



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:29 AM EDT

PDB ID : 6ZMQ / pdb_00006zmq
Title : Cytochrome c Heme Lyase CcmF
Authors : Brausemann, A.; Einsle, O.
Deposited on : 2020-07-03
Resolution : 2.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

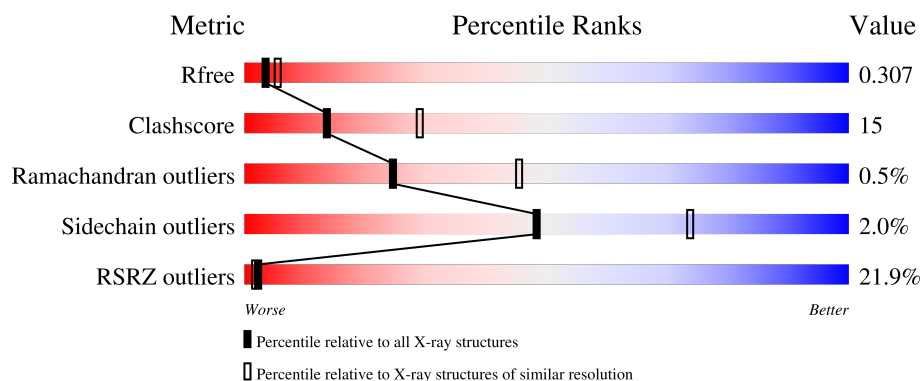
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	660	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4966 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

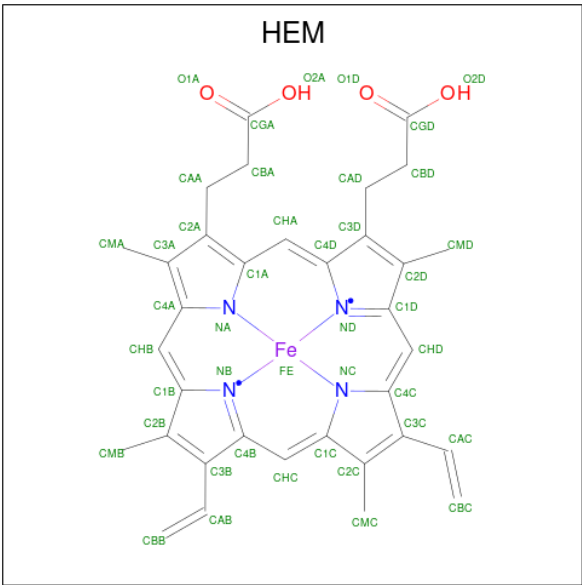
- Molecule 1 is a protein called Cytochrome C-type biogenesis protein ccmF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4636	3107	765	750	14			

There are 17 discrepancies between the modelled and reference sequences:

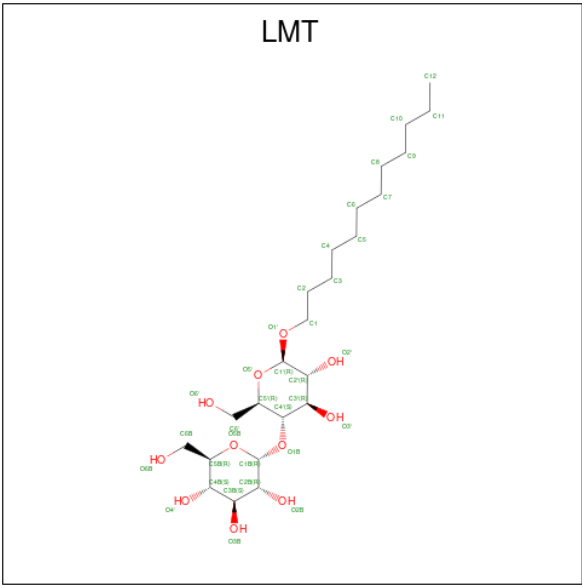
Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	TRP	-	expression tag	UNP Q72IU4
A	-15	SER	-	expression tag	UNP Q72IU4
A	-14	HIS	-	expression tag	UNP Q72IU4
A	-13	PRO	-	expression tag	UNP Q72IU4
A	-12	GLN	-	expression tag	UNP Q72IU4
A	-11	PHE	-	expression tag	UNP Q72IU4
A	-10	GLU	-	expression tag	UNP Q72IU4
A	-9	LYS	-	expression tag	UNP Q72IU4
A	-8	GLY	-	expression tag	UNP Q72IU4
A	-7	ALA	-	expression tag	UNP Q72IU4
A	-6	GLU	-	expression tag	UNP Q72IU4
A	-5	ASN	-	expression tag	UNP Q72IU4
A	-4	LEU	-	expression tag	UNP Q72IU4
A	-3	TYR	-	expression tag	UNP Q72IU4
A	-2	PHE	-	expression tag	UNP Q72IU4
A	-1	GLN	-	expression tag	UNP Q72IU4
A	0	SER	-	expression tag	UNP Q72IU4

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



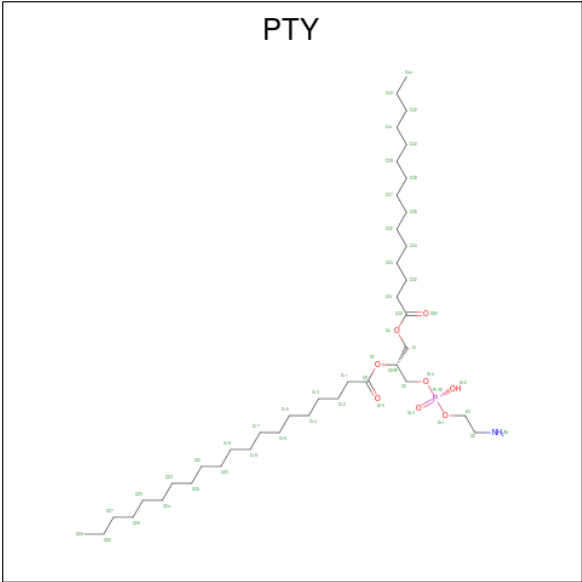
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
4	A	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.72Å 128.27Å 134.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.15 – 2.67 48.15 – 2.67	Depositor EDS
% Data completeness (in resolution range)	44.1 (48.15-2.67) 44.9 (48.15-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.271 , 0.308 0.274 , 0.307	Depositor DCC
R_{free} test set	787 reflections (2.26%)	wwPDB-VP
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 12.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for -h,l,k	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4966	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTY, LMT, 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	0.59	3/4781 (0.1%)	1.07	24/6522 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	566	PRO	N-CA	15.71	1.67	1.47
1	A	257	PHE	C-O	-5.76	1.17	1.24
1	A	261	ALA	C-O	-5.70	1.17	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	PRO	N-CA-C	-12.90	85.89	112.47
1	A	565	TYR	CA-C-N	12.77	135.80	119.84
1	A	565	TYR	C-N-CA	12.77	135.80	119.84
1	A	260	THR	CB-CA-C	8.60	125.46	110.85
1	A	585	TYR	CA-C-N	-8.01	108.19	122.45
1	A	585	TYR	C-N-CA	-8.01	108.19	122.45
1	A	79	LYS	N-CA-C	7.98	123.02	113.28
1	A	585	TYR	CB-CA-C	-7.95	97.81	110.85
1	A	255	THR	CA-CB-OG1	-7.88	97.77	109.60
1	A	566	PRO	CB-CA-C	7.64	124.17	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	GLY	CA-C-O	-6.97	113.68	122.39
1	A	566	PRO	CA-N-CD	-6.68	102.65	112.00
1	A	585	TYR	N-CA-C	-5.67	104.58	112.30
1	A	-1	GLN	N-CA-C	-5.61	99.58	108.73
1	A	521	GLU	N-CA-C	-5.60	108.23	114.62
1	A	595	GLU	N-CA-C	-5.58	100.10	108.96
1	A	540	GLU	CA-C-N	-5.57	112.24	122.27
1	A	540	GLU	C-N-CA	-5.57	112.24	122.27
1	A	518	TYR	CA-CB-CG	5.38	123.58	113.90
1	A	308	VAL	CA-C-N	5.27	124.98	121.13
1	A	308	VAL	C-N-CA	5.27	124.98	121.13
1	A	565	TYR	O-C-N	-5.24	116.73	121.39
1	A	585	TYR	CA-CB-CG	5.20	123.27	113.90
1	A	597	GLY	N-CA-C	5.16	118.88	112.64

