



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:24 pm BST

PDB ID : 6JZS
Title : Structure of the Manganese Protoporphyrin IX-Reconstituted CYP102A1 Haem Domain with N-Abietoyl-L-Tryptophan in complex with Pyridine
Authors : Stanfield, J.K.; Omura, K.; Matsumoto, A.; Kasai, C.; Sugimoto, H.; Shiro, Y.; Watanabe, Y.; Shoji, O.
Deposited on : 2019-05-03
Resolution : 1.68 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 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	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

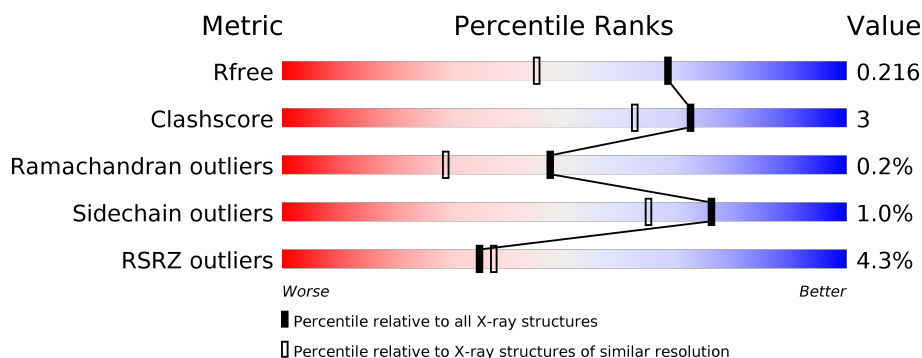
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	494	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>8%</div> </div> </div>
1	C	494	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8245 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 Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	14	0
			3766	2403	637	708	18			
1	C	453	Total	C	N	O	S	0	12	0
			3753	2395	637	703	18			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	expression tag	UNP P14779
A	-30	GLY	-	expression tag	UNP P14779
A	-29	SER	-	expression tag	UNP P14779
A	-28	SER	-	expression tag	UNP P14779
A	-27	HIS	-	expression tag	UNP P14779
A	-26	HIS	-	expression tag	UNP P14779
A	-25	HIS	-	expression tag	UNP P14779
A	-24	HIS	-	expression tag	UNP P14779
A	-23	HIS	-	expression tag	UNP P14779
A	-22	HIS	-	expression tag	UNP P14779
A	-21	SER	-	expression tag	UNP P14779
A	-20	SER	-	expression tag	UNP P14779
A	-19	GLY	-	expression tag	UNP P14779
A	-18	LEU	-	expression tag	UNP P14779
A	-17	VAL	-	expression tag	UNP P14779
A	-16	PRO	-	expression tag	UNP P14779
A	-15	ARG	-	expression tag	UNP P14779
A	-14	GLY	-	expression tag	UNP P14779
A	-13	SER	-	expression tag	UNP P14779
A	-12	HIS	-	expression tag	UNP P14779
A	-11	MET	-	expression tag	UNP P14779
A	-10	ALA	-	expression tag	UNP P14779
A	-9	SER	-	expression tag	UNP P14779
A	-8	GLU	-	expression tag	UNP P14779
A	-7	ASN	-	expression tag	UNP P14779

Continued on next page...

Continued from previous page...

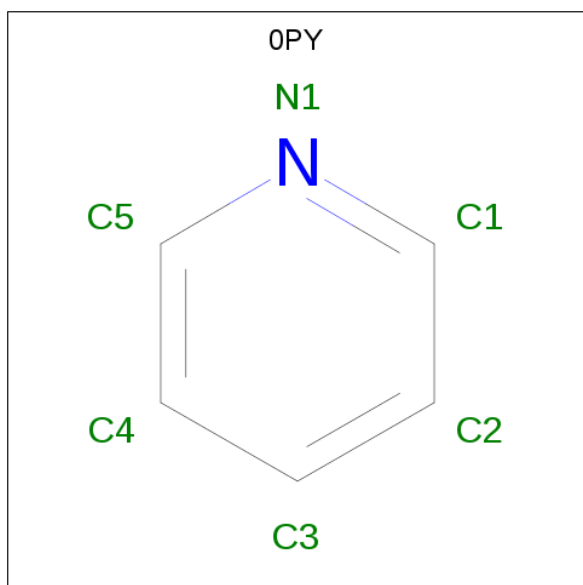
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP P14779
A	-5	TYR	-	expression tag	UNP P14779
A	-4	PHE	-	expression tag	UNP P14779
A	-3	GLN	-	expression tag	UNP P14779
A	-2	GLY	-	expression tag	UNP P14779
A	-1	SER	-	expression tag	UNP P14779
A	457	LEU	-	expression tag	UNP P14779
A	458	PRO	-	expression tag	UNP P14779
A	459	ALA	-	expression tag	UNP P14779
A	460	THR	-	expression tag	UNP P14779
A	461	GLY	-	expression tag	UNP P14779
A	462	GLY	-	expression tag	UNP P14779
C	-31	MET	-	expression tag	UNP P14779
C	-30	GLY	-	expression tag	UNP P14779
C	-29	SER	-	expression tag	UNP P14779
C	-28	SER	-	expression tag	UNP P14779
C	-27	HIS	-	expression tag	UNP P14779
C	-26	HIS	-	expression tag	UNP P14779
C	-25	HIS	-	expression tag	UNP P14779
C	-24	HIS	-	expression tag	UNP P14779
C	-23	HIS	-	expression tag	UNP P14779
C	-22	HIS	-	expression tag	UNP P14779
C	-21	SER	-	expression tag	UNP P14779
C	-20	SER	-	expression tag	UNP P14779
C	-19	GLY	-	expression tag	UNP P14779
C	-18	LEU	-	expression tag	UNP P14779
C	-17	VAL	-	expression tag	UNP P14779
C	-16	PRO	-	expression tag	UNP P14779
C	-15	ARG	-	expression tag	UNP P14779
C	-14	GLY	-	expression tag	UNP P14779
C	-13	SER	-	expression tag	UNP P14779
C	-12	HIS	-	expression tag	UNP P14779
C	-11	MET	-	expression tag	UNP P14779
C	-10	ALA	-	expression tag	UNP P14779
C	-9	SER	-	expression tag	UNP P14779
C	-8	GLU	-	expression tag	UNP P14779
C	-7	ASN	-	expression tag	UNP P14779
C	-6	LEU	-	expression tag	UNP P14779
C	-5	TYR	-	expression tag	UNP P14779
C	-4	PHE	-	expression tag	UNP P14779
C	-3	GLN	-	expression tag	UNP P14779
C	-2	GLY	-	expression tag	UNP P14779

Continued on next page...

