wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 11:59 PM JST

PDB ID	:	7W7D / pdb_00007w7d
Title	:	Heme exporter HrtBA in complex with heme
Authors	:	Hisano, T.; Nakamura, H.; Rahman, M.M.; Tosha, T.; Shiro, Y.; Shirouzu, M.
Deposited on	:	2021-12-04
Resolution	:	3.40 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

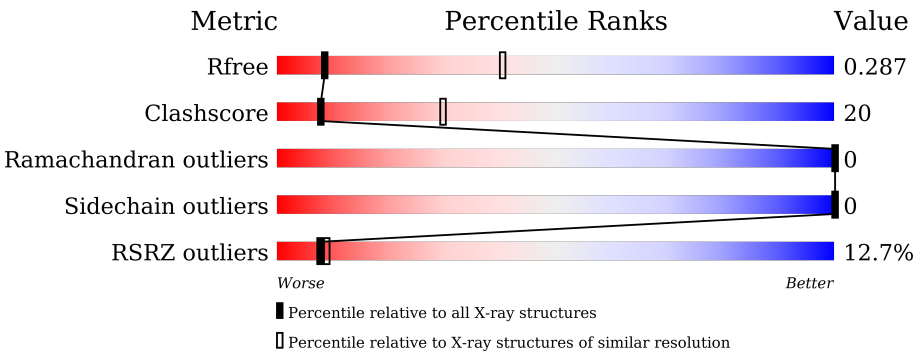
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.40 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 of 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	231	13% 61% 33% 6%
1	C	231	10% 65% 30% 6%
1	E	231	13% 60% 34% 6%
1	G	231	13% 68% 29% .
1	I	231	6% 56% 40% .
1	K	231	11% 60% 35% 5%

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Mol	Chain	Length	Quality of chain
2	B	344	13% 69% 30%
2	D	344	12% 70% 29%
2	F	344	17% 64% 35%
2	H	344	15% 67% 32%
2	J	344	11% 66% 33%
2	L	344	14% 67% 32%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25112 atoms, of which 60 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 Putative ABC transport system, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1618	1010	293	312	3	0	0	0
1	C	218	1634	1019	296	316	3	0	0	0
1	E	217	1629	1016	295	315	3	0	0	0
1	G	225	1693	1059	307	324	3	0	0	0
1	I	221	1652	1031	299	319	3	0	0	0
1	K	219	1639	1022	297	317	3	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	LYS	-	expression tag	UNP Q6NEF2
A	223	LEU	-	expression tag	UNP Q6NEF2
A	224	TRP	-	expression tag	UNP Q6NEF2
A	225	SER	-	expression tag	UNP Q6NEF2
A	226	HIS	-	expression tag	UNP Q6NEF2
A	227	PRO	-	expression tag	UNP Q6NEF2
A	228	GLN	-	expression tag	UNP Q6NEF2
A	229	PHE	-	expression tag	UNP Q6NEF2
A	230	GLU	-	expression tag	UNP Q6NEF2
A	231	LYS	-	expression tag	UNP Q6NEF2
C	222	LYS	-	expression tag	UNP Q6NEF2
C	223	LEU	-	expression tag	UNP Q6NEF2
C	224	TRP	-	expression tag	UNP Q6NEF2
C	225	SER	-	expression tag	UNP Q6NEF2
C	226	HIS	-	expression tag	UNP Q6NEF2
C	227	PRO	-	expression tag	UNP Q6NEF2
C	228	GLN	-	expression tag	UNP Q6NEF2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	229	PHE	-	expression tag	UNP Q6NEF2
C	230	GLU	-	expression tag	UNP Q6NEF2
C	231	LYS	-	expression tag	UNP Q6NEF2
E	222	LYS	-	expression tag	UNP Q6NEF2
E	223	LEU	-	expression tag	UNP Q6NEF2
E	224	TRP	-	expression tag	UNP Q6NEF2
E	225	SER	-	expression tag	UNP Q6NEF2
E	226	HIS	-	expression tag	UNP Q6NEF2
E	227	PRO	-	expression tag	UNP Q6NEF2
E	228	GLN	-	expression tag	UNP Q6NEF2
E	229	PHE	-	expression tag	UNP Q6NEF2
E	230	GLU	-	expression tag	UNP Q6NEF2
E	231	LYS	-	expression tag	UNP Q6NEF2
G	222	LYS	-	expression tag	UNP Q6NEF2
G	223	LEU	-	expression tag	UNP Q6NEF2
G	224	TRP	-	expression tag	UNP Q6NEF2
G	225	SER	-	expression tag	UNP Q6NEF2
G	226	HIS	-	expression tag	UNP Q6NEF2
G	227	PRO	-	expression tag	UNP Q6NEF2
G	228	GLN	-	expression tag	UNP Q6NEF2
G	229	PHE	-	expression tag	UNP Q6NEF2
G	230	GLU	-	expression tag	UNP Q6NEF2
G	231	LYS	-	expression tag	UNP Q6NEF2
I	222	LYS	-	expression tag	UNP Q6NEF2
I	223	LEU	-	expression tag	UNP Q6NEF2
I	224	TRP	-	expression tag	UNP Q6NEF2
I	225	SER	-	expression tag	UNP Q6NEF2
I	226	HIS	-	expression tag	UNP Q6NEF2
I	227	PRO	-	expression tag	UNP Q6NEF2
I	228	GLN	-	expression tag	UNP Q6NEF2
I	229	PHE	-	expression tag	UNP Q6NEF2
I	230	GLU	-	expression tag	UNP Q6NEF2
I	231	LYS	-	expression tag	UNP Q6NEF2
K	222	LYS	-	expression tag	UNP Q6NEF2
K	223	LEU	-	expression tag	UNP Q6NEF2
K	224	TRP	-	expression tag	UNP Q6NEF2
K	225	SER	-	expression tag	UNP Q6NEF2
K	226	HIS	-	expression tag	UNP Q6NEF2
K	227	PRO	-	expression tag	UNP Q6NEF2
K	228	GLN	-	expression tag	UNP Q6NEF2
K	229	PHE	-	expression tag	UNP Q6NEF2
K	230	GLU	-	expression tag	UNP Q6NEF2

