



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 11:11 PM JST

PDB ID : 7XCN / pdb_00007xcn
Title : Crystal structure of the MttB-MttC complex at 2.7 Å resolution
Authors : Li, J.; Chan, M.K.
Deposited on : 2022-03-24
Resolution : 2.70 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 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 : 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

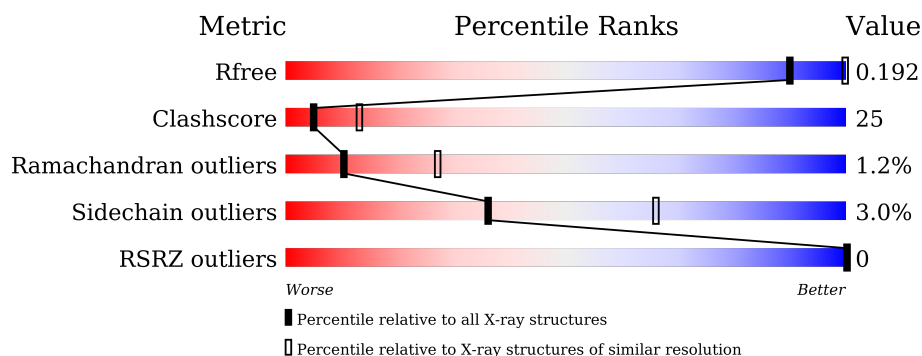
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	503	51% 42% ...
1	B	503	67% 28% ..
1	C	503	67% 29% ..
1	D	503	53% 42% ..
1	E	503	68% 27% ..
1	F	503	65% 31% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	M	224	
2	N	224	
2	O	224	
2	P	224	
2	Q	224	
2	R	224	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33443 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 Trimethylamine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	5	0
			3801	2424	633	722	22			
1	B	494	Total	C	N	O	S	0	8	0
			3843	2446	641	734	22			
1	C	494	Total	C	N	O	S	0	8	0
			3843	2446	641	734	22			
1	D	491	Total	C	N	O	S	0	5	0
			3801	2424	633	722	22			
1	E	494	Total	C	N	O	S	0	8	0
			3843	2446	641	734	22			
1	F	494	Total	C	N	O	S	0	8	0
			3843	2446	641	734	22			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	496	GLY	-	expression tag	UNP A0A0E3QRM4
A	497	GLY	-	expression tag	UNP A0A0E3QRM4
A	498	HIS	-	expression tag	UNP A0A0E3QRM4
A	499	HIS	-	expression tag	UNP A0A0E3QRM4
A	500	HIS	-	expression tag	UNP A0A0E3QRM4
A	501	HIS	-	expression tag	UNP A0A0E3QRM4
A	502	HIS	-	expression tag	UNP A0A0E3QRM4
A	503	HIS	-	expression tag	UNP A0A0E3QRM4
B	496	GLY	-	expression tag	UNP A0A0E3QRM4
B	497	GLY	-	expression tag	UNP A0A0E3QRM4
B	498	HIS	-	expression tag	UNP A0A0E3QRM4
B	499	HIS	-	expression tag	UNP A0A0E3QRM4
B	500	HIS	-	expression tag	UNP A0A0E3QRM4
B	501	HIS	-	expression tag	UNP A0A0E3QRM4
B	502	HIS	-	expression tag	UNP A0A0E3QRM4
B	503	HIS	-	expression tag	UNP A0A0E3QRM4
C	496	GLY	-	expression tag	UNP A0A0E3QRM4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	497	GLY	-	expression tag	UNP A0A0E3QRM4
C	498	HIS	-	expression tag	UNP A0A0E3QRM4
C	499	HIS	-	expression tag	UNP A0A0E3QRM4
C	500	HIS	-	expression tag	UNP A0A0E3QRM4
C	501	HIS	-	expression tag	UNP A0A0E3QRM4
C	502	HIS	-	expression tag	UNP A0A0E3QRM4
C	503	HIS	-	expression tag	UNP A0A0E3QRM4
D	496	GLY	-	expression tag	UNP A0A0E3QRM4
D	497	GLY	-	expression tag	UNP A0A0E3QRM4
D	498	HIS	-	expression tag	UNP A0A0E3QRM4
D	499	HIS	-	expression tag	UNP A0A0E3QRM4
D	500	HIS	-	expression tag	UNP A0A0E3QRM4
D	501	HIS	-	expression tag	UNP A0A0E3QRM4
D	502	HIS	-	expression tag	UNP A0A0E3QRM4
D	503	HIS	-	expression tag	UNP A0A0E3QRM4
E	496	GLY	-	expression tag	UNP A0A0E3QRM4
E	497	GLY	-	expression tag	UNP A0A0E3QRM4
E	498	HIS	-	expression tag	UNP A0A0E3QRM4
E	499	HIS	-	expression tag	UNP A0A0E3QRM4
E	500	HIS	-	expression tag	UNP A0A0E3QRM4
E	501	HIS	-	expression tag	UNP A0A0E3QRM4
E	502	HIS	-	expression tag	UNP A0A0E3QRM4
E	503	HIS	-	expression tag	UNP A0A0E3QRM4
F	496	GLY	-	expression tag	UNP A0A0E3QRM4
F	497	GLY	-	expression tag	UNP A0A0E3QRM4
F	498	HIS	-	expression tag	UNP A0A0E3QRM4
F	499	HIS	-	expression tag	UNP A0A0E3QRM4
F	500	HIS	-	expression tag	UNP A0A0E3QRM4
F	501	HIS	-	expression tag	UNP A0A0E3QRM4
F	502	HIS	-	expression tag	UNP A0A0E3QRM4
F	503	HIS	-	expression tag	UNP A0A0E3QRM4

- Molecule 2 is a protein called Trimethylamine methyltransferase corrinoid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	214	Total	C	N	O	S	0	0	0
			1595	1002	263	323	7			
2	N	212	Total	C	N	O	S	0	0	0
			1576	992	259	318	7			
2	O	214	Total	C	N	O	S	0	0	0
			1595	1002	263	323	7			
2	P	215	Total	C	N	O	S	0	0	0
			1600	1005	264	324	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	211	Total	C	N	O	S	0	0	0
			1571	989	258	317	7			
2	R	214	Total	C	N	O	S	0	0	0
			1595	1002	263	323	7			

There are 42 discrepancies between the modelled and reference sequences:

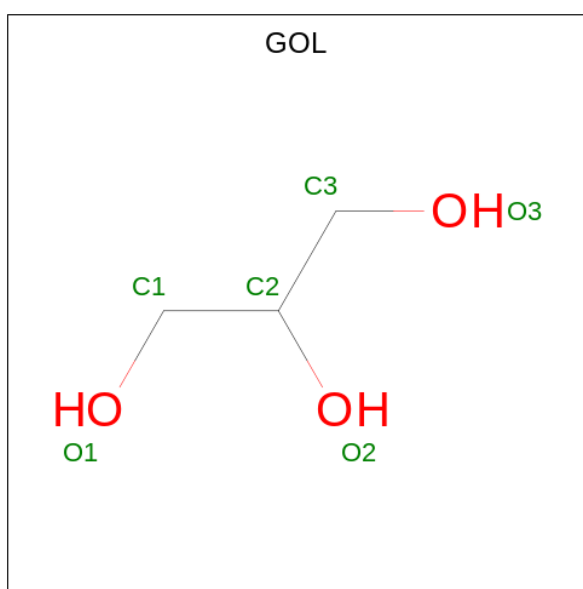
Chain	Residue	Modelled	Actual	Comment	Reference
M	218	GLY	-	expression tag	UNP A0A0E3QQC8
M	219	GLY	-	expression tag	UNP A0A0E3QQC8
M	220	HIS	-	expression tag	UNP A0A0E3QQC8
M	221	HIS	-	expression tag	UNP A0A0E3QQC8
M	222	HIS	-	expression tag	UNP A0A0E3QQC8
M	223	HIS	-	expression tag	UNP A0A0E3QQC8
M	224	HIS	-	expression tag	UNP A0A0E3QQC8
N	218	GLY	-	expression tag	UNP A0A0E3QQC8
N	219	GLY	-	expression tag	UNP A0A0E3QQC8
N	220	HIS	-	expression tag	UNP A0A0E3QQC8
N	221	HIS	-	expression tag	UNP A0A0E3QQC8
N	222	HIS	-	expression tag	UNP A0A0E3QQC8
N	223	HIS	-	expression tag	UNP A0A0E3QQC8
N	224	HIS	-	expression tag	UNP A0A0E3QQC8
O	218	GLY	-	expression tag	UNP A0A0E3QQC8
O	219	GLY	-	expression tag	UNP A0A0E3QQC8
O	220	HIS	-	expression tag	UNP A0A0E3QQC8
O	221	HIS	-	expression tag	UNP A0A0E3QQC8
O	222	HIS	-	expression tag	UNP A0A0E3QQC8
O	223	HIS	-	expression tag	UNP A0A0E3QQC8
O	224	HIS	-	expression tag	UNP A0A0E3QQC8
P	218	GLY	-	expression tag	UNP A0A0E3QQC8
P	219	GLY	-	expression tag	UNP A0A0E3QQC8
P	220	HIS	-	expression tag	UNP A0A0E3QQC8
P	221	HIS	-	expression tag	UNP A0A0E3QQC8
P	222	HIS	-	expression tag	UNP A0A0E3QQC8
P	223	HIS	-	expression tag	UNP A0A0E3QQC8
P	224	HIS	-	expression tag	UNP A0A0E3QQC8
Q	218	GLY	-	expression tag	UNP A0A0E3QQC8
Q	219	GLY	-	expression tag	UNP A0A0E3QQC8
Q	220	HIS	-	expression tag	UNP A0A0E3QQC8
Q	221	HIS	-	expression tag	UNP A0A0E3QQC8
Q	222	HIS	-	expression tag	UNP A0A0E3QQC8
Q	223	HIS	-	expression tag	UNP A0A0E3QQC8

Continued on next page...

