



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2022 – 06:10 PM JST

PDB ID : 7W7B
Title : Heme exporter HrtBA in complex with protoporphyrin IX containing manganese(III), high resolution data
Authors : Hisano, T.; Nakamura, H.; Rahman, M.M.; Tosha, T.; Shirouzu, M.; Shiro, Y.
Deposited on : 2021-12-04
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.28.1
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) : 2.28.1

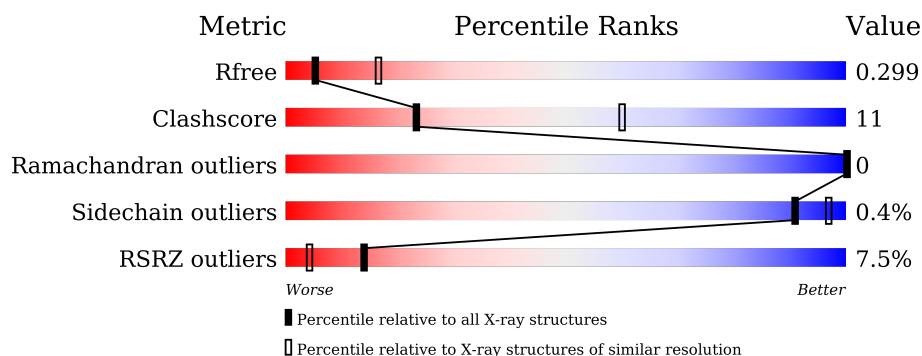
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.






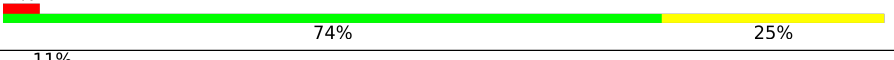
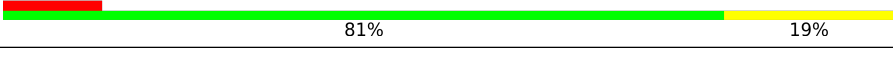
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 $\leq 5\%$. 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	231	<div> <div>4%</div> <div>71% 22% 6%</div> </div>
1	C	231	<div> <div>64% 31% 6%</div> </div>
1	E	231	<div> <div>13%</div> <div>72% 22% 6%</div> </div>
1	G	231	<div> <div>%</div> <div>68% 30% .</div> </div>
1	I	231	<div> <div>71% 25% .</div> </div>
1	K	231	<div> <div>74% 21% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	344	
2	D	344	
2	F	344	
2	H	344	
2	J	344	
2	L	344	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25131 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 Putative ABC transport system, ATP-binding protein.

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

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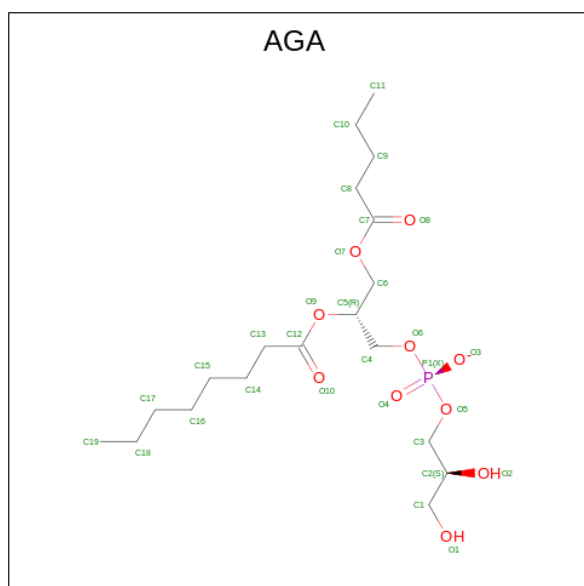
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Chain	Residue	Modelled	Actual	Comment	Reference
K	231	LYS	-	expression tag	UNP Q6NEF2

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

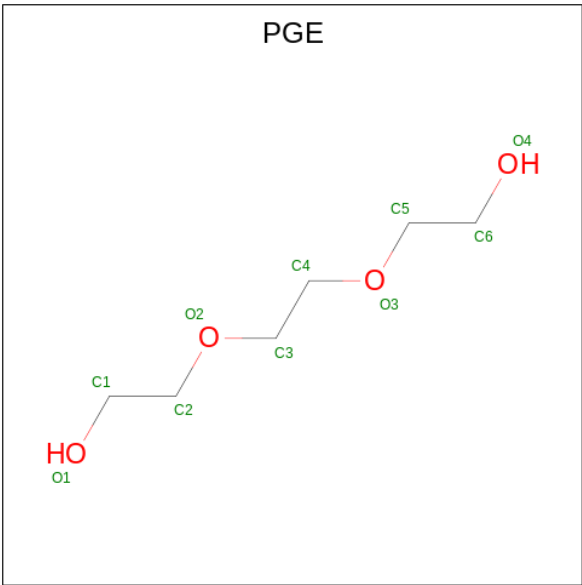
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	341	Total	C	N	O	S	0	1	0
			2518	1617	425	471	5			
2	D	343	Total	C	N	O	S	0	1	0
			2530	1624	427	474	5			
2	F	342	Total	C	N	O	S	0	1	0
			2523	1620	426	472	5			
2	H	341	Total	C	N	O	S	0	0	0
			2510	1612	422	471	5			
2	J	343	Total	C	N	O	S	0	1	0
			2530	1624	427	474	5			
2	L	343	Total	C	N	O	S	0	0	0
			2522	1619	424	474	5			

- Molecule 3 is (1S)-2-[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYL OXY)METHYL]ETHYL OCTANOATE (three-letter code: AGA) (formula: C₁₉H₃₆O₁₀P).



