



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:36 PM UTC

PDB ID : 7XZK / pdb_00007xzk
Title : Crystal Structure of P450BM3 with N-(3-cyclohexylpropanoyl)-L-pipecolyl-L-phenylalanine
Authors : Shoji, O.; Yonemura, K.
Deposited on : 2022-06-02
Resolution : 1.54 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

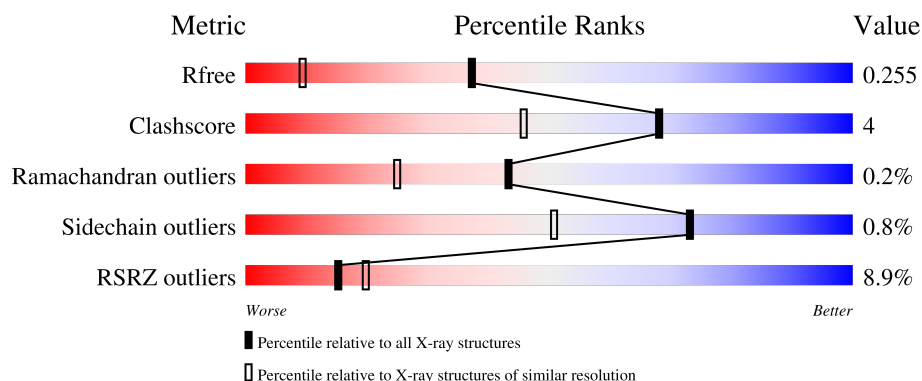
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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.

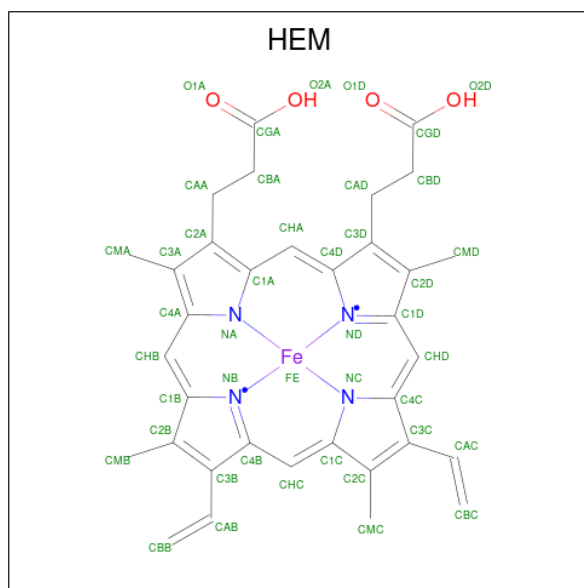
Mol	Chain	Length	Quality of chain
1	A	456	9% 93% 5% ..
1	B	456	9% 91% 9% .

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.

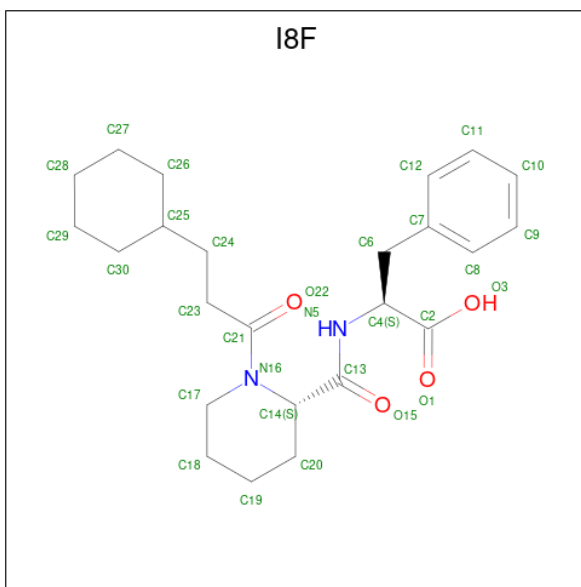
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total 3671	C 2343	N 623	O 688	S 17	0	2	0
1	B	453	Total 3682	C 2351	N 625	O 688	S 18	0	3	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is (2 {S})-2-[[[(2 {S})-1-(3-cyclohexylpropanoyl)piperidin-2-yl]carbonylamino]-3-phenyl-propanoic acid (CCD ID: I8F) (formula: C₂₄H₃₄N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	24	2	4		
3	B	1	Total	C	N	O	0	0
			30	24	2	4		