Continued from previous page...

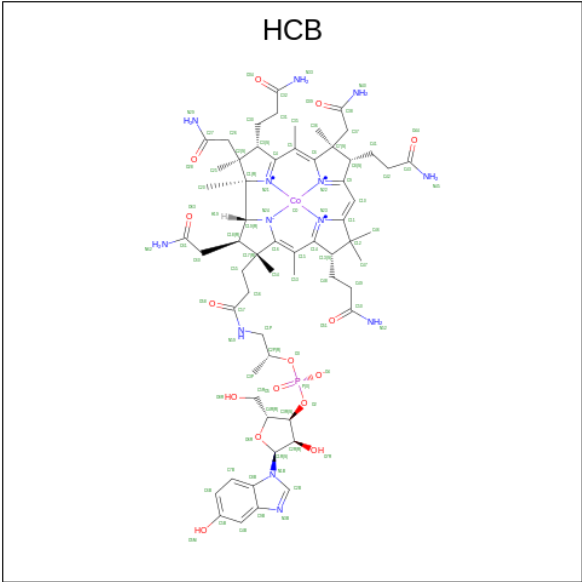
Chain	Residue	Modelled	Actual	Comment	Reference
Q	224	HIS	-	expression tag	UNP A0A0E3QQC8
R	218	GLY	-	expression tag	UNP A0A0E3QQC8
R	219	GLY	-	expression tag	UNP A0A0E3QQC8
R	220	HIS	-	expression tag	UNP A0A0E3QQC8
R	221	HIS	-	expression tag	UNP A0A0E3QQC8
R	222	HIS	-	expression tag	UNP A0A0E3QQC8
R	223	HIS	-	expression tag	UNP A0A0E3QQC8
R	224	HIS	-	expression tag	UNP A0A0E3QQC8

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 5-HYDROXYBENZIMIDAZOLYLCOBAMIDE (CCD ID: HCB) (formula: $C_{60}H_{84}CoN_{13}O_{15}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	M	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
4	N	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
4	O	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
4	P	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
4	Q	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
4	R	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	44	Total	O	0	0
			44	44		
5	B	63	Total	O	0	0
			63	63		
5	C	47	Total	O	0	0
			47	47		
5	D	62	Total	O	0	0
			62	62		
5	E	66	Total	O	0	0
			66	66		
5	F	47	Total	O	0	0
			47	47		

Continued on next page...

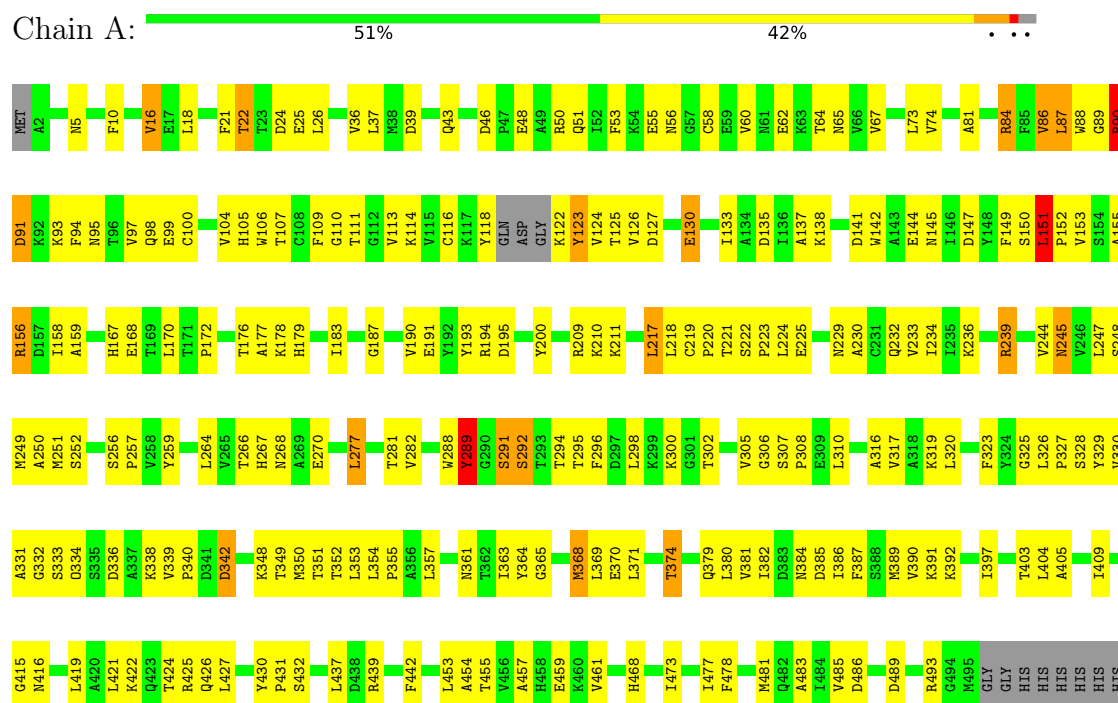
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	5	Total 5	O 5	0	0
5	N	13	Total 13	O 13	0	0
5	O	5	Total 5	O 5	0	0
5	P	6	Total 6	O 6	0	0
5	Q	11	Total 11	O 11	0	0
5	R	4	Total 4	O 4	0	0