Continued from previous page...

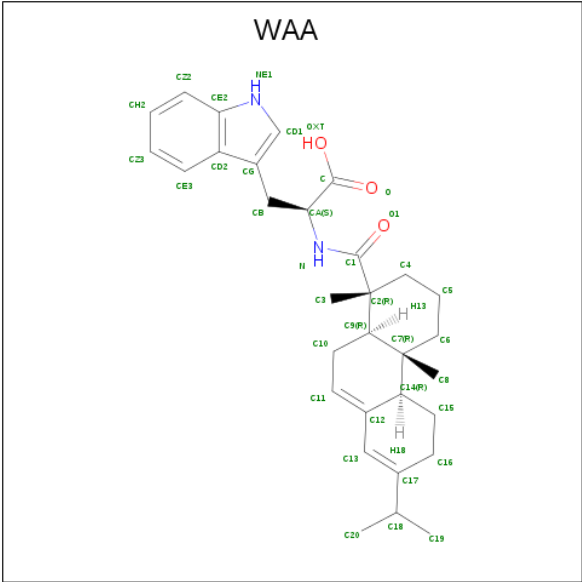
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP P14779
C	457	LEU	-	expression tag	UNP P14779
C	458	PRO	-	expression tag	UNP P14779
C	459	ALA	-	expression tag	UNP P14779
C	460	THR	-	expression tag	UNP P14779
C	461	GLY	-	expression tag	UNP P14779
C	462	GLY	-	expression tag	UNP P14779

- Molecule 2 is pyridine (three-letter code: 0PY) (formula: C₅H₅N).



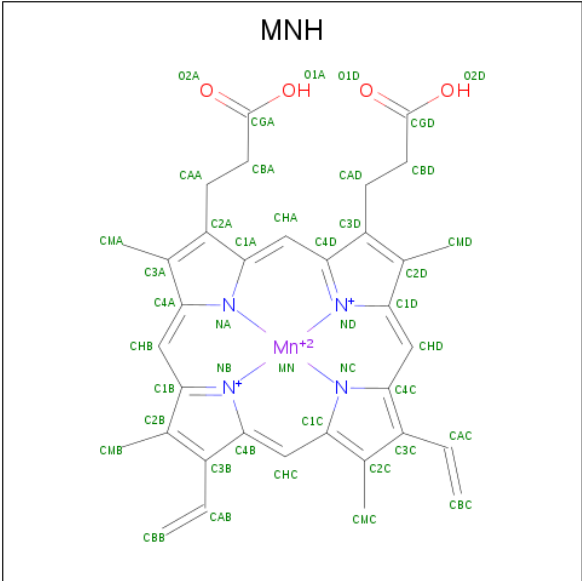
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 6 5 1	0	0
2	C	1	Total C N 6 5 1	0	0
2	C	1	Total C N 6 5 1	0	0

- Molecule 3 is (2S)-2-[[[(1R,4aR,4bR,10aR)-1,4a-dimethyl-7-propan-2-yl-2,3,4,4b,5,6,10,10a-octahydrophenanthren-1-yl]carbonylamino]-3-(1H-indol-3-yl)propanoic acid (three-letter code: WAA) (formula: C₃₁H₄₀N₂O₃) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			36	31	2	3		
3	C	1	Total	C	N	O	0	0
			36	31	2	3		

- Molecule 4 is MANGANESE PROTOPORPHYRIN IX (three-letter code: MNH) (formula: $C_{34}H_{32}MnN_4O_4$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

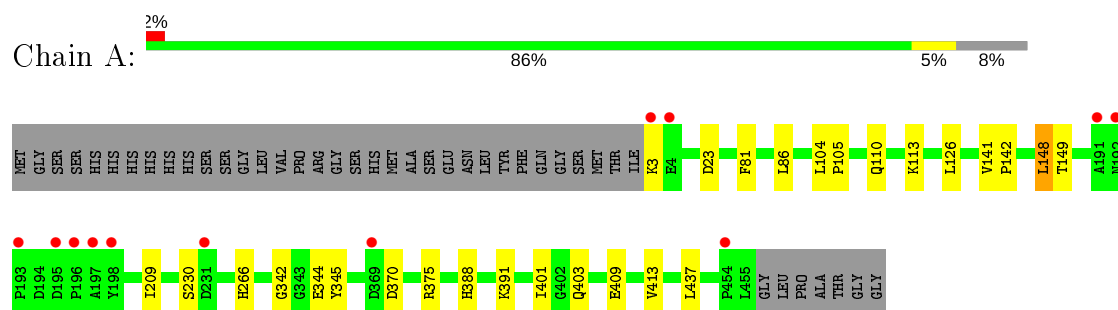
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	267	Total	O	0	0
			267	267		
6	C	259	Total	O	0	0
			259	259		

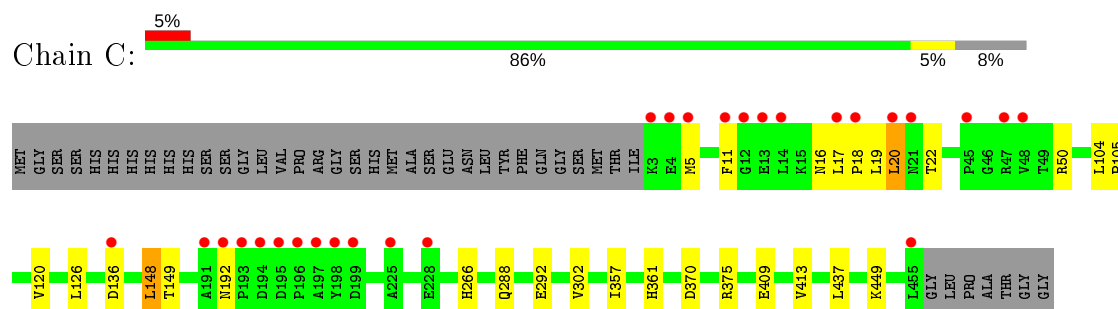
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.72Å 146.13Å 62.48Å 90.00° 96.87° 90.00°	Depositor
Resolution (Å)	47.33 – 1.68 47.29 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.33-1.68) 99.7 (47.29-1.68)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.180 , 0.209 0.188 , 0.216	Depositor DCC
R_{free} test set	5867 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.8	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	0.96	EDS
Total number of atoms	8245	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: MNH, GOL, OPY, WAA

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	0.65	0/3852	0.74	0/5210
1	C	0.67	0/3839	0.75	0/5188
All	All	0.66	0/7691	0.75	0/10398