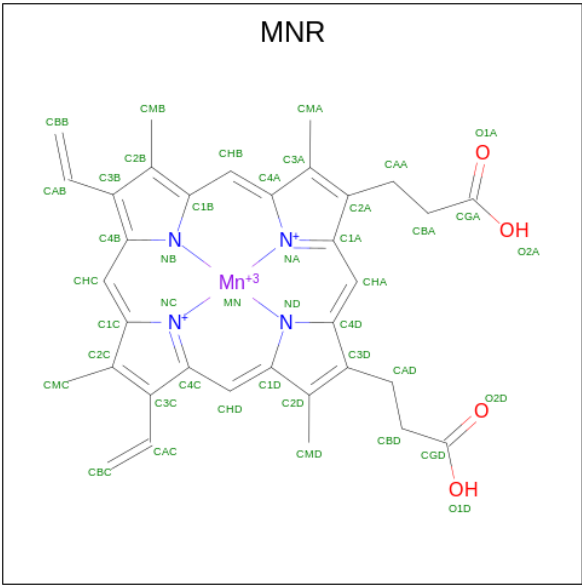
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			23	14	8	1		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



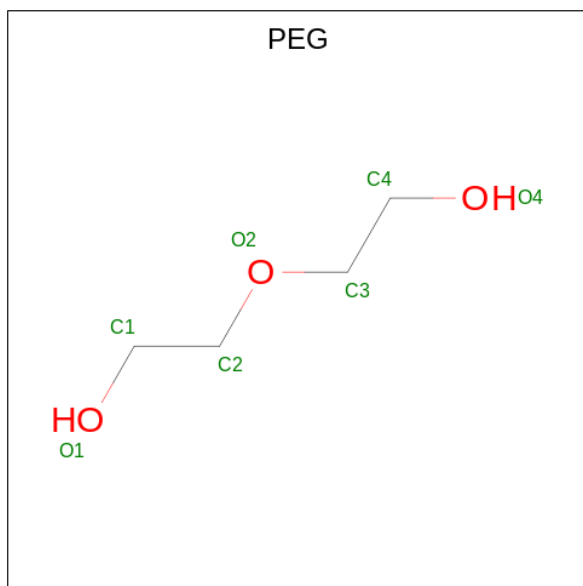
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING MN (three-letter code: MNR) (formula: $C_{34}H_{32}MnN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	Mn	N	O	0
			43	34	1	4	4	
5	H	1	Total	C	Mn	N	O	0
			43	34	1	4	4	

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

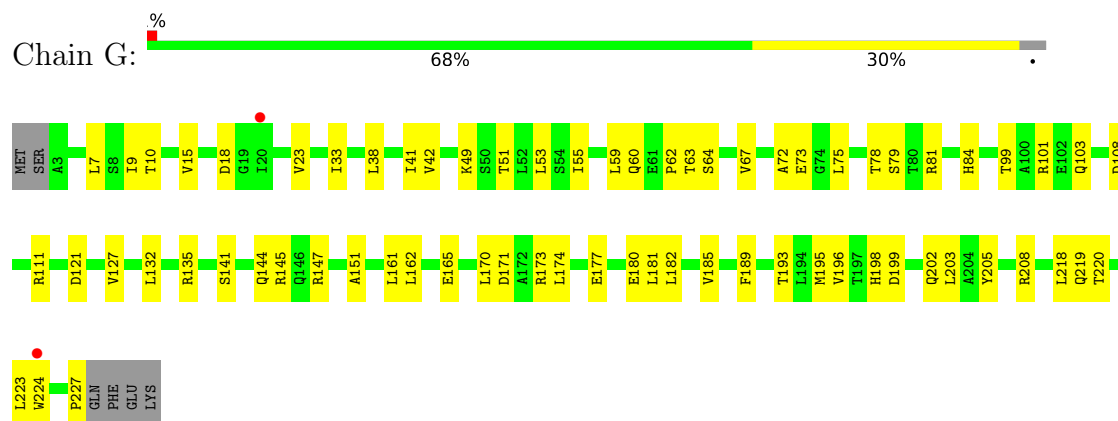


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			7	4	3		
6	H	1	Total	C	O	0	0
			7	4	3		

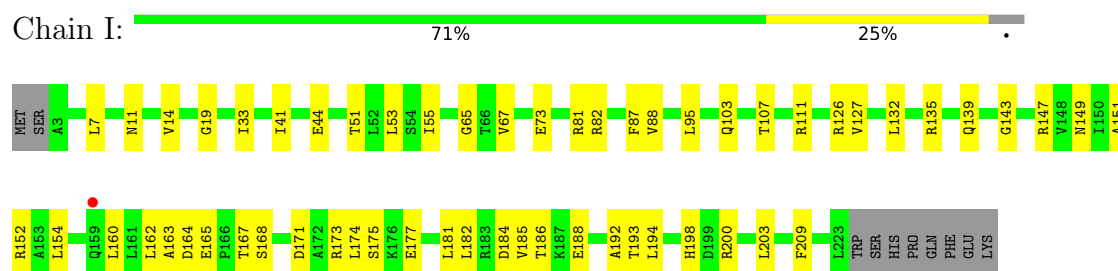
- Molecule 1: Putative ABC transport system, ATP-binding protein



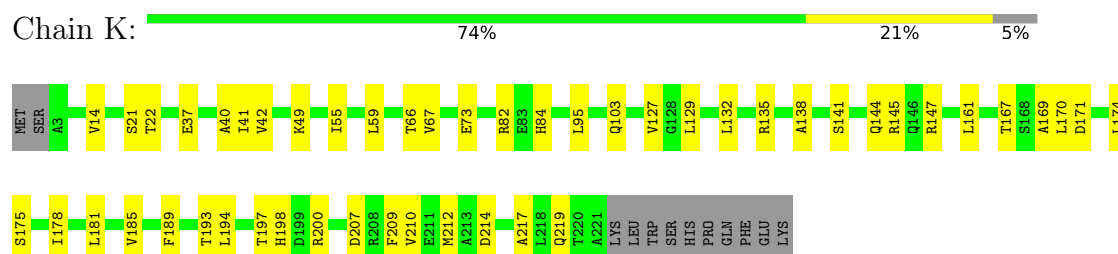
- Molecule 1: Putative ABC transport system, ATP-binding protein



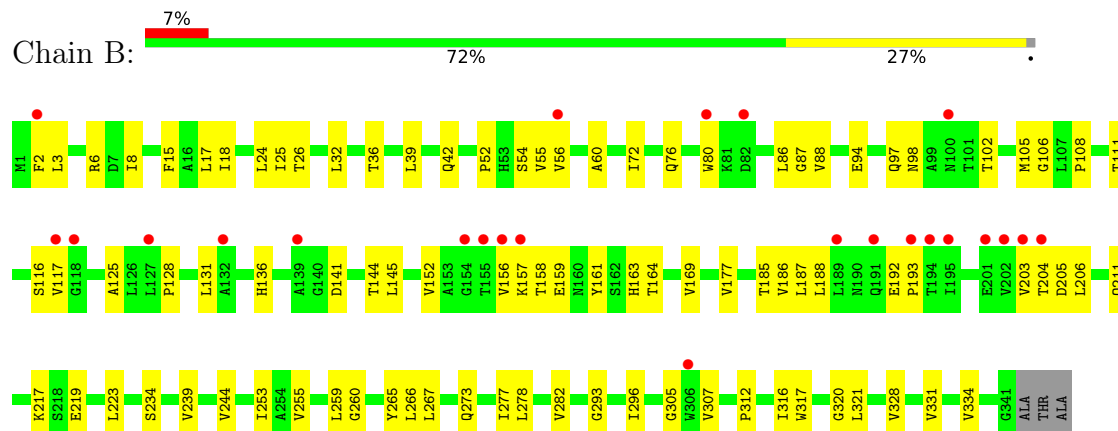
- Molecule 1: Putative ABC transport system, ATP-binding protein