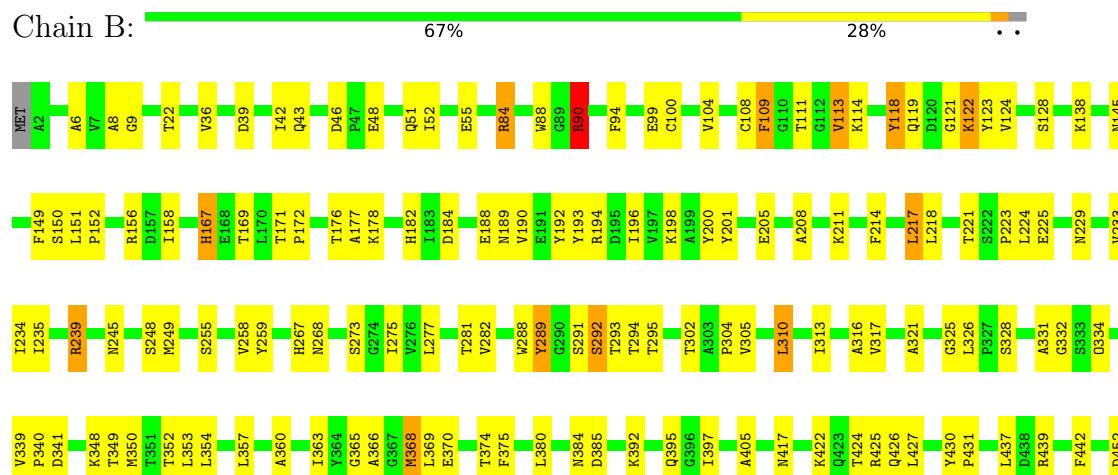
3 Residue-property plots

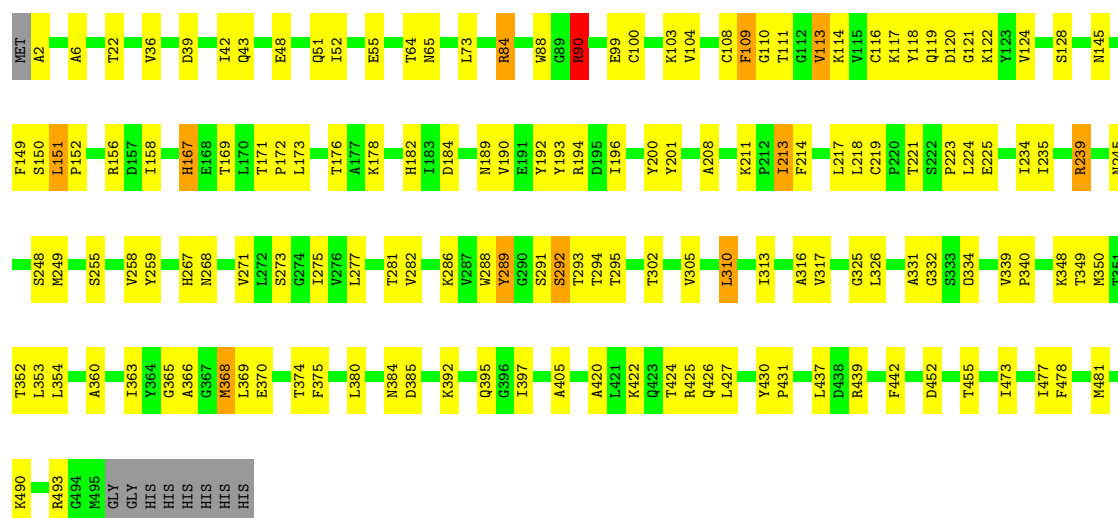
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Trimethylamine methyltransferase



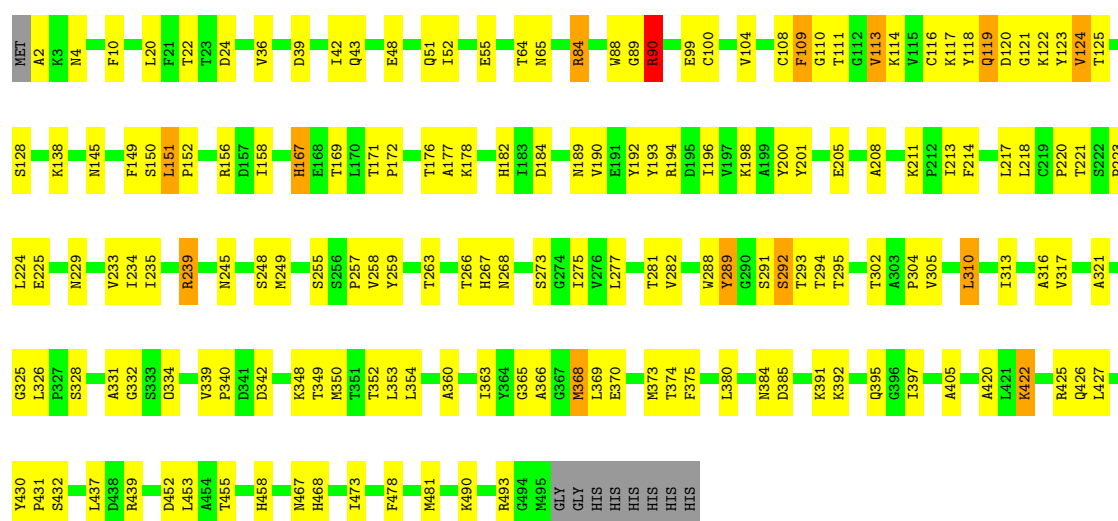
• Molecule 1: Trimethylamine methyltransferase





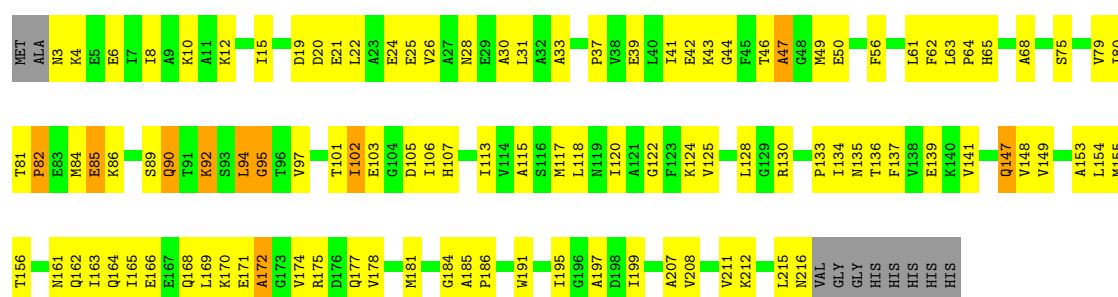
• Molecule 1: Trimethylamine methyltransferase

Chain F: 65% 31% . .

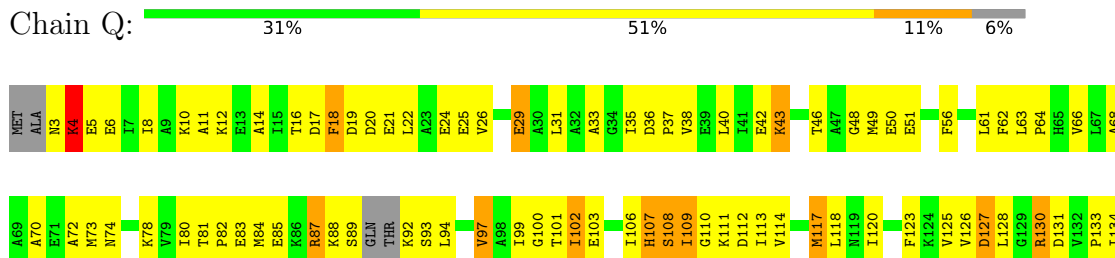


• Molecule 2: Trimethylamine methyltransferase corrinoid protein

Chain M: 47% 44% . .



• Molecule 2: Trimethylamine methyltransferase corrinoid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.43Å 188.14Å 123.95Å 90.00° 119.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-2.70) 94.4 (20.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.238 0.189 , 0.192	Depositor DCC
R_{free} test set	6602 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 7.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.025 for l,k,-h-l 0.025 for -h-l,k,h 0.277 for h,-k,-h-l 0.033 for l,-k,h 0.025 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33443	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: GOL, PYL, HCB

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	0.47	0/3858	0.99	23/5229 (0.4%)
1	B	0.45	0/3902	0.92	9/5291 (0.2%)
1	C	0.44	0/3902	0.93	10/5291 (0.2%)
1	D	0.50	0/3858	1.00	22/5229 (0.4%)
1	E	0.46	0/3902	0.92	9/5291 (0.2%)
1	F	0.42	0/3902	0.92	12/5291 (0.2%)
2	M	0.39	0/1611	0.89	3/2174 (0.1%)
2	N	0.43	0/1591	0.96	6/2145 (0.3%)
2	O	0.37	0/1611	0.93	7/2174 (0.3%)
2	P	0.38	0/1616	0.89	6/2181 (0.3%)
2	Q	0.41	0/1586	0.94	5/2138 (0.2%)
2	R	0.38	0/1611	0.90	1/2174 (0.0%)
All	All	0.44	0/32950	0.94	113/44608 (0.3%)

There are no bond length outliers.

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	289	TYR	N-CA-C	-8.92	94.78	108.96
1	C	224	LEU	N-CA-C	8.76	123.33	111.24
1	D	224	LEU	N-CA-C	8.73	123.53	111.74
1	F	224	LEU	N-CA-C	8.56	123.05	111.24
1	B	224	LEU	N-CA-C	8.54	123.03	111.24

There are no chirality outliers.

There are no planarity outliers.

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	3801	0	3804	208	0
1	B	3843	0	3836	147	0
1	C	3843	0	3836	147	0
1	D	3801	0	3804	197	0
1	E	3843	0	3836	141	0
1	F	3843	0	3836	148	0
2	M	1595	0	1622	119	0
2	N	1576	0	1605	108	0
2	O	1595	0	1622	106	0
2	P	1600	0	1627	99	0
2	Q	1571	0	1600	173	0
2	R	1595	0	1622	113	0
3	A	6	0	8	0	0
3	C	6	0	8	0	0
3	E	6	0	8	3	0
3	F	6	0	8	0	0
4	M	90	0	84	15	0
4	N	90	0	84	11	0
4	O	90	0	84	14	0
4	P	90	0	84	16	0
4	Q	90	0	84	13	0
4	R	90	0	84	17	0
5	A	44	0	0	4	0
5	B	63	0	0	4	0
5	C	47	0	0	6	0
5	D	62	0	0	4	0
5	E	66	0	0	8	0
5	F	47	0	0	2	0
5	M	5	0	0	0	0
5	N	13	0	0	3	0
5	O	5	0	0	0	0
5	P	6	0	0	0	0
5	Q	11	0	0	2	0
5	R	4	0	0	0	0
All	All	33443	0	33186	1656	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 25.