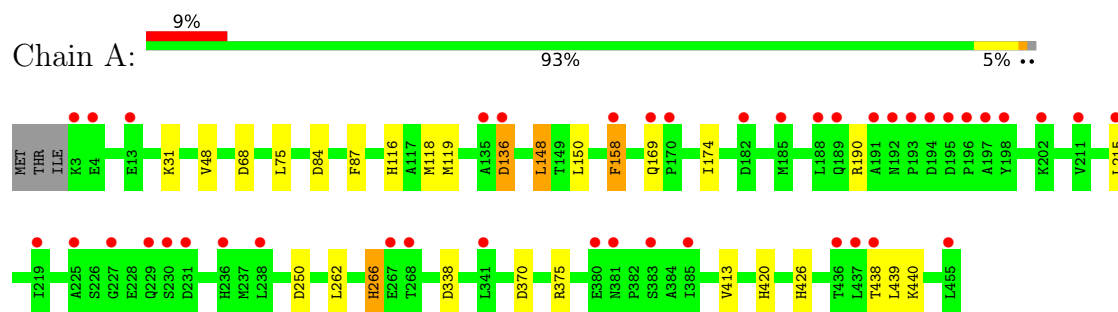
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	309	Total	O	0	0
			309	309		
4	B	295	Total	O	0	0
			295	295		

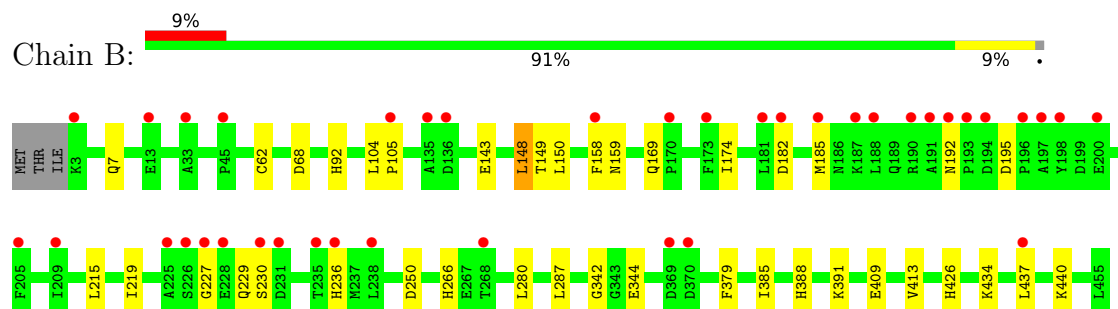
3 Residue-property plots [i](#)

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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.97Å 145.58Å 63.13Å 90.00° 97.03° 90.00°	Depositor
Resolution (Å)	47.48 – 1.54 47.48 – 1.54	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.48-1.54) 99.3 (47.48-1.54)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.211 , 0.242 (Not available) , 0.255	Depositor DCC
R_{free} test set	7616 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8103	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.21% 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: I8F, 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	3/3756 (0.1%)	0.99	4/5076 (0.1%)
1	B	0.63	3/3767 (0.1%)	0.98	3/5089 (0.1%)
All	All	0.63	6/7523 (0.1%)	0.98	7/10165 (0.1%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	420	HIS	CE1-NE2	5.84	1.38	1.32
1	A	266	HIS	CE1-NE2	5.83	1.38	1.32
1	B	388	HIS	CE1-NE2	5.45	1.38	1.32
1	A	426	HIS	CE1-NE2	5.28	1.37	1.32
1	B	92	HIS	CE1-NE2	5.21	1.37	1.32
1	B	426	HIS	CE1-NE2	5.19	1.37	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	GLU	CB-CG-CD	5.69	122.27	112.60
1	B	250	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	68	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	84	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	338	ASP	CA-CB-CG	5.25	117.85	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	68	ASP	CA-CB-CG	5.21	117.81	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	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	3671	0	3633	21	0
1	B	3682	0	3649	27	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
3	A	30	0	0	0	0
3	B	30	0	0	0	0
4	A	309	0	0	7	0
4	B	295	0	0	6	0
All	All	8103	0	7342	53	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 4.