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

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	3766	0	3715	20	0
1	C	3753	0	3708	26	0
2	A	6	0	5	0	0
2	C	12	0	10	1	0
3	A	36	0	0	0	0
3	C	36	0	0	3	0
4	A	43	0	30	5	0
4	C	43	0	30	2	0
5	A	6	0	8	1	0
5	C	18	0	24	1	0
6	A	267	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	259	0	0	2	0
All	All	8245	0	7530	52	0

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

All (52) 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:409[B]:GLU:O	1:A:413[B]:VAL:HG13	1.71	0.91
1:C:16:ASN:O	1:C:19:LEU:HD13	1.73	0.88
1:A:3:LYS:HE2	1:A:344:GLU:OE1	1.78	0.84
4:A:503:MNH:HMC1	4:A:503:MNH:HBC1	1.61	0.82
4:C:504:MNH:HMB1	4:C:504:MNH:HBB1	1.70	0.71
1:C:437[A]:LEU:HD11	3:C:503:WAA:C20	2.21	0.70
4:A:503:MNH:HMB1	4:A:503:MNH:HBB1	1.74	0.69
1:A:149:THR:HA	1:A:409[A]:GLU:OE2	1.98	0.64
1:A:370:ASP:CG	1:A:375:ARG:HH12	2.03	0.61
1:C:19:LEU:N	1:C:19:LEU:HD12	2.16	0.60
4:C:504:MNH:HBC1	4:C:504:MNH:HMC1	1.85	0.59
1:C:148:LEU:HD21	1:C:413[A]:VAL:HG21	1.84	0.58
1:C:437[B]:LEU:H	1:C:437[B]:LEU:HD23	1.71	0.56
1:C:437[A]:LEU:CD1	3:C:503:WAA:C20	2.82	0.56
1:C:5:MET:HE1	1:C:50:ARG:HE	1.71	0.55
1:A:3:LYS:HE3	1:A:345:TYR:OH	2.07	0.55
1:A:437:LEU:HD21	6:A:832:HOH:O	2.07	0.54
1:A:23:ASP:OD2	6:A:601:HOH:O	2.17	0.54
1:C:437[A]:LEU:HD21	2:C:501:OPY:H3	1.90	0.54
1:C:288:GLN:NE2	1:C:292[A]:GLU:HG3	2.22	0.53
1:C:148:LEU:HD13	1:C:413[B]:VAL:HG21	1.91	0.53
5:C:506:GOL:H12	6:C:699:HOH:O	2.10	0.51
1:C:19:LEU:N	1:C:19:LEU:CD1	2.74	0.51
1:A:342:GLY:O	1:A:344:GLU:HG3	2.12	0.49
1:A:401:ILE:CG2	4:A:503:MNH:HMD2	2.42	0.49
1:A:403:GLN:NE2	6:A:605:HOH:O	2.38	0.49
1:A:401:ILE:HG22	4:A:503:MNH:HMD2	1.95	0.48
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.94	0.48
1:C:126[B]:LEU:HD13	1:C:126[B]:LEU:C	2.34	0.48
1:A:148:LEU:HD21	1:A:413[B]:VAL:HG11	1.97	0.47
1:C:148:LEU:CD2	1:C:413[A]:VAL:HG21	2.43	0.47
1:C:437[B]:LEU:HD21	6:C:813:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:LEU:HB3	1:C:18:PRO:HD3	1.98	0.46
1:A:86:LEU:HB2	4:A:503:MNH:HMD1	1.98	0.46
1:C:11:PHE:CE1	1:C:19:LEU:CD1	2.99	0.45
1:C:16:ASN:C	1:C:19:LEU:HD13	2.37	0.45
1:A:141:VAL:HB	1:A:142:PRO:HD3	1.98	0.44
1:A:110:GLN:HE22	1:A:113:LYS:NZ	2.16	0.44
1:C:19:LEU:CD1	1:C:19:LEU:H	2.30	0.44
1:C:149:THR:HA	1:C:409:GLU:OE2	2.17	0.43
5:A:504:GOL:H11	6:A:628:HOH:O	2.19	0.43
1:C:357:ILE:HG22	1:C:361:HIS:CE1	2.54	0.43
1:C:120:VAL:HG11	1:C:302:VAL:HG13	2.00	0.43
1:A:126[B]:LEU:HD13	1:A:126[B]:LEU:C	2.39	0.43
1:A:81:PHE:HB3	1:A:209:ILE:HG12	2.01	0.42
1:C:20:LEU:HD21	3:C:503:WAA:CD1	2.50	0.41
1:C:370:ASP:OD2	1:C:375:ARG:NH1	2.48	0.41
1:C:11:PHE:CE1	1:C:19:LEU:HD12	2.55	0.41
1:A:148:LEU:HD13	1:A:413[A]:VAL:HG21	2.03	0.41
1:A:104:LEU:N	1:A:105:PRO:CD	2.83	0.40
1:C:104:LEU:HB3	1:C:105:PRO:HD3	2.04	0.40
1:C:11:PHE:CE1	1:C:19:LEU:HD11	2.57	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	465/494 (94%)	453 (97%)	11 (2%)	1 (0%)	47	29
1	C	463/494 (94%)	451 (97%)	11 (2%)	1 (0%)	47	29
All	All	928/988 (94%)	904 (97%)	22 (2%)	2 (0%)	47	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	266	HIS
1	A	266	HIS

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	411/429 (96%)	409 (100%)	2 (0%)	88	83
1	C	409/429 (95%)	402 (98%)	7 (2%)	60	43
All	All	820/858 (96%)	811 (99%)	9 (1%)	76	61

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

Mol	Chain	Res	Type
1	A	148	LEU
1	A	230	SER
1	C	20	LEU
1	C	22	THR
1	C	136	ASP
1	C	148	LEU
1	C	192	ASN
1	C	449[A]	LYS
1	C	449[B]	LYS