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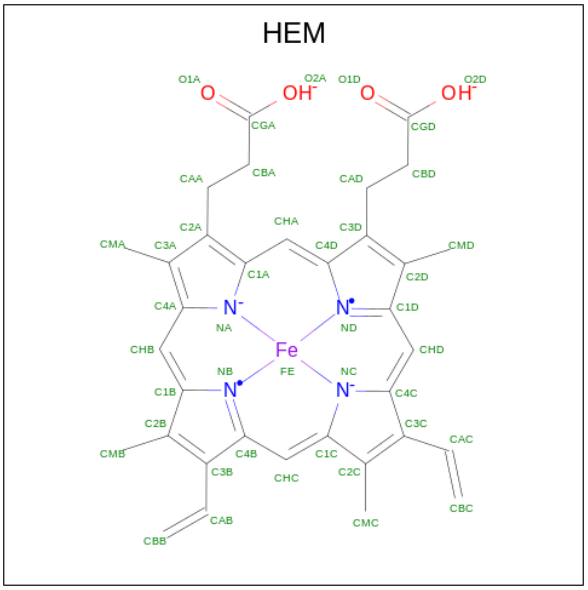
Chain	Residue	Modelled	Actual	Comment	Reference
K	231	LYS	-	expression tag	UNP Q6NEF2

- Molecule 2 is a protein called Putative ABC transport system integral membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	341	2510	1612	422	471	5	0	0	0
2	D	343	2522	1619	424	474	5	0	0	0
2	F	342	2515	1615	423	472	5	0	0	0
2	H	341	2510	1612	422	471	5	0	0	0
2	J	343	2522	1619	424	474	5	0	0	0
2	L	343	2522	1619	424	474	5	0	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



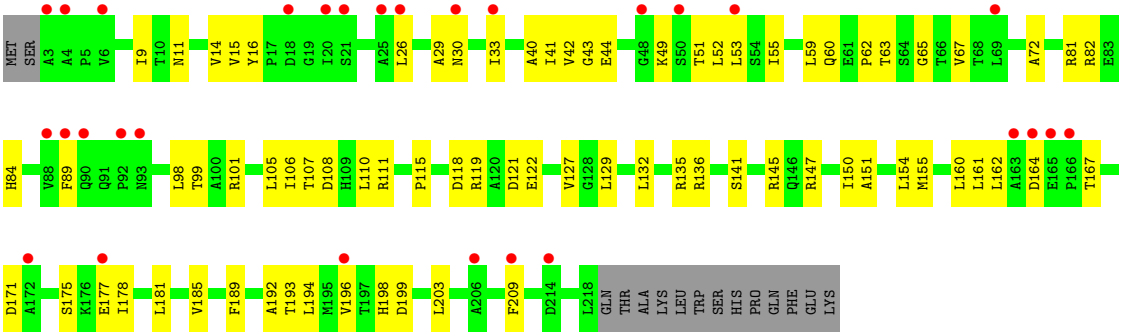
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Fe	H	N	O		
3	D	1	73	34	1	30	4	4	0	0
3	F	1	73	34	1	30	4	4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

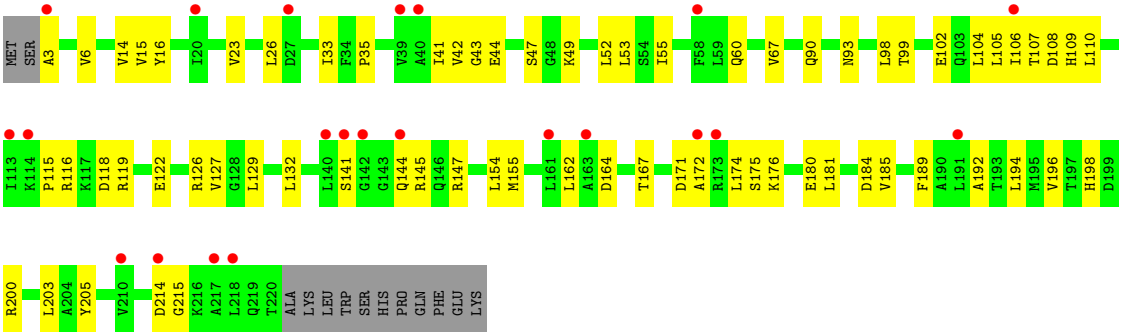
• Molecule 1: Putative ABC transport system, ATP-binding protein

Chain A:



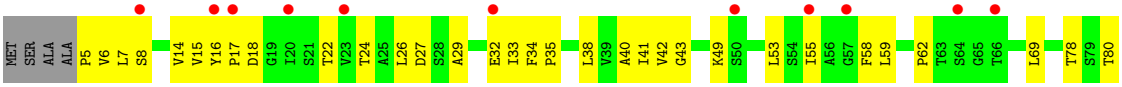
• Molecule 1: Putative ABC transport system, ATP-binding protein

