



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 04:58 AM EDT

PDB ID : 6PM7
Title : The structure of the triclinic crystal form of beef liver catalase at 1.85 Å resolution
Authors : McPherson, A.
Deposited on : 2019-07-01
Resolution : 1.85 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

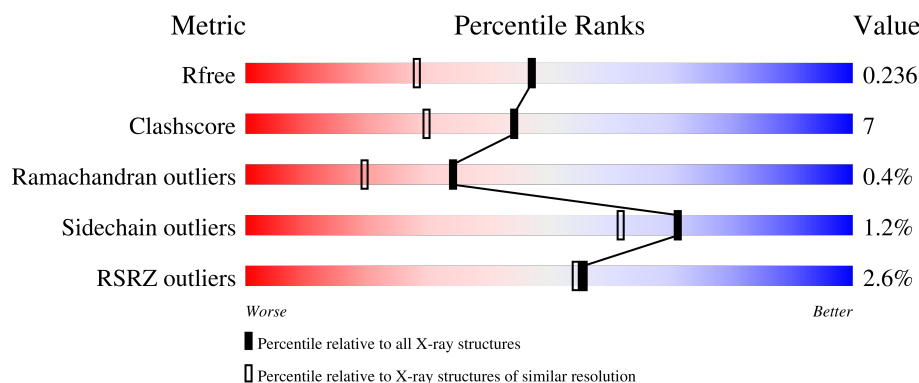
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	527	
1	B	527	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16696 atoms, of which 7783 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 Catalase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	498	Total	C	H	N	O	S	0	0	0
			7842	2543	3834	714	737	14			
1	B	498	Total	C	H	N	O	S	0	1	0
			7848	2545	3837	714	737	15			

There are 4 discrepancies between the modelled and reference sequences:

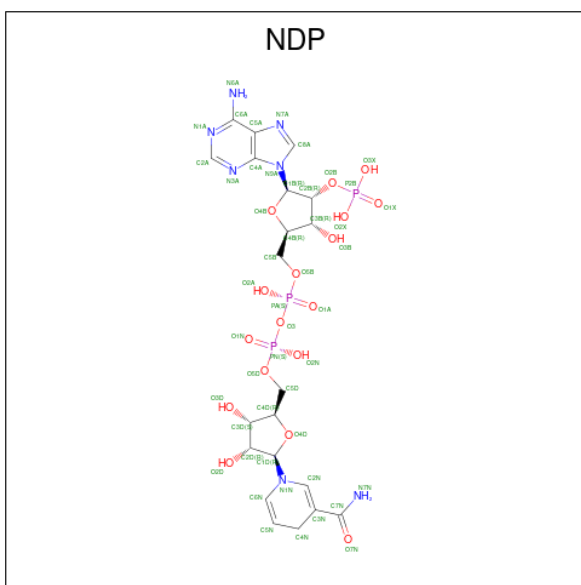
Chain	Residue	Modelled	Actual	Comment	Reference
A	212	ASP	ASN	engineered mutation	UNP P00432
A	225	ASP	ASN	engineered mutation	UNP P00432
B	212	ASP	ASN	engineered mutation	UNP P00432
B	225	ASP	ASN	engineered mutation	UNP P00432

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
2	B	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0
3	B	1	Total 74	C 21	H 26	N 7	O 17	P 3	0	0

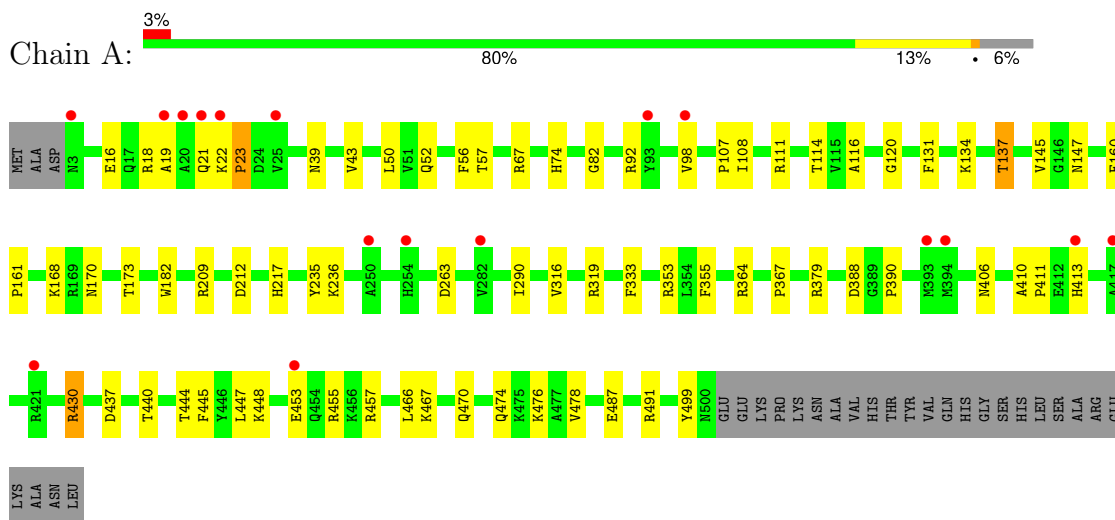
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	295	Total O 295 295	0	0
4	B	413	Total O 417 417	0	4

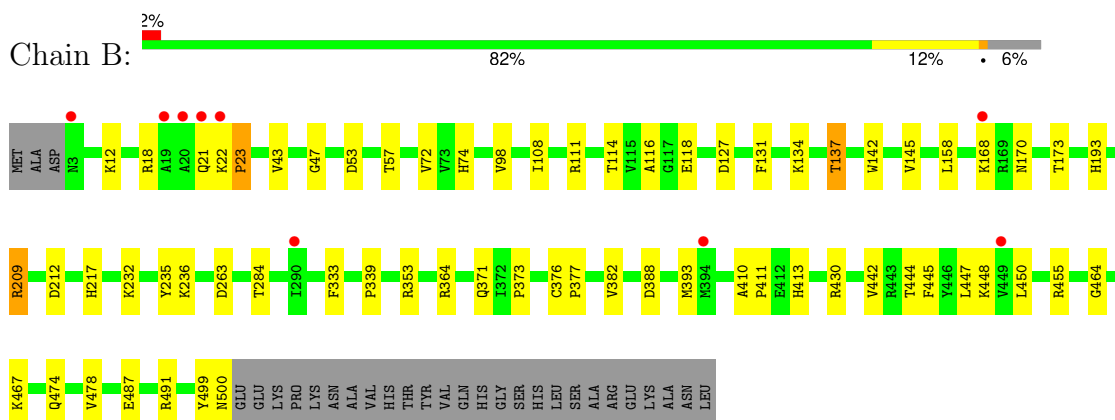
3 Residue-property plots [i](#)