The worst 5 of 1656 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:P:37:PRO:HG2	2:P:90:GLN:HE22	1.13	1.12
2:Q:118:LEU:HD23	2:Q:208:VAL:HG22	1.37	1.07
2:R:94:LEU:HD12	2:R:95:GLY:H	1.11	1.06
2:N:99:ILE:HD11	2:N:115:ALA:HB2	1.38	1.05
2:N:149:VAL:HG23	2:N:178:VAL:HG21	1.38	1.05

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	489/503 (97%)	453 (93%)	35 (7%)	1 (0%)	43	68
1	B	499/503 (99%)	479 (96%)	20 (4%)	0	100	100
1	C	499/503 (99%)	482 (97%)	17 (3%)	0	100	100
1	D	489/503 (97%)	457 (94%)	30 (6%)	2 (0%)	30	54
1	E	499/503 (99%)	475 (95%)	24 (5%)	0	100	100
1	F	499/503 (99%)	469 (94%)	30 (6%)	0	100	100
2	M	212/224 (95%)	191 (90%)	14 (7%)	7 (3%)	3	7
2	N	208/224 (93%)	186 (89%)	15 (7%)	7 (3%)	3	7
2	O	212/224 (95%)	187 (88%)	18 (8%)	7 (3%)	3	7
2	P	213/224 (95%)	187 (88%)	20 (9%)	6 (3%)	4	9
2	Q	207/224 (92%)	155 (75%)	36 (17%)	16 (8%)	1	1
2	R	212/224 (95%)	185 (87%)	22 (10%)	5 (2%)	4	12
All	All	4238/4362 (97%)	3906 (92%)	281 (7%)	51 (1%)	10	27

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4	ASN
2	M	85	GLU
2	O	94	LEU
2	O	95	GLY
2	P	84	MET

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	407/411 (99%)	391 (96%)	16 (4%)	28	57
1	B	411/411 (100%)	399 (97%)	12 (3%)	37	67
1	C	411/411 (100%)	401 (98%)	10 (2%)	43	72
1	D	407/411 (99%)	395 (97%)	12 (3%)	37	67
1	E	411/411 (100%)	403 (98%)	8 (2%)	50	77
1	F	411/411 (100%)	398 (97%)	13 (3%)	34	64
2	M	169/176 (96%)	165 (98%)	4 (2%)	43	72
2	N	166/176 (94%)	159 (96%)	7 (4%)	26	55
2	O	169/176 (96%)	162 (96%)	7 (4%)	27	56
2	P	169/176 (96%)	163 (96%)	6 (4%)	31	60
2	Q	166/176 (94%)	158 (95%)	8 (5%)	23	50
2	R	169/176 (96%)	164 (97%)	5 (3%)	36	66
All	All	3466/3522 (98%)	3358 (97%)	108 (3%)	36	65

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	368	MET
2	M	21	GLU
2	Q	130	ARG
1	F	90	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	151	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	468	HIS
1	E	482	GLN
2	R	216	ASN
2	P	216	ASN
1	E	51	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	GOL	C	601	-	5,5,5	0.34	0	5,5,5	0.49	0
4	HCB	P	301	2	91,100,100	0.96	2 (2%)	146,164,164	1.47	18 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	F	601	-	5,5,5	0.37	0	5,5,5	0.61	0
4	HCB	M	301	2	91,100,100	0.97	2 (2%)	146,164,164	1.45	16 (10%)
4	HCB	N	301	2	91,100,100	1.02	3 (3%)	146,164,164	1.47	18 (12%)
3	GOL	A	601	-	5,5,5	0.32	0	5,5,5	0.89	0
4	HCB	Q	301	2	91,100,100	0.96	2 (2%)	146,164,164	1.48	19 (13%)
4	HCB	R	301	2	91,100,100	1.00	2 (2%)	146,164,164	1.46	18 (12%)
4	HCB	O	301	2	91,100,100	0.99	2 (2%)	146,164,164	1.45	16 (10%)
3	GOL	E	601	-	5,5,5	0.26	0	5,5,5	0.96	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
3	GOL	C	601	-	-	2/4/4/4	-
4	HCB	P	301	2	-	16/56/223/223	0/3/11/11
3	GOL	F	601	-	-	0/4/4/4	-
4	HCB	M	301	2	-	16/56/223/223	0/3/11/11
4	HCB	N	301	2	-	16/56/223/223	0/3/11/11
3	GOL	A	601	-	-	0/4/4/4	-
4	HCB	Q	301	2	-	20/56/223/223	0/3/11/11
4	HCB	R	301	2	-	16/56/223/223	0/3/11/11
4	HCB	O	301	2	-	16/56/223/223	0/3/11/11
3	GOL	E	601	-	-	0/4/4/4	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	301	HCB	C14-N23	4.47	1.42	1.30
4	P	301	HCB	C14-N23	4.44	1.42	1.30
4	M	301	HCB	C14-N23	4.38	1.42	1.30
4	N	301	HCB	C14-N23	4.35	1.42	1.30
4	R	301	HCB	C14-N23	4.35	1.42	1.30

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	301	HCB	C11-N23-C14	8.89	109.67	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	301	HCB	C11-N23-C14	8.74	109.62	106.31
4	P	301	HCB	C11-N23-C14	8.68	109.59	106.31
4	M	301	HCB	C11-N23-C14	8.39	109.48	106.31
4	N	301	HCB	C11-N23-C14	8.35	109.47	106.31

