



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 12:21 AM JST

PDB ID : 7WG0 / pdb_00007wg0
Title : Structure of the Manganese Protoporphyrin IX-Reconstituted CYP102A1
Heme Domain with N-palmitoyl-L-phenylalanine
Authors : Keita, O.; Osami, S.; Yuichiro, A.; Hiroshi, S.
Deposited on : 2021-12-27
Resolution : 2.20 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	:	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

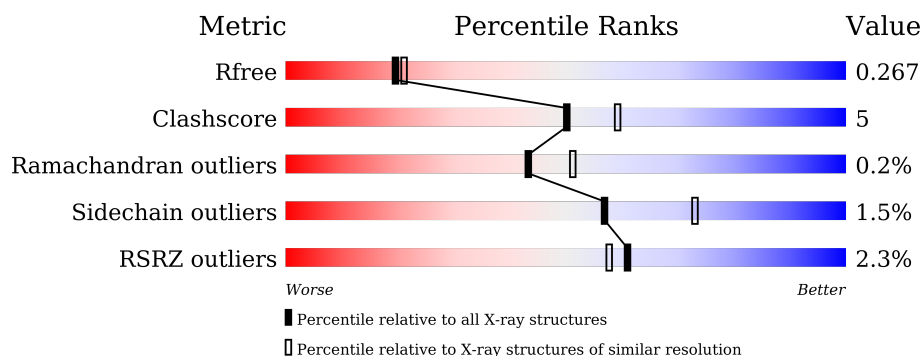
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	483	83% 11% 6%
1	B	483	3% 77% 17% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7835 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	454	Total	C	N	O	S	0	0	0
			3662	2340	622	683	17			
1	B	454	Total	C	N	O	S	0	0	0
			3662	2340	622	683	17			

There are 54 discrepancies between the modelled and reference sequences:

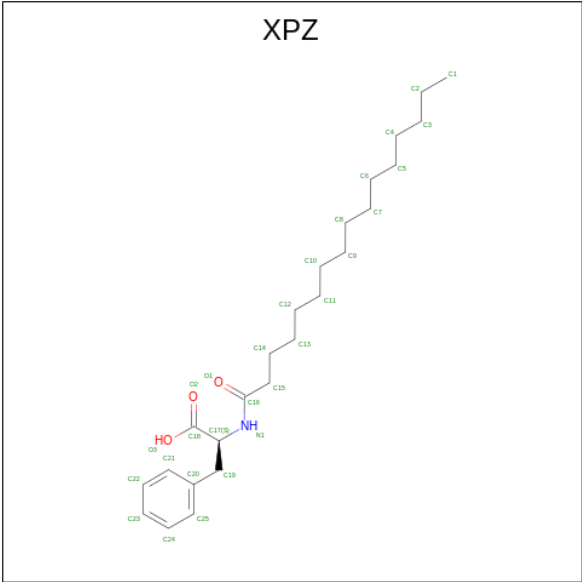
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A1Q8UP87
A	-19	ALA	-	expression tag	UNP A0A1Q8UP87
A	-18	SER	-	expression tag	UNP A0A1Q8UP87
A	-17	HIS	-	expression tag	UNP A0A1Q8UP87
A	-16	HIS	-	expression tag	UNP A0A1Q8UP87
A	-15	HIS	-	expression tag	UNP A0A1Q8UP87
A	-14	HIS	-	expression tag	UNP A0A1Q8UP87
A	-13	HIS	-	expression tag	UNP A0A1Q8UP87
A	-12	HIS	-	expression tag	UNP A0A1Q8UP87
A	-11	SER	-	expression tag	UNP A0A1Q8UP87
A	-10	GLY	-	expression tag	UNP A0A1Q8UP87
A	-9	GLY	-	expression tag	UNP A0A1Q8UP87
A	-8	GLU	-	expression tag	UNP A0A1Q8UP87
A	-7	ASN	-	expression tag	UNP A0A1Q8UP87
A	-6	LEU	-	expression tag	UNP A0A1Q8UP87
A	-5	TYR	-	expression tag	UNP A0A1Q8UP87
A	-4	PHE	-	expression tag	UNP A0A1Q8UP87
A	-3	GLN	-	expression tag	UNP A0A1Q8UP87
A	-2	SER	-	expression tag	UNP A0A1Q8UP87
A	-1	GLY	-	expression tag	UNP A0A1Q8UP87
A	401	PRO	ILE	engineered mutation	UNP A0A1Q8UP87
A	457	LEU	-	expression tag	UNP A0A1Q8UP87
A	458	PRO	-	expression tag	UNP A0A1Q8UP87
A	459	ALA	-	expression tag	UNP A0A1Q8UP87
A	460	THR	-	expression tag	UNP A0A1Q8UP87

Continued on next page...

Continued from previous page...