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: Catalase



• Molecule 1: Catalase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.87Å 140.87Å 101.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	121.99 – 1.85 121.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.5 (121.99-1.85) 98.5 (121.99-1.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.192 , 0.232 0.204 , 0.236	Depositor DCC
R_{free} test set	4940 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16696	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: NDP, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	0/4128	0.76	1/5607 (0.0%)
1	B	0.66	0/4134	0.78	2/5616 (0.0%)
All	All	0.65	0/8262	0.77	3/11223 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	B	209	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	111	ARG	NE-CZ-NH2	-6.11	117.25	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ARG	Mainchain
1	A	430	ARG	Sidechain
1	B	430	ARG	Sidechain

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	4008	3834	3833	53	0
1	B	4011	3837	3838	56	0
2	A	43	30	30	4	0
2	B	43	30	30	4	0
3	A	48	26	26	1	0
3	B	48	26	26	0	0
4	A	295	0	0	9	0
4	B	417	0	0	6	0
All	All	8913	7783	7783	105	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 7.

All (105) 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:170:ASN:HB3	1:A:173:THR:OG1	1.69	0.91
1:B:467:LYS:HD2	1:B:499:TYR:CD1	2.12	0.84
1:A:476:LYS:HE3	4:A:903:HOH:O	1.79	0.82
1:B:284:THR:HG22	4:B:887:HOH:O	1.80	0.81
1:A:57:THR:HG21	4:A:744:HOH:O	1.86	0.75
1:B:98:VAL:CG2	1:B:137:THR:HG21	2.17	0.75
1:A:21:GLN:O	1:A:22:LYS:HB2	1.88	0.74
1:A:430:ARG:HH22	1:B:53:ASP:CG	1.94	0.71
1:B:170:ASN:HB3	1:B:173:THR:OG1	1.93	0.67
1:B:22:LYS:O	1:B:23:PRO:O	2.14	0.66
1:A:476:LYS:CE	4:A:903:HOH:O	2.39	0.65
1:A:430:ARG:NH2	1:B:53:ASP:CG	2.50	0.65
1:A:470:GLN:OE1	1:B:12:LYS:HE2	1.96	0.65
1:B:98:VAL:CG2	1:B:137:THR:CG2	2.75	0.65
1:B:371:GLN:OE1	1:B:393:MET:HB2	1.99	0.62
1:B:98:VAL:HG22	1:B:137:THR:CG2	2.28	0.62
1:B:487:GLU:OE2	1:B:491:ARG:NH2	2.32	0.61
2:B:601:HEM:HBB2	2:B:601:HEM:HMB2	1.83	0.61
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:NH2	1:B:53:ASP:OD2	2.35	0.60
1:A:52:GLN:NE2	4:A:705:HOH:O	2.34	0.59
1:B:21:GLN:O	1:B:22:LYS:HB2	2.02	0.58
1:B:464:GLY:O	1:B:467:LYS:HE3	2.03	0.58
1:A:487:GLU:OE2	1:A:491:ARG:NH2	2.36	0.58
1:B:284:THR:CG2	4:B:887:HOH:O	2.48	0.58
1:B:232:LYS:HD3	4:B:1055:HOH:O	2.03	0.57
2:A:601:HEM:HBC2	2:A:601:HEM:CMC	2.35	0.57
1:B:98:VAL:HG23	4:B:982:HOH:O	2.04	0.56
1:B:209:ARG:HD3	1:B:263:ASP:OD1	2.05	0.56
1:A:319:ARG:NH1	4:A:708:HOH:O	2.38	0.56
1:A:120:GLY:CA	1:B:118:GLU:HG2	2.36	0.56
1:A:67:ARG:HH21	1:B:168:LYS:HE3	1.72	0.54
1:A:406:ASN:HD21	1:A:410:ALA:HB3	1.73	0.54
1:A:430:ARG:NH2	1:B:53:ASP:OD1	2.41	0.54
1:B:18:ARG:HG2	1:B:21:GLN:OE1	2.07	0.54
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.90	0.53
1:A:92:ARG:HG2	4:A:813:HOH:O	2.07	0.53
1:A:107:PRO:HG2	1:A:379:ARG:HD2	1.91	0.52
2:B:601:HEM:HBB2	2:B:601:HEM:CMB	2.39	0.52
1:A:22:LYS:O	1:A:23:PRO:C	2.48	0.52
1:B:22:LYS:O	1:B:23:PRO:C	2.48	0.52