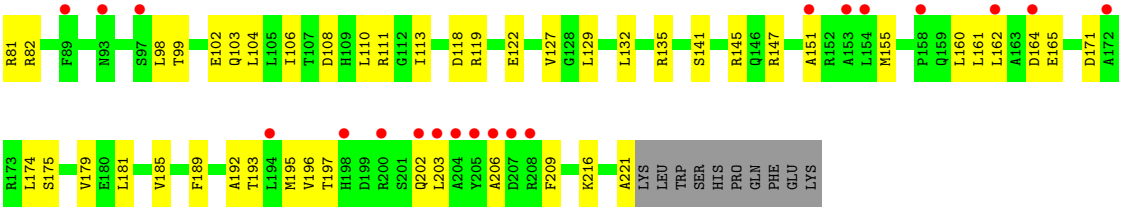
Chain C:



• Molecule 1: Putative ABC transport system, ATP-binding protein

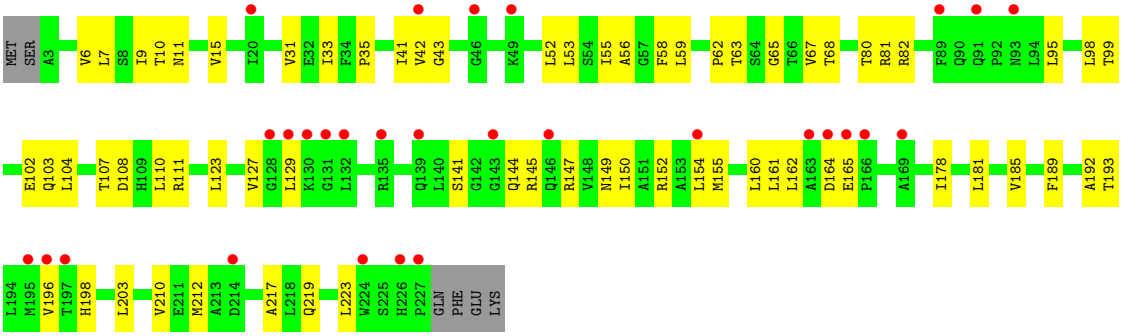
Chain E:





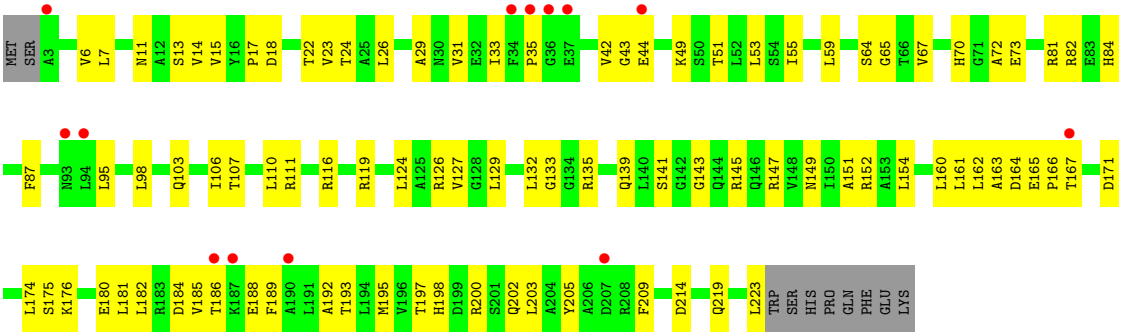
• Molecule 1: Putative ABC transport system, ATP-binding protein

Chain G:



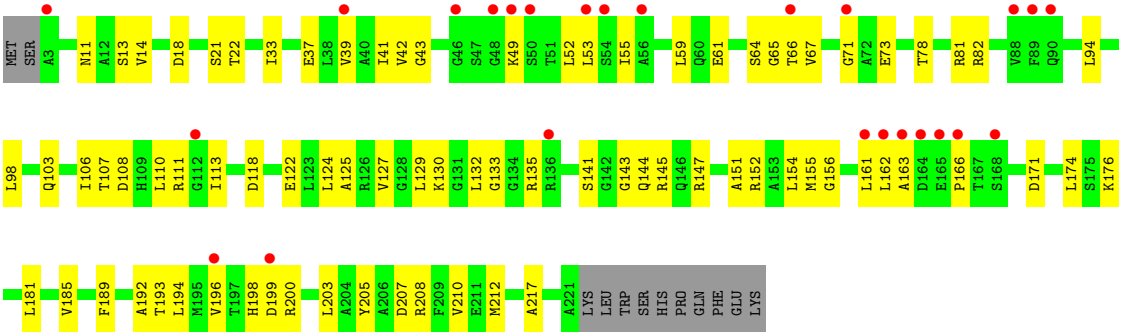
• Molecule 1: Putative ABC transport system, ATP-binding protein

Chain I:



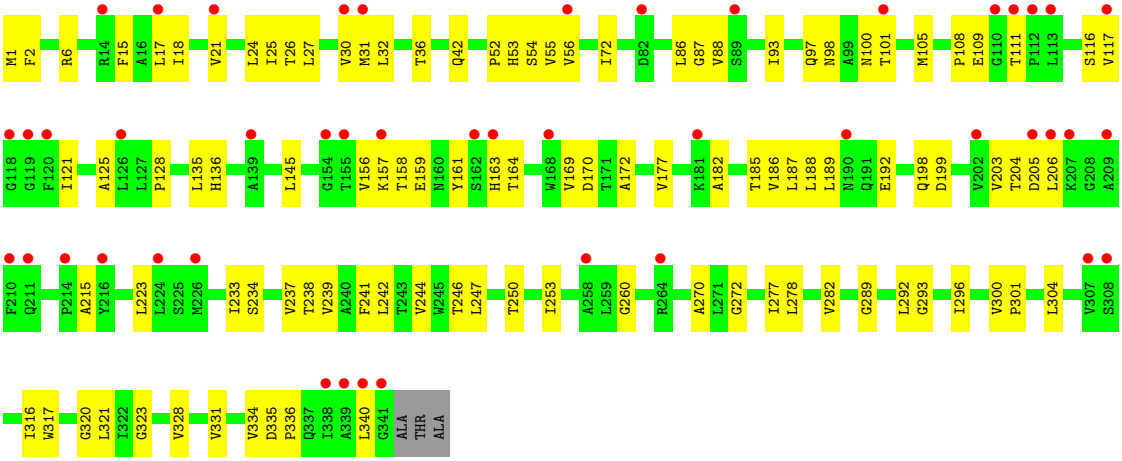
• Molecule 1: Putative ABC transport system, ATP-binding protein