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

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 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	WAA	C	503	-	36,40,40	0.84	0	41,61,61	1.28	5 (12%)
4	MNH	C	504	1	32,50,50	4.50	18 (56%)	19,82,82	3.16	8 (42%)
2	OPY	A	501	-	6,6,6	0.47	0	6,6,6	0.96	0
5	GOL	C	507	-	5,5,5	0.12	0	5,5,5	0.33	0
4	MNH	A	503	1	32,50,50	4.68	18 (56%)	19,82,82	2.79	7 (36%)
5	GOL	A	504	-	5,5,5	0.10	0	5,5,5	0.28	0
3	WAA	A	502	-	36,40,40	0.91	1 (2%)	41,61,61	1.27	6 (14%)
5	GOL	C	505	-	5,5,5	0.10	0	5,5,5	0.29	0
2	OPY	C	502	-	6,6,6	1.07	0	6,6,6	0.64	0
5	GOL	C	506	-	5,5,5	0.09	0	5,5,5	0.24	0
2	OPY	C	501	-	6,6,6	0.70	0	6,6,6	1.05	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	WAA	C	503	-	-	6/17/66/66	0/5/5/5
4	MNH	C	504	1	-	2/10/114/114	-
2	OPY	A	501	-	-	-	0/1/1/1
5	GOL	C	507	-	-	4/4/4/4	-
4	MNH	A	503	1	-	2/10/114/114	-
5	GOL	A	504	-	-	0/4/4/4	-
3	WAA	A	502	-	-	3/17/66/66	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	505	-	-	2/4/4/4	-
2	OPY	C	502	-	-	-	0/1/1/1
5	GOL	C	506	-	-	2/4/4/4	-
2	OPY	C	501	-	-	-	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	MNH	C2D-C3D	14.15	1.45	1.34
4	C	504	MNH	C2D-C3D	13.00	1.44	1.34
4	A	503	MNH	C3C-C2C	-8.22	1.45	1.55
4	C	504	MNH	C3C-C2C	-7.81	1.46	1.55
4	C	504	MNH	C4A-C3A	7.40	1.48	1.38
4	A	503	MNH	C1A-C2A	7.29	1.48	1.38
4	A	503	MNH	C4A-C3A	7.25	1.48	1.38
4	A	503	MNH	CHD-C4C	-7.06	1.42	1.53
4	A	503	MNH	CHC-C1C	-7.02	1.42	1.53
4	C	504	MNH	CHC-C1C	-6.49	1.43	1.53
4	C	504	MNH	C1C-NC	-6.40	1.41	1.49
4	C	504	MNH	C3C-C4C	-6.29	1.47	1.54
4	C	504	MNH	CHD-C4C	-6.19	1.43	1.53
4	A	503	MNH	C3C-C4C	-6.16	1.47	1.54
4	C	504	MNH	C1A-C2A	6.11	1.46	1.38
4	A	503	MNH	CHD-C1D	-6.09	1.43	1.53
4	C	504	MNH	C4C-NC	-5.97	1.42	1.49
4	C	504	MNH	CHD-C1D	-5.55	1.43	1.53
4	A	503	MNH	C1C-NC	-5.37	1.43	1.49
4	A	503	MNH	CHC-C4B	-5.10	1.44	1.53
4	A	503	MNH	C2B-C3B	4.53	1.46	1.35
4	C	504	MNH	CHC-C4B	-4.41	1.45	1.53
4	A	503	MNH	C4C-NC	-3.98	1.44	1.49
4	C	504	MNH	C2B-C3B	3.87	1.45	1.35
4	A	503	MNH	CHB-C4A	-3.61	1.42	1.51
4	C	504	MNH	CHA-C4D	-3.51	1.44	1.53
4	C	504	MNH	CHB-C4A	-3.41	1.42	1.51
4	C	504	MNH	CHB-C1B	-3.18	1.45	1.53
4	A	503	MNH	CHB-C1B	-3.15	1.45	1.53
4	A	503	MNH	C2A-C3A	3.00	1.46	1.37
4	A	503	MNH	CHA-C4D	-2.93	1.45	1.53
4	C	504	MNH	C2C-C1C	-2.77	1.48	1.53
4	A	503	MNH	CHA-C1A	-2.68	1.44	1.51
4	C	504	MNH	C2A-C3A	2.65	1.45	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	504	MNH	CHA-C1A	-2.55	1.45	1.51
3	A	502	WAA	C13-C12	2.16	1.49	1.44
4	A	503	MNH	C2C-C1C	-2.14	1.49	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	504	MNH	CMC-C2C-C3C	7.05	130.09	113.69
4	C	504	MNH	C1C-CHC-C4B	6.18	125.53	112.37
4	A	503	MNH	CMC-C2C-C3C	5.72	126.98	113.69
4	A	503	MNH	C1C-CHC-C4B	4.96	122.95	112.37
4	C	504	MNH	C4C-CHD-C1D	4.92	122.86	112.37
4	C	504	MNH	CBD-CAD-C3D	-4.89	105.69	114.35
4	A	503	MNH	CBD-CAD-C3D	-4.87	105.73	114.35
4	A	503	MNH	C4C-CHD-C1D	4.68	122.34	112.37
4	C	504	MNH	CHB-C4A-C3A	-4.11	122.34	129.45
4	A	503	MNH	CBA-CAA-C2A	-3.79	105.50	112.49
4	C	504	MNH	C2C-C3C-CAC	3.50	130.79	113.83
4	A	503	MNH	C2C-C3C-CAC	3.10	128.84	113.83
4	C	504	MNH	CBA-CAA-C2A	-3.07	106.82	112.49
3	A	502	WAA	C6-C7-C9	3.05	111.76	108.02
3	C	503	WAA	CE3-CD2-CE2	2.98	122.12	118.17
4	A	503	MNH	CHB-C4A-C3A	-2.93	124.37	129.45
3	C	503	WAA	C15-C16-C17	-2.74	107.56	112.33
3	A	502	WAA	CA-N-C1	2.54	125.07	121.66
3	A	502	WAA	CE3-CD2-CE2	2.39	121.34	118.17
3	A	502	WAA	C15-C16-C17	-2.34	108.27	112.33
3	C	503	WAA	CE3-CD2-CG	-2.33	130.14	134.42
3	C	503	WAA	C13-C12-C11	-2.12	118.77	121.77
4	C	504	MNH	CAA-C2A-C1A	2.08	128.76	127.30
3	A	502	WAA	C5-C6-C7	-2.08	110.59	113.17
3	A	502	WAA	CB-CA-N	2.06	112.76	109.01
3	C	503	WAA	C4-C2-C9	2.05	110.68	108.34

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	503	WAA	N-CA-CB-CG
3	C	503	WAA	C-CA-CB-CG
4	C	504	MNH	C4C-C3C-CAC-CBC
4	A	503	MNH	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