1:B:98:VAL:HG22	1:B:137:THR:HG22	1.93	0.51
1:B:18:ARG:CG	1:B:21:GLN:OE1	2.59	0.50
1:A:209:ARG:HB2	4:A:758:HOH:O	2.12	0.50
1:A:355:PHE:CZ	1:B:57:THR:HG23	2.47	0.50
2:B:601:HEM:CMC	2:B:601:HEM:HBC2	2.42	0.50
1:A:98:VAL:HG22	1:A:137:THR:HG21	1.94	0.50
1:B:72:VAL:O	1:B:168:LYS:HE3	2.12	0.49
1:B:444:THR:O	1:B:448:LYS:HB2	2.12	0.49
1:A:147:ASN:ND2	2:A:601:HEM:CAC	2.76	0.49
1:A:437:ASP:OD2	1:A:440:THR:OG1	2.28	0.48
1:A:39:ASN:C	1:B:158:LEU:HD12	2.34	0.48
1:B:98:VAL:HG21	1:B:137:THR:HG21	1.96	0.47
1:A:56:PHE:HB2	1:B:158:LEU:HD21	1.95	0.47
1:A:16:GLU:O	1:A:19:ALA:HB2	2.14	0.47
1:A:74:HIS:HA	1:A:114:THR:O	2.15	0.47
1:B:410:ALA:HB1	1:B:411:PRO:CD	2.45	0.47
1:B:21:GLN:O	1:B:22:LYS:CB	2.63	0.46
1:B:108:ILE:HA	1:B:134:LYS:O	2.16	0.46
1:B:467:LYS:HD2	1:B:499:TYR:CE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:HG2	1:B:21:GLN:CD	2.35	0.46
1:A:467:LYS:HD2	1:A:499:TYR:CD1	2.51	0.46
1:A:82:GLY:HA3	1:A:316:VAL:O	2.15	0.46
1:A:474:GLN:O	1:A:478:VAL:HG23	2.16	0.46
1:A:57:THR:HG22	4:A:981:HOH:O	2.15	0.46
1:B:467:LYS:HD2	1:B:499:TYR:CG	2.48	0.46
2:A:601:HEM:CMB	2:A:601:HEM:HBB2	2.46	0.45
1:A:410:ALA:HB1	1:A:411:PRO:CD	2.47	0.45
1:B:217:HIS:CD2	1:B:353:ARG:HH11	2.35	0.44
1:B:18:ARG:HD3	1:B:21:GLN:OE1	2.17	0.44
1:B:74:HIS:HA	1:B:114:THR:O	2.17	0.44
1:B:474:GLN:O	1:B:478:VAL:HG23	2.17	0.44
1:A:145:VAL:HG22	1:A:333:PHE:HB3	1.99	0.44
1:B:142:TRP:HB2	1:B:339:PRO:HD3	1.99	0.44
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	2.00	0.44
1:A:108:ILE:HA	1:A:134:LYS:O	2.18	0.43
1:A:217:HIS:CD2	1:A:353:ARG:HH11	2.36	0.43
1:A:453:GLU:HB3	1:A:457:ARG:HH21	1.84	0.43
1:B:116:ALA:HA	1:B:168:LYS:HZ3	1.83	0.43
1:B:373:PRO:HA	1:B:376[B]:CYS:SG	2.58	0.43
1:A:445:PHE:HB2	3:A:602:NDP:O2D	2.19	0.43
1:A:447:LEU:O	1:A:455:ARG:NH2	2.51	0.43
1:A:22:LYS:O	1:A:23:PRO:O	2.37	0.43
1:A:116:ALA:O	1:A:168:LYS:NZ	2.46	0.42
1:A:98:VAL:CG2	1:A:137:THR:HG21	2.50	0.42
1:B:445:PHE:CZ	1:B:450:LEU:HD21	2.54	0.42
1:B:193:HIS:HA	1:B:442:VAL:HG22	2.00	0.42
1:A:367:PRO:HG2	1:A:390:PRO:HG2	2.02	0.42
1:B:43:VAL:O	1:B:47:GLY:HA3	2.20	0.42
1:A:367:PRO:HG2	1:A:390:PRO:CG	2.49	0.42
1:B:364:ARG:HD2	4:B:812:HOH:O	2.20	0.42
1:B:377:PRO:HG2	1:B:382:VAL:CG2	2.50	0.42
1:B:447:LEU:O	1:B:455:ARG:NH2	2.53	0.42
1:A:98:VAL:HG22	1:A:137:THR:CG2	2.49	0.41
1:A:43:VAL:HG23	1:A:50:LEU:HD21	2.02	0.41
1:B:474:GLN:OE1	1:B:500:ASN:ND2	2.49	0.41
1:B:21:GLN:HG3	4:B:1065:HOH:O	2.21	0.41
1:A:209:ARG:HD3	1:A:263:ASP:OD2	2.21	0.41
1:B:145:VAL:HG22	1:B:333:PHE:HB3	2.02	0.41
1:A:120:GLY:HA3	1:B:118:GLU:HG2	2.02	0.41
1:A:212:ASP:OD1	1:A:236:LYS:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ARG:HD2	4:A:815:HOH:O	2.21	0.40
1:A:182:TRP:CD2	1:A:466:LEU:HD13	2.56	0.40
1:B:212:ASP:OD1	1:B:236:LYS:HA	2.22	0.40
1:A:444:THR:O	1:A:448:LYS:HB2	2.21	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	496/527 (94%)	474 (96%)	20 (4%)	2 (0%)	34	19
1	B	497/527 (94%)	480 (97%)	15 (3%)	2 (0%)	34	19
All	All	993/1054 (94%)	954 (96%)	35 (4%)	4 (0%)	34	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ASP
1	B	23	PRO
1	B	388	ASP
1	A	23	PRO