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

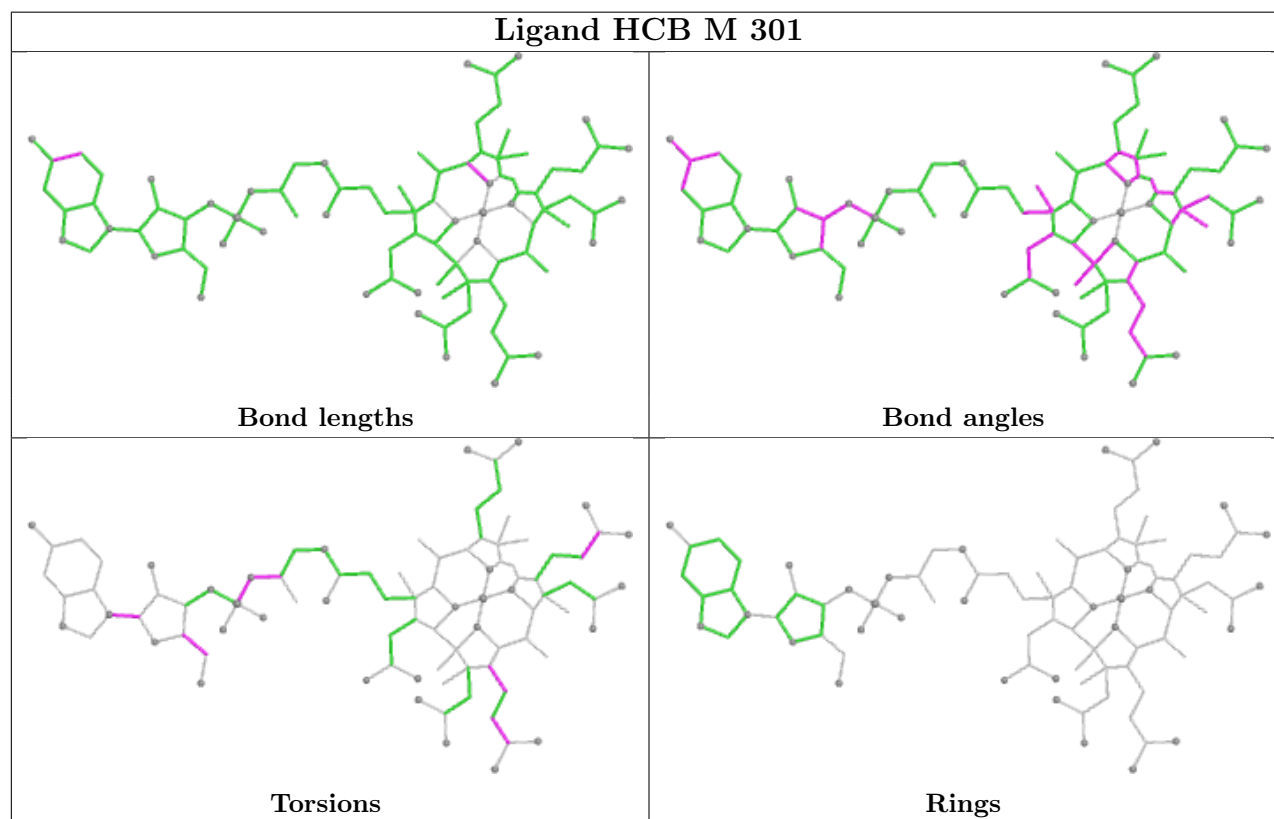
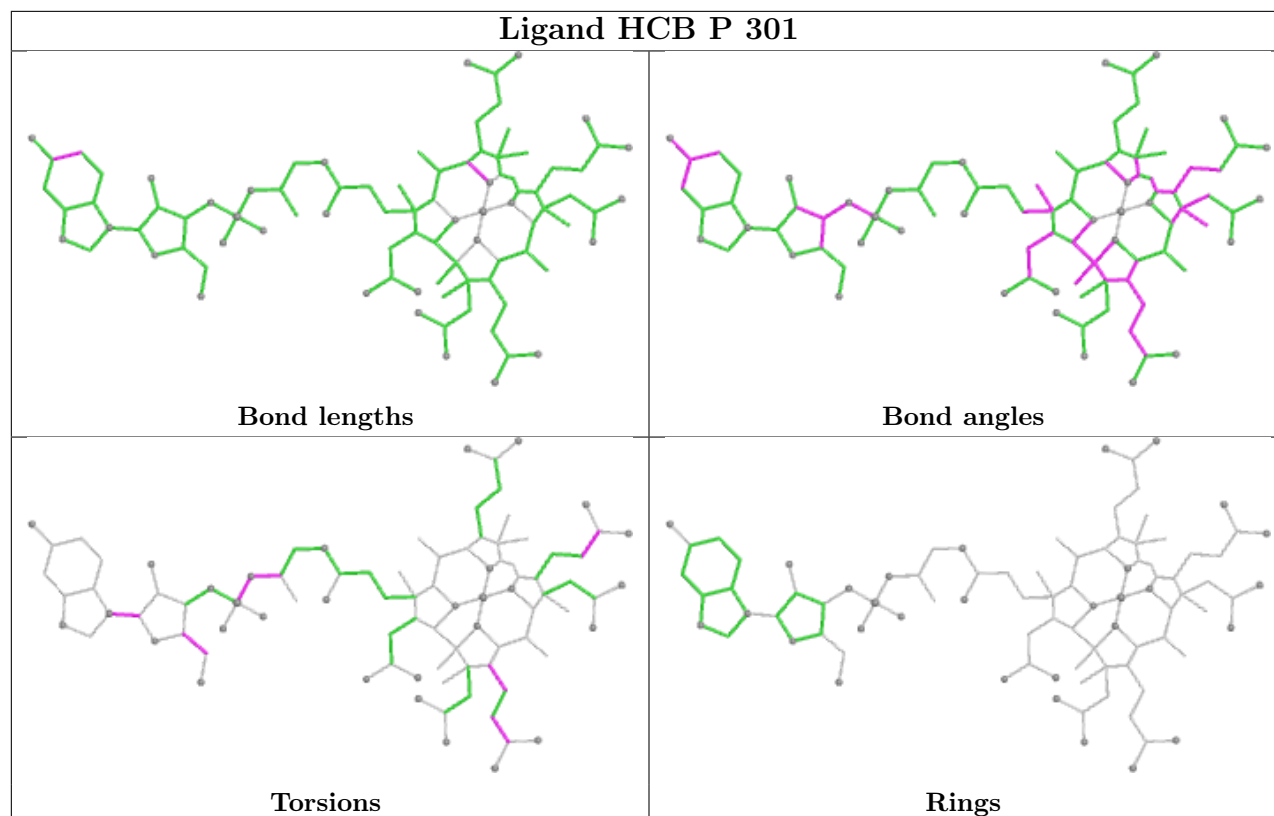
Mol	Chain	Res	Type	Atoms
4	M	301	HCB	C2-C3-C30-C31
4	M	301	HCB	C4-C3-C30-C31
4	M	301	HCB	C1P-C2P-O3-P
4	M	301	HCB	C3P-C2P-O3-P
4	M	301	HCB	C2P-O3-P-O4

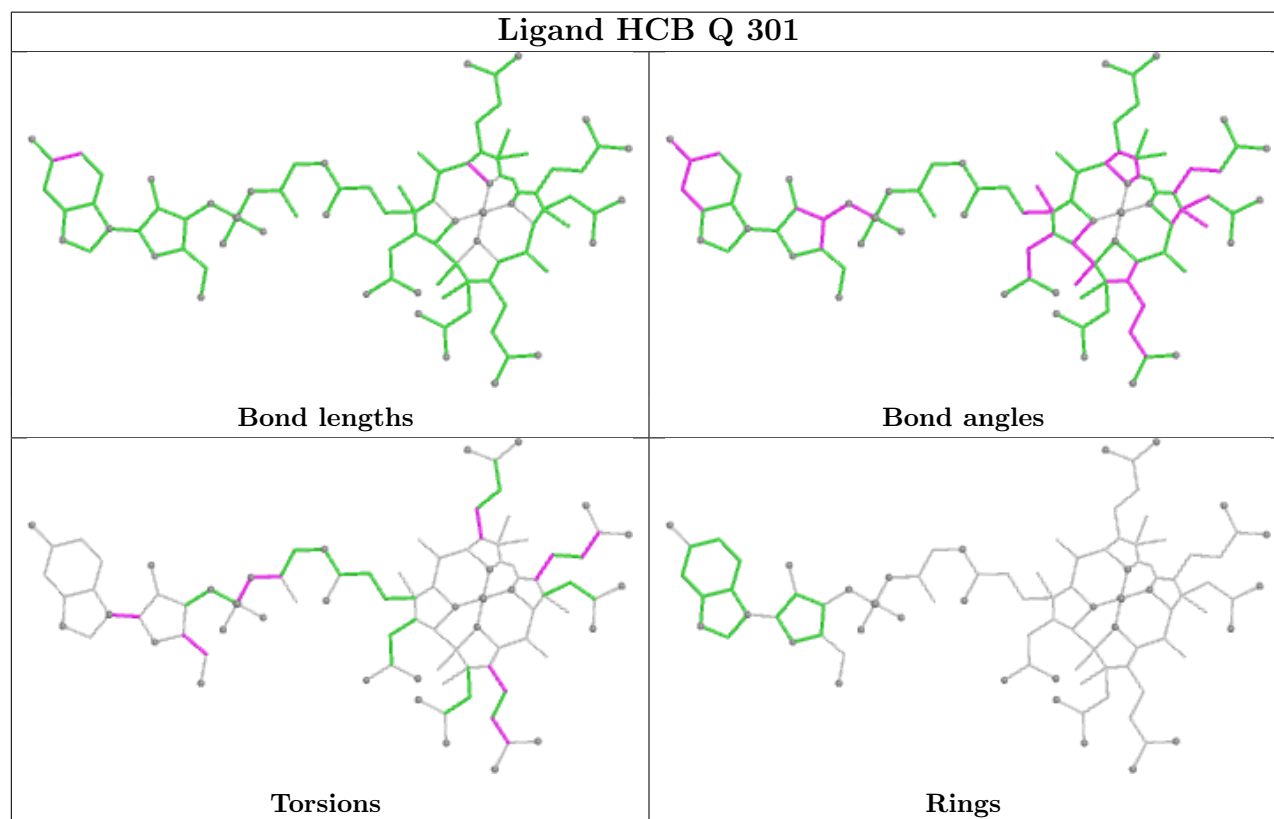
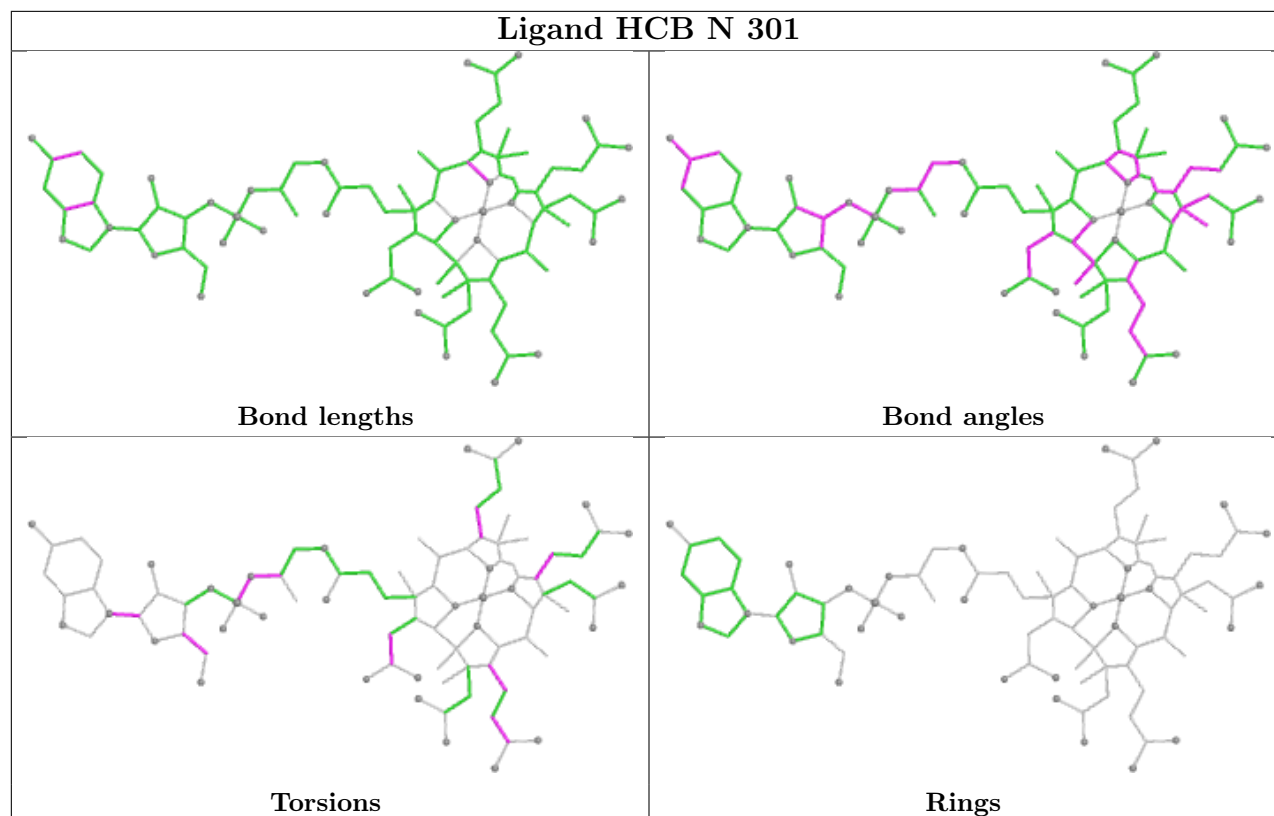
There are no ring outliers.