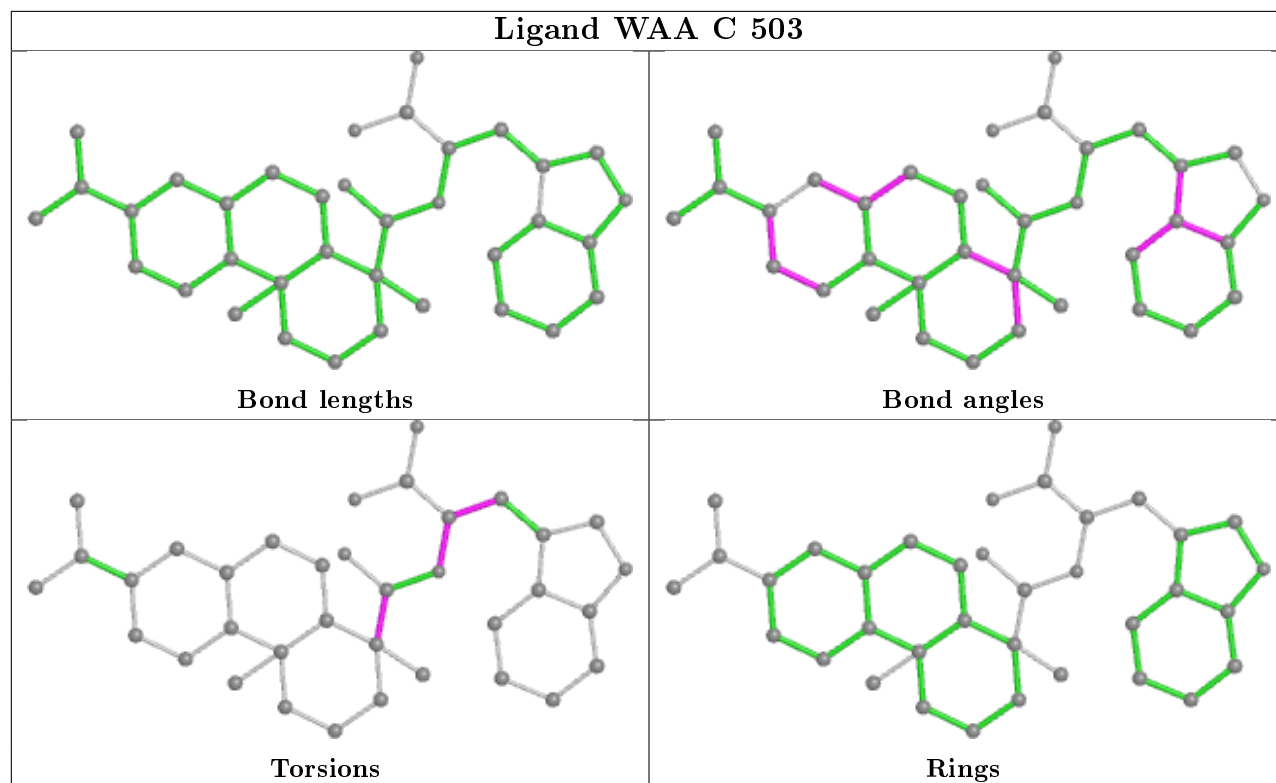
Mol	Chain	Res	Type	Atoms
5	C	505	GOL	O1-C1-C2-C3
5	C	507	GOL	O1-C1-C2-C3
5	C	507	GOL	C1-C2-C3-O3
5	C	506	GOL	C1-C2-C3-O3
5	C	506	GOL	O2-C2-C3-O3
5	C	505	GOL	O1-C1-C2-O2
5	C	507	GOL	O2-C2-C3-O3
4	C	504	MNH	C2C-C3C-CAC-CBC
4	A	503	MNH	C2C-C3C-CAC-CBC
3	A	502	WAA	C-CA-N-C1
3	C	503	WAA	O1-C1-C2-C3
3	A	502	WAA	O1-C1-C2-C3
5	C	507	GOL	O1-C1-C2-O2
3	C	503	WAA	CB-CA-N-C1
3	C	503	WAA	C-CA-N-C1
3	C	503	WAA	N-C1-C2-C3
3	A	502	WAA	N-C1-C2-C3

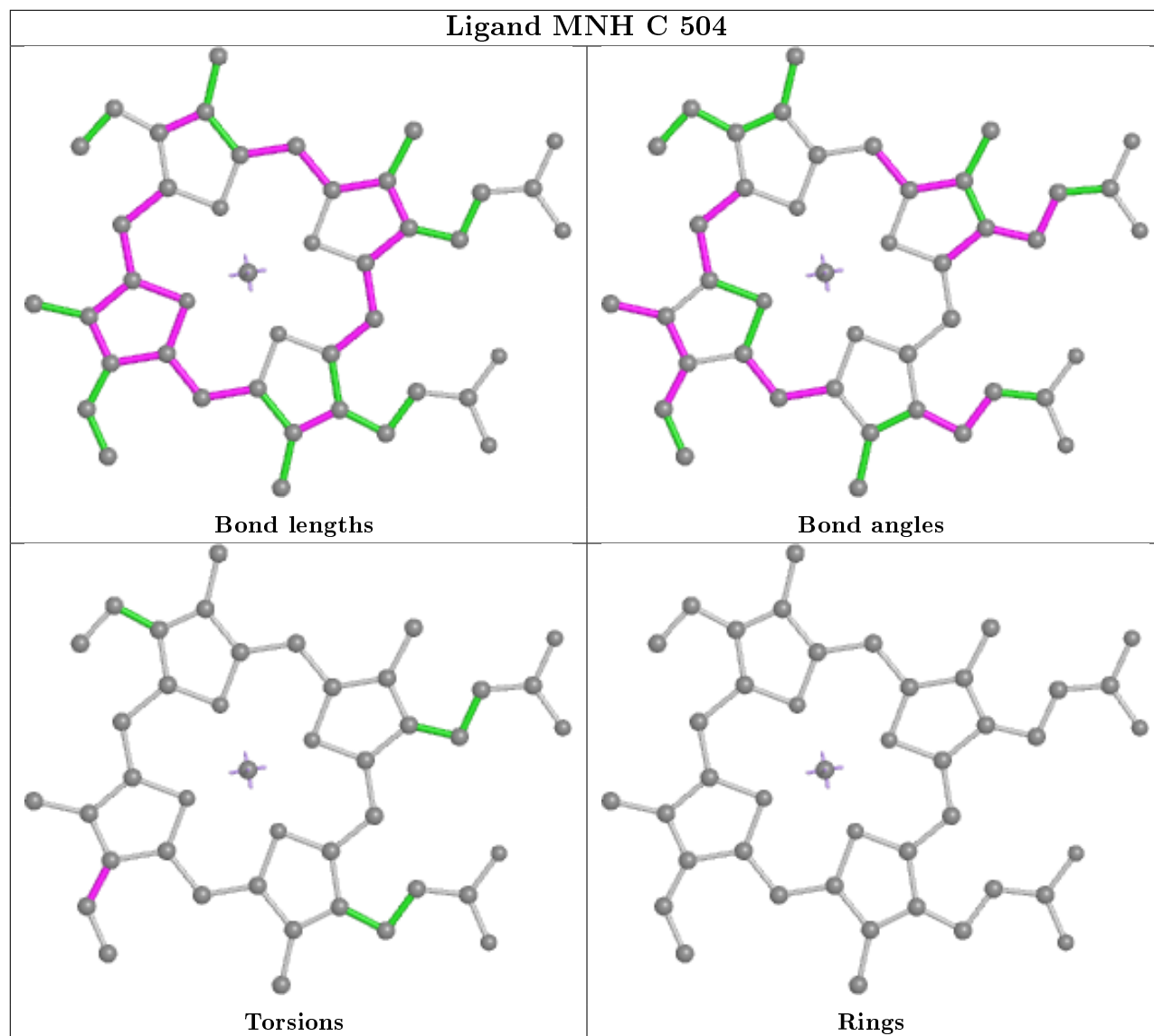
There are no ring outliers.