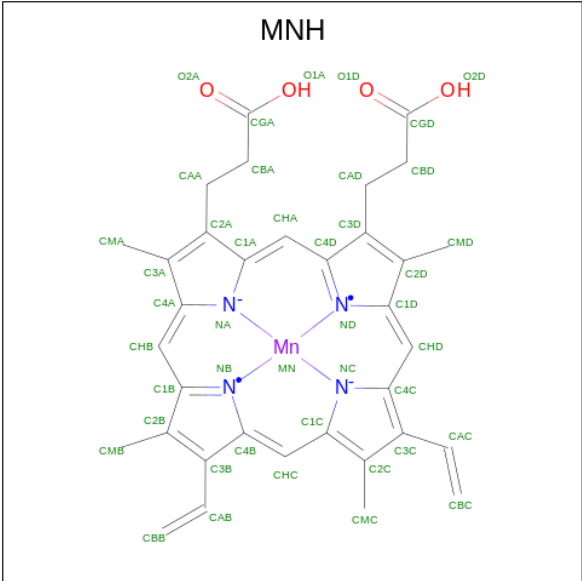
Chain	Residue	Modelled	Actual	Comment	Reference
A	461	GLY	-	expression tag	UNP A0A1Q8UP87
A	462	GLY	-	expression tag	UNP A0A1Q8UP87
B	-20	MET	-	initiating methionine	UNP A0A1Q8UP87
B	-19	ALA	-	expression tag	UNP A0A1Q8UP87
B	-18	SER	-	expression tag	UNP A0A1Q8UP87
B	-17	HIS	-	expression tag	UNP A0A1Q8UP87
B	-16	HIS	-	expression tag	UNP A0A1Q8UP87
B	-15	HIS	-	expression tag	UNP A0A1Q8UP87
B	-14	HIS	-	expression tag	UNP A0A1Q8UP87
B	-13	HIS	-	expression tag	UNP A0A1Q8UP87
B	-12	HIS	-	expression tag	UNP A0A1Q8UP87
B	-11	SER	-	expression tag	UNP A0A1Q8UP87
B	-10	GLY	-	expression tag	UNP A0A1Q8UP87
B	-9	GLY	-	expression tag	UNP A0A1Q8UP87
B	-8	GLU	-	expression tag	UNP A0A1Q8UP87
B	-7	ASN	-	expression tag	UNP A0A1Q8UP87
B	-6	LEU	-	expression tag	UNP A0A1Q8UP87
B	-5	TYR	-	expression tag	UNP A0A1Q8UP87
B	-4	PHE	-	expression tag	UNP A0A1Q8UP87
B	-3	GLN	-	expression tag	UNP A0A1Q8UP87
B	-2	SER	-	expression tag	UNP A0A1Q8UP87
B	-1	GLY	-	expression tag	UNP A0A1Q8UP87
B	401	PRO	ILE	engineered mutation	UNP A0A1Q8UP87
B	457	LEU	-	expression tag	UNP A0A1Q8UP87
B	458	PRO	-	expression tag	UNP A0A1Q8UP87
B	459	ALA	-	expression tag	UNP A0A1Q8UP87
B	460	THR	-	expression tag	UNP A0A1Q8UP87
B	461	GLY	-	expression tag	UNP A0A1Q8UP87
B	462	GLY	-	expression tag	UNP A0A1Q8UP87

- Molecule 2 is (2 {S})-2-(hexadecanoylamino)-3-phenyl-propanoic acid (CCD ID: XPZ) (formula: C₂₅H₄₁NO₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	25	1	3		
2	B	1	Total	C	N	O	0	0
			29	25	1	3		

- Molecule 3 is MANGANESE PROTOPORPHYRIN IX (CCD ID: MNH) (formula: $C_{34}H_{32}MnN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

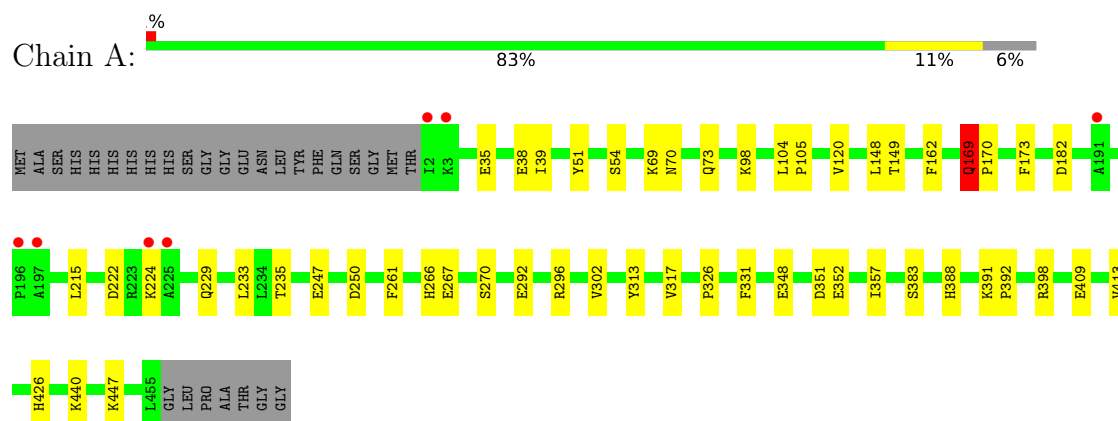
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	203	Total	O	0	0
			203	203		
4	B	164	Total	O	0	0
			164	164		

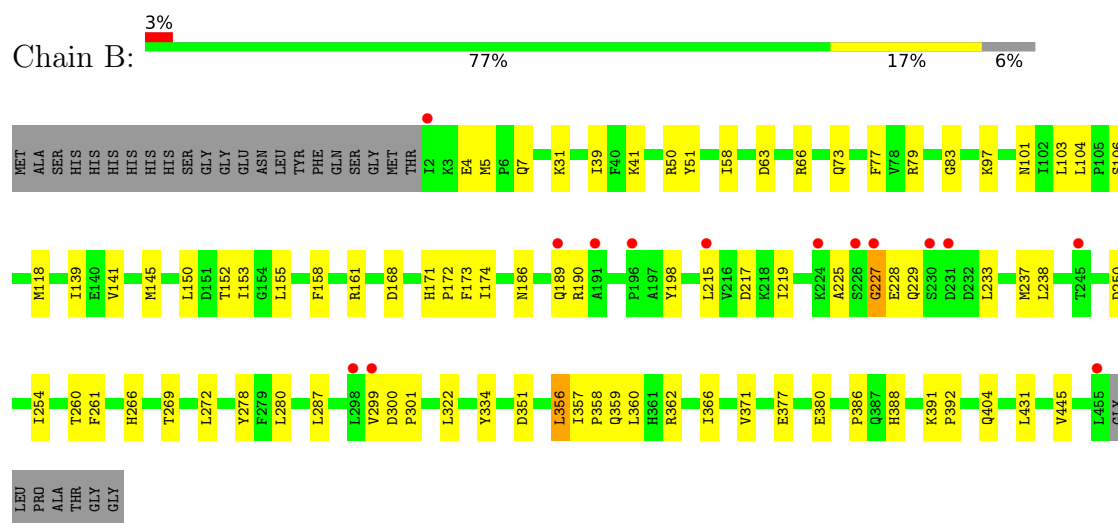
3 Residue-property plots [i](#)