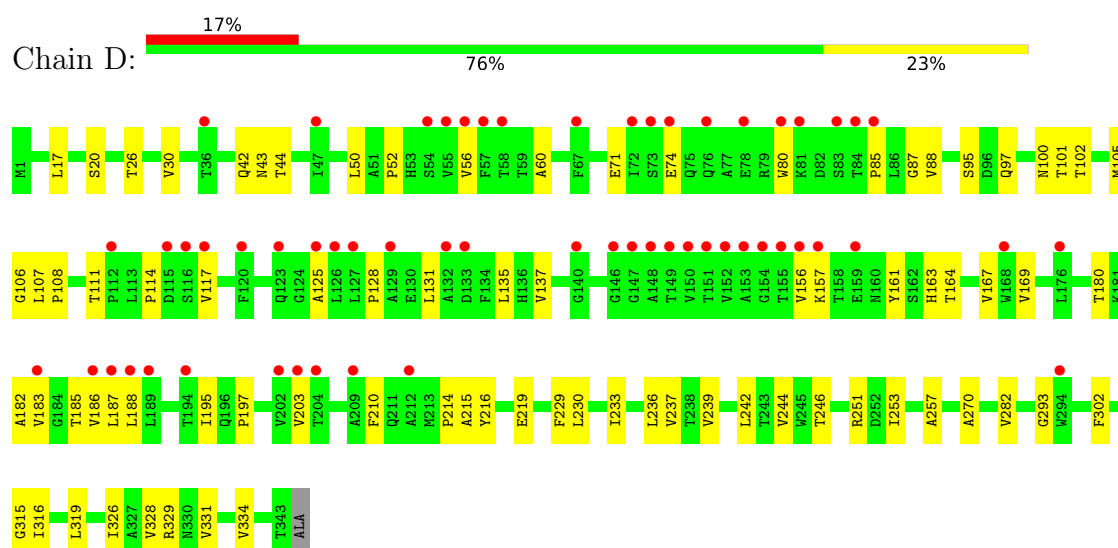
- Molecule 1: Putative ABC transport system, ATP-binding protein



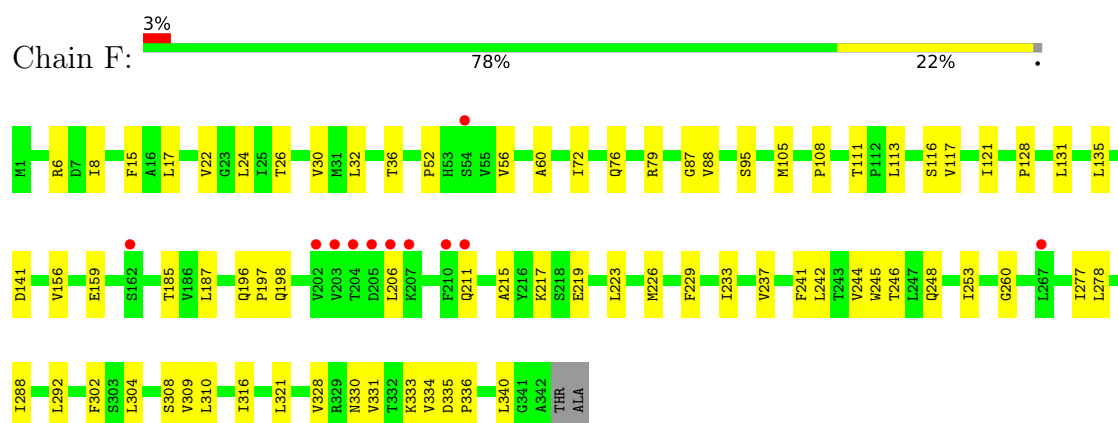
- Molecule 2: Putative ABC transport system integral membrane protein



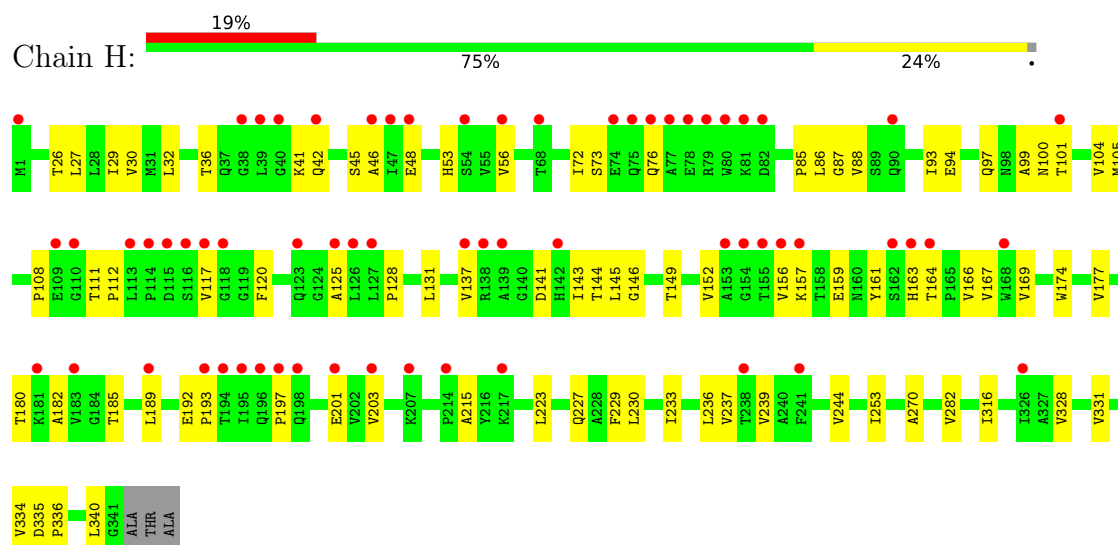
- Molecule 2: Putative ABC transport system integral membrane protein