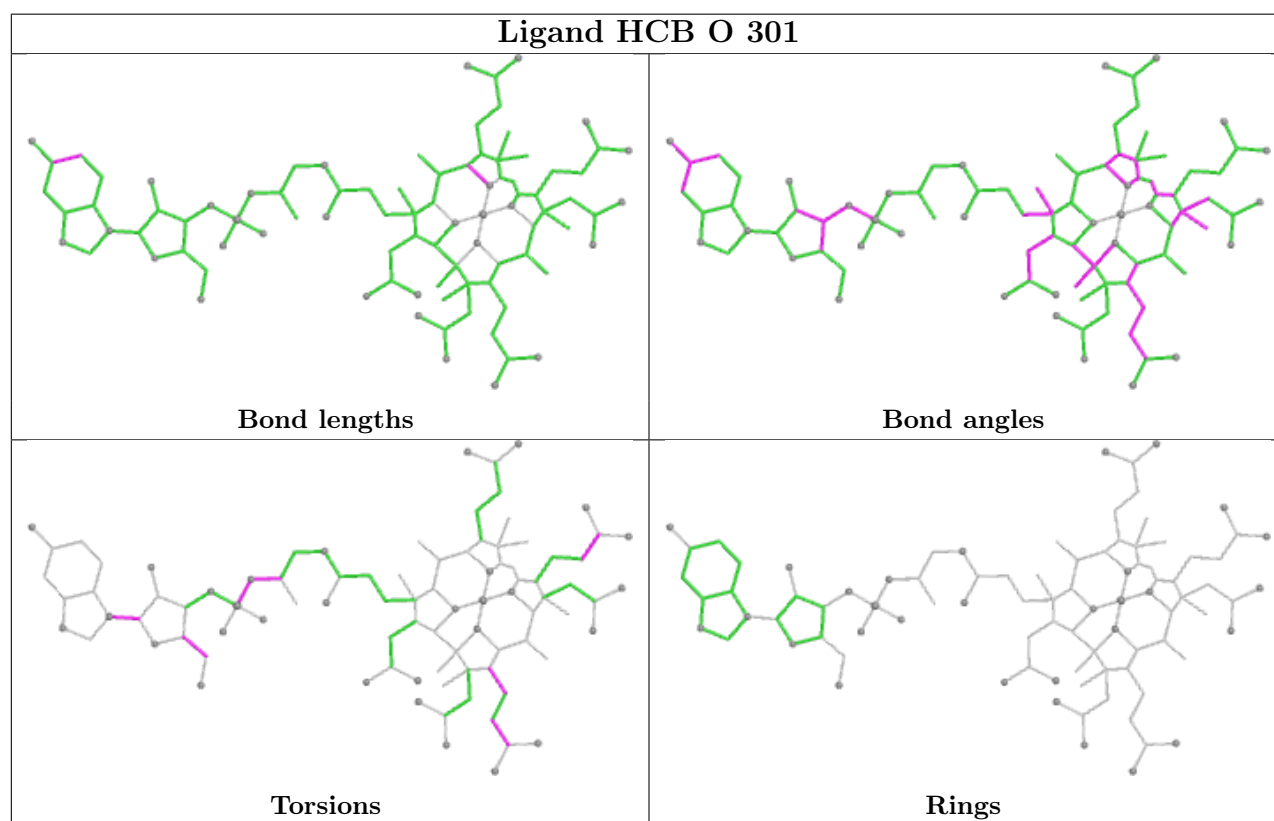
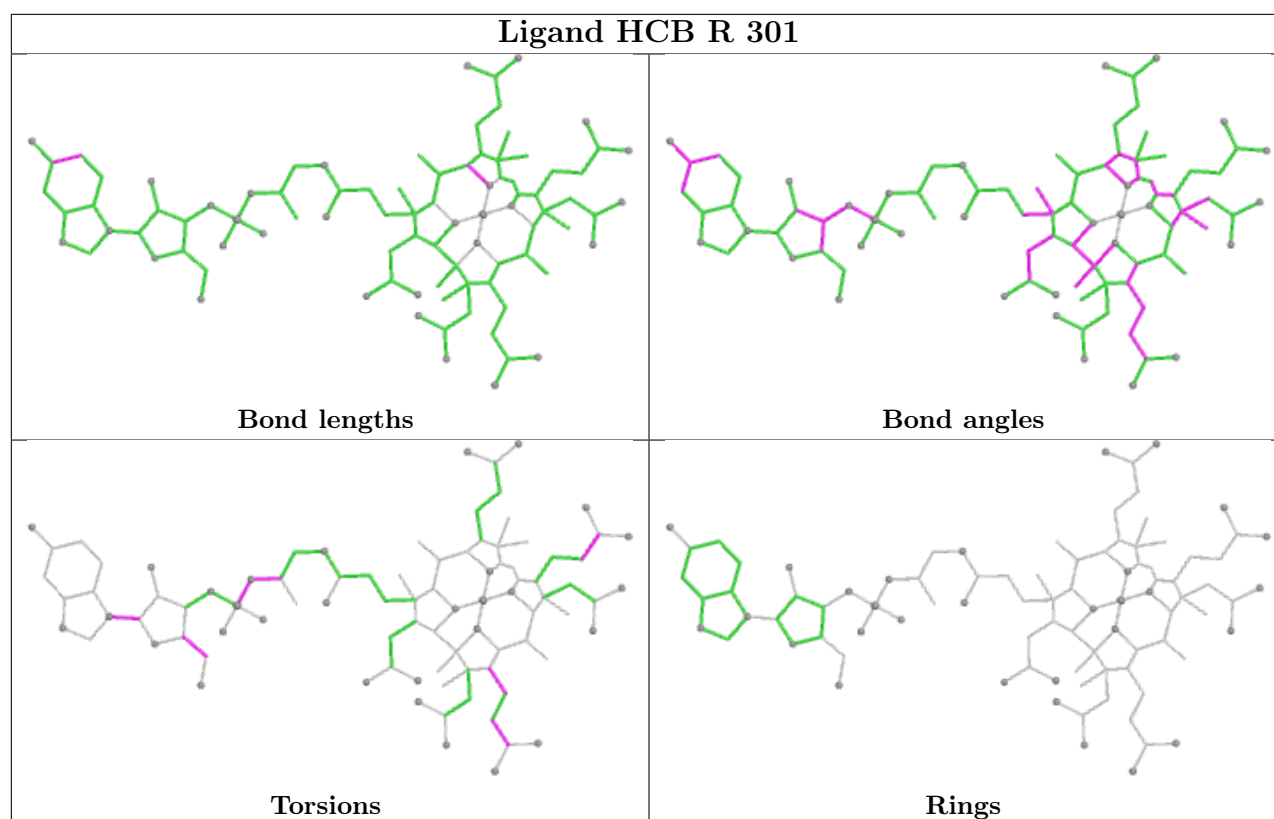
7 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	301	HCB	16	0
4	M	301	HCB	15	0
4	N	301	HCB	11	0
4	Q	301	HCB	13	0
4	R	301	HCB	17	0
4	O	301	HCB	14	0
3	E	601	GOL	3	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 [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	490/503 (97%)	-1.72	0 100 100	16, 39, 62, 103	5 (1%)
1	B	493/503 (98%)	-1.73	0 100 100	11, 33, 57, 85	8 (1%)
1	C	493/503 (98%)	-1.73	0 100 100	15, 35, 59, 92	8 (1%)
1	D	490/503 (97%)	-1.74	0 100 100	13, 36, 59, 95	5 (1%)
1	E	493/503 (98%)	-1.75	0 100 100	12, 31, 53, 86	8 (1%)
1	F	493/503 (98%)	-1.72	0 100 100	15, 38, 62, 93	8 (1%)
2	M	214/224 (95%)	-1.58	0 100 100	35, 66, 92, 129	0
2	N	212/224 (94%)	-1.64	0 100 100	27, 60, 84, 95	0
2	O	214/224 (95%)	-1.60	0 100 100	33, 68, 98, 125	0
2	P	215/224 (95%)	-1.58	0 100 100	31, 62, 90, 115	0
2	Q	211/224 (94%)	-1.49	0 100 100	31, 76, 111, 123	0
2	R	214/224 (95%)	-1.58	0 100 100	36, 66, 93, 121	0
All	All	4232/4362 (97%)	-1.69	0 100 100	11, 42, 85, 129	42 (0%)