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

- Molecule 1: 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.78Å 127.89Å 148.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.52 – 2.20 48.52 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.52-2.20) 100.0 (48.52-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.208 , 0.267 0.214 , 0.267	Depositor DCC
R_{free} test set	3001 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7835	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6943e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: XPZ, MNH

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	1.10	0/3748	1.47	6/5068 (0.1%)
1	B	1.10	0/3748	1.49	7/5068 (0.1%)
All	All	1.10	0/7496	1.48	13/10136 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	ASP	CA-CB-CG	7.20	119.80	112.60
1	A	169	GLN	CB-CA-C	5.69	117.61	108.91
1	B	152	THR	CA-CB-OG1	-5.69	101.06	109.60
1	A	331	PHE	CA-CB-CG	5.66	119.46	113.80
1	B	168	ASP	N-CA-C	-5.66	106.22	113.23
1	B	217	ASP	O-C-N	5.61	128.07	122.12
1	B	269	THR	CA-C-N	5.50	127.58	120.44
1	B	269	THR	C-N-CA	5.50	127.58	120.44
1	A	222	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	227	GLY	CA-C-O	-5.06	117.69	122.39
1	A	224	LYS	CA-C-N	5.05	127.31	120.65
1	A	224	LYS	C-N-CA	5.05	127.31	120.65
1	A	250	ASP	CA-CB-CG	5.04	117.64	112.60

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	3662	0	3631	26	0
1	B	3662	0	3631	49	0
2	A	29	0	0	0	0
2	B	29	0	0	1	0
3	A	43	0	30	3	0
3	B	43	0	30	1	0
4	A	203	0	0	0	0
4	B	164	0	0	1	0
All	All	7835	0	7322	79	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 5.

All (79) 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:B:63:ASP:OD2	1:B:66:ARG:HD3	1.93	0.69
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.76	0.67
3:A:502:MNH:HBB1	3:A:502:MNH:HMB1	1.79	0.64
1:A:70:ASN:ND2	1:A:352:GLU:OE2	2.29	0.63
1:A:162:PHE:HE1	1:A:215:LEU:HD21	1.64	0.62
1:A:292:GLU:OE1	1:A:296:ARG:NH1	2.33	0.62
1:B:118:MET:HE2	1:B:155:LEU:HG	1.81	0.61
1:B:377:GLU:O	1:B:380:GLU:HG3	2.01	0.60
1:A:38:GLU:HB2	1:A:54:SER:HB3	1.85	0.59
1:B:227:GLY:O	1:B:229:GLN:HG2	2.05	0.57
1:A:409:GLU:O	1:A:413:VAL:HG12	2.05	0.56
1:B:158:PHE:HB3	1:B:219:ILE:CG2	2.38	0.54
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.43	0.53
1:A:98:LYS:HE3	1:A:247:GLU:HB2	1.89	0.53
1:B:189:GLN:HA	1:B:189:GLN:OE1	2.07	0.52
1:A:229:GLN:HA	1:A:235:THR:HG23	1.91	0.52
1:A:120:VAL:HG11	1:A:302:VAL:HG13	1.93	0.51
1:B:5:MET:SD	1:B:50:ARG:HG2	2.51	0.51
1:B:141:VAL:O	1:B:145:MET:HG2	2.11	0.51
1:A:326:PRO:HG3	1:A:357:ILE:HG22	1.96	0.48
1:A:69:LYS:HD3	1:A:398:ARG:CZ	2.43	0.48
1:A:313:TYR:O	1:A:317:VAL:HG23	2.14	0.48