Chain K:



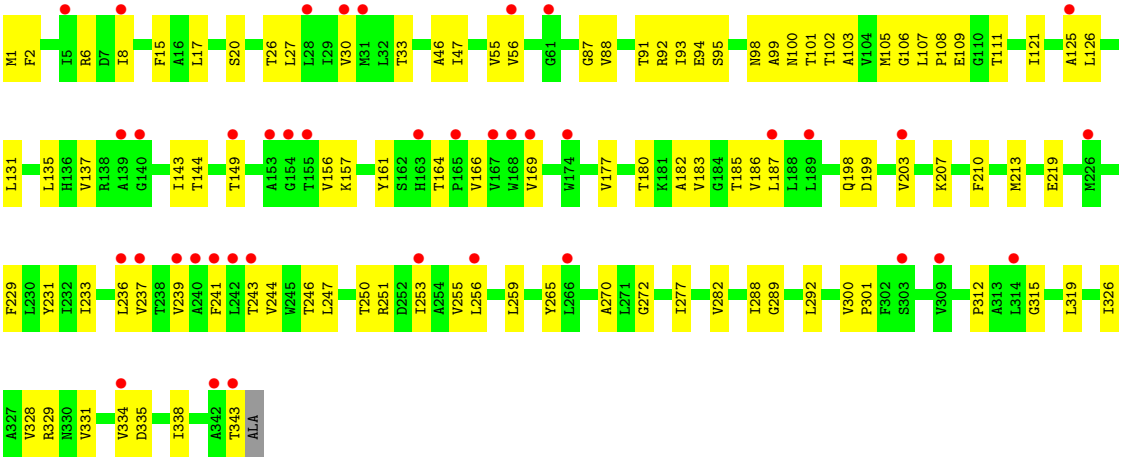
• Molecule 2: Putative ABC transport system integral membrane protein

Chain B:



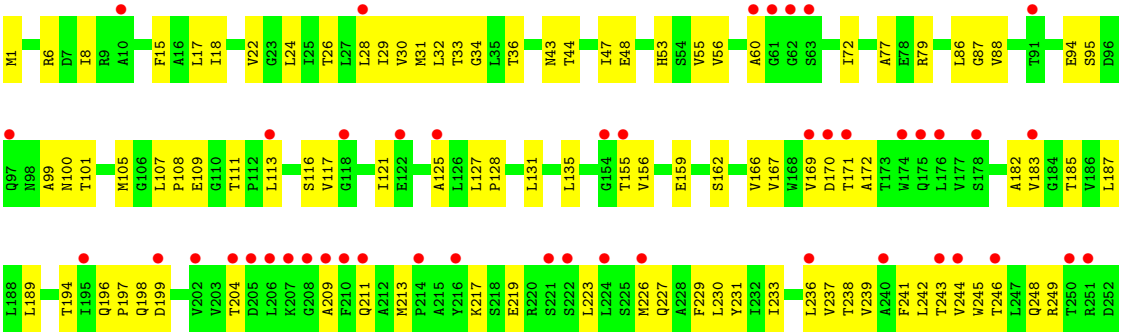
• Molecule 2: Putative ABC transport system integral membrane protein

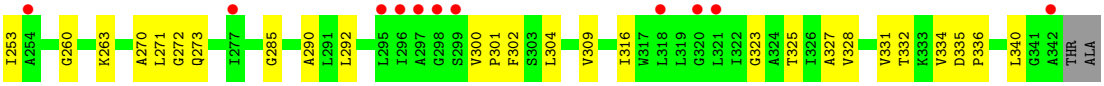
Chain D:



• Molecule 2: Putative ABC transport system integral membrane protein

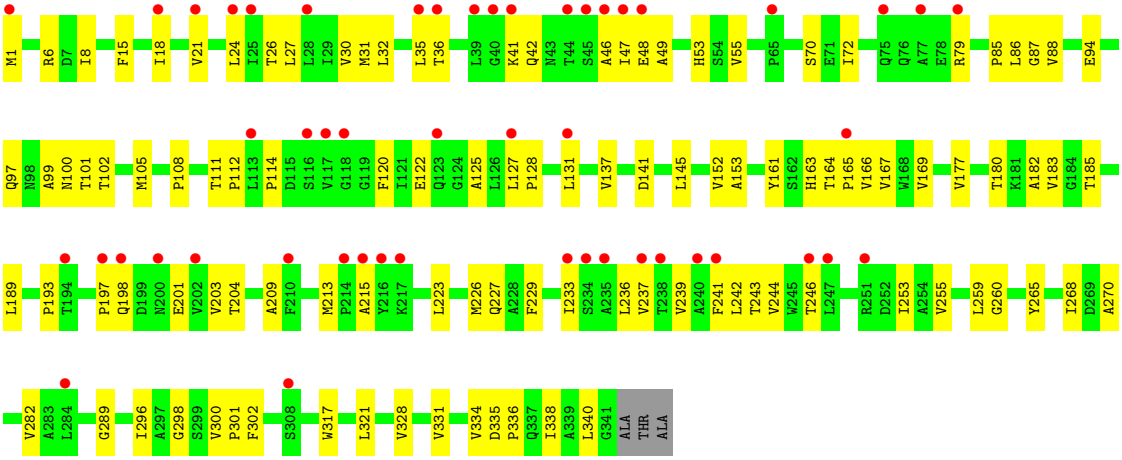
Chain F:





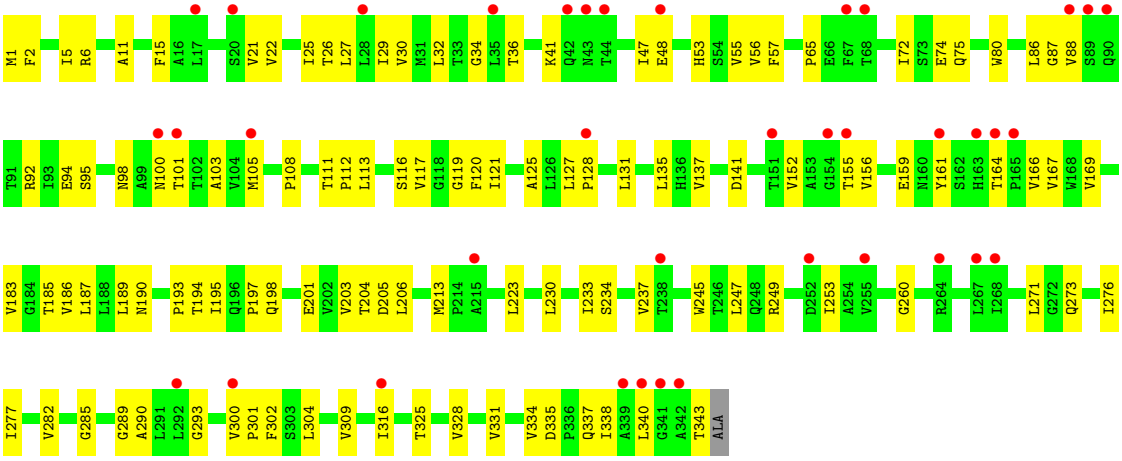
• Molecule 2: Putative ABC transport system integral membrane protein

Chain H:



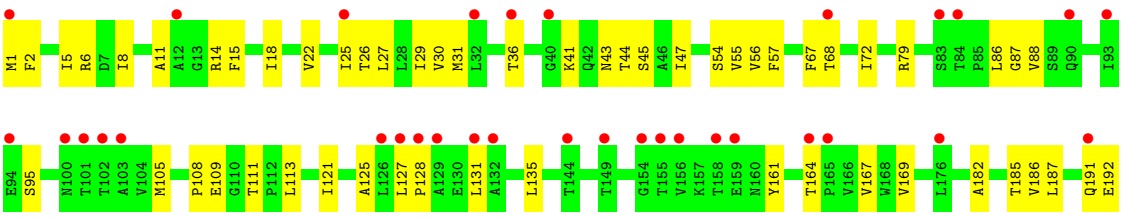
• Molecule 2: Putative ABC transport system integral membrane protein

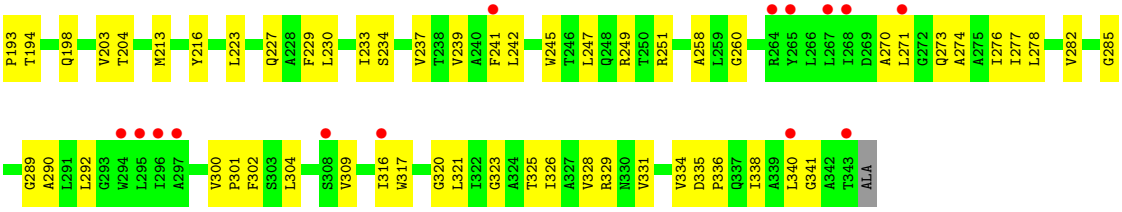
Chain J:



• Molecule 2: Putative ABC transport system integral membrane protein

Chain L:




P193 T194 Q198 V203 T204 M213 Y216 L223 Q227 A228 F229 L230 I233 S234 V237 T238 V239 A240 F241 L242 W245 T246 L247 Q248 R249 T250 R251 A258 L259 G260 R264 Y265 L266 L267 I268 D269 A270 L271 G272 Q273 A274 A275 I276 I277 L278 V282 G285
G289 A290 L291 L292 G293 W294 L295 I296 A297 V300 P301 F302 S303 L304 S308 V309 I316 W317 G320 L321 I322 G323 A324 T325 I326 A327 V328 R329 N330 V331 V334 D335 P336 Q337 I338 A339 L340 G341 A342 T343 ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	82.58Å 135.03Å 160.97Å 112.49° 100.41° 93.78°	Depositor
Resolution (Å)	49.29 – 3.40 49.29 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.29-3.40) 85.5 (49.29-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.53 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.255 , 0.285 0.257 , 0.287	Depositor DCC
R_{free} test set	2948 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å^2)	103.8	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 72.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25112	wwPDB-VP
Average B, all atoms (Å^2)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: HEM

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	0.12	0/1637	0.27	0/2216
1	C	0.13	0/1653	0.28	0/2238
1	E	0.09	0/1648	0.26	0/2230
1	G	0.13	0/1716	0.29	0/2325
1	I	0.14	0/1671	0.28	0/2263
1	K	0.16	0/1658	0.30	0/2245
2	B	0.12	0/2556	0.25	0/3495
2	D	0.09	0/2568	0.21	0/3512
2	F	0.11	0/2561	0.24	0/3502
2	H	0.08	0/2556	0.21	0/3495
2	J	0.10	0/2568	0.23	0/3512
2	L	0.11	0/2568	0.24	0/3512
All	All	0.11	0/25360	0.25	0/34545

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	1618	0	1664	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1634	0	1679	74	0
1	E	1629	0	1675	75	0
1	G	1693	0	1737	62	0
1	I	1652	0	1697	87	0
1	K	1639	0	1684	80	0
2	B	2510	0	2588	94	0
2	D	2522	0	2600	88	0
2	F	2515	0	2593	123	0
2	H	2510	0	2588	108	0
2	J	2522	0	2600	94	0
2	L	2522	0	2600	95	0
3	D	43	30	30	7	0
3	F	43	30	30	9	0
All	All	25052	60	25765	1004	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 20.

