08	124.68	109.75

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	B	203	OZ2	CG2
12	A	306	UMQ	C5
12	A	306	UMQ	C2
12	A	306	UMQ	C1
14	B	201	CLA	NC

5 of 122 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	B	203	OZ2	O1B-C1B-O2G-C2G
15	B	203	OZ2	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
15	B	203	OZ2	CG1-CG2-CG3-OG3
9	C	301	HEM	C2D-C3D-CAD-CBD
9	C	301	HEM	C4D-C3D-CAD-CBD

There are no ring outliers.

9 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	301	HEM	6	0
12	A	306	UMQ	1	0
14	B	201	CLA	1	0
9	A	303	HEM	8	0
16	D	201	1E2	2	0
9	A	301	HEM	7	0
12	A	308	UMQ	1	0
15	G	102	OZ2	1	0
9	A	302	HEM	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand OZ2 B 203

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand OZ2 C 303

Bond lengths

Bond angles

Torsions

Rings

Ligand UMQ A 306

Bond lengths

Bond angles

Torsions

Rings

Ligand 8K6 A 305

Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 201

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 303

Bond lengths

Bond angles

Torsions

Rings

Ligand UMQ A 307

Bond lengths

Bond angles

Torsions

Rings

Ligand 1E2 D 201

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UMQ A 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR G 101

Bond lengths

Bond angles

Torsions

Rings

Ligand OZ2 G 102

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 302

Bond lengths

Bond angles

Torsions

Rings

5.7　Other polymers (i)

There are no such residues in this entry.

5.8　Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	213/215 (99%)	0.08	0	100	100	47, 65, 96, 135	0
2	B	159/160 (99%)	0.21	8 (5%)	28	19	51, 85, 126, 184	0
3	C	288/289 (99%)	0.93	66 (22%)	0	0	58, 95, 219, 257	1 (0%)
4	D	38/179 (21%)	0.53	6 (15%)	2	1	51, 76, 168, 214	0
5	E	28/32 (87%)	0.25	3 (10%)	6	3	83, 95, 118, 139	0
6	F	31/35 (88%)	0.32	2 (6%)	18	11	72, 87, 125, 131	0
7	G	35/37 (94%)	1.08	7 (20%)	1	0	62, 84, 193, 242	0
8	H	28/29 (96%)	0.12	0	100	100	67, 76, 99, 122	0
All	All	820/976 (84%)	0.49	92 (11%)	5	3	47, 84, 185, 257	1 (0%)

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	206	THR	11.1
3	C	220	SER	9.7
3	C	219	VAL	9.3
7	G	35	LEU	7.2
7	G	36	GLY	7.2