All (53) 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:116:HIS:HA	4:A:814:HOH:O	1.66	0.95
1:B:385:ILE:HD12	4:B:822:HOH:O	1.70	0.90
1:A:440:LYS:HB3	4:A:675:HOH:O	1.79	0.81
1:A:119:MET:HB2	4:A:814:HOH:O	1.80	0.81
1:B:182:ASP:HB3	4:B:838:HOH:O	1.80	0.80
1:B:215:LEU:HD13	4:B:617:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:MET:SD	4:A:814:HOH:O	2.55	0.64
1:B:185:MET:HE3	1:B:437:LEU:HA	1.80	0.63
2:A:501:HEM:HBC2	2:A:501:HEM:HMC1	1.82	0.62
1:B:185:MET:HE3	1:B:437:LEU:HB2	1.84	0.59
1:B:227:GLY:O	1:B:229:GLN:NE2	2.36	0.58
1:A:158:PHE:HZ	1:A:262:LEU:HD21	1.67	0.57
1:A:215:LEU:HD12	4:A:786:HOH:O	2.03	0.57
1:B:185:MET:HE3	1:B:437:LEU:CA	2.35	0.57
1:A:158:PHE:CZ	1:A:262:LEU:HD21	2.41	0.56
2:B:501:HEM:HMC1	2:B:501:HEM:HBC2	1.89	0.55
1:A:169:GLN:HE21	1:B:169:GLN:HE22	1.54	0.55
1:A:150:LEU:HD11	1:A:174:ILE:HD11	1.87	0.55
1:A:370:ASP:OD2	1:A:375:ARG:NH1	2.38	0.52
1:B:185:MET:HE3	1:B:437:LEU:CB	2.39	0.52
1:A:136:ASP:OD1	1:A:136:ASP:N	2.41	0.51
1:A:150:LEU:HD21	1:A:174:ILE:HG13	1.93	0.51
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.91	0.51
1:A:440:LYS:CD	4:A:884:HOH:O	2.58	0.51
1:B:379:PHE:CE1	1:B:385:ILE:HD11	2.46	0.50
1:B:236:HIS:HB3	4:B:706:HOH:O	2.12	0.49
1:B:150:LEU:HD11	1:B:174:ILE:HD11	1.95	0.49
1:B:434:LYS:HD3	1:B:440:LYS:HE2	1.94	0.48
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.43	0.48
2:B:501:HEM:HMB2	2:B:501:HEM:HBB2	1.96	0.47
1:A:118:MET:HA	1:A:118:MET:HE2	1.96	0.47
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.96	0.47
1:A:75:LEU:HD21	1:A:87:PHE:CZ	2.51	0.46
1:B:379:PHE:CE1	1:B:385:ILE:CD1	2.99	0.46
1:B:440:LYS:HB3	4:B:737:HOH:O	2.15	0.45
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.46	0.45
1:B:104:LEU:N	1:B:105:PRO:HD2	2.32	0.45
1:B:192:ASN:O	1:B:195:ASP:HB2	2.19	0.43
1:A:440:LYS:HD2	4:A:884:HOH:O	2.18	0.43
1:B:379:PHE:CD1	1:B:385:ILE:HD11	2.54	0.43
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.50	0.42
1:A:438:THR:OG1	1:A:439:LEU:N	2.52	0.42
1:B:7:GLN:HB2	4:B:783:HOH:O	2.20	0.42
1:A:158:PHE:CZ	1:A:262:LEU:HD11	2.53	0.42
1:B:342:GLY:O	1:B:344:GLU:HG3	2.19	0.42
1:B:158:PHE:CD1	1:B:158:PHE:N	2.88	0.41
1:B:158:PHE:CD2	1:B:219:ILE:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASN:ND2	1:B:230:SER:OG	2.54	0.41
1:B:149:THR:HA	1:B:409:GLU:OE2	2.20	0.41
1:A:158:PHE:HZ	1:A:262:LEU:HD11	1.86	0.41
1:B:62:CYS:SG	1:B:391:LYS:HE2	2.61	0.41
1:B:280:LEU:HD22	1:B:287:LEU:HA	2.02	0.40
1:A:158:PHE:CD1	1:A:158:PHE:N	2.90	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	453/456 (99%)	439 (97%)	13 (3%)	1 (0%)	43	25
1	B	454/456 (100%)	443 (98%)	10 (2%)	1 (0%)	43	25
All	All	907/912 (100%)	882 (97%)	23 (2%)	2 (0%)	43	25