5.3.2 Protein sidechains [i](#)

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	430/454 (95%)	425 (99%)	5 (1%)	71	62
1	B	431/454 (95%)	426 (99%)	5 (1%)	71	62
All	All	861/908 (95%)	851 (99%)	10 (1%)	71	62

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	PHE
1	A	137	THR
1	A	235	TYR
1	A	290	ILE
1	A	413	HIS
1	B	127	ASP
1	B	131	PHE
1	B	137	THR
1	B	235	TYR
1	B	413	HIS

Sometimes 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 ⓘ

There are no monosaccharides 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	NDP	A	602	-	47,52,52	0.81	2 (4%)	61,80,80	0.72	1 (1%)
2	HEM	A	601	1	42,50,50	1.24	5 (11%)	46,82,82	1.82	14 (30%)
2	HEM	B	601	1	42,50,50	1.29	5 (11%)	46,82,82	2.23	14 (30%)
3	NDP	B	602	-	47,52,52	0.76	1 (2%)	61,80,80	0.80	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	A	602	-	-	12/30/77/77	0/5/5/5
2	HEM	A	601	1	-	2/12/54/54	-
2	HEM	B	601	1	-	2/12/54/54	-
3	NDP	B	602	-	-	6/30/77/77	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C4D-ND	-3.93	1.33	1.40
2	A	601	HEM	C1B-NB	-3.20	1.34	1.40
2	B	601	HEM	CHB-C1B	2.96	1.41	1.34
2	A	601	HEM	C4D-ND	-2.67	1.35	1.40
2	B	601	HEM	C1B-NB	-2.58	1.35	1.40
2	B	601	HEM	C1D-ND	-2.53	1.33	1.38
3	A	602	NDP	PN-O3	2.47	1.62	1.59
2	A	601	HEM	CHA-C4D	2.40	1.40	1.34
2	A	601	HEM	C4B-NB	-2.19	1.34	1.38
3	A	602	NDP	PA-O3	2.19	1.61	1.59
3	B	602	NDP	PA-O3	2.19	1.61	1.59
2	A	601	HEM	CHB-C1B	2.15	1.39	1.34
2	B	601	HEM	C4B-NB	-2.05	1.34	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	HEM	CHC-C4B-NB	7.20	132.18	124.44
2	B	601	HEM	C1B-NB-C4B	5.21	111.38	105.21
2	A	601	HEM	CHC-C4B-NB	4.75	129.54	124.44
2	B	601	HEM	CHD-C1D-ND	4.51	129.28	124.44
2	B	601	HEM	C3B-C4B-NB	-4.44	106.28	109.47
2	A	601	HEM	CHD-C1D-ND	4.35	129.12	124.44
2	B	601	HEM	CAD-C3D-C4D	3.64	131.04	124.70
2	B	601	HEM	CHD-C1D-C2D	-3.57	119.39	125.03
3	B	602	NDP	P2B-O2B-C2B	-3.32	114.56	123.43
2	B	601	HEM	O2D-CGD-CBD	3.25	124.27	114.00
2	A	601	HEM	CHD-C1D-C2D	-3.25	119.90	125.03
2	A	601	HEM	CHA-C4D-ND	3.11	128.23	124.37
2	A	601	HEM	CBA-CAA-C2A	-3.06	107.39	112.54
2	B	601	HEM	CHB-C1B-NB	3.01	128.10	124.37
2	A	601	HEM	C1B-NB-C4B	3.00	108.76	105.21
2	A	601	HEM	CHB-C1B-NB	2.81	127.86	124.37
2	B	601	HEM	CHA-C4D-ND	2.74	127.77	124.37
2	A	601	HEM	CAD-C3D-C4D	2.71	129.41	124.70
2	A	601	HEM	O2D-CGD-CBD	2.61	122.26	114.00
2	B	601	HEM	CAD-C3D-C2D	-2.56	123.08	127.87
2	B	601	HEM	C4A-C3A-C2A	2.36	108.64	107.00
3	B	602	NDP	C5A-C6A-N6A	2.29	123.80	120.31
2	A	601	HEM	CHA-C4D-C3D	-2.18	121.20	125.23
2	A	601	HEM	CMC-C2C-C3C	2.15	128.98	124.68
2	A	601	HEM	C3B-C4B-NB	-2.14	107.93	109.47
2	A	601	HEM	O2A-CGA-O1A	-2.11	117.90	123.33
2	B	601	HEM	CHA-C4D-C3D	-2.09	121.38	125.23
3	A	602	NDP	P2B-O2B-C2B	-2.09	117.86	123.43
2	A	601	HEM	O1D-CGD-CBD	-2.04	116.64	123.09
2	B	601	HEM	CHC-C4B-C3B	-2.02	121.48	124.57
2	B	601	HEM	O1D-CGD-CBD	-2.02	116.70	123.09

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NDP	C5B-O5B-PA-O1A
3	A	602	NDP	C5B-O5B-PA-O3
3	A	602	NDP	C5D-O5D-PN-O3
3	A	602	NDP	C5D-O5D-PN-O1N
3	B	602	NDP	C5D-O5D-PN-O1N
3	B	602	NDP	C2N-C3N-C7N-N7N
3	A	602	NDP	C1B-C2B-O2B-P2B

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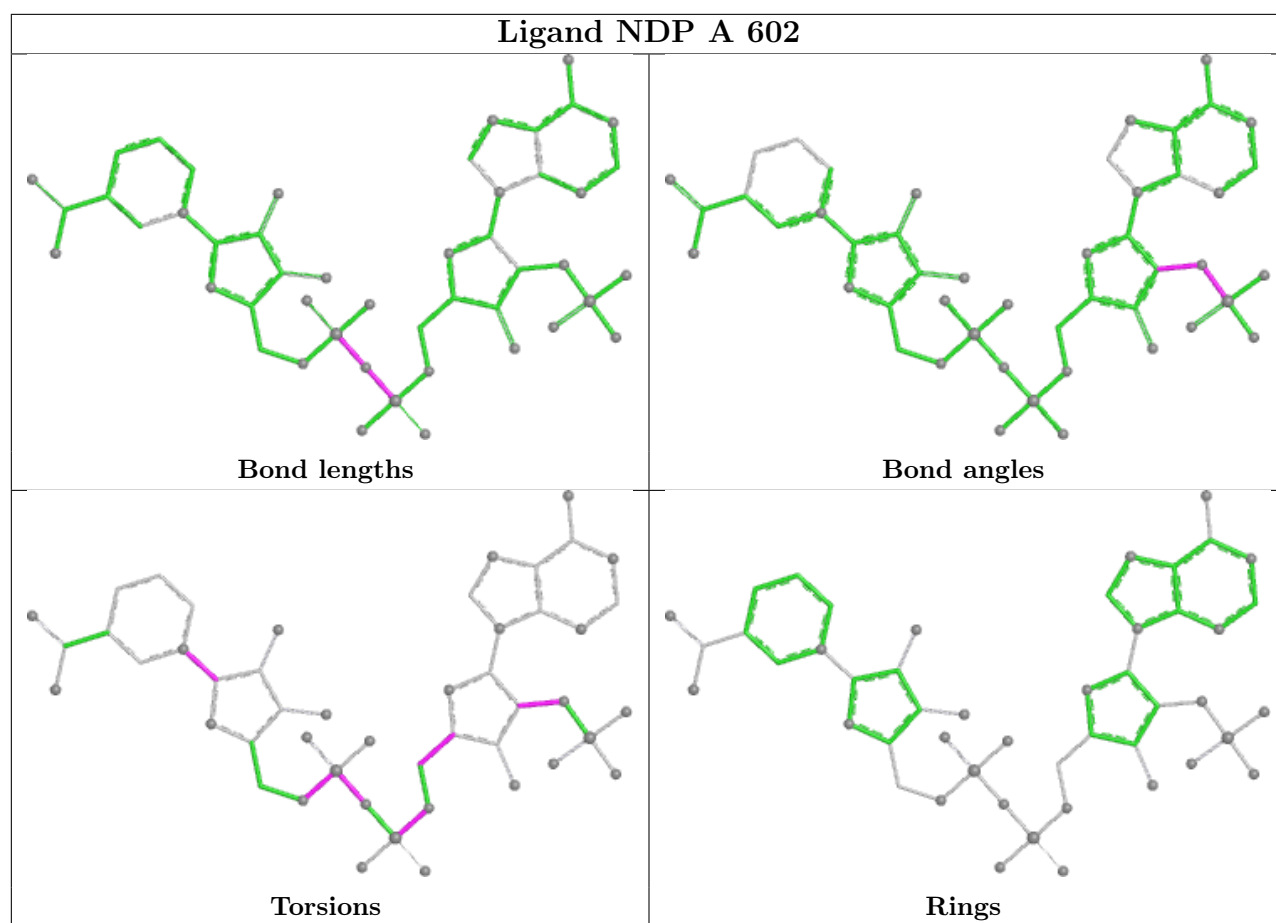
Mol	Chain	Res	Type	Atoms
3	A	602	NDP	C3B-C2B-O2B-P2B
3	A	602	NDP	O4B-C4B-C5B-O5B
3	A	602	NDP	C3B-C4B-C5B-O5B
3	A	602	NDP	PA-O3-PN-O2N
3	A	602	NDP	O4D-C1D-N1N-C6N
3	B	602	NDP	O4D-C1D-N1N-C6N
3	A	602	NDP	C5B-O5B-PA-O2A
3	B	602	NDP	C2B-O2B-P2B-O3X
2	A	601	HEM	CAD-CBD-CGD-O2D
2	A	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	CAD-CBD-CGD-O1D
2	B	601	HEM	CAD-CBD-CGD-O2D
3	A	602	NDP	PA-O3-PN-O1N
3	B	602	NDP	PA-O3-PN-O1N
3	B	602	NDP	PA-O3-PN-O2N