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 (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	UMQ	A	306	34/34	0.68	0.39	85,138,194,197	0
11	8K6	A	305	18/18	0.71	0.45	96,120,123,123	0
15	OZ2	C	303	38/48	0.75	0.34	54,108,185,186	0
17	OCT	F	101	8/8	0.78	0.47	102,123,135,135	0
12	UMQ	A	307	34/34	0.81	0.47	115,144,174,177	0
15	OZ2	G	102	44/48	0.81	0.27	58,102,166,169	0
12	UMQ	A	308	34/34	0.83	0.38	109,146,192,197	0
10	MYS	A	304	15/15	0.85	0.26	77,94,102,102	0
18	BCR	G	101	40/40	0.86	0.33	68,95,177,180	0
16	1E2	D	201	23/23	0.91	0.17	104,110,123,134	0
15	OZ2	B	203	32/48	0.93	0.17	91,97,127,128	0
14	CLA	B	201	65/65	0.93	0.23	68,98,132,135	0
13	CD	C	302	1/1	0.94	0.17	142,142,142,142	0
9	HEM	A	303	43/43	0.96	0.26	50,74,88,89	0
9	HEM	C	301	43/43	0.97	0.20	76,82,98,107	0
13	CD	B	202	1/1	0.98	0.22	124,124,124,124	0
9	HEM	A	302	43/43	0.98	0.27	51,64,74,79	0
9	HEM	A	301	43/43	0.98	0.25	38,50,63,75	0
13	CD	A	309	1/1	0.99	0.20	85,85,85,85	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UMQ A 306:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
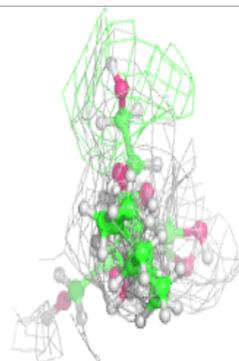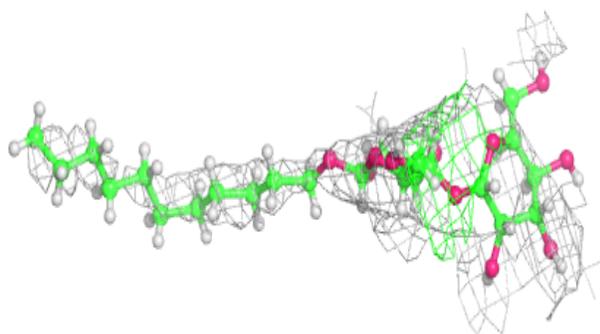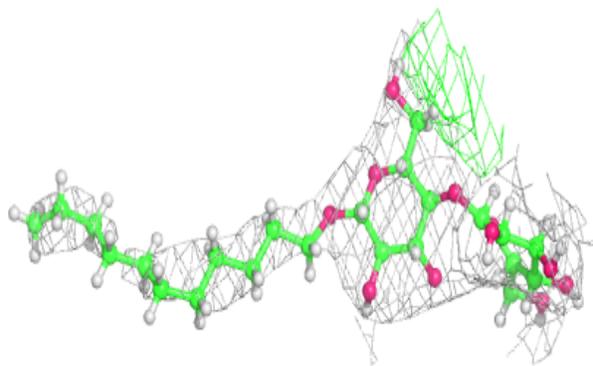
Electron density around 8K6 A 305:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
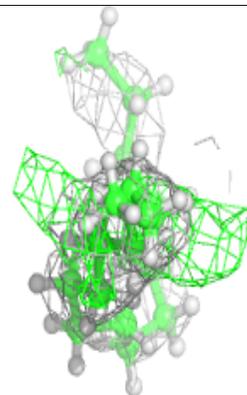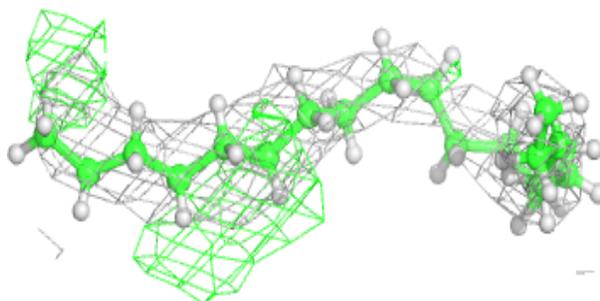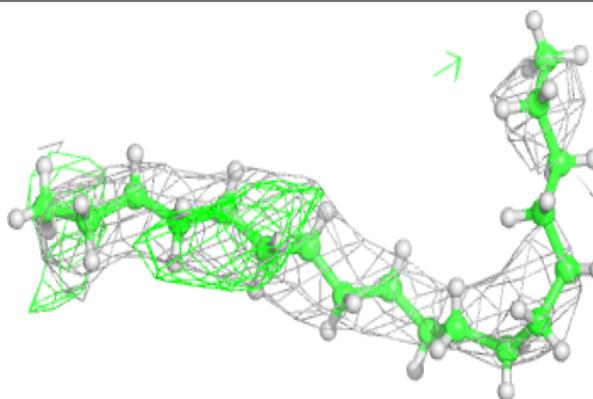
Electron density around OZ2 C 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
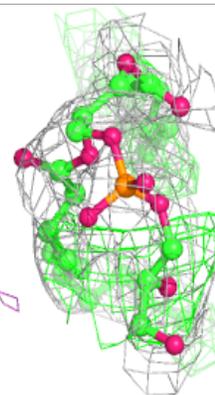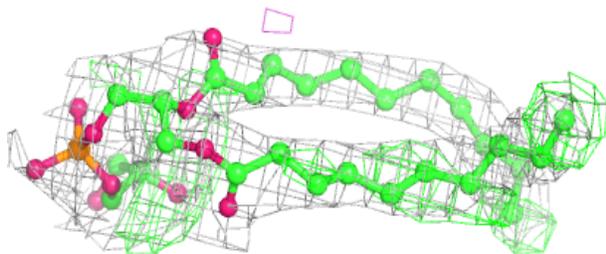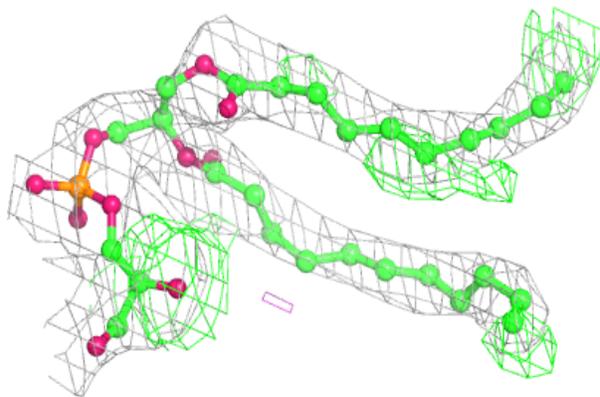
Electron density around UMQ A 307:

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mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
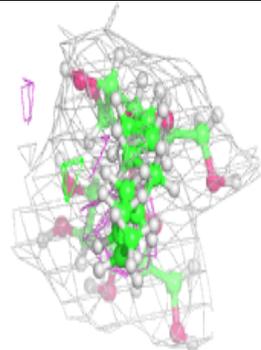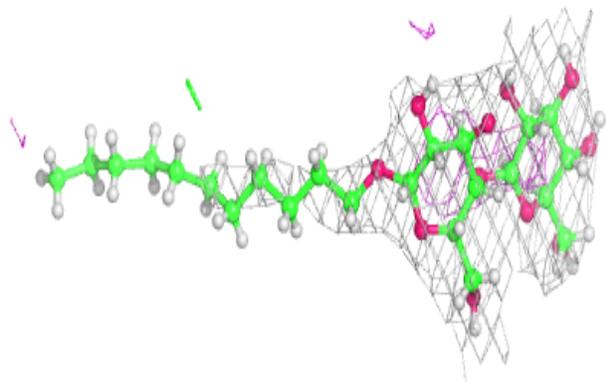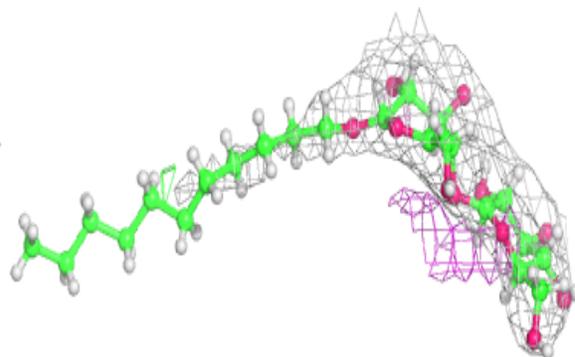
Electron density around OZ2 G 102:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
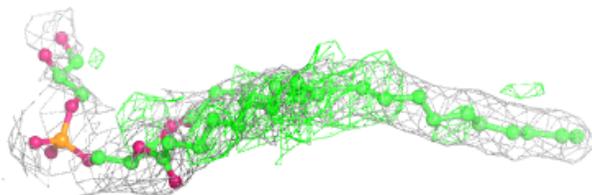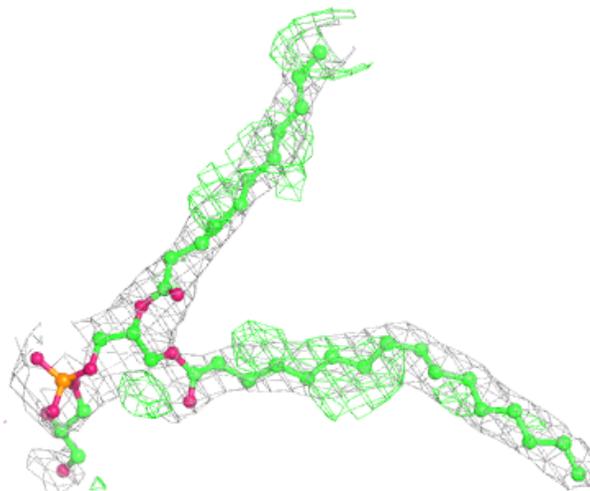
Electron density around UMQ A 308:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