1:B:73:GLN:HG3	1:B:77:PHE:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.94	0.47
1:B:272:LEU:HD13	1:B:322:LEU:HG	1.95	0.47
3:A:502:MNH:HMC1	3:A:502:MNH:HBC1	1.96	0.47
1:B:238:LEU:HD23	1:B:254:ILE:HD13	1.95	0.47
1:B:366:ILE:HD12	1:B:386:PRO:HG2	1.97	0.47
1:B:63:ASP:OD2	1:B:66:ARG:CD	2.60	0.47
1:B:300:ASP:HB3	1:B:301:PRO:CD	2.44	0.47
1:B:97:LYS:HE2	1:B:101:ASN:OD1	2.15	0.46
1:B:260:THR:HA	2:B:501:XPZ:C1	2.46	0.46
1:B:7:GLN:HG3	1:B:41:LYS:O	2.17	0.45
1:B:233:LEU:HD21	1:B:261:PHE:CD2	2.52	0.45
1:B:280:LEU:HD22	1:B:287:LEU:HA	1.98	0.45
1:B:190:ARG:HG2	1:B:198:TYR:CZ	2.52	0.45
1:B:103:LEU:HD21	1:B:237:MET:HG2	1.98	0.44
1:B:362:ARG:HA	1:B:371:VAL:CG2	2.47	0.44
1:B:362:ARG:HA	1:B:371:VAL:HG21	2.00	0.44
1:B:161:ARG:HD3	4:B:655:HOH:O	2.17	0.44
1:B:227:GLY:O	1:B:229:GLN:N	2.50	0.44
1:B:31:LYS:HE3	1:B:31:LYS:HB2	1.69	0.44
1:B:173:PHE:CD1	1:B:215:LEU:HD22	2.53	0.44
1:B:150:LEU:HD22	1:B:174:ILE:CG1	2.48	0.44
1:B:139:ILE:O	1:B:445:VAL:HA	2.17	0.44
1:B:118:MET:HE2	1:B:155:LEU:CG	2.48	0.43
1:A:229:GLN:HA	1:A:235:THR:CG2	2.49	0.43
1:A:267:GLU:O	1:A:270:SER:HB3	2.18	0.43
1:B:300:ASP:N	1:B:300:ASP:OD1	2.50	0.43
1:A:233:LEU:HD21	1:A:261:PHE:CD1	2.53	0.43
1:B:391:LYS:N	1:B:392:PRO:CD	2.81	0.43
1:A:348:GLU:O	1:A:351:ASP:HB2	2.19	0.43
1:B:150:LEU:HD22	1:B:174:ILE:HG13	1.99	0.43
1:B:334:TYR:HA	1:B:351:ASP:O	2.18	0.43
1:B:171:HIS:ND1	1:B:172:PRO:HD2	2.33	0.43
1:B:158:PHE:HB3	1:B:219:ILE:HG23	2.01	0.42
3:B:502:MNH:HBC1	3:B:502:MNH:HMC1	2.01	0.42
1:A:391:LYS:N	1:A:392:PRO:CD	2.82	0.42
1:B:39:ILE:HA	1:B:51:TYR:O	2.19	0.42
1:B:79:ARG:HG3	1:B:83:GLY:O	2.19	0.42
1:B:357:ILE:N	1:B:358:PRO:CD	2.82	0.42
1:B:359:GLN:O	1:B:360:LEU:C	2.63	0.42
1:A:149:THR:C	1:A:266:HIS:HB2	2.45	0.42
1:B:189:GLN:OE1	1:B:189:GLN:CA	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:TYR:CZ	1:B:431:LEU:HB2	2.55	0.42
1:A:426:HIS:CD2	1:A:447:LYS:HE3	2.55	0.42
1:B:104:LEU:HD23	1:B:104:LEU:HA	1.86	0.42
1:A:173:PHE:CD1	1:A:215:LEU:HD22	2.55	0.41
3:A:502:MNH:HBC1	3:A:502:MNH:CMC	2.50	0.41
1:B:58:ILE:HD12	1:B:360:LEU:HD13	2.02	0.41
1:A:169:GLN:HG3	1:A:170:PRO:HD2	2.02	0.41
1:A:267:GLU:OE1	1:A:440:LYS:HE3	2.21	0.41
1:A:39:ILE:HA	1:A:51:TYR:O	2.21	0.41
1:B:300:ASP:HB3	1:B:301:PRO:HD2	2.02	0.40
1:B:174:ILE:HD11	1:B:266:HIS:NE2	2.36	0.40
1:B:153:ILE:HD12	1:B:153:ILE:HA	1.92	0.40
1:B:356:LEU:HD23	1:B:356:LEU:HA	1.99	0.40
1:A:267:GLU:OE1	1:A:440:LYS:CE	2.69	0.40
1:A:104:LEU:N	1:A:105:PRO:CD	2.85	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	452/483 (94%)	426 (94%)	26 (6%)	0	100	100
1	B	452/483 (94%)	437 (97%)	13 (3%)	2 (0%)	30	34
All	All	904/966 (94%)	863 (96%)	39 (4%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	GLU
1	B	225	ALA