There are no RSRZ outliers to report.

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

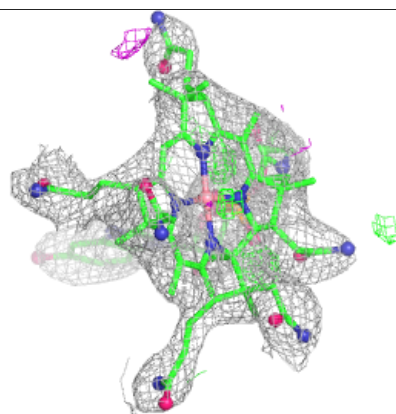
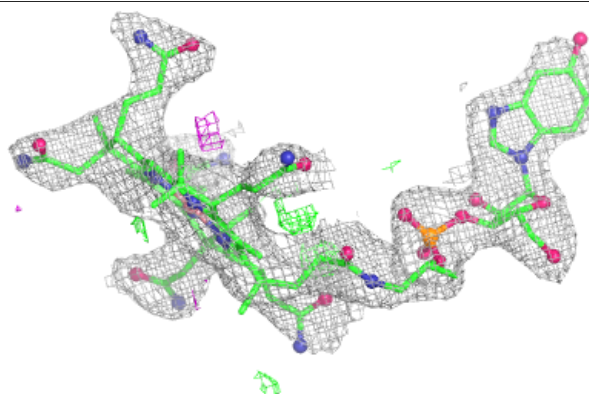
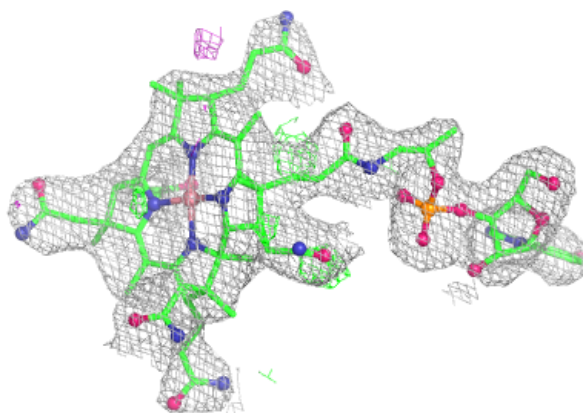
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	A	601	6/6	0.98	0.07	64,76,82,90	0
3	GOL	C	601	6/6	0.99	0.07	59,73,74,74	0
3	GOL	E	601	6/6	0.99	0.04	56,61,70,74	0
3	GOL	F	601	6/6	0.99	0.04	53,66,72,80	0
4	HCB	M	301	90/90	0.99	0.03	30,53,70,84	0
4	HCB	O	301	90/90	0.99	0.03	27,48,67,73	0
4	HCB	P	301	90/90	0.99	0.03	24,48,66,72	0
4	HCB	Q	301	90/90	0.99	0.04	35,67,100,109	0
4	HCB	R	301	90/90	0.99	0.03	30,51,62,70	0
4	HCB	N	301	90/90	1.00	0.03	16,54,67,95	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.

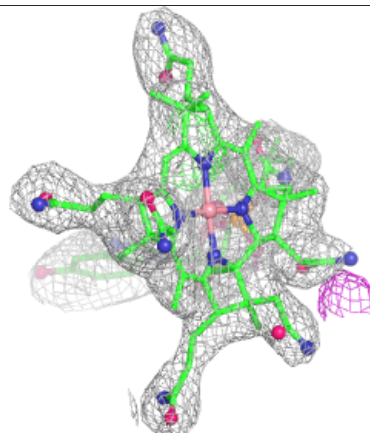
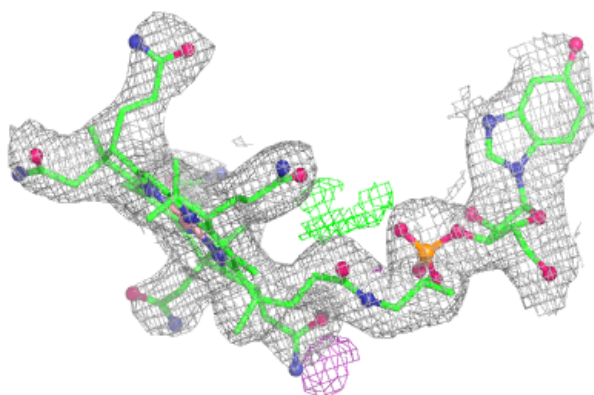
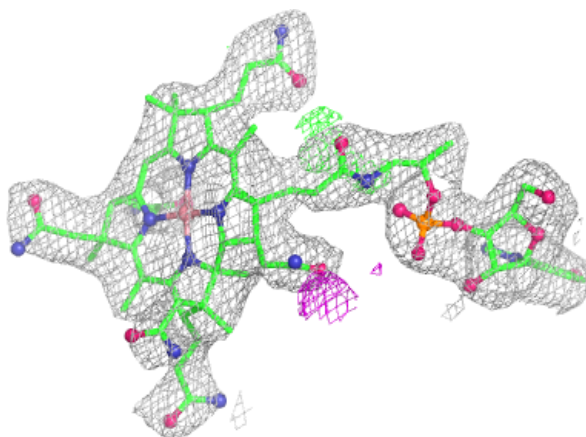
Electron density around HCB M 301:

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

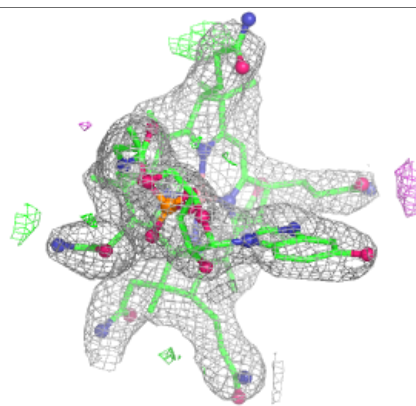
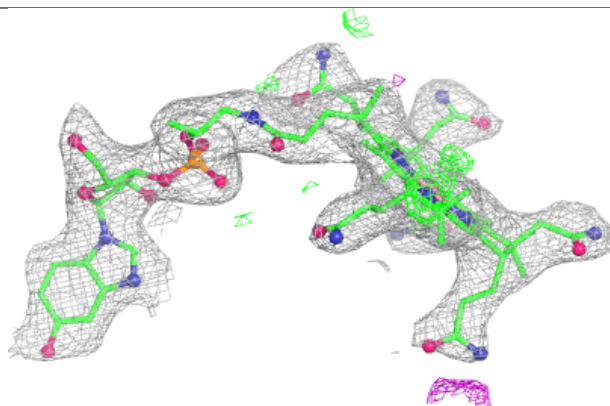
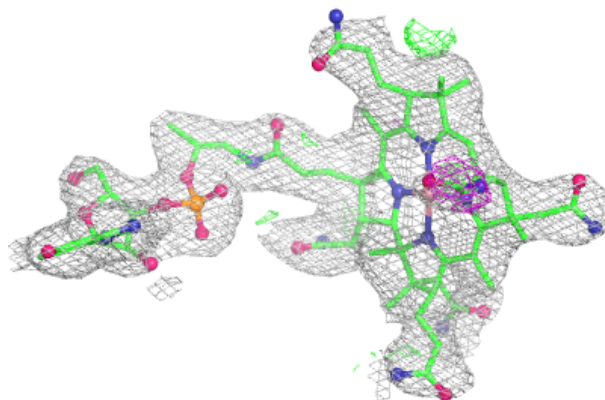