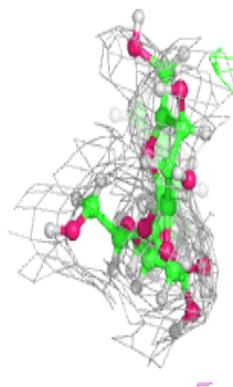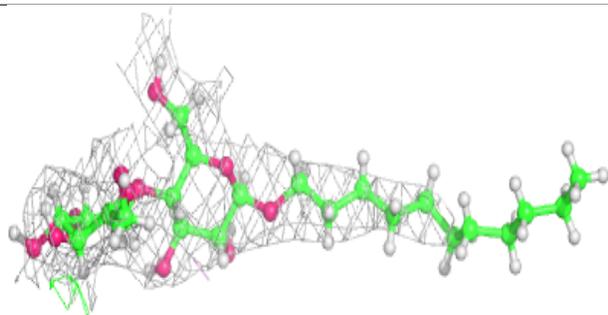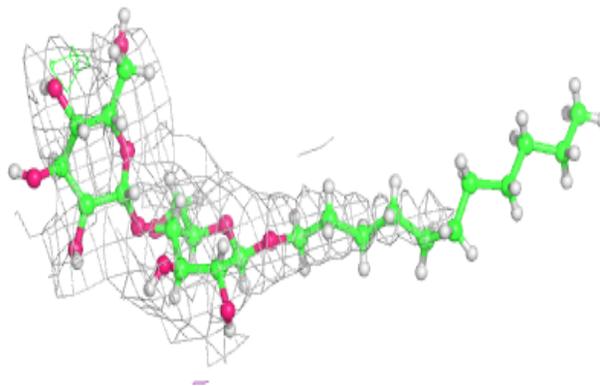
Electron density around BCR G 101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
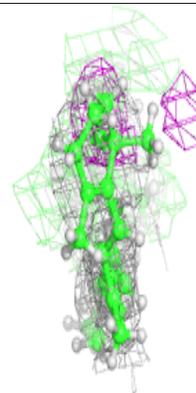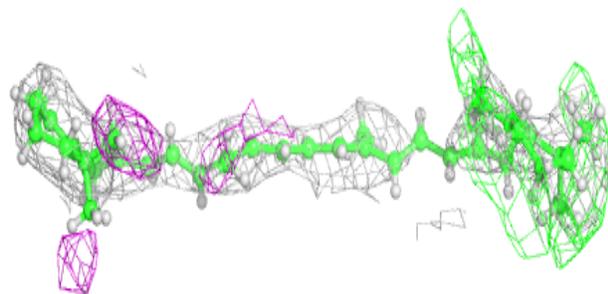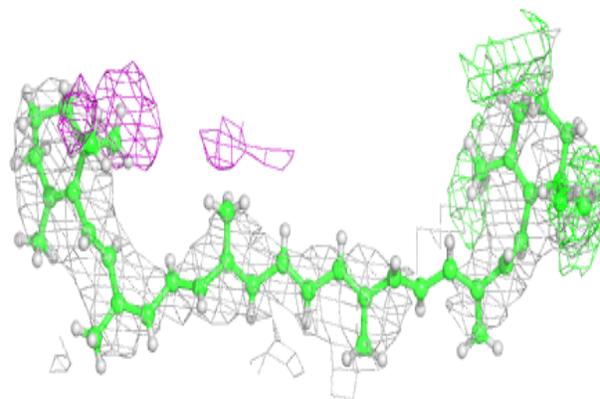
Electron density around 1E2 D 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
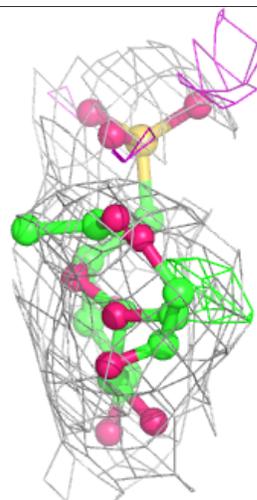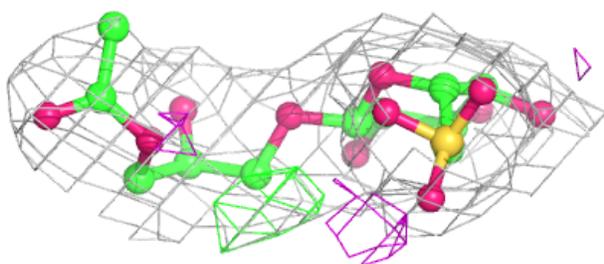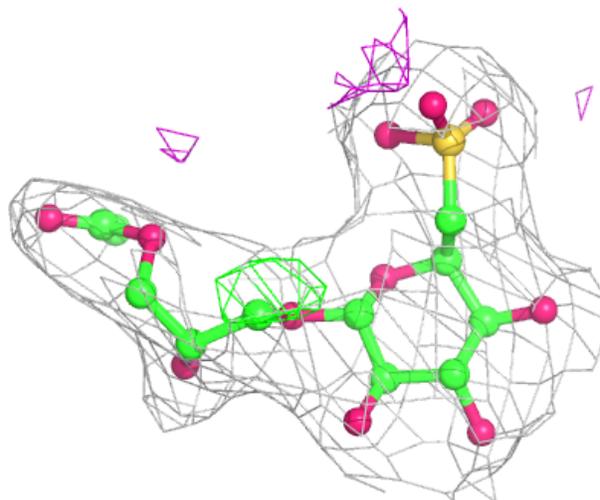