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	398/419 (95%)	392 (98%)	6 (2%)	57	73
1	B	398/419 (95%)	392 (98%)	6 (2%)	57	73
All	All	796/838 (95%)	784 (98%)	12 (2%)	57	73

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	73	GLN
1	A	148	LEU
1	A	169	GLN
1	A	182	ASP
1	A	383	SER
1	B	4	GLU
1	B	106	SER
1	B	186	ASN
1	B	299	VAL
1	B	356	LEU
1	B	404	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	73	GLN
1	A	236	HIS
1	A	239	ASN
1	A	285	HIS
1	A	381	ASN
1	B	70	ASN
1	B	109	GLN
1	B	186	ASN
1	B	381	ASN

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 ⓘ

4 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	MNH	B	502	1	46,50,50	2.02	14 (30%)	59,82,82	3.09	26 (44%)
2	XPZ	A	501	-	29,29,29	0.49	0	33,33,33	1.25	4 (12%)
3	MNH	A	502	1	46,50,50	2.09	16 (34%)	59,82,82	2.64	22 (37%)
2	XPZ	B	501	-	29,29,29	0.56	0	33,33,33	1.58	6 (18%)

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	MNH	B	502	1	-	2/14/94/94	-
2	XPZ	A	501	-	-	12/27/27/27	0/1/1/1
3	MNH	A	502	1	-	2/14/94/94	-
2	XPZ	B	501	-	-	13/27/27/27	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	MNH	C2A-C3A	4.68	1.46	1.36
3	B	502	MNH	C3B-C2B	4.30	1.46	1.37
3	A	502	MNH	CHB-C1B	4.20	1.48	1.39
3	B	502	MNH	C3D-C2D	4.18	1.45	1.36
3	B	502	MNH	C1A-C2A	4.10	1.52	1.45
3	A	502	MNH	CHD-C1D	4.00	1.46	1.38
3	B	502	MNH	CHB-C4A	4.00	1.46	1.38
3	A	502	MNH	C4C-NC	3.97	1.45	1.39
3	A	502	MNH	C3B-C2B	3.86	1.45	1.37
3	A	502	MNH	C3D-C2D	3.74	1.44	1.36
3	B	502	MNH	C2A-C3A	3.63	1.44	1.36
3	B	502	MNH	CHB-C1B	3.63	1.47	1.39
3	B	502	MNH	C1A-NA	3.62	1.45	1.39
3	B	502	MNH	CHC-C1C	3.33	1.46	1.39
3	A	502	MNH	CHA-C1A	3.30	1.44	1.38
3	A	502	MNH	C4A-NA	3.09	1.44	1.39
3	A	502	MNH	C1C-NC	2.76	1.43	1.39
3	B	502	MNH	C4A-NA	2.65	1.43	1.39
3	B	502	MNH	CHA-C1A	2.64	1.43	1.38
3	A	502	MNH	CHB-C4A	2.61	1.43	1.38
3	A	502	MNH	CHC-C4B	2.58	1.43	1.38
3	A	502	MNH	C1A-NA	2.43	1.43	1.39
3	B	502	MNH	CHC-C4B	2.43	1.43	1.38
3	B	502	MNH	CHD-C1D	2.39	1.43	1.38
3	A	502	MNH	CHC-C1C	2.39	1.44	1.39
3	A	502	MNH	C1D-C2D	2.35	1.49	1.44
3	A	502	MNH	CHA-C4D	2.30	1.44	1.39
3	B	502	MNH	C4A-C3A	2.28	1.49	1.45
3	B	502	MNH	CHD-C4C	2.23	1.44	1.39
3	A	502	MNH	CBD-CGD	2.06	1.55	1.50

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	MNH	C3D-C4D-ND	7.69	115.73	109.79
3	B	502	MNH	C3B-C2B-C1B	-7.67	100.80	106.49
3	B	502	MNH	C2D-C1D-ND	7.47	116.99	109.84
3	B	502	MNH	C3A-C4A-NA	7.46	116.28	109.94
3	A	502	MNH	C3D-C4D-ND	7.39	115.49	109.79
3	B	502	MNH	C2A-C1A-NA	7.24	115.52	110.02
3	A	502	MNH	C2C-C1C-NC	7.21	119.02	109.89
3	B	502	MNH	C2C-C1C-NC	6.07	117.57	109.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	MNH	C3B-C2B-C1B	-5.87	102.13	106.49
3	B	502	MNH	C2B-C1B-NB	5.49	116.15	109.88
3	A	502	MNH	C2A-C1A-NA	5.42	114.13	110.02
3	A	502	MNH	C3A-C4A-NA	5.12	114.29	109.94
3	A	502	MNH	C3C-C2C-C1C	-4.34	101.92	107.16
3	A	502	MNH	C4B-C3B-C2B	-4.24	103.75	107.11
3	B	502	MNH	C3C-C2C-C1C	-4.15	102.16	107.16
3	A	502	MNH	C2B-C1B-NB	3.93	114.37	109.88
3	B	502	MNH	CHB-C1B-C2B	-3.83	119.00	124.98
3	A	502	MNH	C2D-C1D-ND	3.79	113.47	109.84
3	B	502	MNH	CHB-C4A-NA	-3.61	120.55	124.40
3	B	502	MNH	C4B-C3B-C2B	-3.56	104.29	107.11
2	B	501	XPZ	C19-C17-C18	3.55	118.98	110.42
3	A	502	MNH	CHA-C4D-ND	-3.46	121.54	124.47
3	B	502	MNH	O2A-CGA-CBA	-3.33	112.38	123.08
2	B	501	XPZ	C18-C17-N1	3.31	118.39	110.55
3	B	502	MNH	C1D-C2D-C3D	-3.18	103.61	106.96
2	B	501	XPZ	C20-C19-C17	3.13	122.01	113.39
3	A	502	MNH	CAD-C3D-C4D	3.12	130.11	124.66
3	B	502	MNH	O1D-CGD-CBD	-3.07	113.22	123.08
3	B	502	MNH	CMD-C2D-C1D	3.05	129.68	125.04
2	B	501	XPZ	C21-C20-C25	3.05	122.96	118.17
3	A	502	MNH	CHB-C1B-C2B	-2.96	120.36	124.98
3	A	502	MNH	CMB-C2B-C1B	2.85	129.39	125.04
2	A	501	XPZ	O3-C18-C17	2.85	122.87	113.40
3	A	502	MNH	CMA-C3A-C4A	2.81	129.66	124.71
3	B	502	MNH	CHA-C1A-NA	-2.81	121.41	124.40
3	B	502	MNH	C1A-C2A-C3A	-2.80	103.48	107.13
2	B	501	XPZ	O3-C18-C17	2.79	122.69	113.40
3	B	502	MNH	CAA-C2A-C1A	2.77	130.12	124.89
3	A	502	MNH	CHC-C1C-C2C	-2.77	119.43	127.24
3	B	502	MNH	CAD-C3D-C4D	2.72	129.42	124.66
3	A	502	MNH	CAA-C2A-C1A	2.64	129.87	124.89
3	A	502	MNH	CMD-C2D-C1D	2.59	128.99	125.04
2	B	501	XPZ	C19-C20-C21	-2.57	115.80	120.91
3	B	502	MNH	CHD-C1D-C2D	-2.57	119.59	126.73
3	B	502	MNH	CHA-C4D-C3D	-2.52	121.13	124.84
3	B	502	MNH	O1A-CGA-CBA	2.45	121.91	114.03
3	B	502	MNH	C4C-CHD-C1D	-2.45	120.53	126.34
3	A	502	MNH	O1D-CGD-CBD	-2.45	115.21	123.08
3	B	502	MNH	O2D-CGD-CBD	2.37	121.64	114.03
3	A	502	MNH	CBA-CAA-C2A	-2.33	106.15	112.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	XPZ	C18-C17-N1	2.33	116.07	110.55
3	A	502	MNH	CHC-C4B-C3B	-2.32	117.71	126.11
2	A	501	XPZ	C20-C19-C17	2.18	119.39	113.39
3	B	502	MNH	CHC-C1C-C2C	-2.17	121.09	127.24
2	A	501	XPZ	C14-C15-C16	-2.16	107.19	113.26
3	A	502	MNH	O2A-CGA-CBA	-2.08	116.40	123.08
3	A	502	MNH	CHB-C4A-NA	-2.04	122.23	124.40
3	B	502	MNH	CMB-C2B-C3B	2.03	133.28	128.30

There are no chirality outliers.