Electron density around HCB O 301:

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

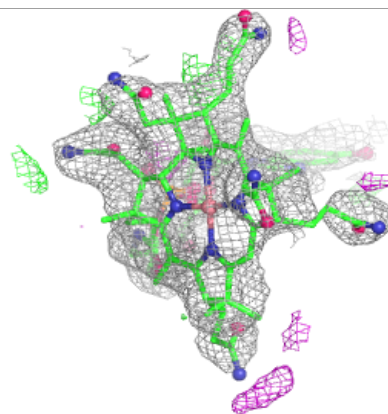
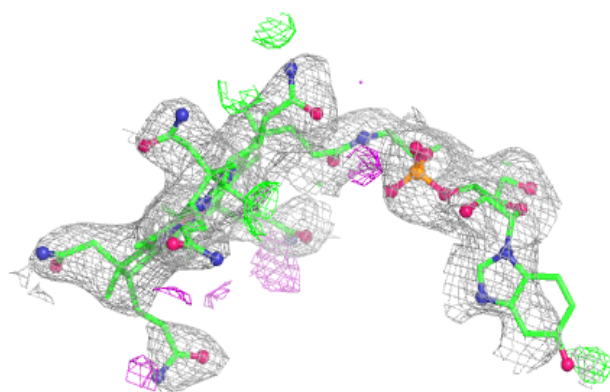
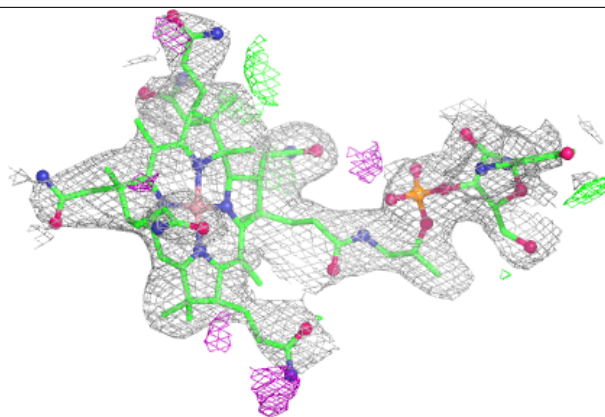
**Electron density around HCB P 301:**

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



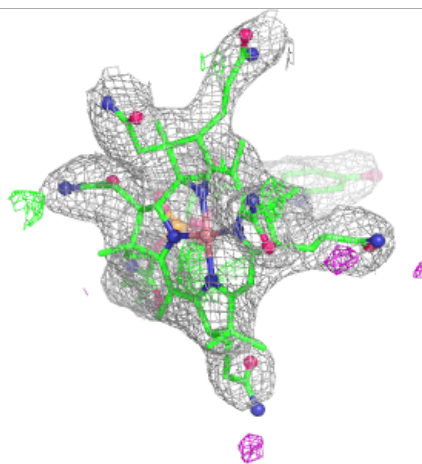
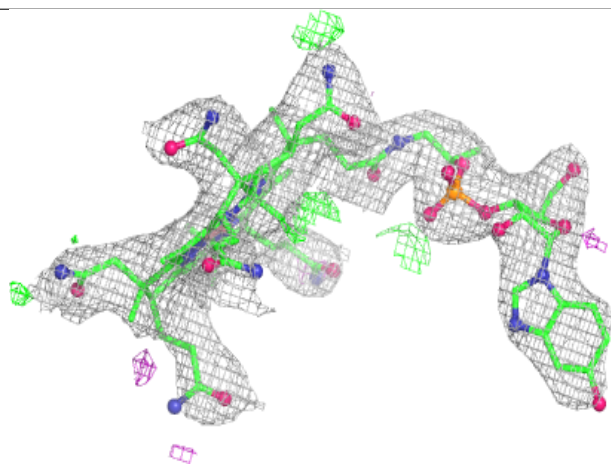
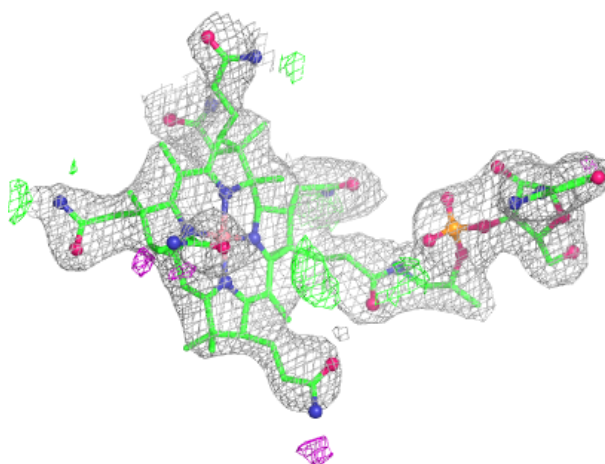
Electron density around HCB Q 301:

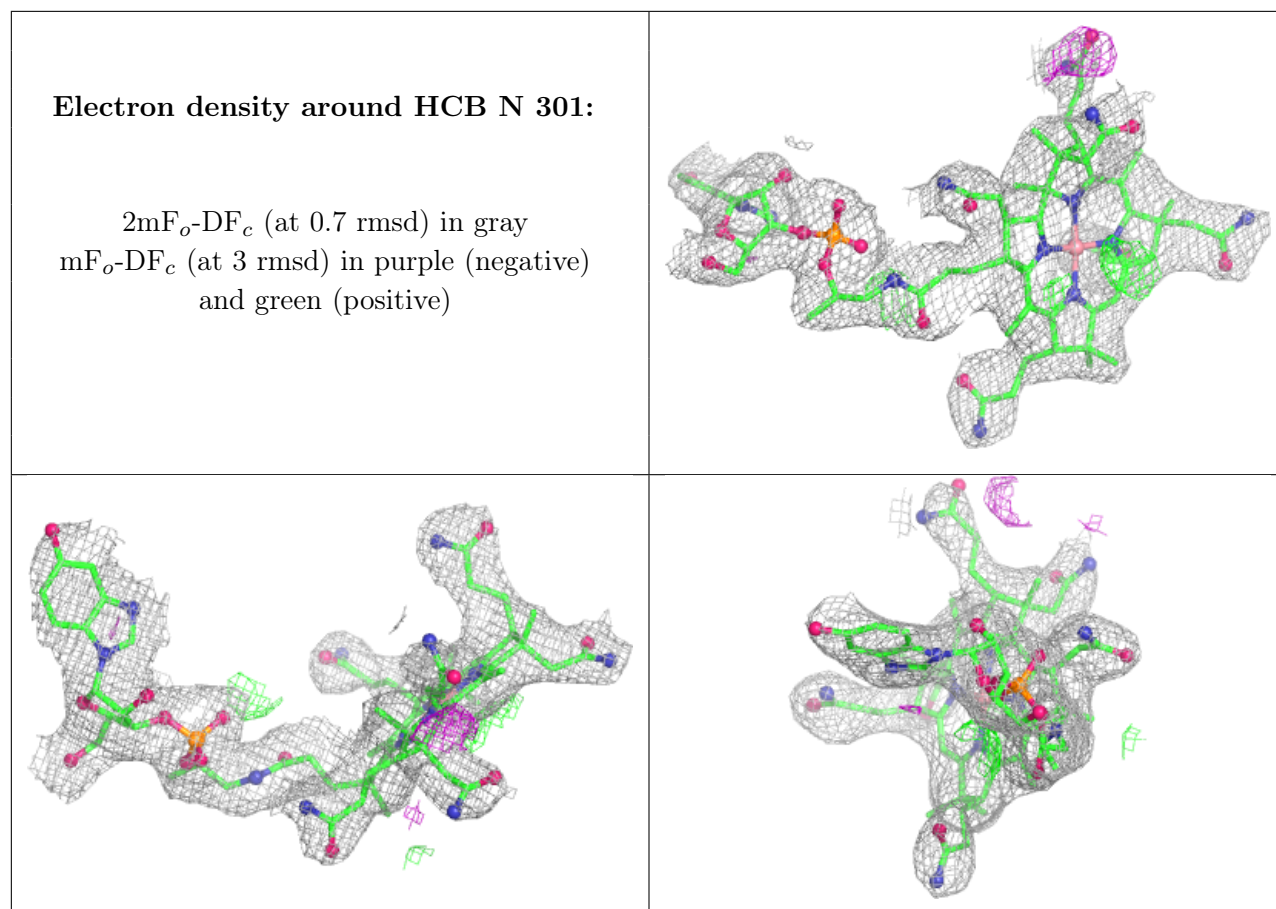
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HCB R 301:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.