6 monomers are involved in 13 short contacts:

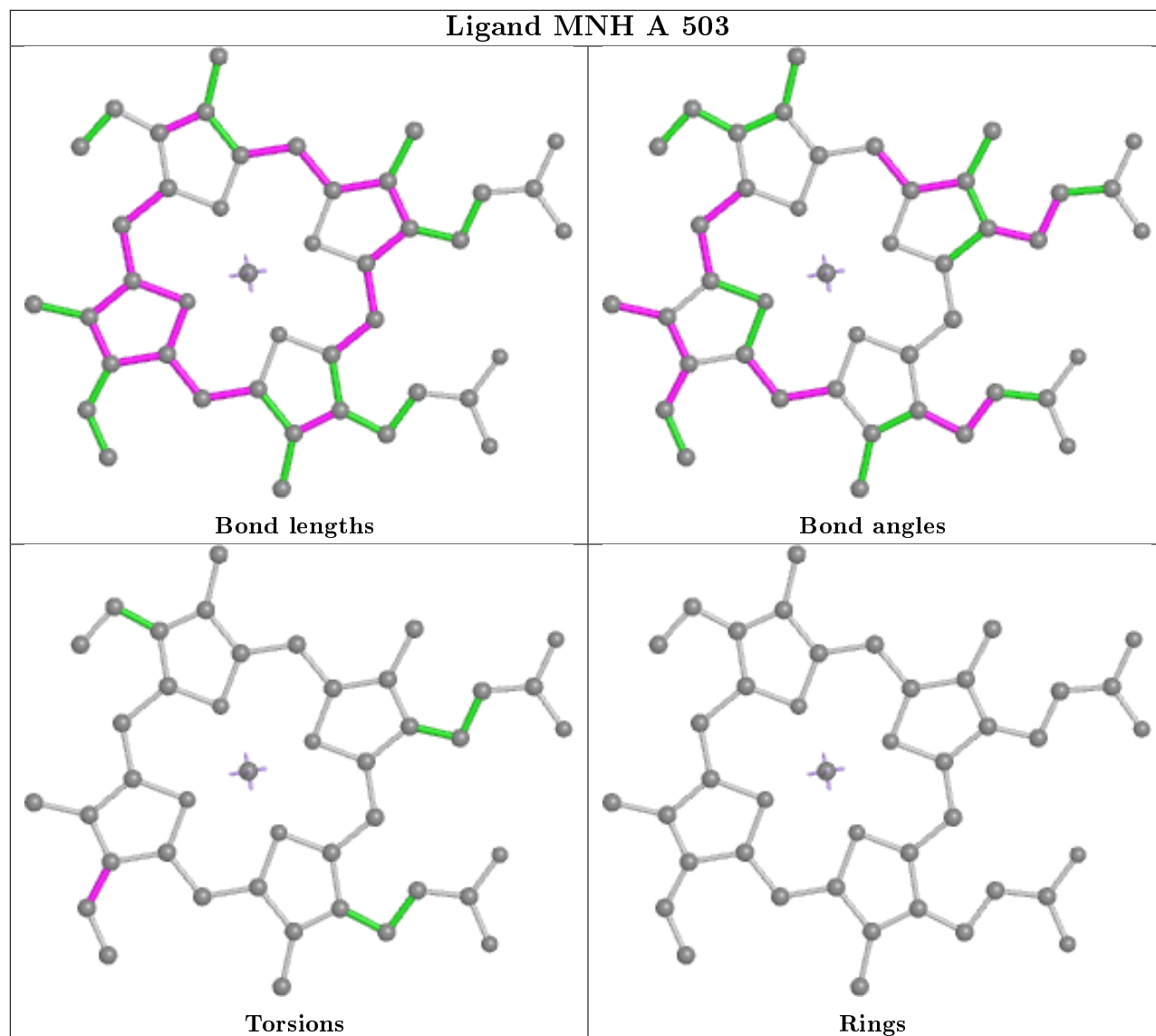
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	WAA	3	0
4	C	504	MNH	2	0
4	A	503	MNH	5	0
5	A	504	GOL	1	0
5	C	506	GOL	1	0
2	C	501	OPY	1	0