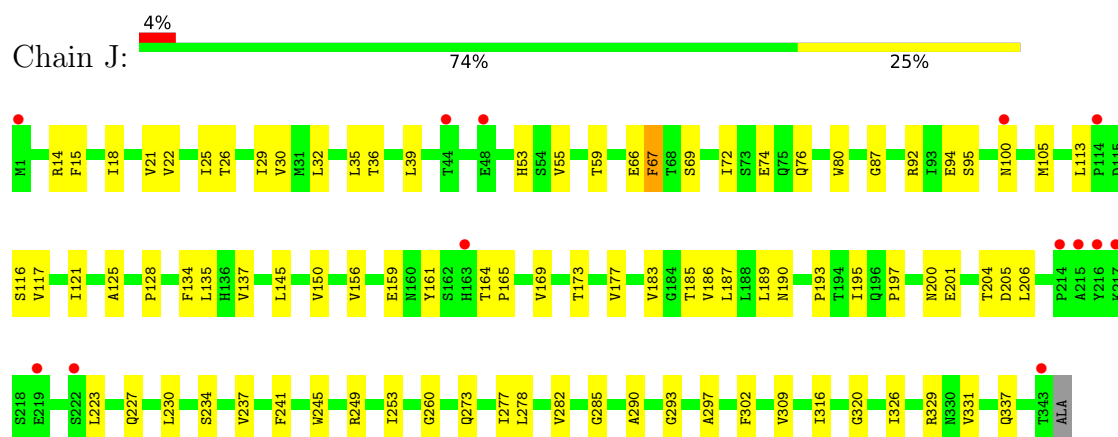
• Molecule 2: Putative ABC transport system integral membrane protein



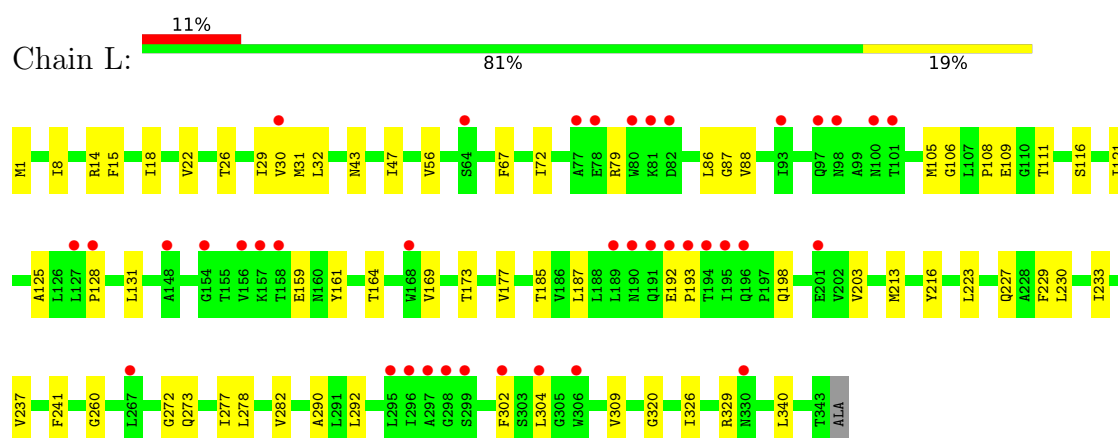
• Molecule 2: Putative ABC transport system integral membrane protein



• Molecule 2: Putative ABC transport system integral membrane protein



- Molecule 2: Putative ABC transport system integral membrane protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.00Å 133.49Å 159.34Å 111.65° 99.69° 94.64°	Depositor
Resolution (Å)	49.39 – 3.00 49.39 – 2.99	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.39-3.00) 80.2 (49.39-2.99)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.26 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.266 , 0.299 0.266 , 0.299	Depositor DCC
R_{free} test set	3785 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	25131	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: AGA, PEG, PGE, MNR

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	0/1637	0.54	0/2216
1	C	0.29	0/1653	0.54	0/2238
1	E	0.26	0/1648	0.50	0/2230
1	G	0.30	0/1716	0.52	0/2325
1	I	0.30	0/1671	0.53	0/2263
1	K	0.29	0/1658	0.53	0/2245
2	B	0.26	0/2567	0.51	0/3509
2	D	0.29	0/2579	0.53	0/3526
2	F	0.26	0/2572	0.50	0/3516
2	H	0.27	0/2556	0.52	0/3495
2	J	0.27	0/2579	0.50	0/3526
2	L	0.26	0/2568	0.50	0/3512
All	All	0.28	0/25404	0.52	0/34601

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	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1634	0	1679	53	0
1	E	1629	0	1675	37	0
1	G	1693	0	1737	45	0
1	I	1652	0	1697	46	0
1	K	1639	0	1684	36	0
2	B	2518	0	2601	75	0
2	D	2530	0	2613	58	0
2	F	2523	0	2606	56	0
2	H	2510	0	2588	61	0
2	J	2530	0	2613	59	0
2	L	2522	0	2600	42	0
3	B	23	0	19	2	0
4	B	10	0	14	1	0
5	D	43	0	30	8	0
5	H	43	0	30	5	0
6	D	7	0	10	0	0
6	H	7	0	10	0	0
All	All	25131	0	25870	575	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 11.

The worst 5 of 575 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)
2:F:79:ARG:HH12	2:F:198:GLN:HB2	1.31	0.93
1:I:198:HIS:HB3	1:K:198:HIS:CE1	2.07	0.90
1:A:53:LEU:HD11	1:A:162:LEU:HB3	1.56	0.87
1:E:59:LEU:HD13	2:F:340:LEU:HD11	1.55	0.86
1:E:127:VAL:HG13	1:E:181:LEU:HD21	1.58	0.86

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%)	208 (97%)	6 (3%)	0	100	100
1	C	216/231 (94%)	210 (97%)	6 (3%)	0	100	100
1	E	215/231 (93%)	208 (97%)	7 (3%)	0	100	100
1	G	223/231 (96%)	216 (97%)	7 (3%)	0	100	100
1	I	219/231 (95%)	211 (96%)	8 (4%)	0	100	100
1	K	217/231 (94%)	210 (97%)	7 (3%)	0	100	100
2	B	340/344 (99%)	334 (98%)	6 (2%)	0	100	100
2	D	342/344 (99%)	336 (98%)	6 (2%)	0	100	100
2	F	341/344 (99%)	331 (97%)	10 (3%)	0	100	100
2	H	339/344 (98%)	331 (98%)	8 (2%)	0	100	100
2	J	342/344 (99%)	332 (97%)	10 (3%)	0	100	100
2	L	341/344 (99%)	335 (98%)	6 (2%)	0	100	100
All	All	3349/3450 (97%)	3262 (97%)	87 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/186 (92%)	171 (99%)	1 (1%)	86	95
1	C	174/186 (94%)	172 (99%)	2 (1%)	73	90
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%)	174 (99%)	1 (1%)	86	95
1	K	174/186 (94%)	173 (99%)	1 (1%)	86	95
2	B	265/265 (100%)	265 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	266/265 (100%)	266 (100%)	0	100	100
2	F	265/265 (100%)	263 (99%)	2 (1%)	81	93
2	H	264/265 (100%)	264 (100%)	0	100	100
2	J	266/265 (100%)	264 (99%)	2 (1%)	81	93
2	L	265/265 (100%)	264 (100%)	1 (0%)	91	97
All	All	2640/2706 (98%)	2630 (100%)	10 (0%)	91	97