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	565	TYR	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4636	0	4702	142	0
2	A	43	0	30	5	0
3	A	70	0	91	1	0
4	A	200	0	316	9	0
5	A	17	0	0	1	0
All	All	4966	0	5139	147	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 15.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LYS:NZ	1:A:530:MET:HE3	1.73	1.02
1:A:554:ARG:HH21	1:A:554:ARG:HG2	1.24	1.02
1:A:515:LYS:HZ3	1:A:530:MET:HE3	1.25	0.98
1:A:586:TYR:OH	1:A:606:VAL:CG1	2.11	0.98
1:A:270:PHE:CE1	1:A:350:LEU:HG	1.99	0.97
1:A:76:HIS:ND1	1:A:79:LYS:HB2	1.83	0.94
1:A:586:TYR:OH	1:A:606:VAL:HG13	1.72	0.89
1:A:76:HIS:CG	1:A:79:LYS:HB2	2.08	0.87
1:A:541:GLY:O	1:A:543:ARG:N	2.09	0.85
1:A:80:ASP:HB2	1:A:542:ARG:HH22	1.42	0.84
1:A:270:PHE:CZ	1:A:350:LEU:HB2	2.15	0.81
1:A:612:TRP:HA	1:A:615:VAL:HG12	1.61	0.80
1:A:343:LEU:HD23	1:A:413:ARG:HH21	1.45	0.79
1:A:80:ASP:HB2	1:A:542:ARG:NH2	1.97	0.77
1:A:343:LEU:HD23	1:A:413:ARG:NH2	1.99	0.77
1:A:515:LYS:NZ	1:A:530:MET:CE	2.50	0.75
1:A:554:ARG:HG2	1:A:554:ARG:NH2	1.96	0.75
1:A:80:ASP:H	1:A:542:ARG:NH2	1.87	0.73
1:A:499:MET:O	1:A:503:ILE:HG13	1.88	0.73
1:A:545:ALA:HB1	1:A:563:HIS:NE2	2.04	0.72
1:A:270:PHE:CE1	1:A:350:LEU:CG	2.72	0.72
1:A:590:MET:HG3	1:A:604:LEU:HD23	1.73	0.71
1:A:417:GLU:CD	1:A:418:VAL:HG22	2.16	0.70
1:A:80:ASP:CB	1:A:542:ARG:HH22	2.03	0.70
1:A:515:LYS:HZ3	1:A:530:MET:CE	2.03	0.70
1:A:594:ARG:HG3	1:A:594:ARG:HH21	1.58	0.69
1:A:120:ARG:HB2	1:A:192:ALA:HB1	1.74	0.69
1:A:562:LEU:H	1:A:562:LEU:HD23	1.58	0.68
1:A:311:ALA:HA	4:A:704:PTY:H132	1.77	0.67
1:A:594:ARG:HG3	1:A:594:ARG:NH2	2.10	0.67
1:A:564:PHE:CE1	1:A:574:ALA:HB1	2.30	0.66
1:A:275:PHE:HB2	1:A:327:LEU:CD1	2.26	0.66
1:A:120:ARG:NH2	1:A:201:THR:HG23	2.10	0.66
1:A:536:ARG:H	1:A:547:GLU:HB2	1.61	0.66
1:A:541:GLY:C	1:A:543:ARG:H	2.03	0.66
1:A:554:ARG:HH21	1:A:554:ARG:CG	2.04	0.64
1:A:142:ILE:HD11	1:A:307:PRO:HG2	1.83	0.61
1:A:168:MET:HA	1:A:171:VAL:HG22	1.83	0.61
1:A:80:ASP:H	1:A:542:ARG:HH22	1.49	0.59
1:A:257:PHE:HB2	1:A:277:PHE:HB3	1.85	0.58
1:A:529:ARG:O	1:A:529:ARG:HG3	2.03	0.58
1:A:550:LEU:HD11	1:A:602:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:N	1:A:542:ARG:HH22	2.03	0.57
1:A:114:LYS:HZ1	1:A:125:LEU:HD21	1.69	0.57
1:A:227:TRP:HD1	1:A:231:VAL:HB	1.69	0.57
1:A:549:LEU:HD12	1:A:549:LEU:H	1.68	0.57
1:A:417:GLU:OE2	1:A:418:VAL:HG22	2.04	0.56
1:A:515:LYS:HZ1	1:A:530:MET:HE3	1.64	0.56
1:A:586:TYR:HD1	1:A:587:PHE:H	1.52	0.56
1:A:69:LEU:HB2	1:A:72:VAL:HG12	1.89	0.55
1:A:417:GLU:CD	1:A:418:VAL:CG2	2.79	0.55
1:A:485:ARG:O	1:A:489:SER:HB3	2.07	0.54
1:A:506:SER:HA	1:A:608:PRO:HD2	1.90	0.54
1:A:270:PHE:HE1	1:A:350:LEU:HG	1.65	0.53
1:A:275:PHE:HB2	1:A:327:LEU:HD12	1.90	0.53
1:A:258:LEU:HD21	2:A:701:HEM:HBD1	1.91	0.53
1:A:594:ARG:HD3	1:A:596:LYS:HE2	1.90	0.53
1:A:417:GLU:OE1	1:A:418:VAL:HG22	2.09	0.53
1:A:130:GLY:HA3	4:A:704:PTY:H232	1.90	0.52
1:A:592:PHE:HE1	1:A:600:ALA:HB1	1.75	0.52
1:A:9:LEU:O	1:A:13:LEU:HB2	2.09	0.52
1:A:516:THR:HA	1:A:601:SER:HA	1.91	0.52
1:A:586:TYR:OH	1:A:606:VAL:HG12	2.05	0.52
1:A:515:LYS:HZ1	1:A:530:MET:CE	2.20	0.52
1:A:62:LEU:HD23	1:A:76:HIS:NE2	2.25	0.51
1:A:373:VAL:O	1:A:374:GLU:HG3	2.09	0.51
1:A:270:PHE:HB3	1:A:273:TRP:HB2	1.93	0.51
1:A:559:ARG:HE	1:A:561:ARG:HE	1.58	0.51
1:A:591:ASP:HB3	1:A:603:ARG:HB3	1.93	0.51
1:A:-9:LYS:HD3	1:A:-8:GLY:H	1.75	0.50
1:A:402:LEU:HA	1:A:405:VAL:HG12	1.93	0.50
1:A:499:MET:HE3	1:A:503:ILE:HD11	1.93	0.50
1:A:596:LYS:HD2	1:A:599:TRP:HE1	1.77	0.50
1:A:541:GLY:C	1:A:543:ARG:N	2.62	0.50
1:A:563:HIS:HB3	1:A:577:VAL:HG23	1.94	0.50
1:A:167:TRP:O	1:A:170:ALA:HB3	2.12	0.50
1:A:415:ARG:HH21	1:A:417:GLU:HB3	1.75	0.50
1:A:84:VAL:HA	1:A:87:VAL:HG22	1.93	0.50
1:A:589:LEU:HB3	1:A:605:ILE:HG13	1.93	0.50
4:A:705:PTY:H211	4:A:705:PTY:H351	1.93	0.49
1:A:203:VAL:HA	1:A:206:THR:HG22	1.95	0.49
1:A:59:GLU:HG2	1:A:89:PRO:HG2	1.94	0.49
1:A:62:LEU:CD2	1:A:76:HIS:CD2	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:SER:O	1:A:572:LEU:N	2.46	0.49
1:A:185:VAL:HG11	1:A:209:TRP:CD1	2.48	0.48
1:A:586:TYR:CZ	1:A:606:VAL:HG13	2.49	0.48
1:A:175:LEU:HD11	4:A:706:PTY:H442	1.94	0.48
1:A:62:LEU:HD23	1:A:76:HIS:CD2	2.49	0.48
1:A:71:TYR:HE1	1:A:92:ALA:HB3	1.78	0.48
1:A:417:GLU:OE2	1:A:418:VAL:CG2	2.62	0.47
1:A:583:ASN:HB2	1:A:586:TYR:HB3	1.97	0.47
1:A:80:ASP:OD2	1:A:542:ARG:NH1	2.43	0.47
1:A:512:GLU:HB2	1:A:605:ILE:HG22	1.96	0.47
1:A:264:GLN:OE1	1:A:274:ASN:ND2	2.47	0.47
1:A:263:VAL:HG23	1:A:349:LEU:HD12	1.96	0.47
1:A:185:VAL:HG13	1:A:186:PRO:HD2	1.97	0.47
1:A:288:GLY:O	1:A:292:THR:HG23	2.15	0.47
1:A:239:ALA:HB3	1:A:244:GLU:HG3	1.96	0.46
1:A:581:PRO:CD	1:A:590:MET:HE1	2.44	0.46
1:A:612:TRP:CA	1:A:615:VAL:HG12	2.41	0.46
1:A:15:LEU:HD22	1:A:19:LEU:HD12	1.97	0.46
1:A:576:LYS:HD3	1:A:593:ASP:H	1.81	0.46
1:A:180:PHE:HB2	1:A:285:THR:HG22	1.98	0.46
1:A:207:ARG:NH1	2:A:701:HEM:O1D	2.49	0.45
1:A:263:VAL:CG2	1:A:349:LEU:HD12	2.47	0.45
4:A:705:PTY:H391	4:A:705:PTY:H241	1.98	0.45
1:A:586:TYR:HD1	1:A:587:PHE:N	2.13	0.45
1:A:581:PRO:HD2	1:A:590:MET:HE1	1.99	0.45
4:A:706:PTY:H221	4:A:706:PTY:H252	1.75	0.45
1:A:230:GLU:HA	1:A:578:ILE:HD11	1.99	0.45
1:A:570:SER:OG	1:A:571:PRO:HD2	2.17	0.45
1:A:344:SER:OG	1:A:413:ARG:N	2.48	0.44
1:A:93:LEU:HD11	1:A:308:VAL:HG11	2.00	0.44
1:A:549:LEU:HD12	1:A:549:LEU:N	2.31	0.44
1:A:84:VAL:O	1:A:88:THR:OG1	2.25	0.44
1:A:117:ASP:OD1	1:A:198:ARG:NH1	2.50	0.44
1:A:259:HIS:NE2	2:A:701:HEM:C4B	2.78	0.44
1:A:72:VAL:O	1:A:76:HIS:N	2.51	0.44
1:A:326:LEU:HA	1:A:329:ARG:HG2	2.00	0.44
1:A:263:VAL:O	1:A:267:ARG:N	2.51	0.44
1:A:244:GLU:OE1	1:A:293:ARG:NH1	2.51	0.43
1:A:275:PHE:CB	1:A:327:LEU:CD1	2.94	0.43
1:A:507:GLN:HG3	4:A:707:PTY:H331	2.00	0.43
1:A:76:HIS:ND1	1:A:79:LYS:CB	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:TYR:CD1	1:A:587:PHE:N	2.86	0.42
1:A:432:GLY:HA3	1:A:450:GLY:HA2	2.01	0.42
4:A:706:PTY:H332	4:A:706:PTY:H182	2.01	0.42
1:A:215:GLY:HA2	1:A:218:THR:HG22	2.01	0.42
1:A:180:PHE:HA	1:A:285:THR:HG21	2.01	0.42
1:A:275:PHE:CB	1:A:327:LEU:HD12	2.49	0.42
1:A:356:PHE:HZ	2:A:701:HEM:HMC1	1.84	0.42
1:A:270:PHE:CE1	1:A:350:LEU:CD2	3.03	0.42
1:A:496:VAL:HG23	2:A:701:HEM:CBC	2.50	0.42
1:A:546:VAL:HG23	1:A:564:PHE:HB3	2.00	0.41
1:A:208:TRP:NE1	4:A:706:PTY:O11	2.49	0.41
1:A:41:ARG:NH1	5:A:801:HOH:O	2.52	0.41
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.80	0.41
1:A:199:TYR:CZ	1:A:330:VAL:HG21	2.56	0.41
1:A:408:LEU:HD12	1:A:425:LEU:HD11	2.02	0.41
1:A:194:MET:HE3	1:A:326:LEU:HB2	2.03	0.41
1:A:554:ARG:HB3	1:A:555:PHE:H	1.67	0.41
1:A:164:GLN:HB2	1:A:165:ASN:H	1.60	0.41
1:A:22:LEU:HD23	1:A:126:ALA:O	2.22	0.40
1:A:545:ALA:HB1	1:A:563:HIS:CD2	2.56	0.40
1:A:166:HIS:CG	1:A:231:VAL:HG11	2.57	0.40
1:A:326:LEU:HD22	1:A:329:ARG:HE	1.87	0.40
3:A:702:LMT:H3'	3:A:702:LMT:H1B	1.72	0.40