All (29) torsion outliers are listed below:

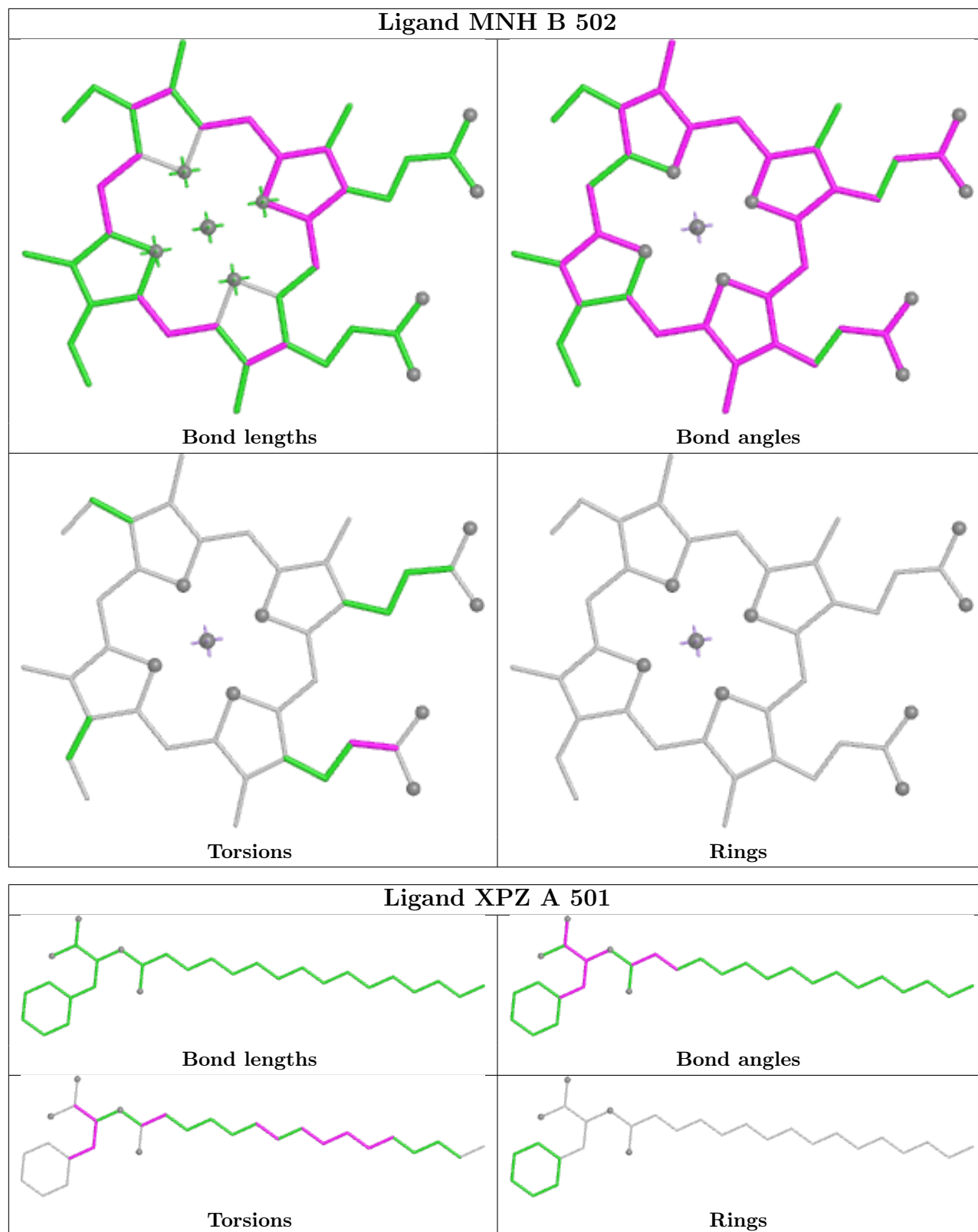
Mol	Chain	Res	Type	Atoms
2	A	501	XPZ	C7-C8-C9-C10
2	B	501	XPZ	N1-C17-C19-C20
2	B	501	XPZ	C13-C14-C15-C16
2	B	501	XPZ	C6-C7-C8-C9
2	A	501	XPZ	C6-C7-C8-C9
2	A	501	XPZ	C4-C5-C6-C7
2	A	501	XPZ	C9-C10-C11-C12
2	B	501	XPZ	C4-C5-C6-C7
2	B	501	XPZ	C18-C17-C19-C20
2	A	501	XPZ	C5-C6-C7-C8
2	A	501	XPZ	C17-C19-C20-C21
2	A	501	XPZ	C17-C19-C20-C25
2	B	501	XPZ	C17-C19-C20-C21
2	B	501	XPZ	C17-C19-C20-C25
2	A	501	XPZ	C19-C17-C18-O2
2	B	501	XPZ	C19-C17-C18-O3
2	A	501	XPZ	C19-C17-C18-O3
2	B	501	XPZ	C19-C17-C18-O2
2	B	501	XPZ	C14-C15-C16-N1
3	B	502	MNH	CAD-CBD-CGD-O1D
3	A	502	MNH	CAD-CBD-CGD-O1D
2	A	501	XPZ	N1-C17-C19-C20
3	B	502	MNH	CAD-CBD-CGD-O2D
3	A	502	MNH	CAD-CBD-CGD-O2D
2	B	501	XPZ	C11-C12-C13-C14
2	B	501	XPZ	C14-C15-C16-O1
2	B	501	XPZ	C7-C8-C9-C10
2	A	501	XPZ	C14-C15-C16-N1
2	A	501	XPZ	C14-C15-C16-O1