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	302	PHE
1	K	197	THR
2	L	67	PHE
2	F	141	ASP
2	F	226	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	337	GLN
2	H	53	HIS
2	J	43	ASN
1	K	84	HIS
1	K	198	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

6 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
6	PEG	D	402	-	6,6,6	0.13	0	5,5,5	0.07	0
3	AGA	B	501	-	22,22,29	0.49	0	26,27,35	0.72	1 (3%)
5	MNR	H	401	2	29,50,50	3.42	15 (51%)	17,82,82	2.38	6 (35%)
6	PEG	H	402	-	6,6,6	0.12	0	5,5,5	0.06	0
5	MNR	D	401	2	29,50,50	3.37	15 (51%)	17,82,82	2.23	5 (29%)
4	PGE	B	502	-	9,9,9	0.16	0	8,8,8	0.11	0

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
6	PEG	D	402	-	-	0/4/4/4	-
3	AGA	B	501	-	-	4/24/24/34	-
5	MNR	H	401	2	-	3/8/94/94	-
6	PEG	H	402	-	-	2/4/4/4	-
5	MNR	D	401	2	-	3/8/94/94	-
4	PGE	B	502	-	-	1/7/7/7	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	401	MNR	C1D-C2D	5.85	1.46	1.38
5	D	401	MNR	C1B-C2B	5.69	1.45	1.38
5	D	401	MNR	C1D-C2D	5.60	1.45	1.38
5	D	401	MNR	C4D-C3D	5.55	1.45	1.38
5	H	401	MNR	C1B-C2B	5.49	1.45	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	401	MNR	CAD-C3D-C4D	-5.93	123.13	127.30
5	D	401	MNR	CAD-C3D-C4D	-5.42	123.49	127.30
5	H	401	MNR	CHC-C4B-C3B	-4.61	123.34	129.55
5	D	401	MNR	CHC-C4B-C3B	-4.43	123.60	129.55
5	H	401	MNR	CBD-CAD-C3D	4.00	119.87	112.49

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

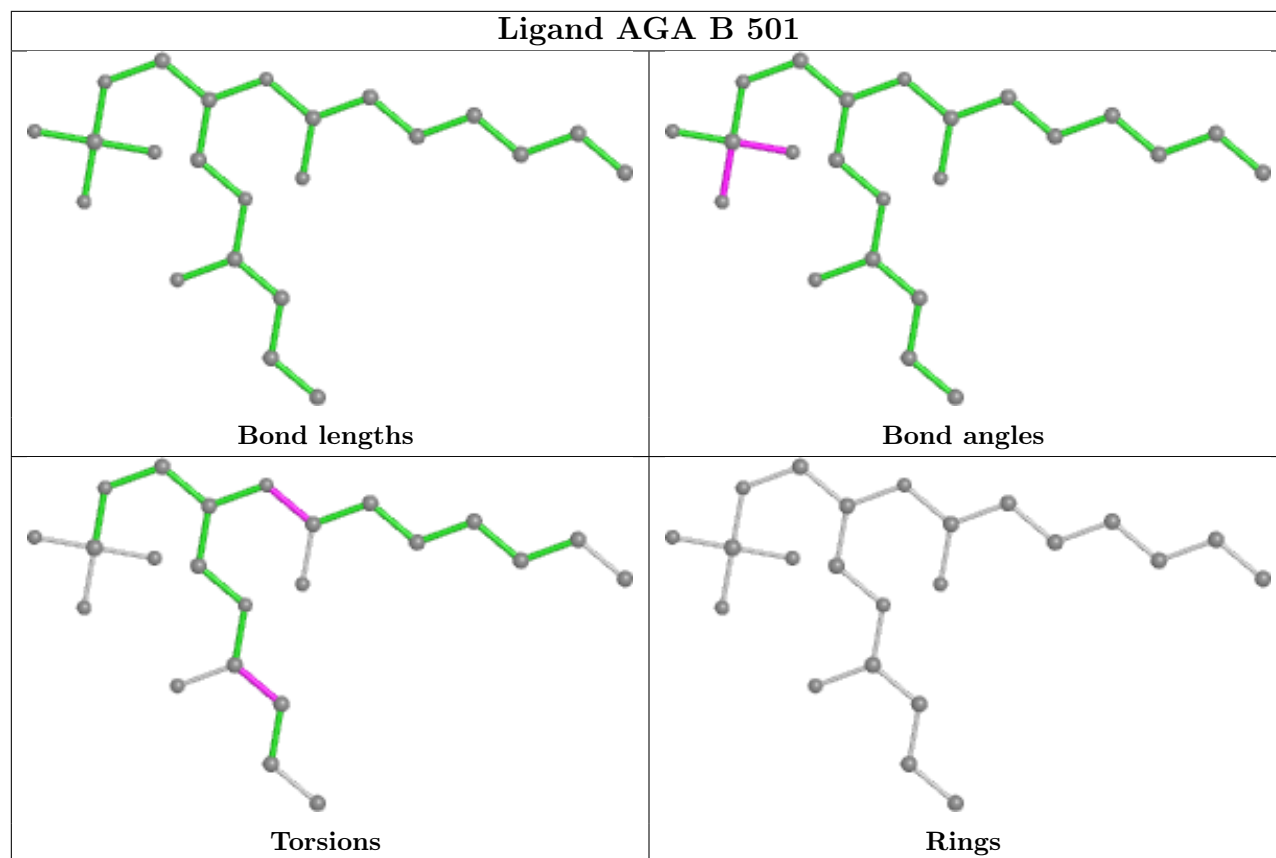
Mol	Chain	Res	Type	Atoms
5	D	401	MNR	C2D-C3D-CAD-CBD
5	D	401	MNR	C4D-C3D-CAD-CBD
5	H	401	MNR	C2D-C3D-CAD-CBD
5	H	401	MNR	C4D-C3D-CAD-CBD
3	B	501	AGA	C13-C12-O9-C5

There are no ring outliers.