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	577/660 (87%)	542 (94%)	32 (6%)	3 (0%)	24	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	ARG
1	A	554	ARG
1	A	593	ASP

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	456/510 (89%)	447 (98%)	9 (2%)	48 74

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	164	GLN
1	A	491	VAL
1	A	496	VAL
1	A	542	ARG
1	A	553	ASP
1	A	554	ARG
1	A	594	ARG
1	A	595	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	132	GLN

5.3.3 RNA ⓘ

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](#)

7 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	$\# Z > 2$
4	PTY	A	707	-	49,49,49	0.90	4 (8%)	52,54,54	1.08	2 (3%)
4	PTY	A	705	-	49,49,49	0.92	4 (8%)	52,54,54	0.98	2 (3%)
3	LMT	A	703	-	36,36,36	1.15	4 (11%)	47,47,47	1.40	7 (14%)
3	LMT	A	702	-	36,36,36	1.19	8 (22%)	47,47,47	1.68	11 (23%)
2	HEM	A	701	1	50,50,50	1.84	13 (26%)	67,82,82	1.88	13 (19%)
4	PTY	A	706	-	49,49,49	0.94	3 (6%)	52,54,54	1.15	2 (3%)
4	PTY	A	704	-	49,49,49	0.95	3 (6%)	52,54,54	1.09	2 (3%)