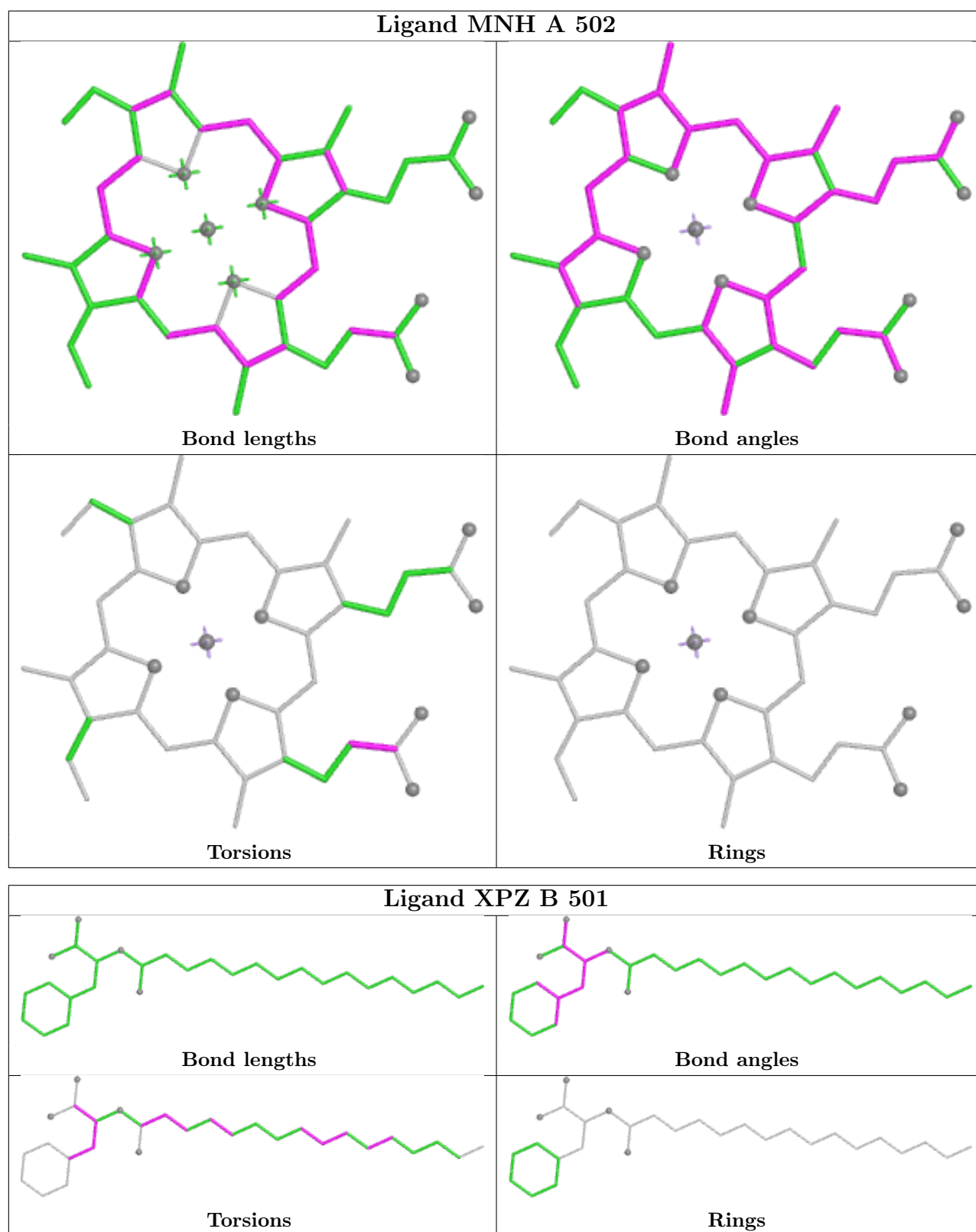
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	MNH	1	0
3	A	502	MNH	3	0
2	B	501	XPZ	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.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	454/483 (93%)	-0.20	7 (1%) 72 69	22, 33, 65, 93	0
1	B	454/483 (93%)	-0.04	14 (3%) 51 48	20, 34, 66, 100	0
All	All	908/966 (93%)	-0.12	21 (2%) 61 58	20, 33, 66, 100	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	4.1
1	B	2	ILE	4.0
1	A	196	PRO	2.9
1	B	230	SER	2.9
1	B	189	GLN	2.9
1	B	191	ALA	2.8
1	B	227	GLY	2.8
1	B	215	LEU	2.5
1	B	226	SER	2.4
1	A	224	LYS	2.3
1	A	191	ALA	2.3
1	B	455	LEU	2.2
1	B	224	LYS	2.2
1	B	231	ASP	2.2
1	B	196	PRO	2.2
1	B	298	LEU	2.2
1	B	299	VAL	2.2
1	A	225	ALA	2.2
1	A	3	LYS	2.1
1	B	245	THR	2.1
1	A	197	ALA	2.1

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](#)