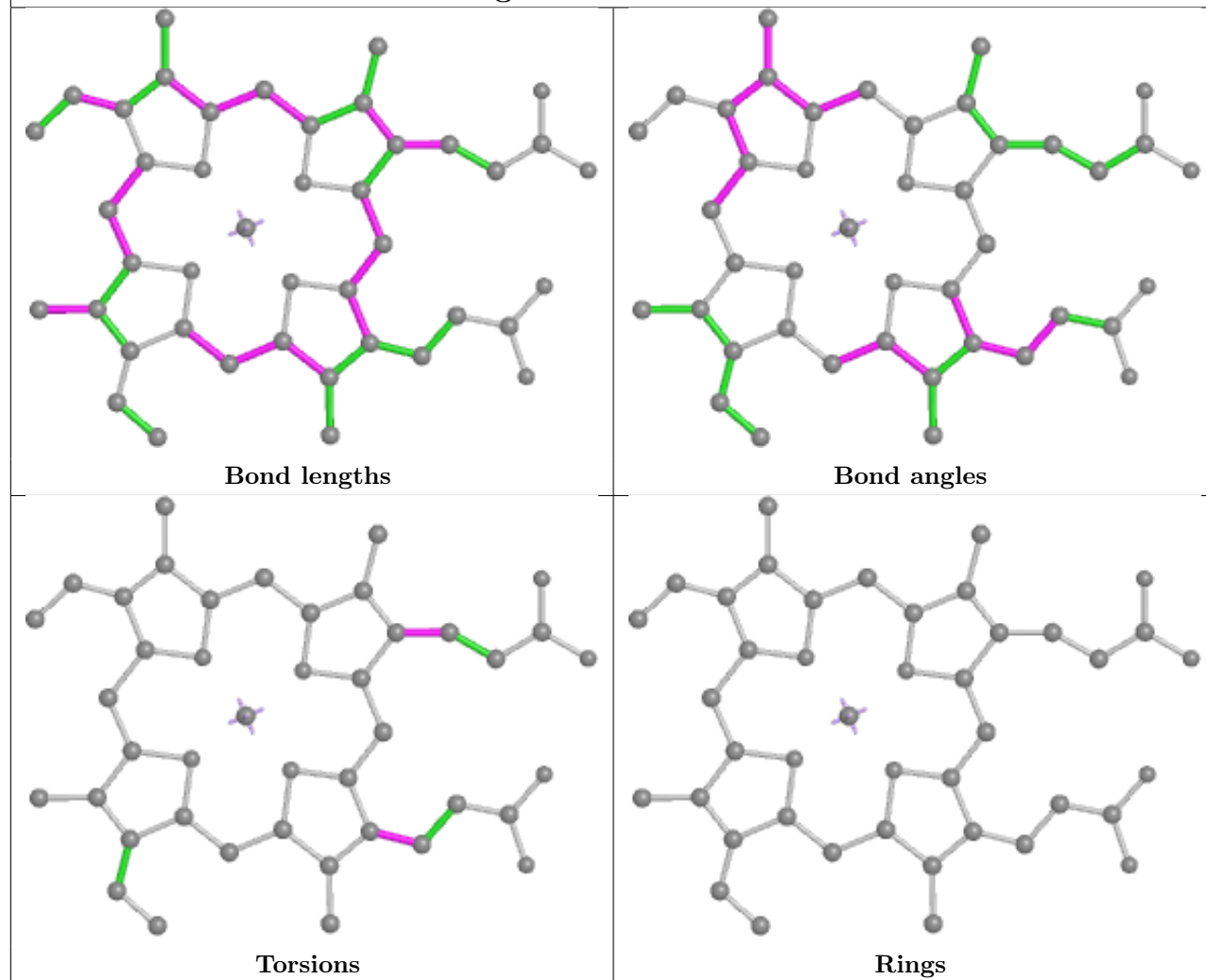
4 monomers are involved in 16 short contacts:

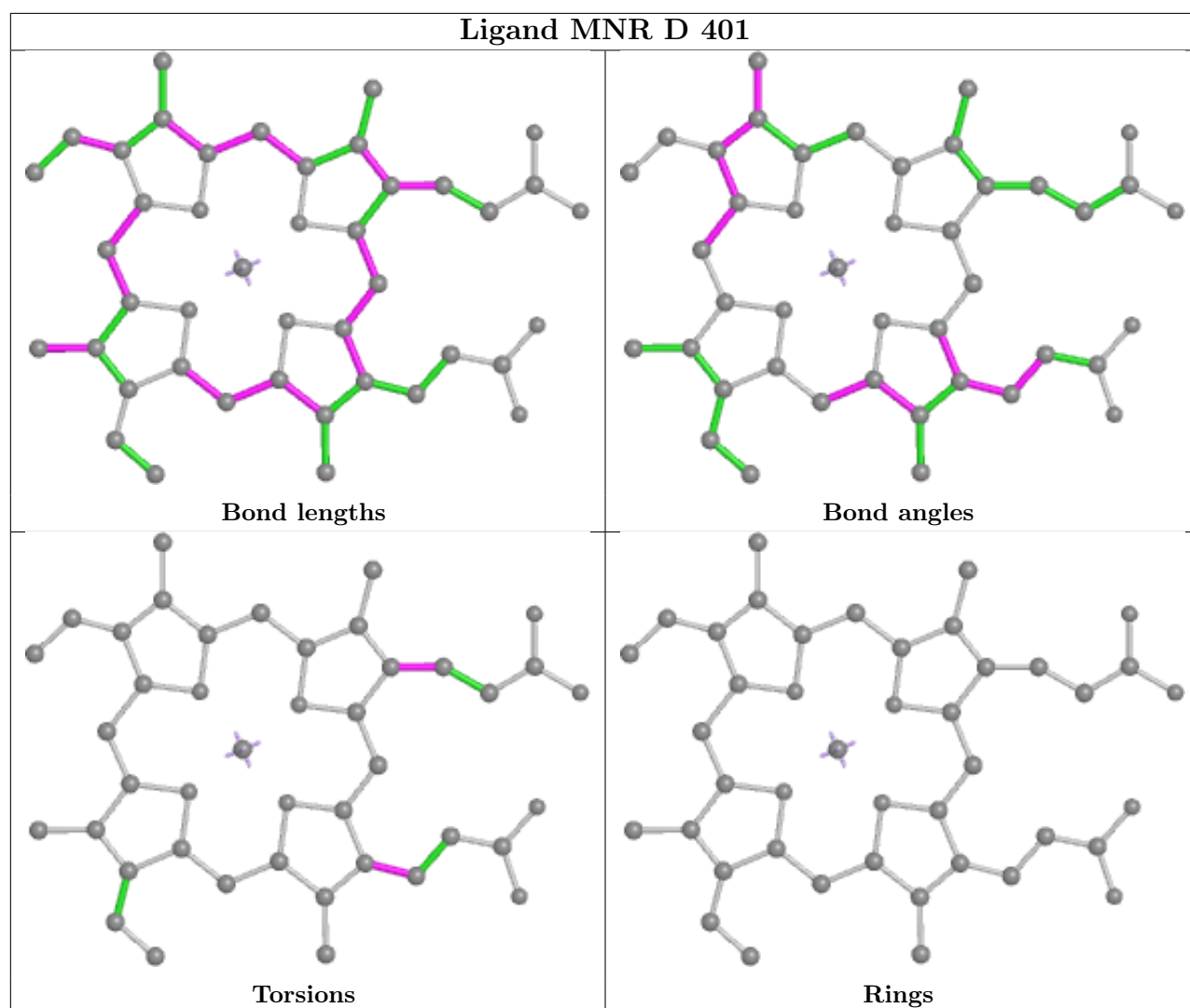
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	AGA	2	0
5	H	401	MNR	5	0
5	D	401	MNR	8	0
4	B	502	PGE	1	0