All (2) Ramachandran outliers are listed below:

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

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	399/400 (100%)	394 (99%)	5 (1%)	61	31
1	B	400/400 (100%)	399 (100%)	1 (0%)	86	74
All	All	799/800 (100%)	793 (99%)	6 (1%)	73	51

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	48	VAL
1	A	136	ASP
1	A	148	LEU
1	A	158	PHE
1	B	148	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	192	ASN
1	A	204	GLN
1	A	236	HIS
1	A	285	HIS
1	A	387	GLN
1	B	70	ASN
1	B	73	GLN
1	B	159	ASN
1	B	169	GLN
1	B	189	GLN
1	B	204	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	I8F	B	502	-	32,32,32	0.69	1 (3%)	41,42,42	0.96	2 (4%)
2	HEM	A	501	1	50,50,50	1.75	10 (20%)	67,82,82	1.80	17 (25%)
3	I8F	A	502	-	32,32,32	0.65	0	41,42,42	0.96	1 (2%)
2	HEM	B	501	1	50,50,50	1.65	9 (18%)	67,82,82	1.68	17 (25%)

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	I8F	B	502	-	-	2/25/44/44	0/3/3/3
2	HEM	A	501	1	-	3/14/54/54	-
3	I8F	A	502	-	-	3/25/44/44	0/3/3/3
2	HEM	B	501	1	-	4/14/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C1B-NB	-5.33	1.31	1.40
2	A	501	HEM	FE-NB	4.97	2.10	1.94
2	B	501	HEM	FE-NB	4.70	2.09	1.94
2	A	501	HEM	C1B-NB	-4.34	1.32	1.40
2	A	501	HEM	FE-NC	4.04	2.08	1.95
2	B	501	HEM	FE-NC	3.45	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C1C-NC	-3.29	1.33	1.39
2	B	501	HEM	C1D-C2D	3.12	1.50	1.44
2	B	501	HEM	C1C-NC	-3.04	1.33	1.39
2	A	501	HEM	CMD-C2D	2.61	1.56	1.50
2	A	501	HEM	C1C-C2C	-2.60	1.40	1.45
2	A	501	HEM	C3B-C4B	2.39	1.49	1.44
2	B	501	HEM	FE-NA	2.23	2.02	1.95
2	B	501	HEM	C4D-C3D	2.20	1.48	1.45
2	A	501	HEM	CHB-C1B	2.15	1.42	1.38
2	A	501	HEM	C4D-ND	-2.08	1.36	1.40
2	B	501	HEM	CHA-C4D	2.06	1.42	1.38
2	B	501	HEM	C4B-NB	-2.06	1.34	1.38
2	A	501	HEM	C4B-NB	-2.03	1.34	1.38
3	B	502	I8F	O3-C2	-2.02	1.24	1.30