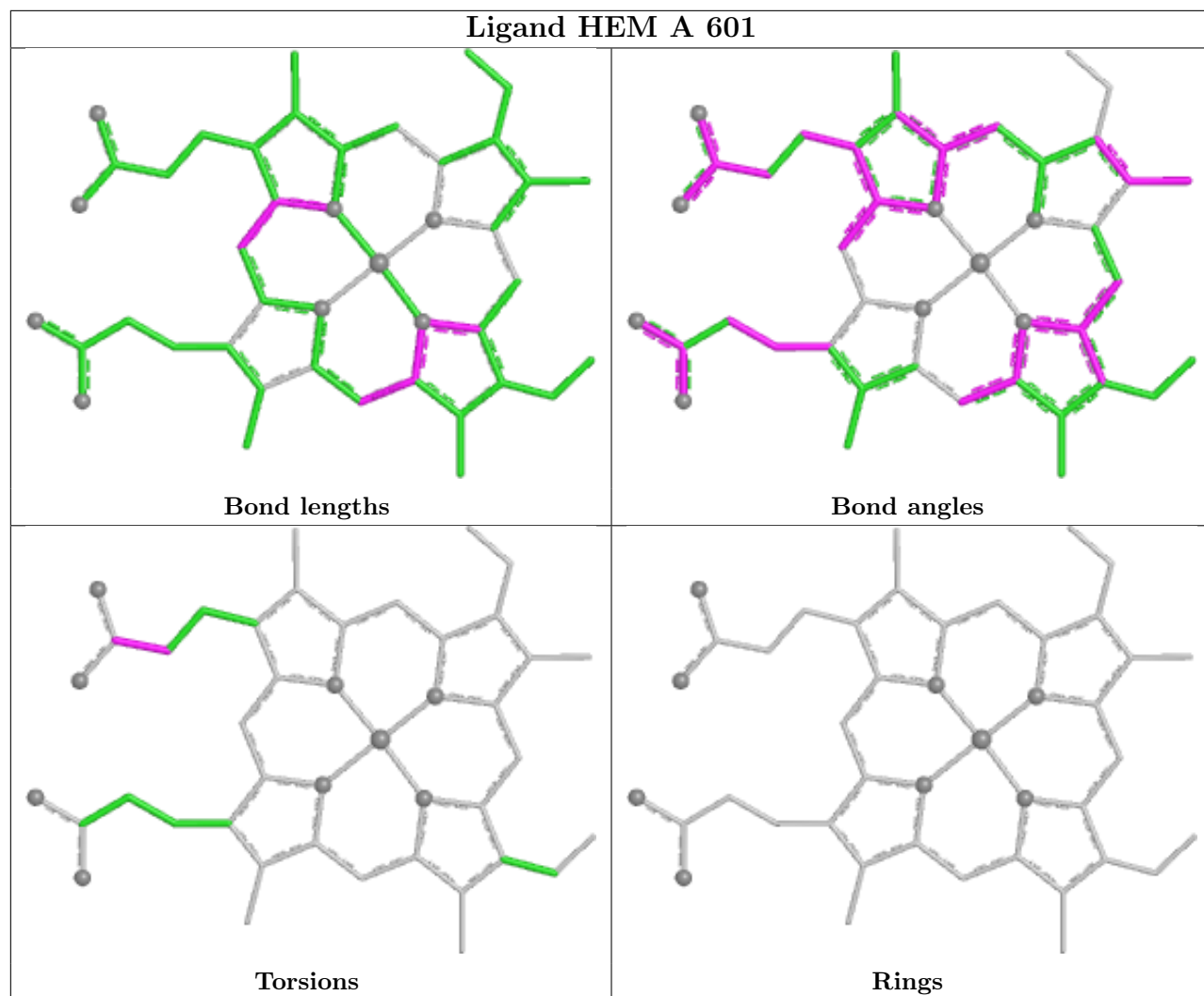
There are no ring outliers.