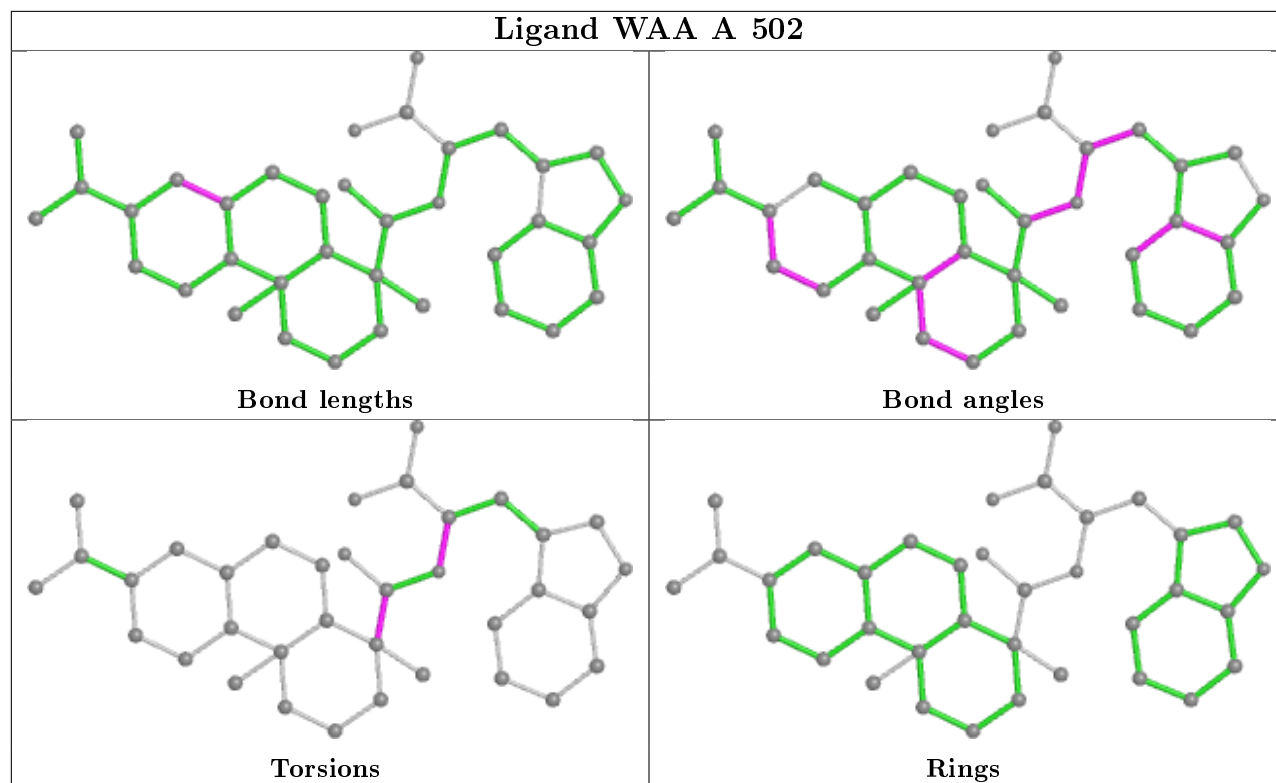
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 MNH A 503





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	453/494 (91%)	-0.16	12 (2%) 56 58	17, 25, 52, 95	0
1	C	453/494 (91%)	-0.06	27 (5%) 21 22	18, 27, 53, 84	0
All	All	906/988 (91%)	-0.11	39 (4%) 35 37	17, 26, 53, 95	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	ALA	6.9
1	C	191	ALA	5.4
1	A	197	ALA	5.3
1	C	4	GLU	5.0
1	C	3	LYS	4.7
1	C	17	LEU	4.3
1	A	193	PRO	4.3
1	A	196	PRO	4.1
1	A	192	ASN	4.1
1	C	5	MET	4.0
1	A	454	PRO	3.5
1	A	3	LYS	3.1
1	C	196	PRO	3.0
1	C	455	LEU	2.9
1	C	12	GLY	2.8
1	A	231	ASP	2.8
1	C	194	ASP	2.8
1	C	192	ASN	2.7
1	C	198	TYR	2.6
1	A	4	GLU	2.6
1	A	198	TYR	2.6
1	C	48	VAL	2.5
1	C	21	ASN	2.4
1	C	13	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	136	ASP	2.3
1	C	11	PHE	2.3
1	C	195	ASP	2.2
1	C	193	PRO	2.2
1	C	225	ALA	2.2
1	C	228	GLU	2.2
1	A	369	ASP	2.2
1	C	20	LEU	2.2
1	C	14	LEU	2.1
1	C	18	PRO	2.1
1	C	197	ALA	2.1
1	C	45	PRO	2.1
1	A	195	ASP	2.0
1	C	199	ASP	2.0
1	C	47	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

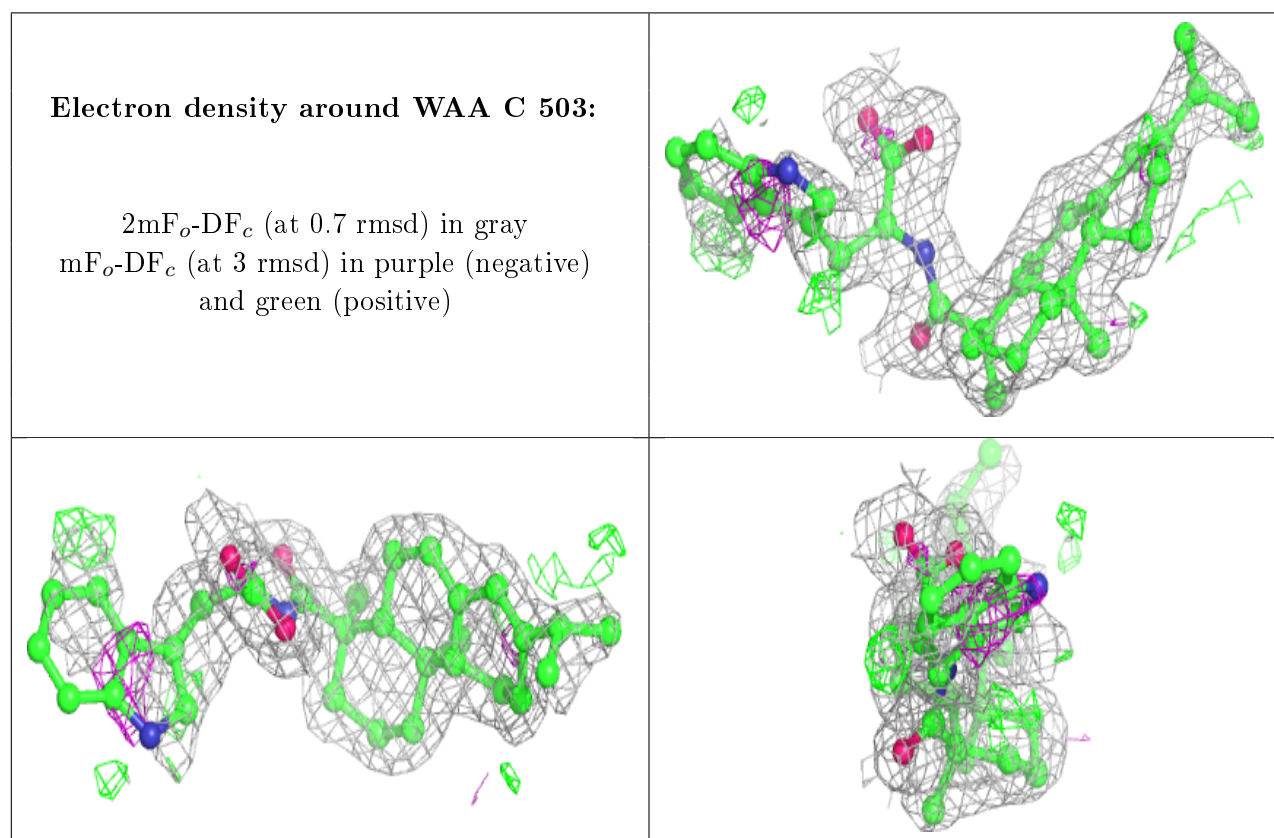
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	C	507	6/6	0.81	0.16	55,56,57,58	0
5	GOL	C	506	6/6	0.82	0.24	52,55,58,62	0
5	GOL	C	505	6/6	0.83	0.16	59,66,68,70	0
2	0PY	C	502	6/6	0.88	0.27	41,42,43,43	0
3	WAA	C	503	36/36	0.88	0.14	27,36,72,74	0
3	WAA	A	502	36/36	0.91	0.11	27,32,45,47	0
5	GOL	A	504	6/6	0.93	0.11	37,44,47,50	0
2	0PY	C	501	6/6	0.94	0.09	29,30,32,33	0

Continued on next page...