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 than 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 MNR H 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%)	0.03	9 (4%) 36 14	94, 115, 134, 152	0
1	C	218/231 (94%)	-0.21	0 100 100	75, 100, 120, 134	0
1	E	217/231 (93%)	0.56	30 (13%) 2 1	110, 147, 192, 290	0
1	G	225/231 (97%)	-0.20	2 (0%) 84 63	82, 108, 145, 171	0
1	I	221/231 (95%)	-0.18	1 (0%) 91 75	79, 99, 117, 130	0
1	K	219/231 (94%)	-0.22	0 100 100	77, 92, 114, 151	0
2	B	341/344 (99%)	0.23	24 (7%) 16 5	98, 120, 183, 228	0
2	D	343/344 (99%)	0.84	58 (16%) 1 0	95, 160, 220, 246	0
2	F	342/344 (99%)	0.10	11 (3%) 47 20	110, 133, 173, 202	0
2	H	341/344 (99%)	0.81	64 (18%) 1 0	109, 176, 221, 267	0
2	J	343/344 (99%)	-0.02	13 (3%) 40 16	94, 149, 187, 241	0
2	L	343/344 (99%)	0.39	39 (11%) 5 1	86, 144, 191, 215	0
All	All	3369/3450 (97%)	0.22	251 (7%) 14 4	75, 128, 195, 290	0

The worst 5 of 251 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	154	GLY	12.1
2	D	155	THR	8.9
2	D	187	LEU	7.4
1	E	21	SER	6.9
2	J	100	ASN	6.8

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](#)

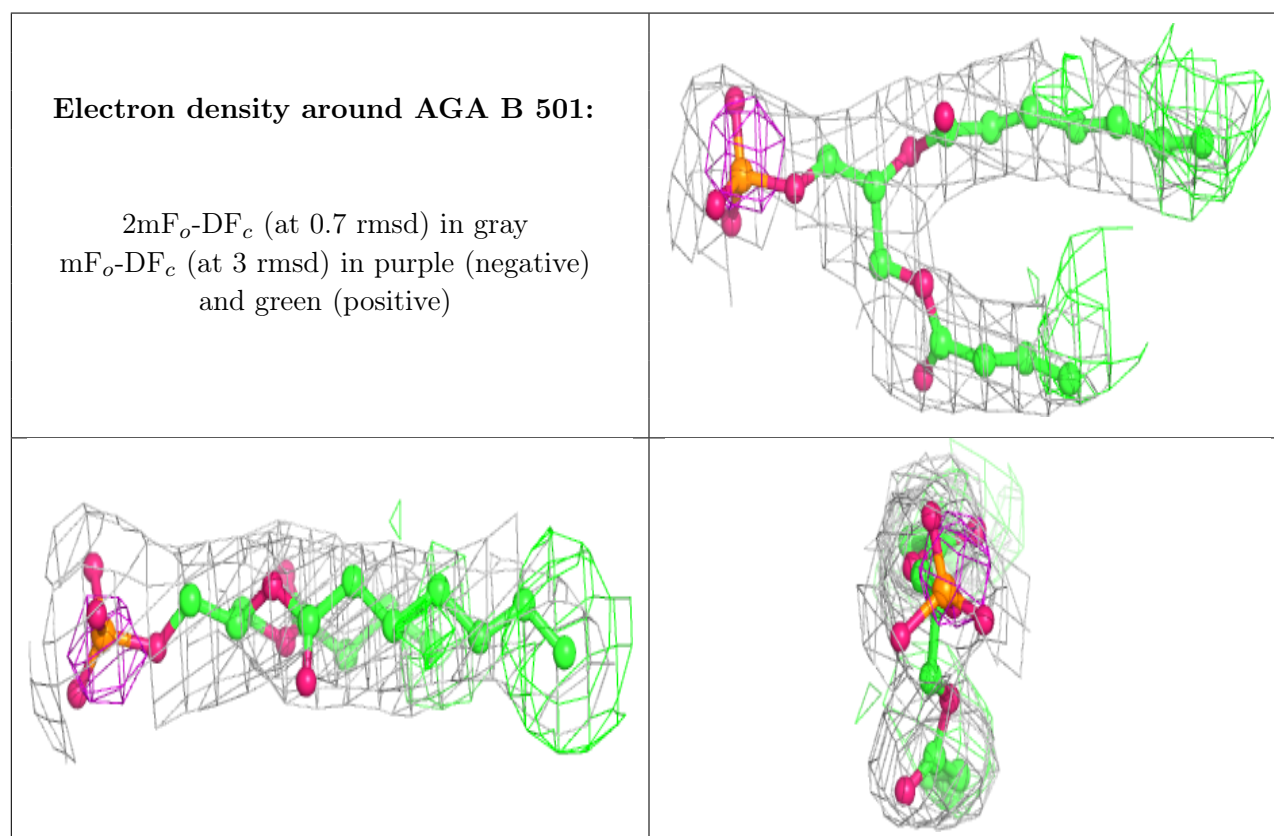
There are no monosaccharides in this entry.