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C3B-C4B-NB	-5.68	105.39	109.47
2	A	501	HEM	C1B-NB-C4B	4.96	111.08	105.21
2	B	501	HEM	C1B-NB-C4B	4.74	110.82	105.21
2	B	501	HEM	O2A-CGA-CBA	4.25	127.44	114.00
2	B	501	HEM	CHC-C4B-NB	4.03	128.76	124.42
2	A	501	HEM	CHD-C4C-NC	3.88	128.68	124.45
2	A	501	HEM	O2A-CGA-CBA	3.66	125.56	114.00
2	B	501	HEM	CHA-C4D-C3D	-3.62	118.55	125.23
2	B	501	HEM	CHA-C4D-ND	3.20	128.33	124.37
2	B	501	HEM	CHD-C4C-NC	3.15	127.89	124.45
2	A	501	HEM	C4C-NC-C1C	2.99	110.70	105.82
2	A	501	HEM	CHC-C4B-NB	2.90	127.54	124.42
2	A	501	HEM	C3D-C4D-ND	2.85	113.29	110.17
2	B	501	HEM	O2A-CGA-O1A	-2.72	116.34	123.33
2	A	501	HEM	O2A-CGA-O1A	-2.68	116.43	123.33
2	B	501	HEM	C4C-NC-C1C	2.66	110.16	105.82
2	A	501	HEM	CBD-CAD-C3D	-2.66	105.19	112.53
2	A	501	HEM	CHD-C1D-C2D	-2.65	120.85	125.03
2	A	501	HEM	CHD-C1D-ND	2.61	127.23	124.42
2	A	501	HEM	CAD-C3D-C4D	2.54	129.13	124.70
2	A	501	HEM	CHA-C4D-C3D	-2.50	120.61	125.23
2	B	501	HEM	C2D-C1D-ND	2.46	112.74	109.90
3	A	502	I8F	C24-C23-C21	-2.42	110.21	113.39
2	A	501	HEM	CHA-C1A-NA	2.36	128.15	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	CHB-C1B-NB	2.32	127.24	124.37
2	A	501	HEM	C3B-C2B-C1B	-2.32	104.67	106.41
2	B	501	HEM	CAD-C3D-C4D	2.31	128.73	124.70
2	B	501	HEM	CMD-C2D-C1D	2.31	128.64	125.03
2	B	501	HEM	C1D-C2D-C3D	-2.26	104.60	106.98
2	B	501	HEM	C3B-C4B-NB	-2.23	107.87	109.47
3	B	502	I8F	C24-C25-C26	-2.18	106.57	112.05
2	B	501	HEM	O1A-CGA-CBA	-2.17	116.20	123.09
2	B	501	HEM	CHB-C1B-NB	2.11	126.98	124.37
2	B	501	HEM	C1A-CHA-C4D	-2.11	121.28	126.25
3	B	502	I8F	C18-C17-N16	-2.09	107.41	110.65
2	A	501	HEM	C1A-CHA-C4D	-2.08	121.36	126.25
2	B	501	HEM	C3D-C4D-ND	2.05	112.41	110.17

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	I8F	C21-C23-C24-C25
3	A	502	I8F	C23-C24-C25-C26
3	B	502	I8F	C21-C23-C24-C25
3	A	502	I8F	C23-C24-C25-C30
3	B	502	I8F	C23-C24-C25-C26
2	B	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAD-CBD-CGD-O2D
2	B	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAD-CBD-CGD-O1D
2	B	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O2A