Continued from previous page...

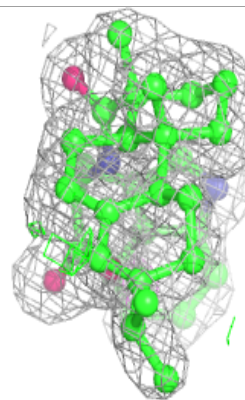
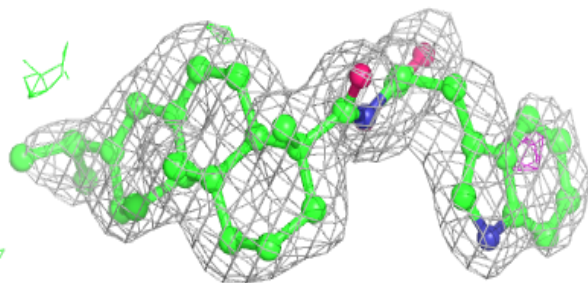
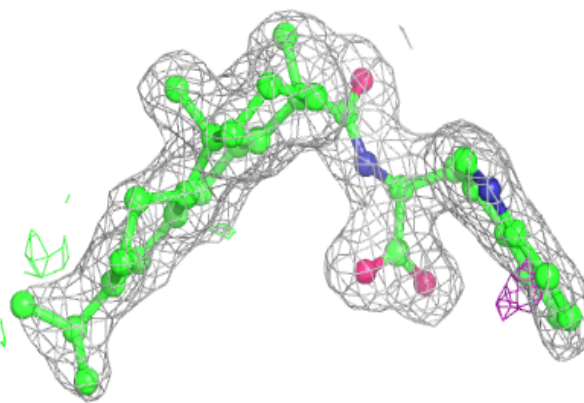
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	OPY	A	501	6/6	0.96	0.08	29,30,32,32	0
4	MNH	C	504	43/43	0.99	0.07	16,17,20,22	0
4	MNH	A	503	43/43	0.99	0.07	16,17,20,24	0

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.



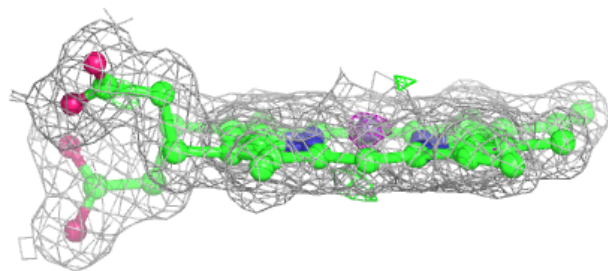
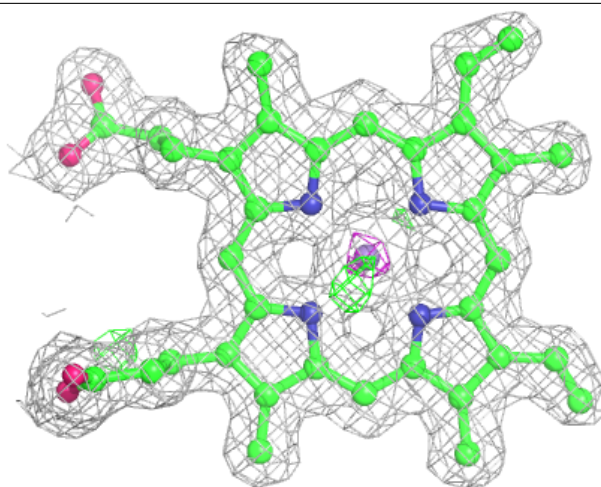
Electron density around WAA A 502:

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



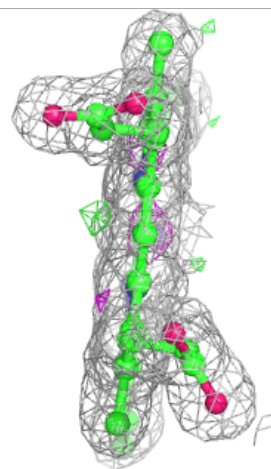
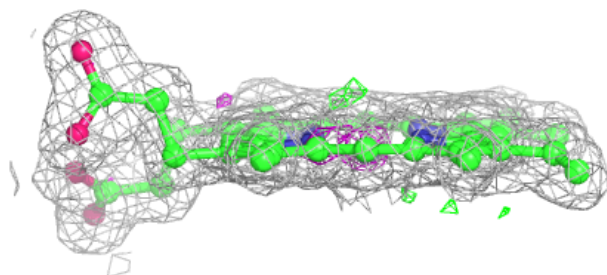
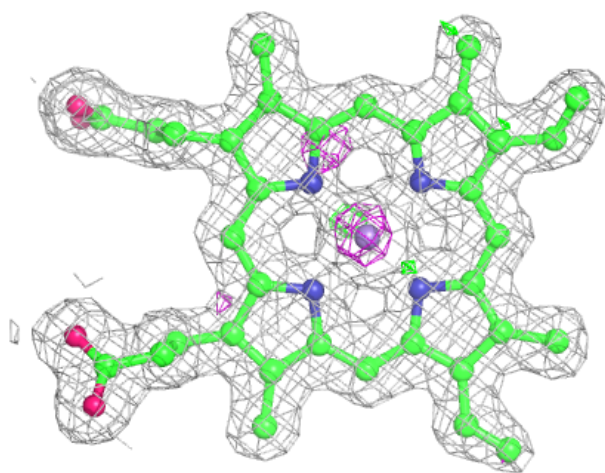
Electron density around MNH C 504:

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



Electron density around MNH A 503:

$2mF_o-DF_c$ (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.