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
4	PTY	A	707	-	-	16/53/53/53	-
4	PTY	A	705	-	-	23/53/53/53	-
3	LMT	A	703	-	-	12/21/61/61	0/2/2/2
3	LMT	A	702	-	-	11/21/61/61	0/2/2/2
2	HEM	A	701	1	-	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PTY	A	706	-	-	26/53/53/53	-
4	PTY	A	704	-	-	27/53/53/53	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	HEM	FE-ND	5.02	2.10	1.94
2	A	701	HEM	FE-NB	4.56	2.08	1.94
2	A	701	HEM	CBB-CAB	3.95	1.49	1.30
2	A	701	HEM	CBC-CAC	3.79	1.48	1.30
2	A	701	HEM	C4D-ND	-3.57	1.34	1.40
2	A	701	HEM	C1D-ND	-3.33	1.32	1.38
2	A	701	HEM	FE-NC	3.11	2.05	1.95
4	A	704	PTY	O7-C8	2.82	1.42	1.34
2	A	701	HEM	C1B-NB	-2.81	1.35	1.40
2	A	701	HEM	C1C-C2C	-2.71	1.40	1.45
4	A	706	PTY	O4-C30	2.70	1.41	1.33
4	A	707	PTY	O7-C6	-2.60	1.40	1.46
3	A	703	LMT	O3'-C3'	-2.58	1.36	1.43
4	A	705	PTY	O7-C6	-2.50	1.40	1.46
4	A	704	PTY	O4-C30	2.48	1.40	1.33
4	A	705	PTY	O4-C30	2.44	1.40	1.33
4	A	707	PTY	O4-C30	2.42	1.40	1.33
4	A	706	PTY	O7-C6	-2.40	1.40	1.46
3	A	702	LMT	O3'-C3'	-2.40	1.37	1.43
3	A	703	LMT	O3B-C3B	-2.37	1.37	1.43
2	A	701	HEM	C3C-C4C	-2.36	1.41	1.46
4	A	705	PTY	O7-C8	2.31	1.40	1.34
3	A	702	LMT	C3'-C4'	2.30	1.58	1.52
3	A	702	LMT	O3B-C3B	-2.30	1.37	1.43
3	A	702	LMT	O2B-C2B	-2.29	1.37	1.43
2	A	701	HEM	FE-NA	2.28	2.02	1.95
4	A	706	PTY	O7-C8	2.25	1.40	1.34
3	A	703	LMT	O2'-C2'	-2.25	1.37	1.43
3	A	702	LMT	C4'-C5'	2.21	1.58	1.52
3	A	702	LMT	O2'-C2'	-2.21	1.37	1.43
4	A	704	PTY	O4-C1	-2.20	1.40	1.45
3	A	703	LMT	O2B-C2B	-2.19	1.37	1.43
4	A	705	PTY	O4-C1	-2.19	1.40	1.45
4	A	707	PTY	O7-C8	2.18	1.40	1.34
4	A	707	PTY	O4-C1	-2.18	1.40	1.45
2	A	701	HEM	C4B-NB	-2.15	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	HEM	C4D-C3D	2.05	1.48	1.45
3	A	702	LMT	C3'-C2'	2.02	1.57	1.52
3	A	702	LMT	O4'-C4B	-2.01	1.38	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	HEM	CHC-C4B-NB	6.25	131.15	124.42
2	A	701	HEM	CHD-C4C-NC	5.07	129.98	124.45
4	A	704	PTY	O7-C8-C11	4.84	121.94	111.48
2	A	701	HEM	C1B-NB-C4B	4.58	110.63	105.21
3	A	702	LMT	C1B-O5B-C5B	4.15	121.82	113.72
4	A	706	PTY	O7-C8-C11	4.03	120.20	111.48
2	A	701	HEM	C4D-ND-C1D	3.95	109.88	105.21
3	A	702	LMT	O5B-C5B-C4B	3.93	116.78	109.70
3	A	702	LMT	O5'-C5'-C4'	3.82	117.62	109.72
3	A	703	LMT	C3'-C4'-C5'	-3.75	102.61	110.93
4	A	705	PTY	O7-C8-C11	3.71	119.50	111.48
4	A	707	PTY	O7-C8-C11	3.65	119.37	111.48
2	A	701	HEM	CHB-C1B-NB	3.56	128.78	124.37
3	A	703	LMT	C1B-O5B-C5B	3.54	120.64	113.72
2	A	701	HEM	C3B-C4B-NB	-3.49	106.96	109.47
3	A	702	LMT	C3B-C4B-C5B	-3.34	104.18	110.23
4	A	706	PTY	O4-C30-C31	3.32	121.94	111.83
2	A	701	HEM	CHA-C1A-NA	3.16	129.59	123.86
3	A	702	LMT	C2'-C3'-C4'	3.08	116.67	109.68
3	A	702	LMT	O1B-C4'-C3'	2.95	114.72	107.23
3	A	702	LMT	O1'-C1'-C2'	2.93	112.72	108.27
3	A	703	LMT	O5B-C1B-C2B	2.85	116.22	110.37
4	A	707	PTY	O4-C30-C31	2.80	120.36	111.83
4	A	705	PTY	O4-C30-C31	2.75	120.22	111.83
3	A	702	LMT	O5B-C1B-C2B	2.71	115.95	110.37
2	A	701	HEM	C4C-C3C-C2C	2.71	109.16	106.81
2	A	701	HEM	CBB-CAB-C3B	-2.61	114.49	127.53
3	A	703	LMT	O5B-C5B-C4B	2.60	114.38	109.70
4	A	704	PTY	O4-C30-C31	2.52	119.53	111.83
2	A	701	HEM	C2A-C1A-NA	-2.50	107.38	110.15
3	A	703	LMT	C3B-C4B-C5B	-2.45	105.80	110.23
3	A	703	LMT	C4B-C3B-C2B	2.39	115.03	110.83
3	A	702	LMT	C1B-O1B-C4'	2.37	123.59	117.98
2	A	701	HEM	C1C-CHC-C4B	-2.36	121.00	126.02
2	A	701	HEM	C3B-C2B-C1B	2.31	108.15	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	LMT	C1'-O5'-C5'	2.31	118.23	113.72
3	A	703	LMT	C1B-C2B-C3B	2.18	114.59	110.01
2	A	701	HEM	CMC-C2C-C1C	2.14	128.50	124.73
3	A	702	LMT	O5B-C5B-C6B	2.11	111.67	106.44

There are no chirality outliers.

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	HEM	C2B-C3B-CAB-CBB
2	A	701	HEM	C4B-C3B-CAB-CBB
2	A	701	HEM	C2C-C3C-CAC-CBC
2	A	701	HEM	C4C-C3C-CAC-CBC
3	A	703	LMT	C2'-C1'-O1'-C1
3	A	703	LMT	O5'-C1'-O1'-C1
4	A	704	PTY	N1-C2-C3-O11
4	A	704	PTY	C3-O11-P1-O14
4	A	704	PTY	C5-O14-P1-O11
4	A	704	PTY	C5-O14-P1-O12
4	A	705	PTY	C5-O14-P1-O11
4	A	705	PTY	C5-O14-P1-O12
4	A	705	PTY	C5-O14-P1-O13
4	A	706	PTY	N1-C2-C3-O11
4	A	707	PTY	O10-C8-O7-C6
3	A	702	LMT	C3'-C4'-O1B-C1B
4	A	704	PTY	O30-C30-O4-C1
4	A	707	PTY	C11-C8-O7-C6
4	A	704	PTY	C31-C30-O4-C1
3	A	702	LMT	C4'-C5'-C6'-O6'
4	A	706	PTY	C31-C30-O4-C1
3	A	702	LMT	O5'-C5'-C6'-O6'
4	A	706	PTY	C11-C8-O7-C6
4	A	706	PTY	O30-C30-O4-C1
4	A	706	PTY	O10-C8-O7-C6
4	A	705	PTY	C16-C17-C18-C19
3	A	702	LMT	O1'-C1-C2-C3
3	A	702	LMT	C1-C2-C3-C4
4	A	705	PTY	C11-C8-O7-C6
4	A	705	PTY	C15-C16-C17-C18
4	A	707	PTY	C19-C20-C21-C22
4	A	707	PTY	C13-C14-C15-C16
3	A	702	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
4	A	705	PTY	C21-C22-C23-C24
4	A	706	PTY	C11-C12-C13-C14
4	A	705	PTY	C40-C41-C42-C43
4	A	706	PTY	C31-C32-C33-C34
4	A	707	PTY	C24-C25-C26-C27
4	A	706	PTY	C35-C36-C37-C38
4	A	704	PTY	C37-C38-C39-C40
4	A	704	PTY	C23-C24-C25-C26
4	A	704	PTY	C35-C36-C37-C38
4	A	706	PTY	C39-C40-C41-C42
4	A	706	PTY	C34-C35-C36-C37
4	A	704	PTY	C14-C15-C16-C17
4	A	705	PTY	O10-C8-O7-C6
3	A	703	LMT	O1'-C1-C2-C3
4	A	707	PTY	C8-C11-C12-C13
4	A	707	PTY	C33-C34-C35-C36
3	A	703	LMT	C2B-C1B-O1B-C4'
4	A	706	PTY	C12-C13-C14-C15
3	A	702	LMT	O5B-C5B-C6B-O6B
3	A	703	LMT	C6-C7-C8-C9
4	A	705	PTY	C22-C23-C24-C25
4	A	705	PTY	C31-C32-C33-C34
4	A	707	PTY	C38-C39-C40-C41
3	A	703	LMT	O5B-C5B-C6B-O6B
3	A	702	LMT	C5-C6-C7-C8
4	A	704	PTY	C11-C12-C13-C14
4	A	704	PTY	C39-C40-C41-C42
3	A	702	LMT	C2-C3-C4-C5
4	A	704	PTY	C41-C42-C43-C44
4	A	704	PTY	C19-C20-C21-C22
4	A	705	PTY	C17-C18-C19-C20
4	A	706	PTY	C26-C27-C28-C29
4	A	706	PTY	C33-C34-C35-C36
4	A	707	PTY	C31-C30-O4-C1
3	A	703	LMT	C5-C6-C7-C8
4	A	707	PTY	C23-C24-C25-C26
4	A	705	PTY	C39-C40-C41-C42
4	A	704	PTY	O14-C5-C6-O7
4	A	704	PTY	C24-C25-C26-C27
4	A	705	PTY	C37-C38-C39-C40
3	A	702	LMT	C7-C8-C9-C10
3	A	703	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	A	702	LMT	C4-C5-C6-C7
4	A	706	PTY	C24-C25-C26-C27
4	A	707	PTY	O30-C30-O4-C1
4	A	706	PTY	O4-C1-C6-O7
4	A	704	PTY	O14-C5-C6-C1
4	A	704	PTY	C6-C5-O14-P1
4	A	706	PTY	C32-C33-C34-C35
4	A	704	PTY	C12-C13-C14-C15
4	A	707	PTY	C34-C35-C36-C37
4	A	704	PTY	C3-O11-P1-O13
4	A	704	PTY	C5-O14-P1-O13
4	A	705	PTY	C3-O11-P1-O13
4	A	706	PTY	C3-O11-P1-O13
4	A	706	PTY	C5-O14-P1-O12
4	A	705	PTY	C34-C35-C36-C37
4	A	705	PTY	C32-C33-C34-C35
3	A	703	LMT	O5B-C1B-O1B-C4'
4	A	704	PTY	C13-C14-C15-C16
4	A	706	PTY	O4-C1-C6-C5
4	A	707	PTY	O4-C30-C31-C32
4	A	706	PTY	C40-C41-C42-C43
3	A	703	LMT	C1-C2-C3-C4
4	A	704	PTY	C15-C16-C17-C18
2	A	701	HEM	CAD-CBD-CGD-O1D
2	A	701	HEM	CAA-CBA-CGA-O1A
4	A	704	PTY	C34-C35-C36-C37
4	A	705	PTY	C25-C26-C27-C28
4	A	704	PTY	C20-C21-C22-C23
3	A	703	LMT	C9-C10-C11-C12
4	A	704	PTY	C33-C34-C35-C36
4	A	705	PTY	C26-C27-C28-C29
2	A	701	HEM	CAD-CBD-CGD-O2D
4	A	706	PTY	C25-C26-C27-C28
3	A	703	LMT	C4-C5-C6-C7
4	A	705	PTY	C14-C15-C16-C17
4	A	706	PTY	C38-C39-C40-C41
2	A	701	HEM	CAA-CBA-CGA-O2A
4	A	704	PTY	C8-C11-C12-C13
4	A	706	PTY	C23-C24-C25-C26
4	A	707	PTY	C36-C37-C38-C39
4	A	705	PTY	C24-C25-C26-C27
4	A	705	PTY	C20-C21-C22-C23