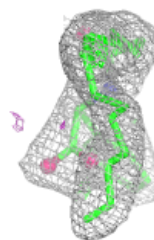
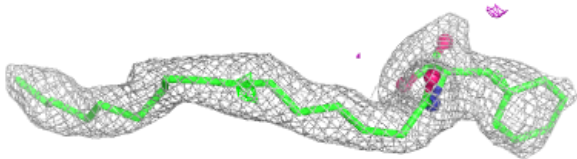
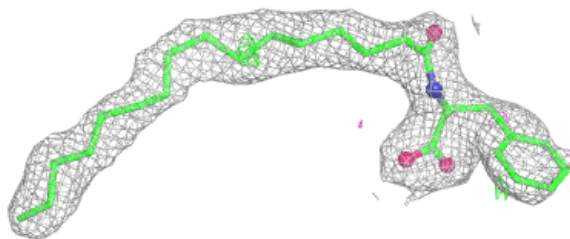
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XPZ	A	501	29/29	0.92	0.11	34,41,51,53	0
2	XPZ	B	501	29/29	0.92	0.13	39,44,52,53	0
3	MNH	A	502	43/43	0.98	0.06	24,26,27,30	0
3	MNH	B	502	43/43	0.99	0.05	19,20,21,22	0

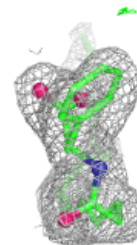
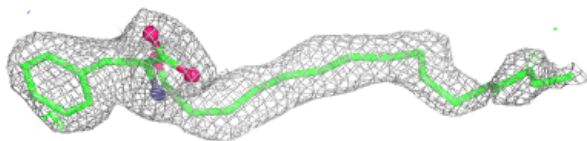
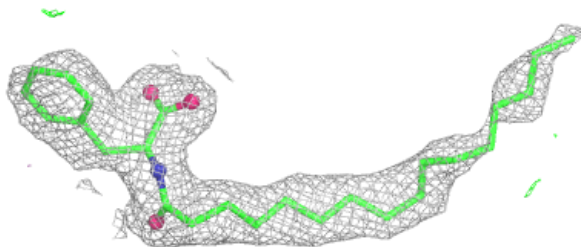
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XPZ A 501:

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

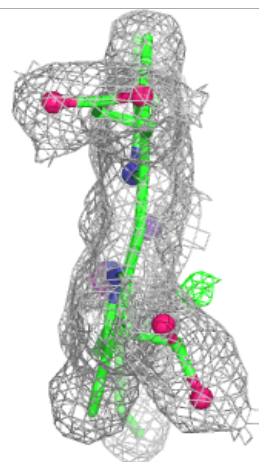
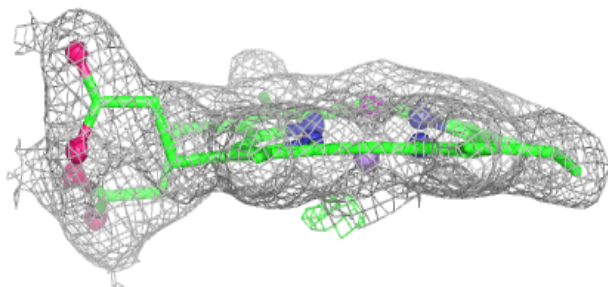
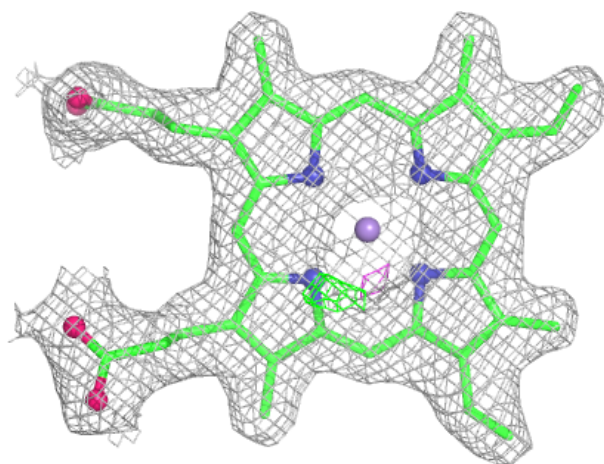
**Electron density around XPZ B 501:**

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



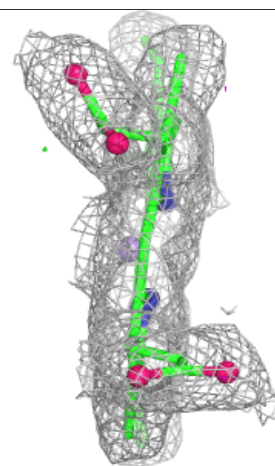
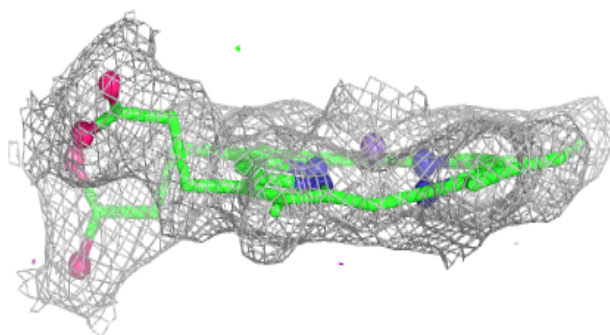
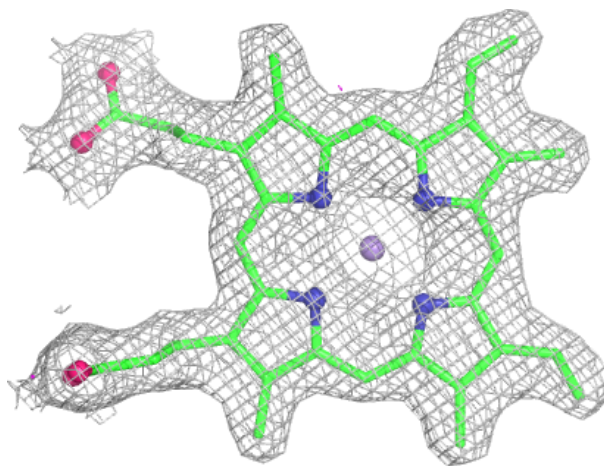
Electron density around MNH A 502:

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



Electron density around MNH B 502:

$2mF_o-DF_c$ (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.