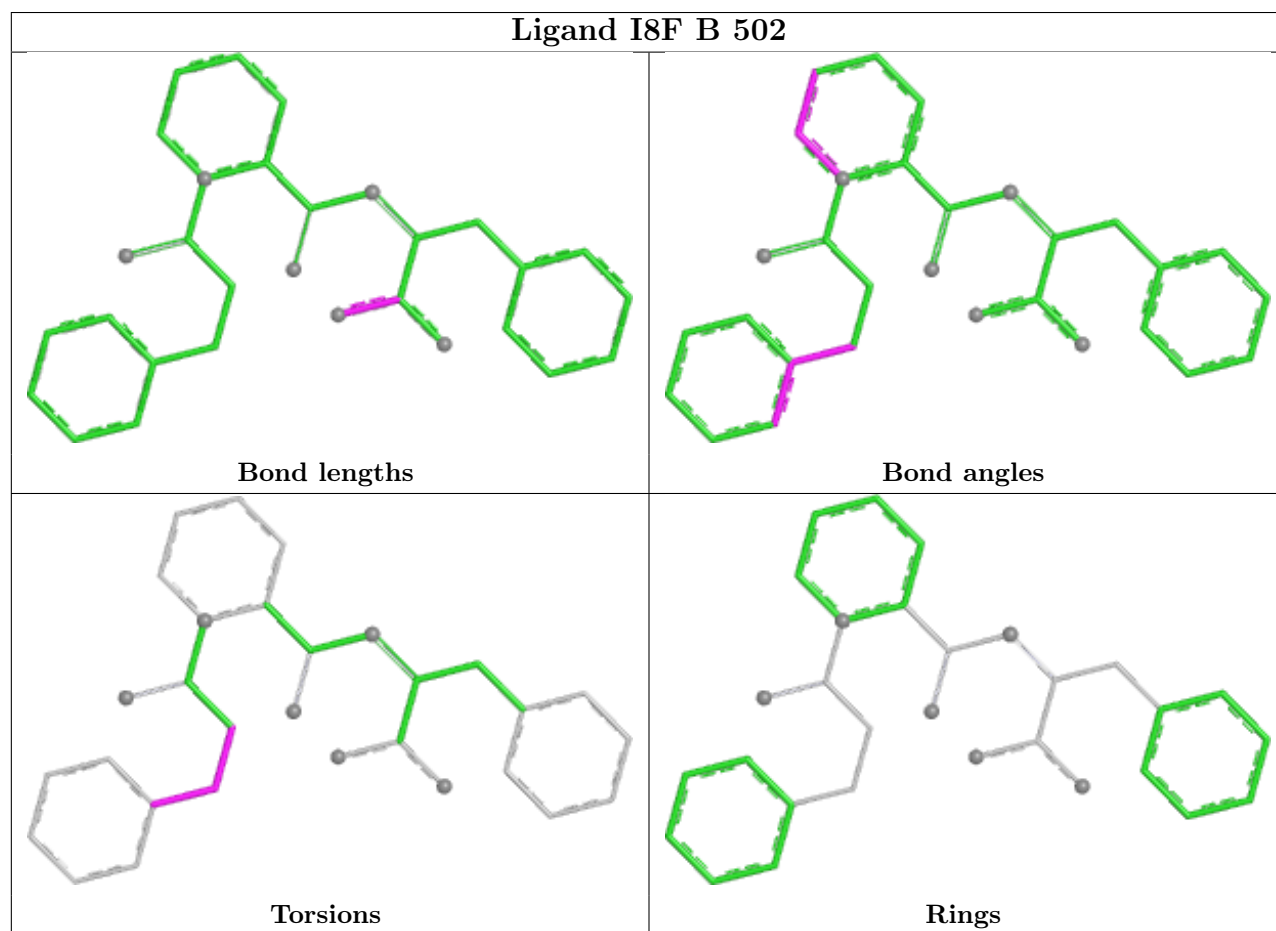
There are no ring outliers.