The worst 5 of 1004 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:E:26:LEU:HD11	1:E:29:ALA:HB2	1.27	1.16
2:L:31:MET:HE1	2:L:292:LEU:HD23	1.36	1.03
2:D:1:MET:HE1	2:D:272:GLY:HA3	1.41	1.02
1:I:127:VAL:HG13	1:I:181:LEU:HD21	1.40	1.01
2:D:253:ILE:HD13	2:D:331:VAL:HG23	1.41	1.01

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	214/231 (93%)	211 (99%)	3 (1%)	0	100	100
1	C	216/231 (94%)	212 (98%)	4 (2%)	0	100	100
1	E	215/231 (93%)	212 (99%)	3 (1%)	0	100	100
1	G	223/231 (96%)	220 (99%)	3 (1%)	0	100	100
1	I	219/231 (95%)	217 (99%)	2 (1%)	0	100	100
1	K	217/231 (94%)	214 (99%)	3 (1%)	0	100	100
2	B	339/344 (98%)	333 (98%)	6 (2%)	0	100	100
2	D	341/344 (99%)	334 (98%)	7 (2%)	0	100	100
2	F	340/344 (99%)	335 (98%)	5 (2%)	0	100	100
2	H	339/344 (98%)	331 (98%)	8 (2%)	0	100	100
2	J	341/344 (99%)	333 (98%)	8 (2%)	0	100	100
2	L	341/344 (99%)	335 (98%)	6 (2%)	0	100	100
All	All	3345/3450 (97%)	3287 (98%)	58 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	172/186 (92%)	172 (100%)	0	100	100
1	C	174/186 (94%)	174 (100%)	0	100	100
1	E	174/186 (94%)	174 (100%)	0	100	100
1	G	180/186 (97%)	180 (100%)	0	100	100
1	I	175/186 (94%)	175 (100%)	0	100	100
1	K	174/186 (94%)	174 (100%)	0	100	100
2	B	264/265 (100%)	264 (100%)	0	100	100
2	D	265/265 (100%)	265 (100%)	0	100	100
2	F	264/265 (100%)	264 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	264/265 (100%)	264 (100%)	0	100	100
2	J	265/265 (100%)	265 (100%)	0	100	100
2	L	265/265 (100%)	265 (100%)	0	100	100
All	All	2636/2706 (97%)	2636 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	11	ASN
2	J	90	GLN
1	I	149	ASN
2	J	98	ASN
2	D	191	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	HEM	F	401	2	50,50,50	1.39	8 (16%)	66,82,82	1.39	11 (16%)
3	HEM	D	401	2	50,50,50	1.42	8 (16%)	66,82,82	1.38	8 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	F	401	2	-	4/14/54/54	-
3	HEM	D	401	2	-	5/14/54/54	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	HEM	FE-NA	3.60	2.07	1.95
3	D	401	HEM	FE-ND	3.59	2.06	1.94
3	F	401	HEM	FE-NC	3.48	2.06	1.95
3	F	401	HEM	FE-NB	3.32	2.05	1.94
3	F	401	HEM	FE-ND	3.25	2.04	1.94

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	401	HEM	C1B-NB-C4B	3.29	108.47	105.07
3	F	401	HEM	C1B-NB-C4B	3.16	108.33	105.07
3	D	401	HEM	C4D-ND-C1D	3.13	108.31	105.07
3	F	401	HEM	C4D-ND-C1D	3.07	108.24	105.07
3	D	401	HEM	C4C-NC-C1C	3.05	108.33	105.35

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	HEM	C2A-CAA-CBA-CGA
3	F	401	HEM	CAA-CBA-CGA-O1A
3	D	401	HEM	CAA-CBA-CGA-O2A
3	D	401	HEM	CAD-CBD-CGD-O2D
3	D	401	HEM	CAD-CBD-CGD-O1D