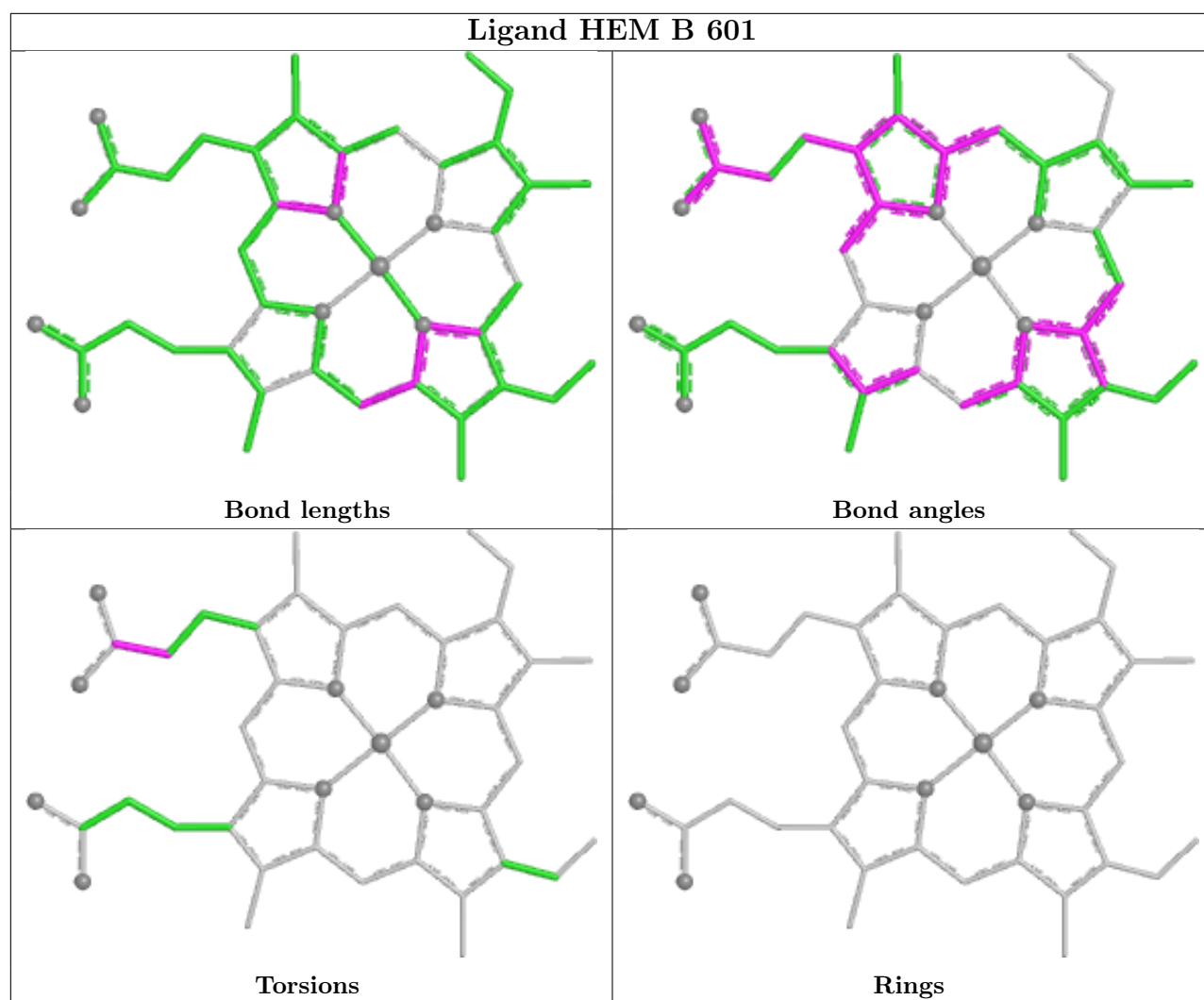
3 monomers are involved in 9 short contacts:

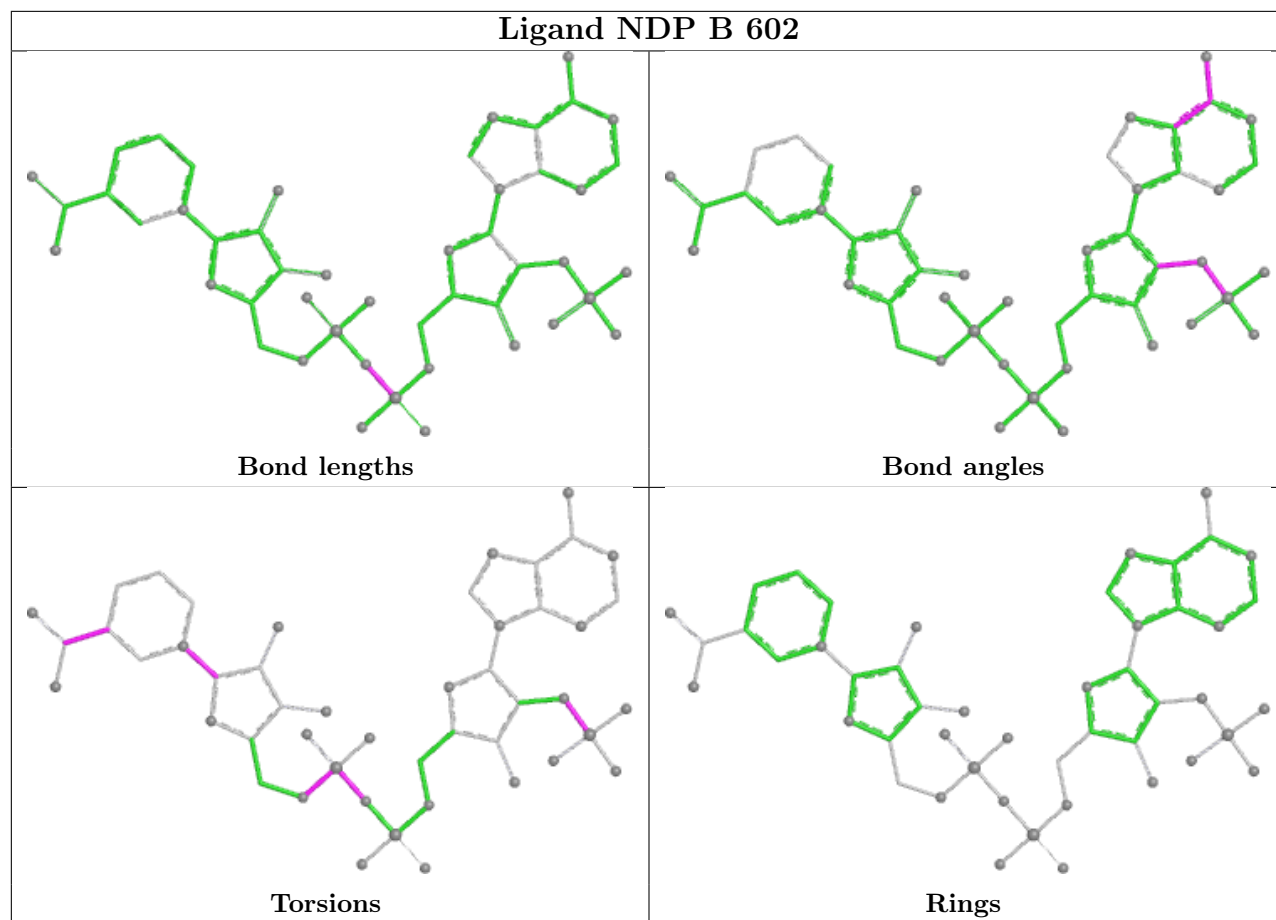
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NDP	1	0
2	A	601	HEM	4	0
2	B	601	HEM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	498/527 (94%)	0.31	17 (3%) 45 42	40, 59, 80, 126	0
1	B	498/527 (94%)	0.20	9 (1%) 68 68	36, 49, 73, 108	0
All	All	996/1054 (94%)	0.25	26 (2%) 56 54	36, 55, 78, 126	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	GLN	6.6
1	A	19	ALA	5.7
1	B	19	ALA	5.6
1	A	22	LYS	4.9
1	B	22	LYS	4.7
1	A	21	GLN	4.4
1	B	20	ALA	4.2
1	A	282	VAL	3.9
1	A	254	HIS	3.6
1	A	394	MET	3.1
1	A	3	ASN	3.0
1	A	93	TYR	2.8
1	A	20	ALA	2.6
1	A	417	ALA	2.6
1	B	290	ILE	2.5
1	A	25	VAL	2.5
1	A	413	HIS	2.2
1	A	393	MET	2.2
1	B	449	VAL	2.2
1	A	250	ALA	2.2
1	B	394	MET	2.1
1	B	3	ASN	2.1
1	B	168	LYS	2.1
1	A	98	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	421	ARG	2.1
1	A	453	GLU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