Electron density around OZ2 B 203:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
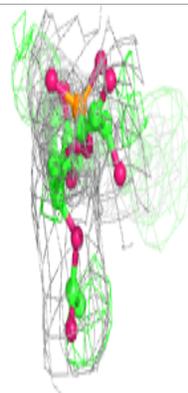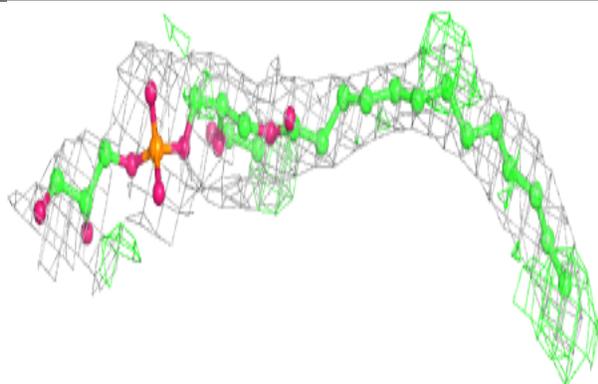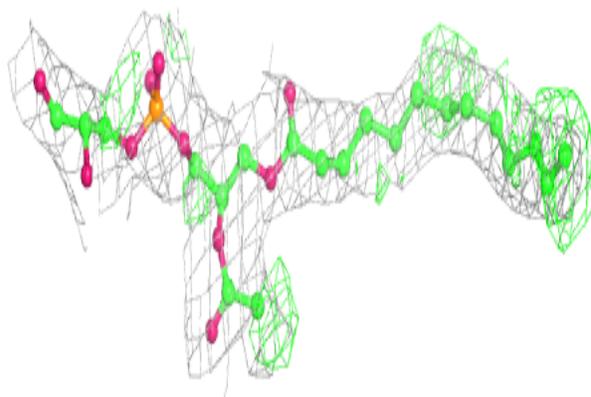
Electron density around CLA B 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
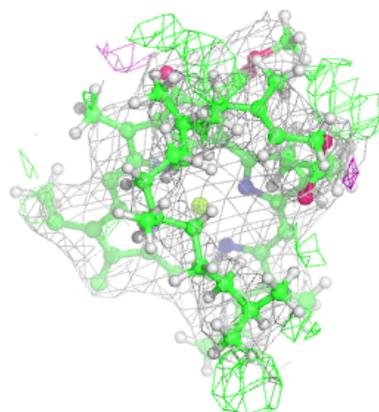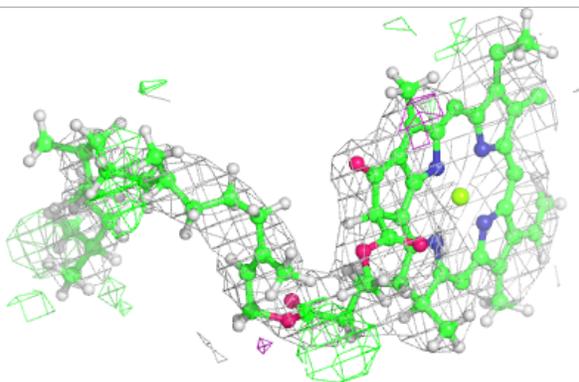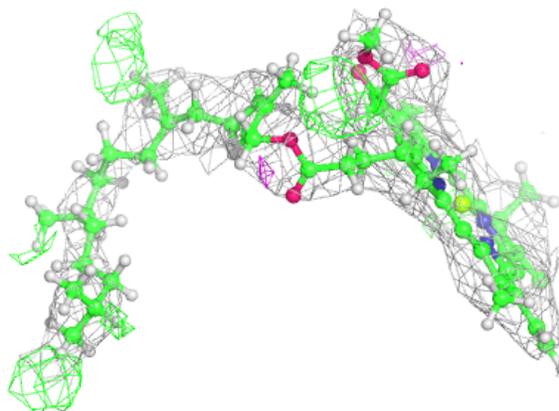
Electron density around HEM A 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