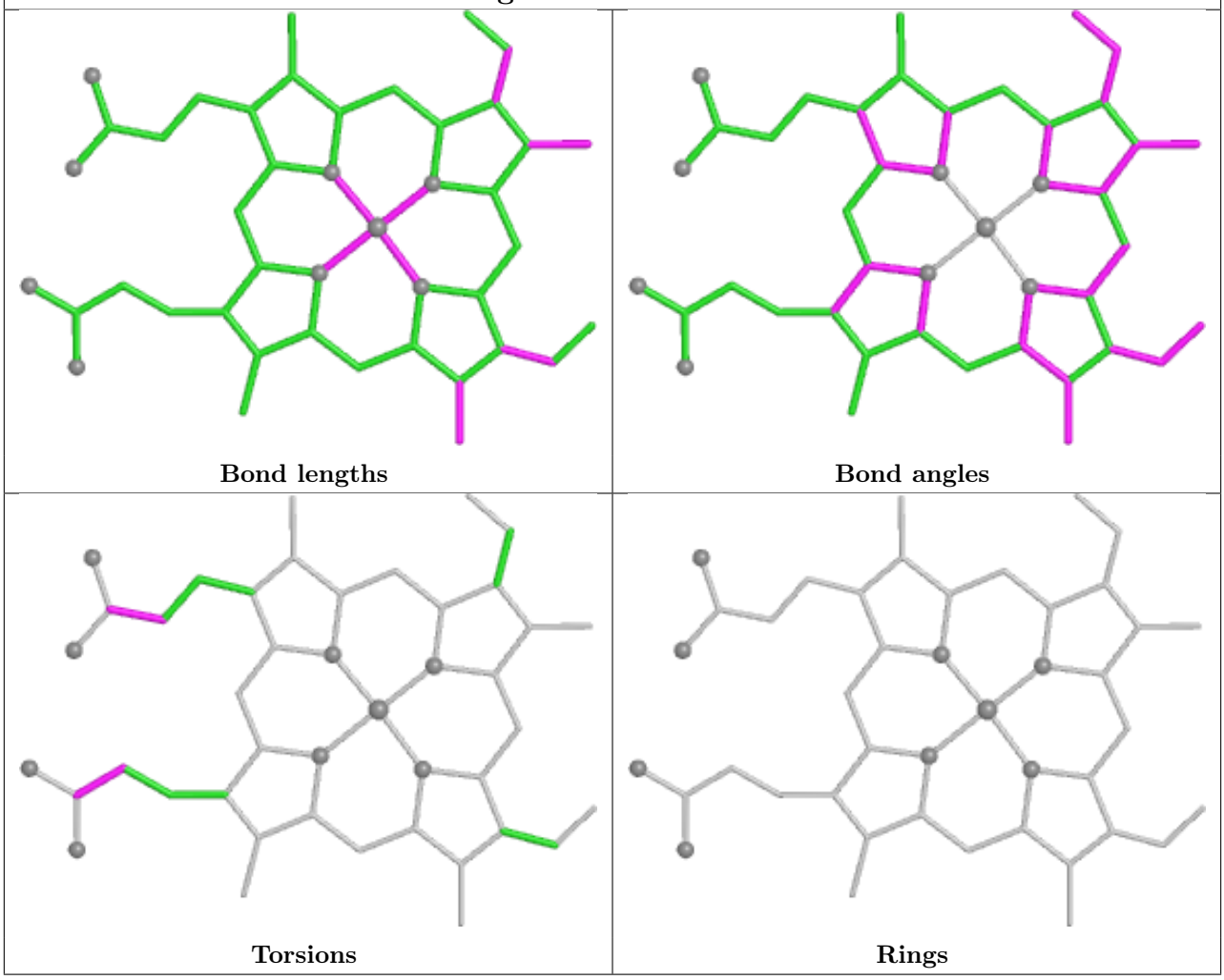
There are no ring outliers.

2 monomers are involved in 16 short contacts:

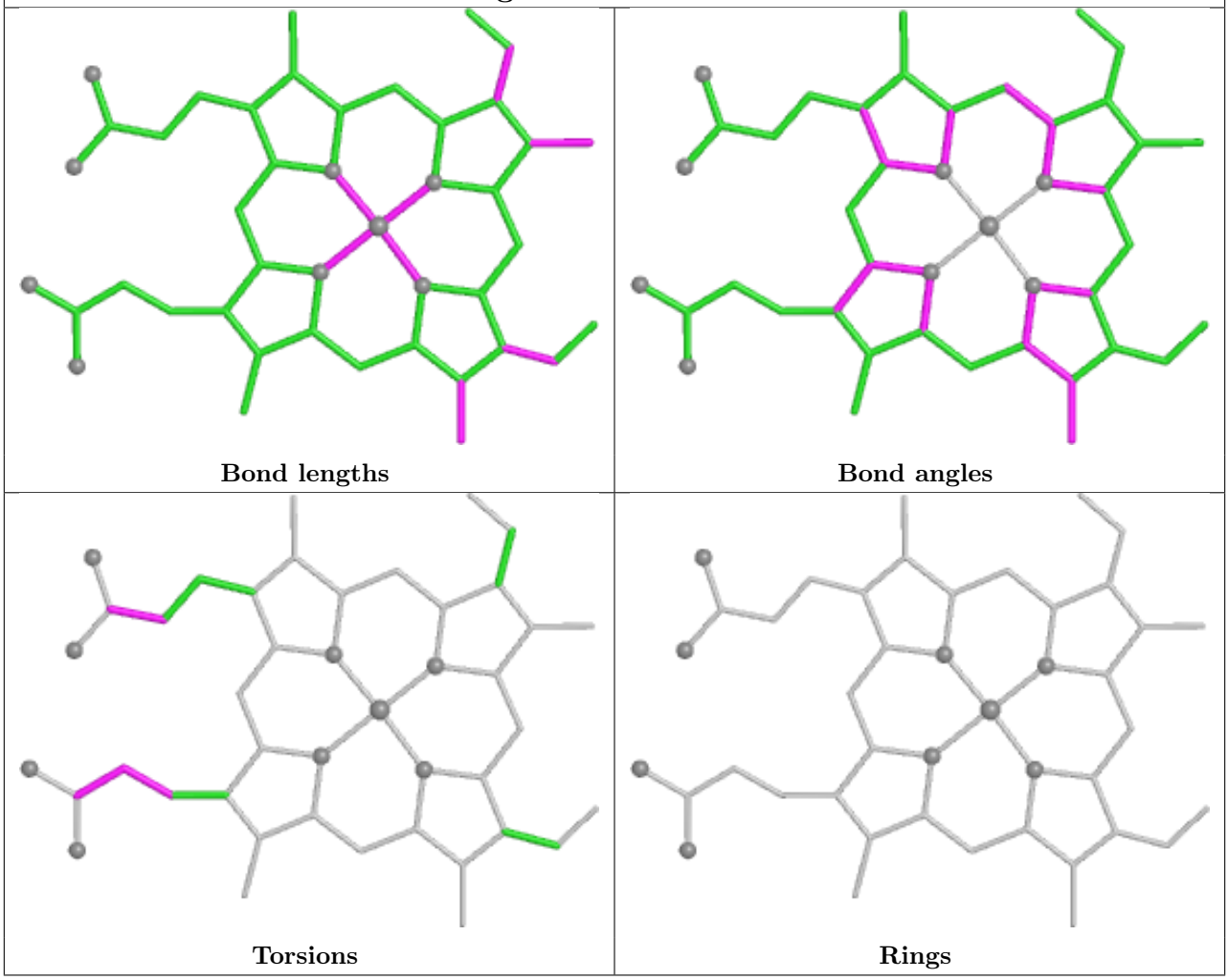
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	HEM	9	0
3	D	401	HEM	7	0