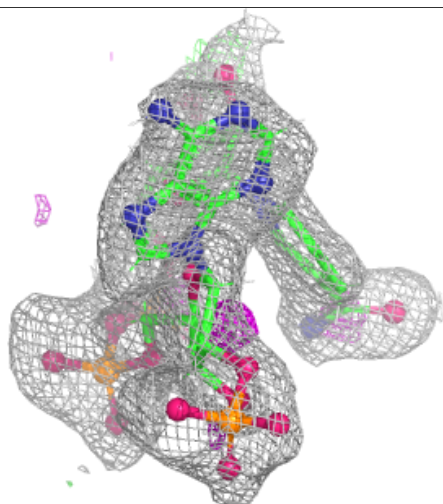
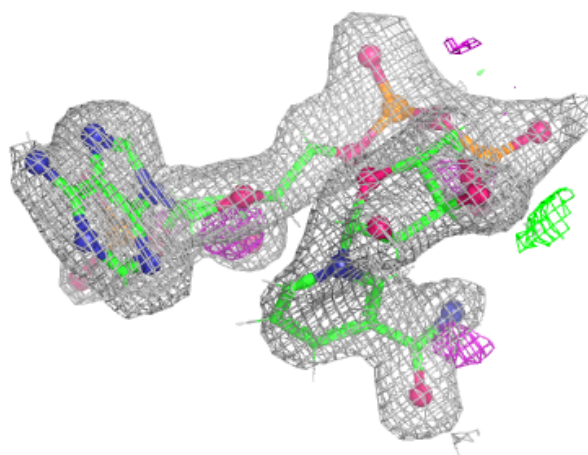
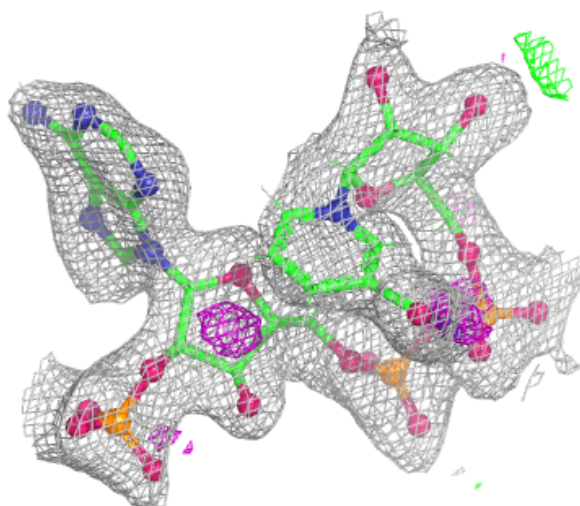
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NDP	B	602	48/48	0.87	0.16	56,67,78,88	0
3	NDP	A	602	48/48	0.89	0.18	62,73,88,93	0
2	HEM	A	601	43/43	0.96	0.14	43,51,74,82	0
2	HEM	B	601	43/43	0.96	0.11	38,43,63,73	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.

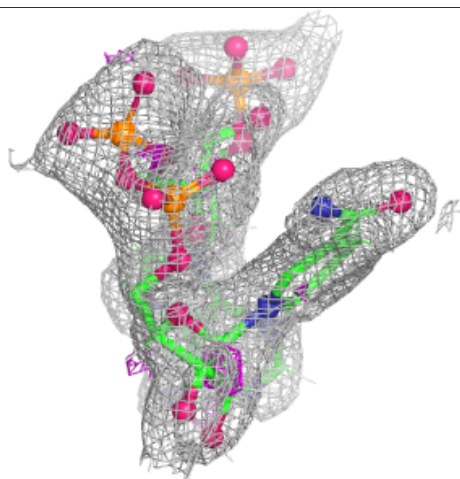
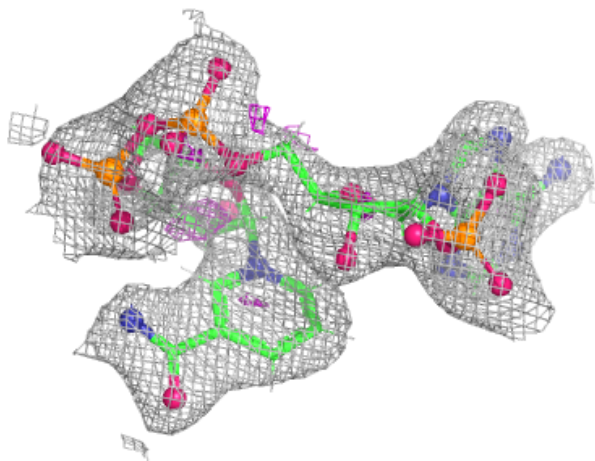
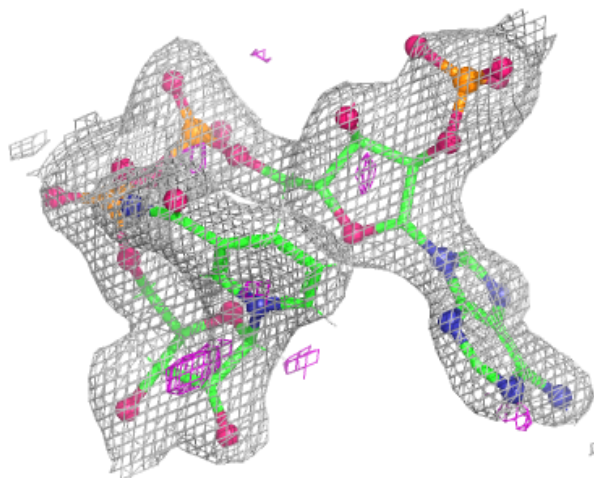
Electron density around NDP B 602:

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



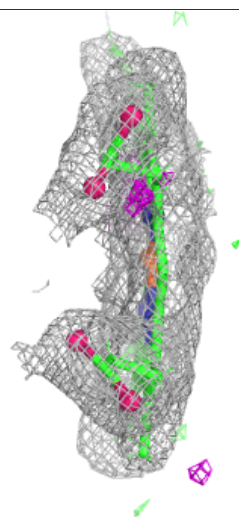
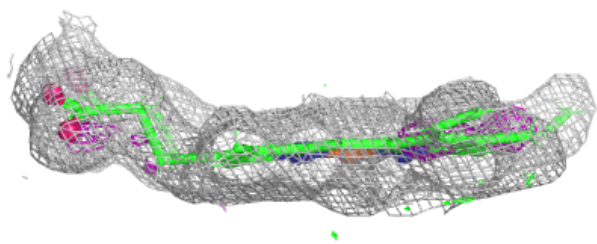
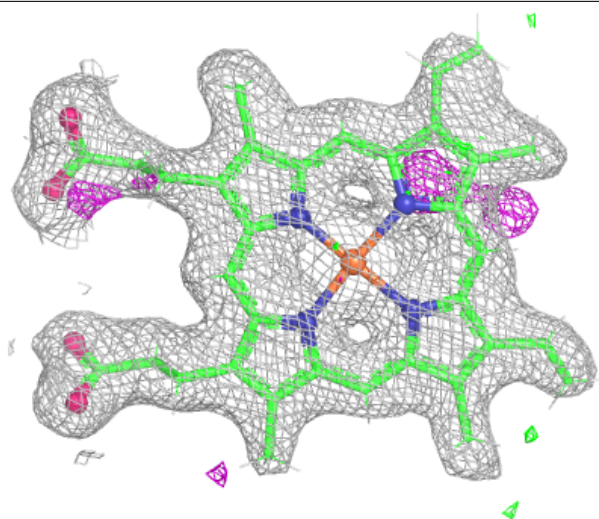
Electron density around NDP A 602:

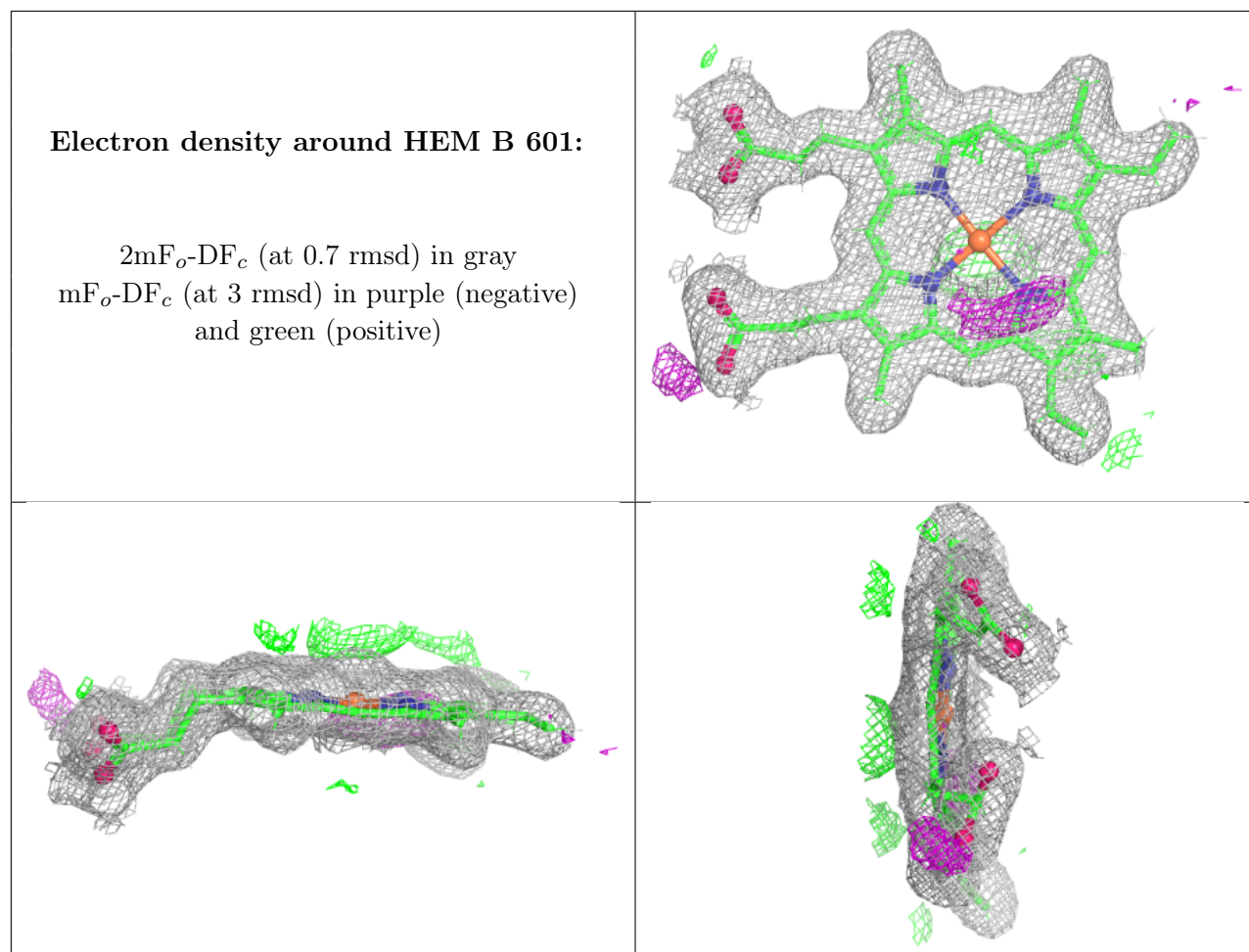
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 601:

$2mF_o-DF_c$ (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.