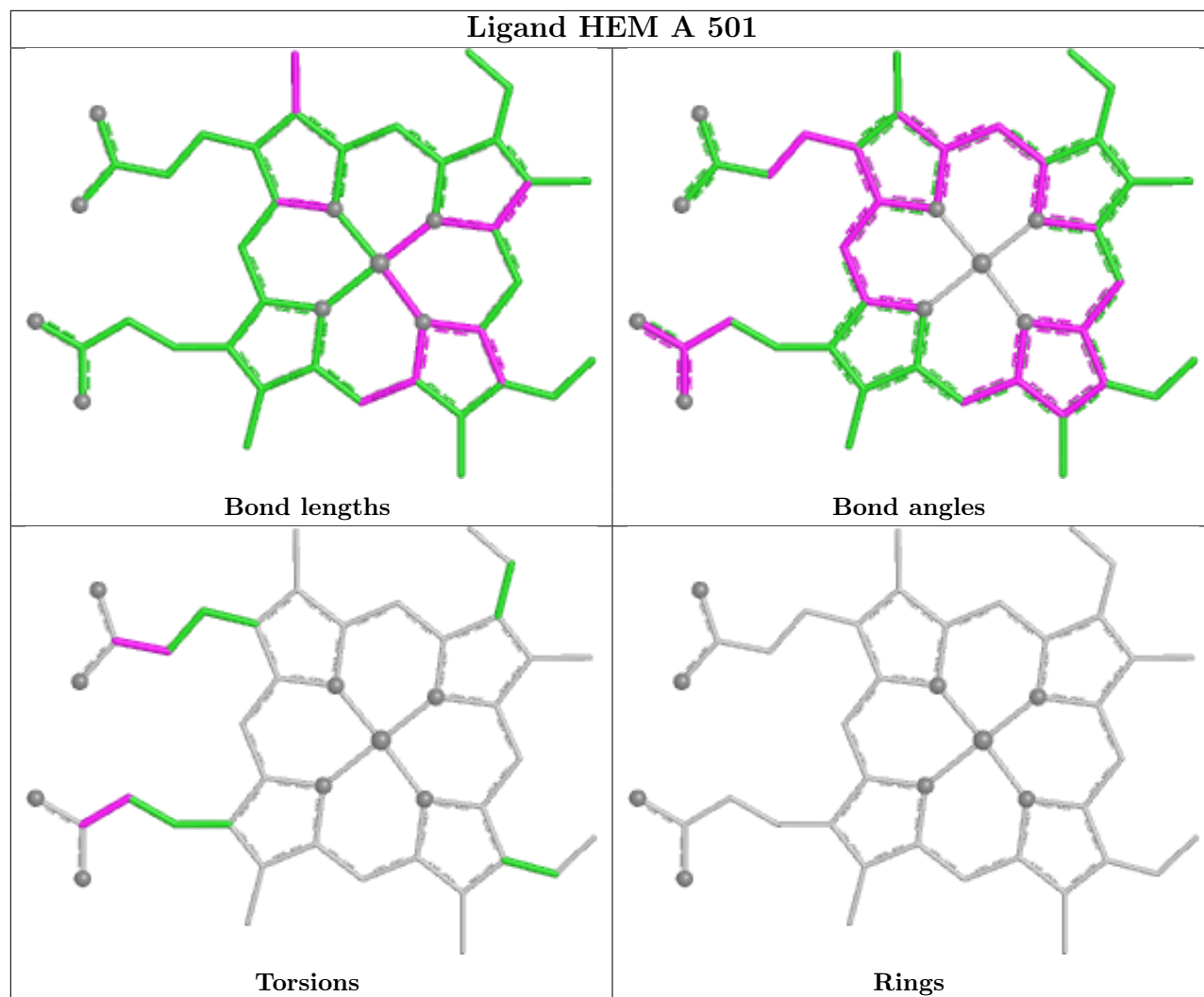
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	2	0
2	B	501	HEM	4	0