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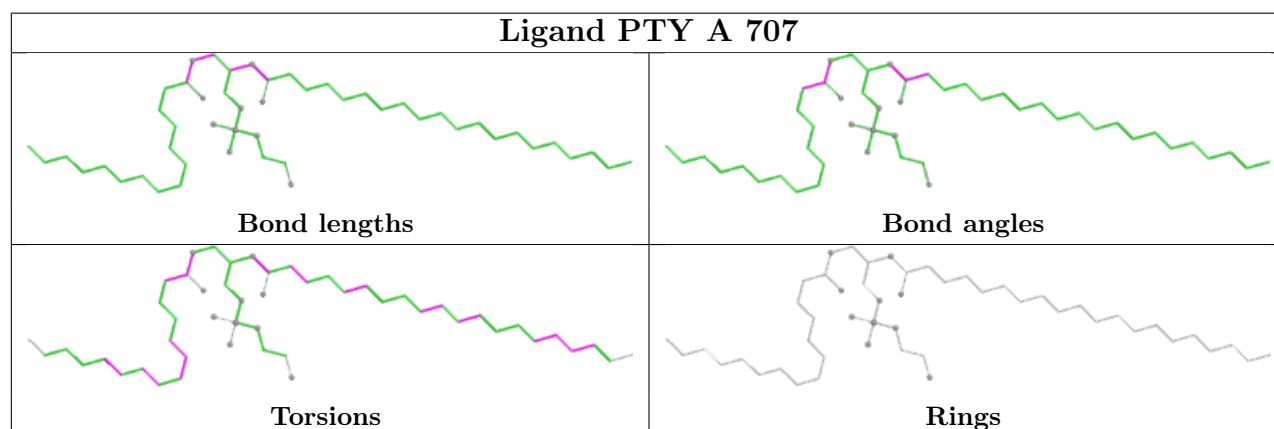
Mol	Chain	Res	Type	Atoms
4	A	706	PTY	C22-C23-C24-C25
4	A	705	PTY	C13-C14-C15-C16
4	A	707	PTY	C17-C18-C19-C20
4	A	706	PTY	C37-C38-C39-C40
4	A	706	PTY	C20-C21-C22-C23
4	A	707	PTY	C25-C26-C27-C28

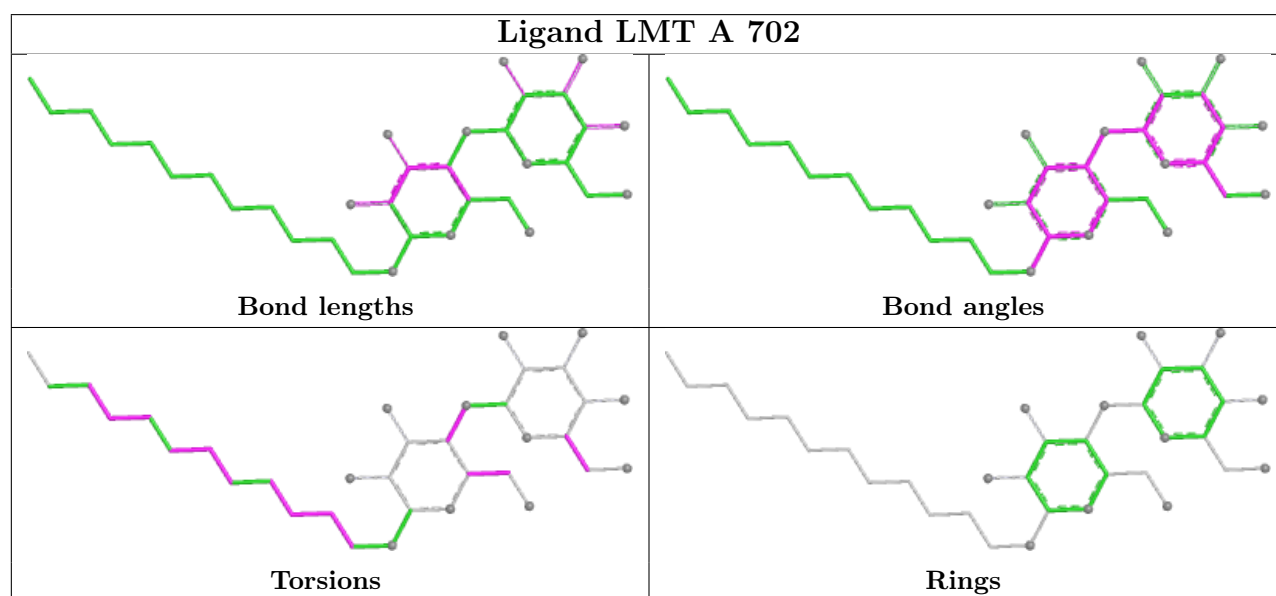
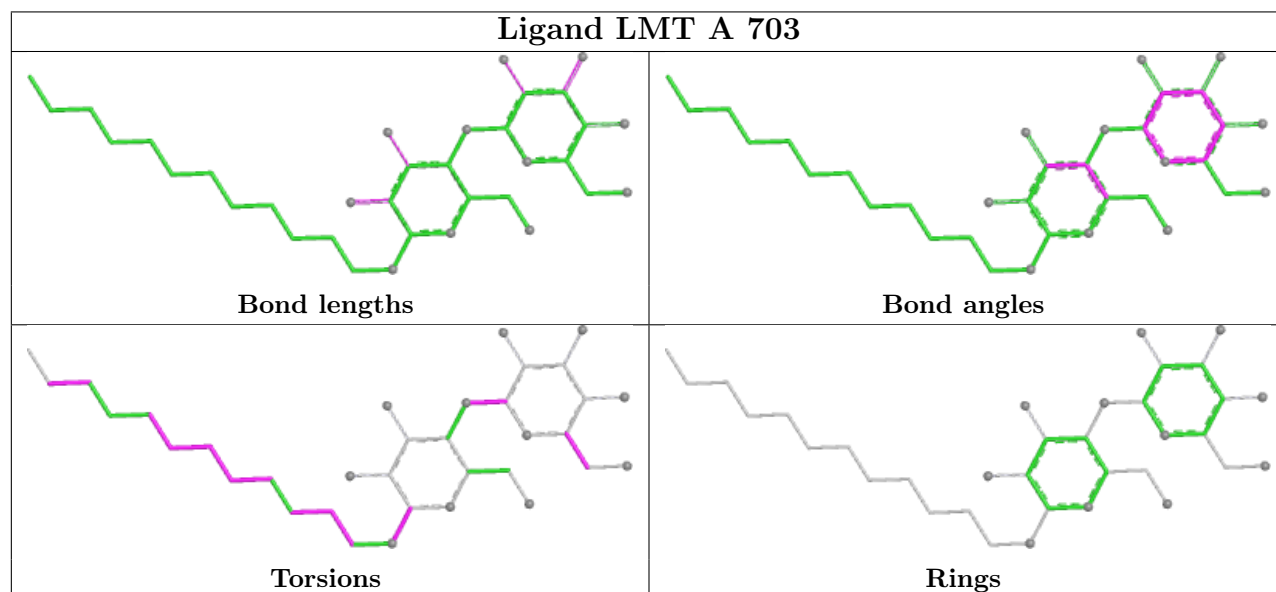
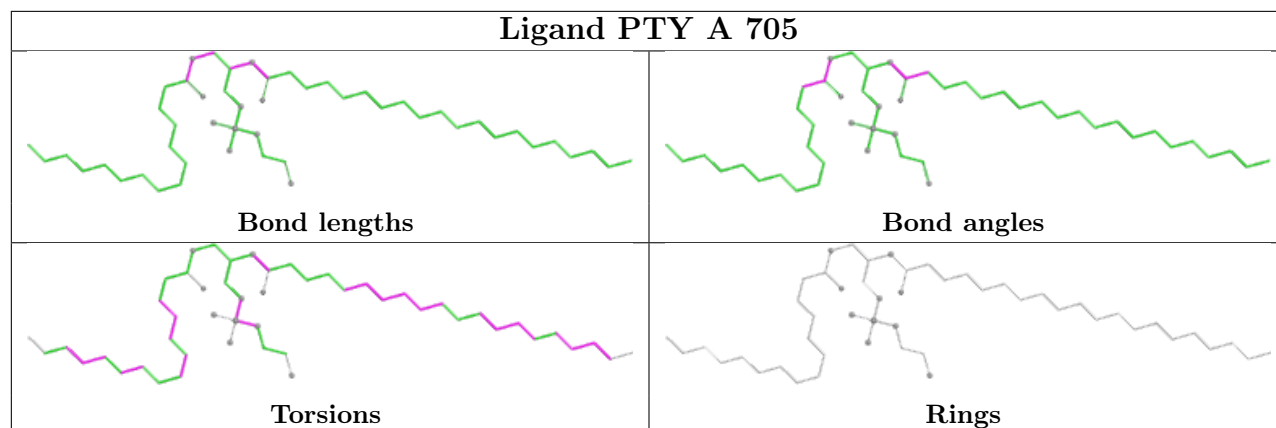
There are no ring outliers.