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 HEM F 401



Ligand HEM D 401



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	216/231 (93%)	0.70	29 (13%)	7	8	110, 140, 164, 193	0
1	C	218/231 (94%)	0.57	22 (10%)	12	12	98, 137, 164, 180	0
1	E	217/231 (93%)	0.74	31 (14%)	6	8	126, 193, 245, 288	0
1	G	225/231 (97%)	0.82	29 (12%)	7	9	102, 149, 223, 263	0
1	I	221/231 (95%)	0.33	13 (5%)	28	22	102, 130, 156, 170	0
1	K	219/231 (94%)	0.58	25 (11%)	10	10	90, 122, 151, 225	0
2	B	341/344 (99%)	0.79	46 (13%)	7	8	108, 153, 213, 268	0
2	D	343/344 (99%)	0.80	40 (11%)	9	10	115, 203, 284, 307	0
2	F	342/344 (99%)	0.83	57 (16%)	4	6	128, 160, 221, 310	0
2	H	341/344 (99%)	0.83	50 (14%)	6	7	144, 202, 253, 283	0
2	J	343/344 (99%)	0.69	38 (11%)	10	11	108, 190, 244, 279	0
2	L	343/344 (99%)	0.76	47 (13%)	6	8	112, 168, 218, 251	0
All	All	3369/3450 (97%)	0.72	427 (12%)	8	9	90, 158, 240, 310	0

The worst 5 of 427 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	164	ASP	9.8
2	B	154	GLY	9.1
1	G	164	ASP	8.6
1	G	196	VAL	8.5
2	H	241	PHE	7.7

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 oligosaccharides in this entry.

6.4 Ligands (i)

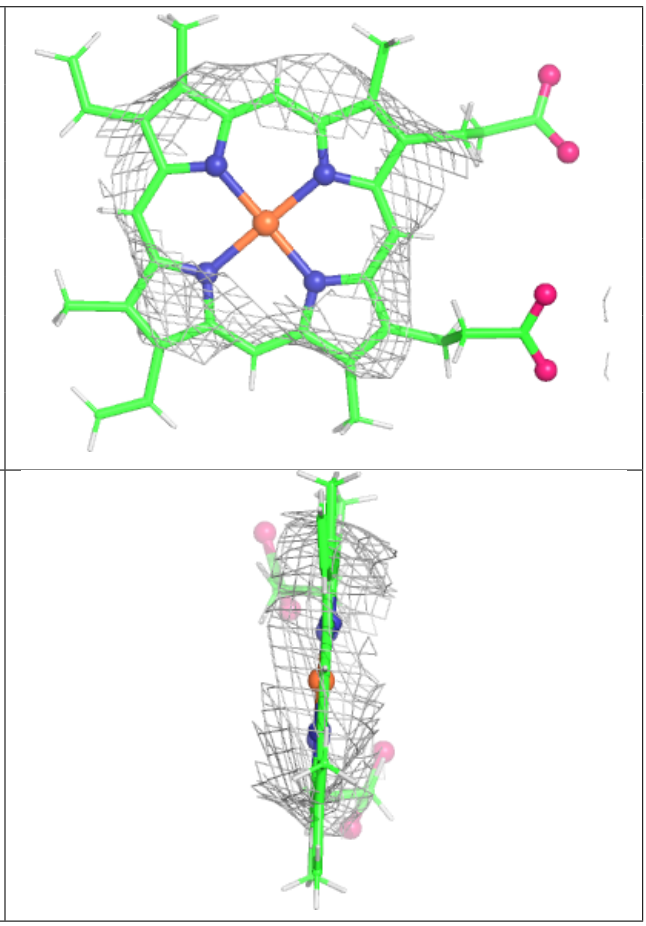
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

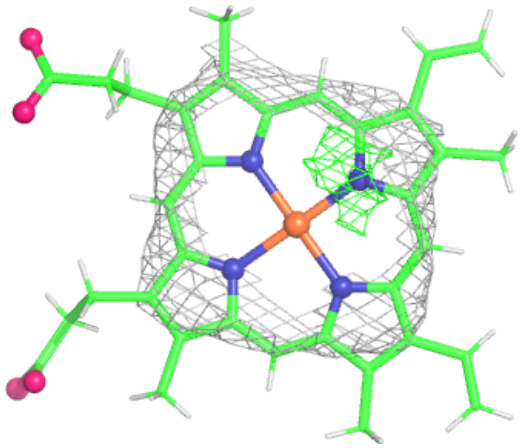
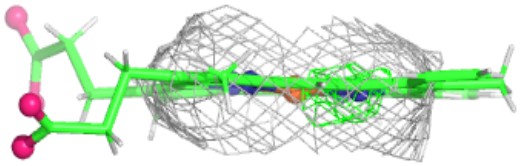
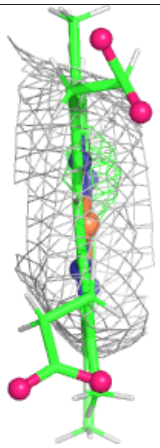
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEM	F	401	43/43	0.90	0.19	208,288,288,288	73
3	HEM	D	401	43/43	0.95	0.25	208,268,268,268	73

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 HEM F 401:

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 D 401: 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.