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.

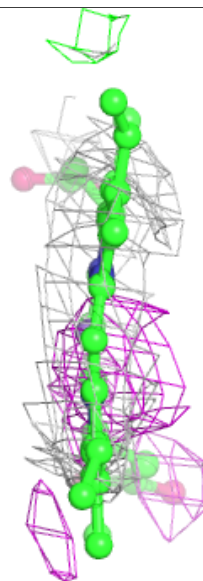
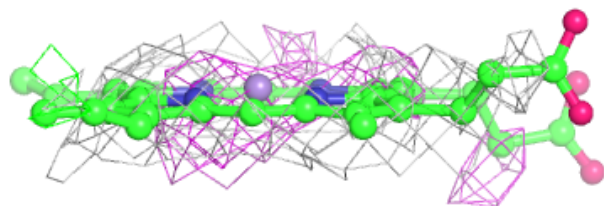
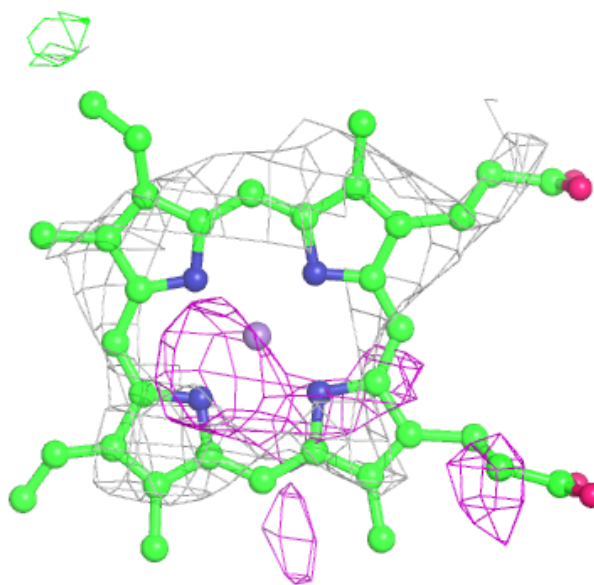
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PGE	B	502	10/10	0.71	0.29	132,132,132,132	0
3	AGA	B	501	23/30	0.76	0.21	142,142,142,142	0
6	PEG	H	402	7/7	0.80	0.29	172,172,172,172	0
6	PEG	D	402	7/7	0.84	0.41	172,172,172,172	0
5	MNR	H	401	43/43	0.86	0.35	179,179,179,179	0
5	MNR	D	401	43/43	0.93	0.26	119,119,119,119	0

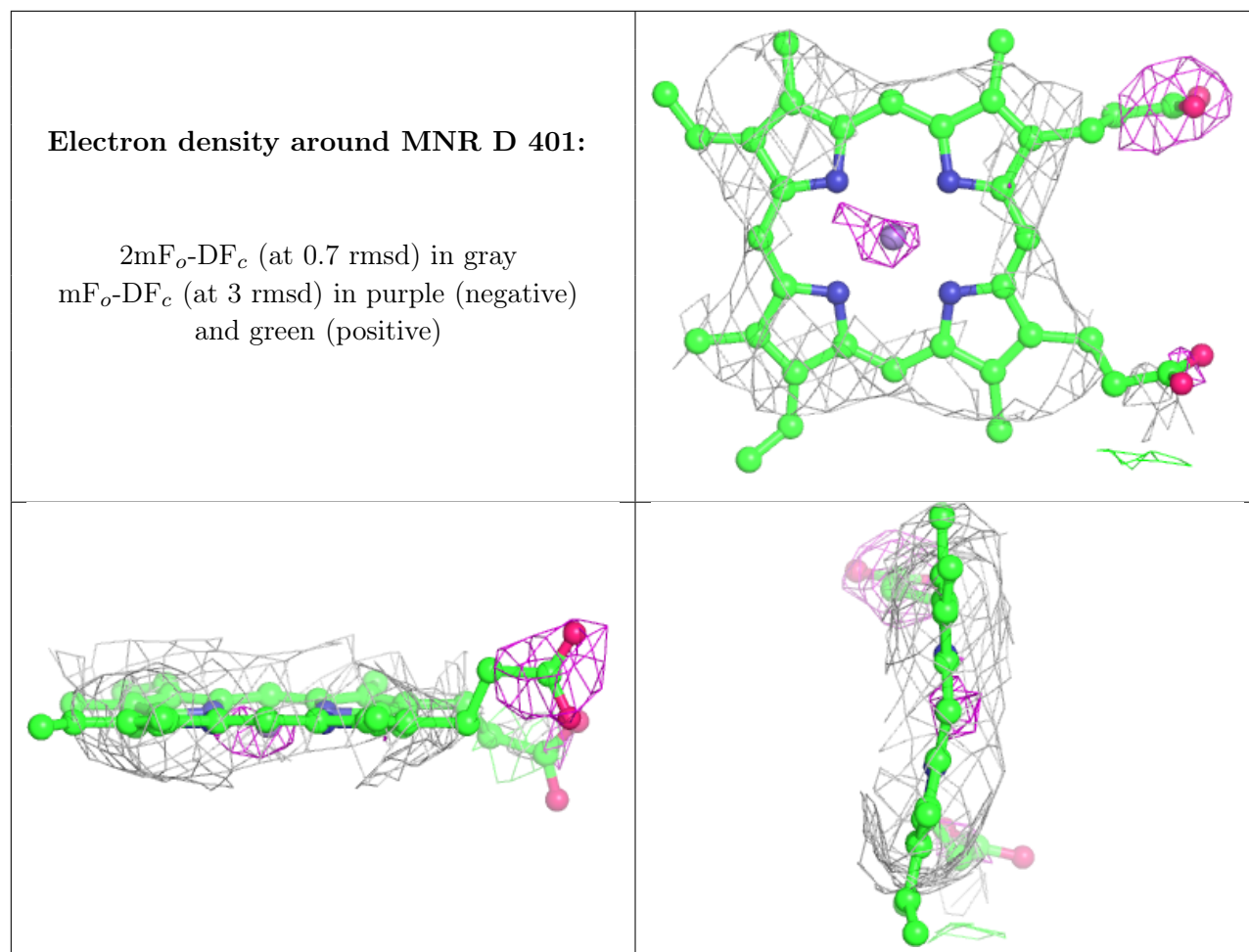
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around MNR H 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.