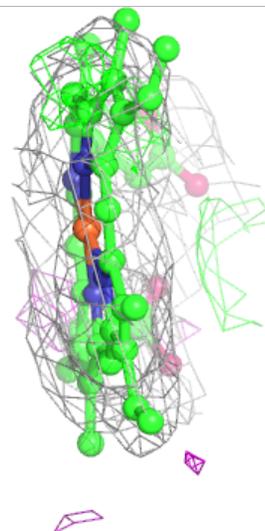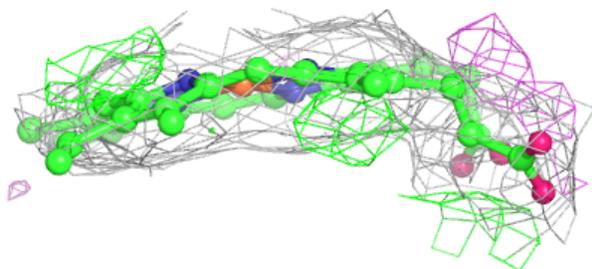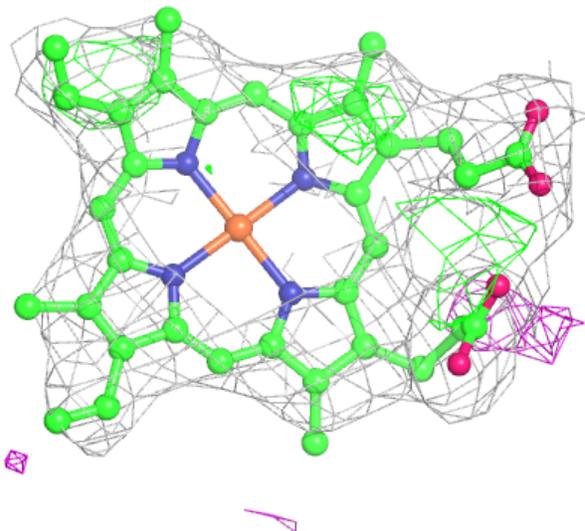
Electron density around HEM C 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
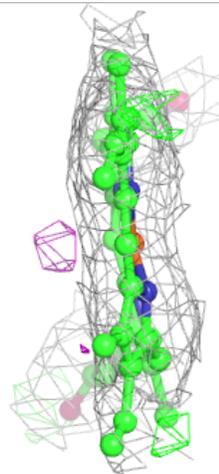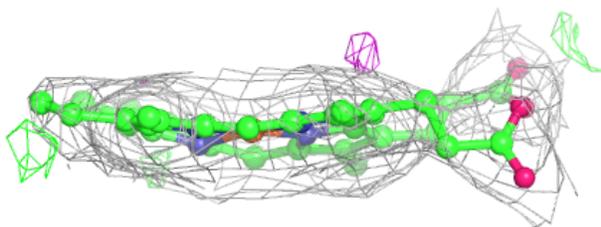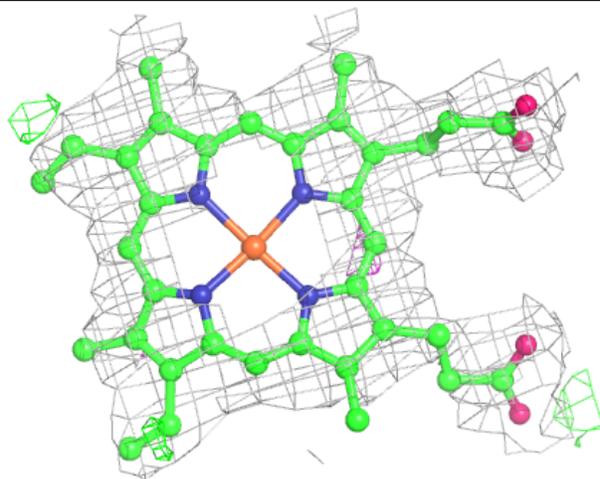
Electron density around HEM A 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEM A 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.