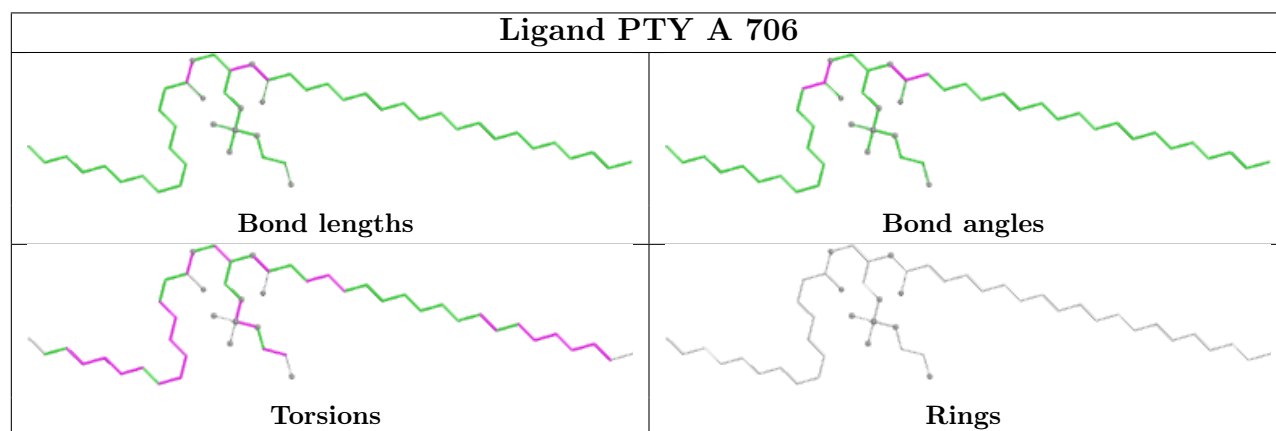
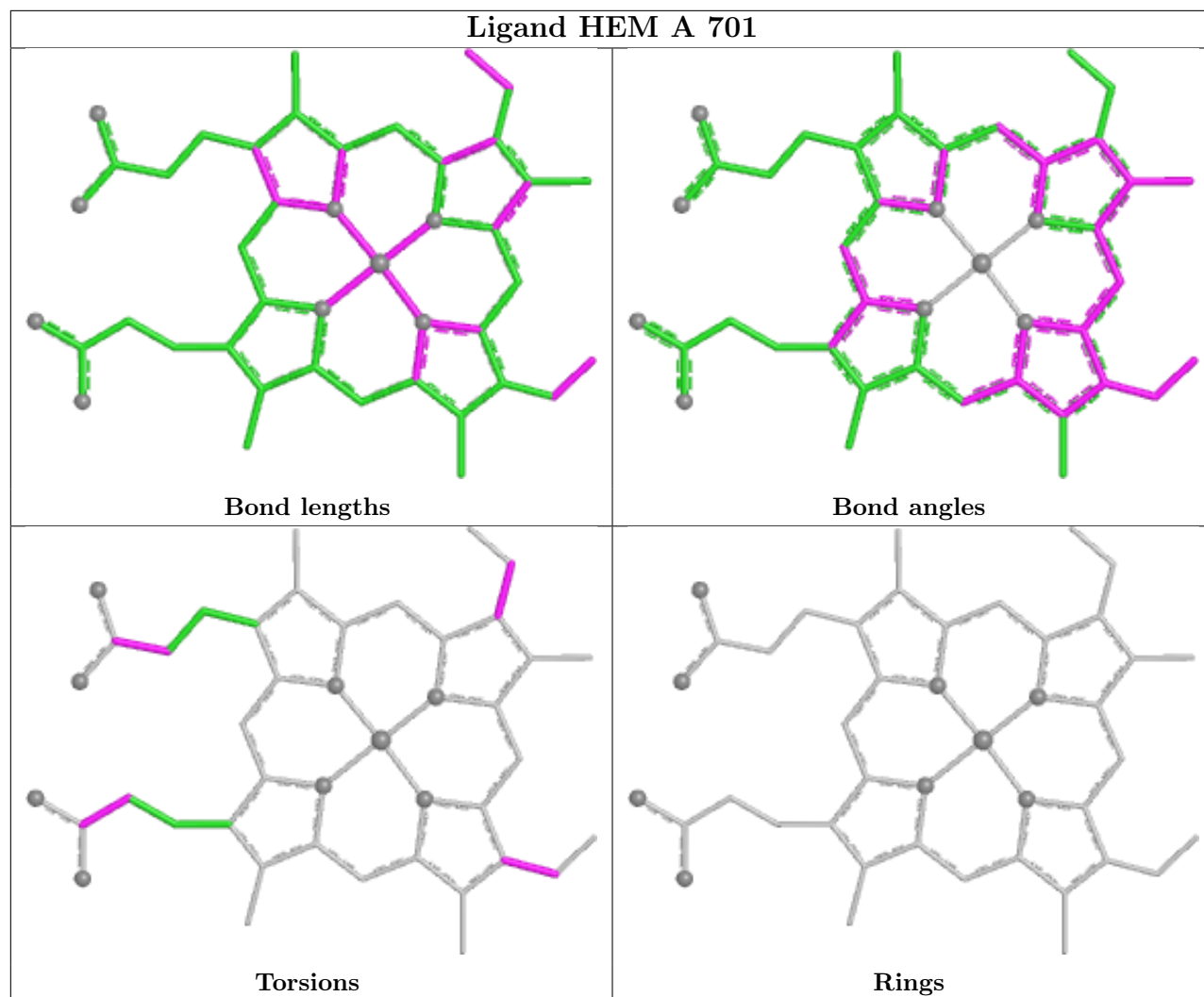
6 monomers are involved in 15 short contacts:

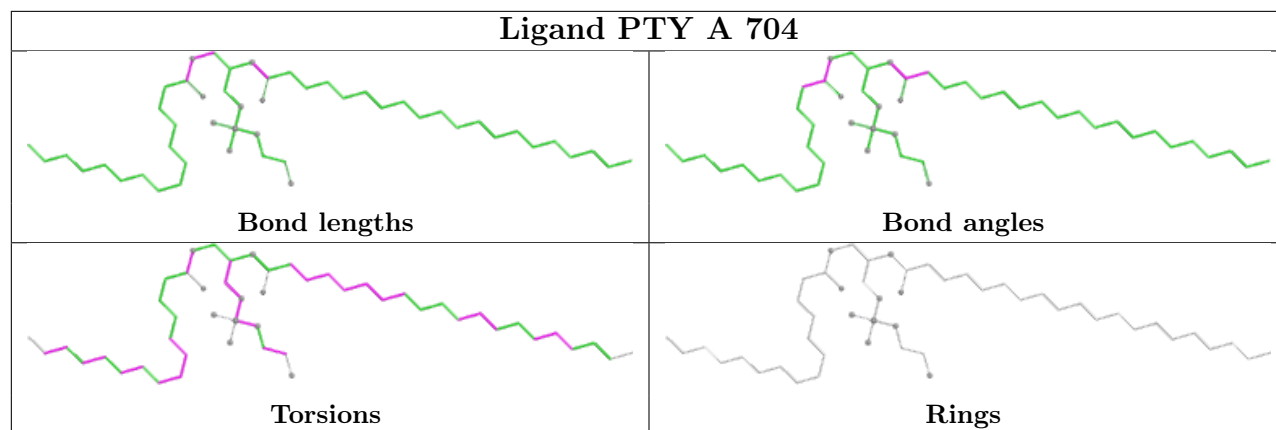
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	707	PTY	1	0
4	A	705	PTY	2	0
3	A	702	LMT	1	0
2	A	701	HEM	5	0
4	A	706	PTY	4	0
4	A	704	PTY	2	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	589/660 (89%)	1.19	129 (21%) 2 2	28, 55, 100, 138	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	VAL	9.6
1	A	533	GLN	8.1
1	A	412	ARG	7.7
1	A	417	GLU	7.2
1	A	163	LEU	6.8
1	A	534	GLY	6.5
1	A	419	LEU	6.4
1	A	535	VAL	5.9
1	A	559	ARG	5.9
1	A	414	ALA	5.4
1	A	518	TYR	5.3
1	A	267	ARG	4.9
1	A	599	TRP	4.5
1	A	538	LEU	4.4
1	A	357	ALA	4.4
1	A	579	TYR	4.4
1	A	411	TRP	4.2
1	A	64	VAL	4.1
1	A	585	TYR	4.1
1	A	554	ARG	4.0
1	A	558	VAL	3.9
1	A	215	GLY	3.9
1	A	537	ALA	3.8
1	A	268	GLY	3.8
1	A	329	ARG	3.8
1	A	182	GLY	3.7
1	A	539	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	204	GLU	3.6
1	A	540	GLU	3.6
1	A	570	SER	3.5
1	A	420	ARG	3.5
1	A	212	ILE	3.5
1	A	522	ALA	3.5
1	A	62	LEU	3.5
1	A	200	GLN	3.5
1	A	544	PHE	3.5
1	A	211	LEU	3.5
1	A	78	THR	3.4
1	A	-4	LEU	3.4
1	A	355	PHE	3.4
1	A	561	ARG	3.4
1	A	523	TRP	3.4
1	A	101	GLY	3.4
1	A	552	THR	3.3
1	A	107	TYR	3.3
1	A	413	ARG	3.3
1	A	94	GLU	3.2
1	A	448	ALA	3.2
1	A	198	ARG	3.1
1	A	13	LEU	3.1
1	A	65	HIS	3.1
1	A	324	LEU	3.1
1	A	320	THR	3.0
1	A	77	SER	3.0
1	A	629	TRP	3.0
1	A	148	THR	3.0
1	A	213	ALA	3.0
1	A	575	PRO	2.9
1	A	499	MET	2.9
1	A	306	GLY	2.9
1	A	536	ARG	2.9
1	A	249	ILE	2.9
1	A	218	THR	2.9
1	A	67	PHE	2.9
1	A	269	ALA	2.8
1	A	480	PHE	2.8
1	A	237	TYR	2.8
1	A	168	MET	2.8
1	A	234	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	565	TYR	2.8
1	A	623	GLY	2.7
1	A	531	THR	2.7
1	A	528	VAL	2.7
1	A	93	LEU	2.7
1	A	164	GLN	2.6
1	A	10	GLY	2.6
1	A	270	PHE	2.6
1	A	621	ALA	2.6
1	A	210	THR	2.5
1	A	356	PHE	2.5
1	A	33	ASP	2.5
1	A	3	PRO	2.5
1	A	-7	ALA	2.4
1	A	141	THR	2.4
1	A	488	GLY	2.4
1	A	181	VAL	2.4
1	A	624	THR	2.4
1	A	551	LYS	2.4
1	A	216	PHE	2.4
1	A	176	MET	2.4
1	A	-9	LYS	2.4
1	A	450	GLY	2.4
1	A	208	TRP	2.3
1	A	415	ARG	2.3
1	A	271	LYS	2.3
1	A	178	LEU	2.3
1	A	284	ALA	2.3
1	A	586	TYR	2.3
1	A	102	LEU	2.3
1	A	386	PRO	2.2
1	A	543	ARG	2.2
1	A	246	ALA	2.2
1	A	549	LEU	2.2
1	A	167	TRP	2.2
1	A	239	ALA	2.2
1	A	597	GLY	2.2
1	A	364	VAL	2.2
1	A	545	ALA	2.1
1	A	105	THR	2.1
1	A	99	LEU	2.1
1	A	103	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	511	LEU	2.1
1	A	-2	PHE	2.1
1	A	481	LEU	2.1
1	A	184	SER	2.1
1	A	360	ALA	2.1
1	A	201	THR	2.1
1	A	567	GLN	2.1
1	A	179	GLY	2.1
1	A	584	ASP	2.0
1	A	60	TRP	2.0
1	A	569	ASN	2.0
1	A	235	GLY	2.0
1	A	207	ARG	2.0
1	A	566	PRO	2.0
1	A	422	LEU	2.0
1	A	526	GLY	2.0
1	A	486	ARG	2.0
1	A	492	VAL	2.0

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	LMT	A	702	35/35	0.47	0.17	44,77,96,98	35
4	PTY	A	706	50/50	0.65	0.20	30,64,107,130	0
4	PTY	A	707	50/50	0.71	0.21	33,65,103,112	1
4	PTY	A	704	50/50	0.72	0.17	29,68,109,116	1
3	LMT	A	703	35/35	0.78	0.14	25,88,125,129	0

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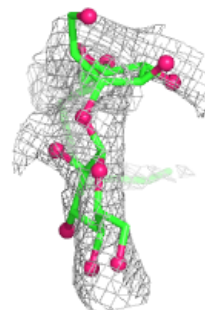
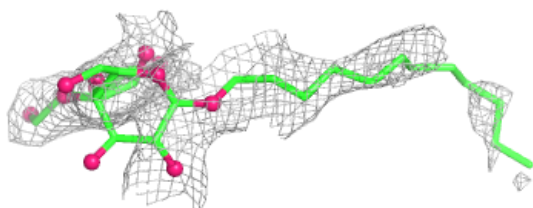
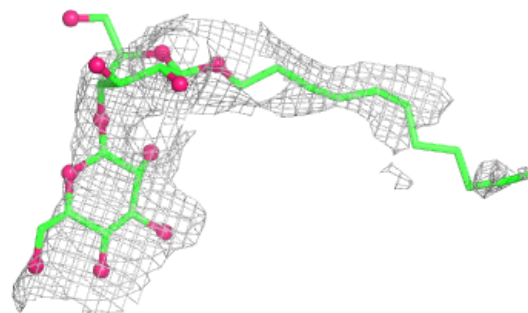
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PTY	A	705	50/50	0.86	0.15	26,48,76,87	0
2	HEM	A	701	43/43	0.95	0.11	20,45,63,78	0

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.

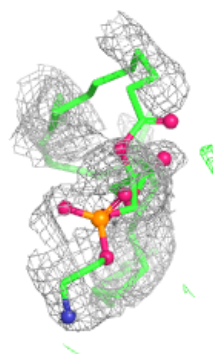
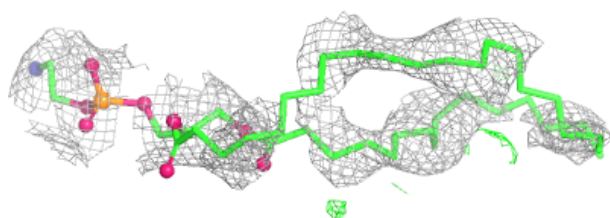
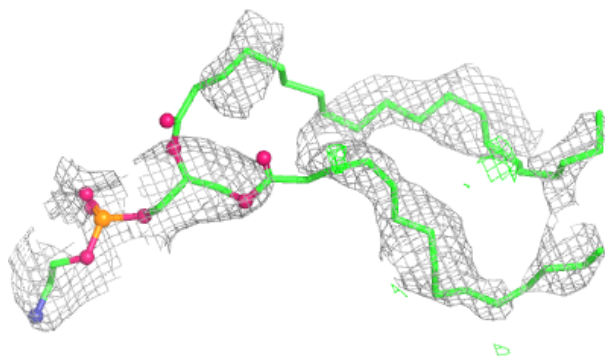
Electron density around LMT A 702:

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

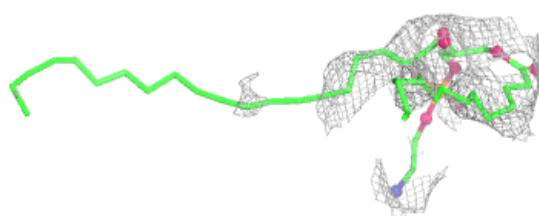
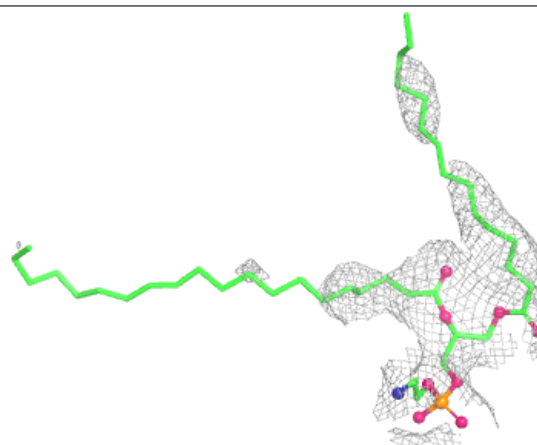


Electron density around PTY A 706:

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

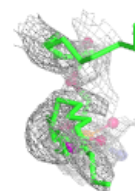
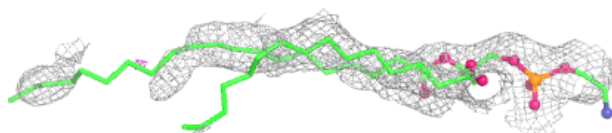
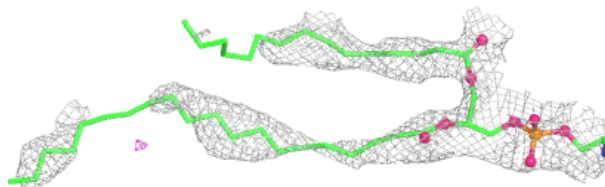
**Electron density around PTY A 707:**

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

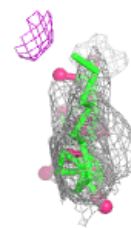
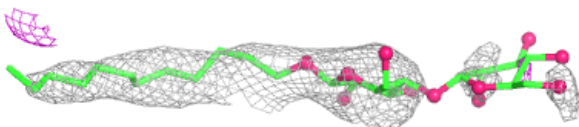
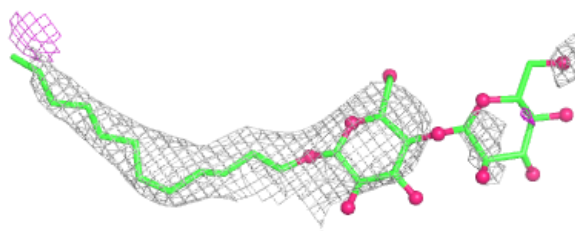


Electron density around PTY A 704:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

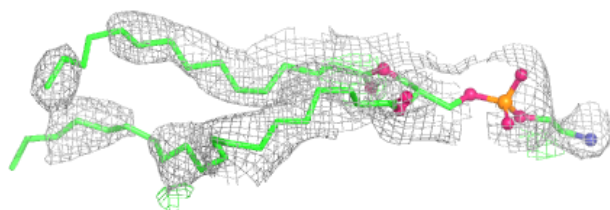
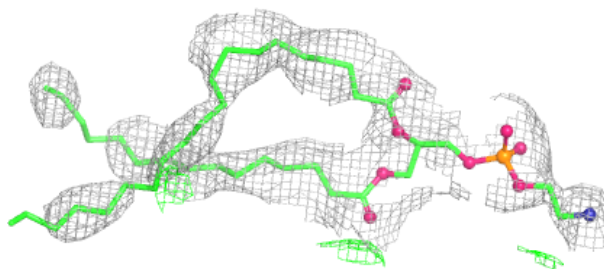
**Electron density around LMT A 703:**

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



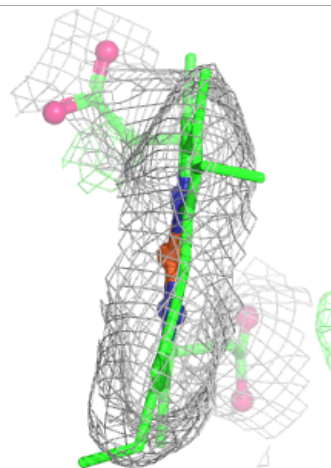
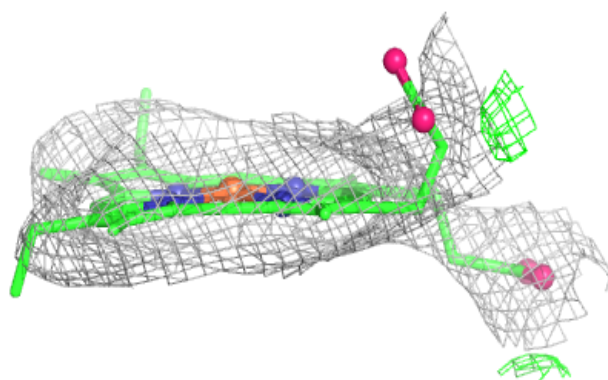
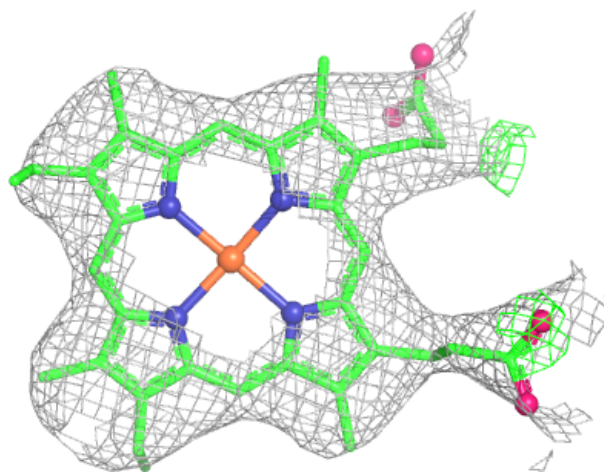
Electron density around PTY A 705:

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



Electron density around HEM A 701:

$2mF_o-DF_c$ (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.