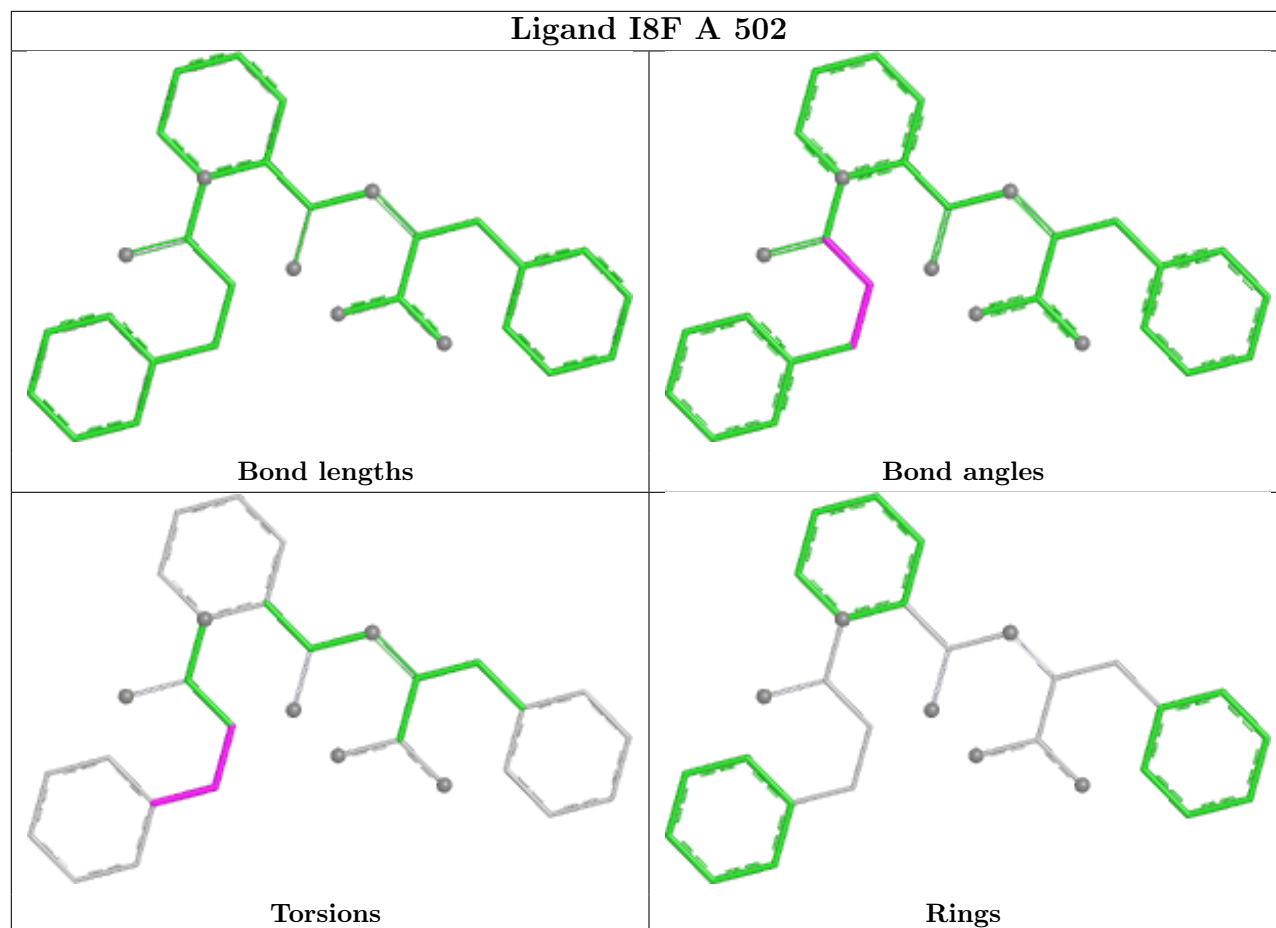
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

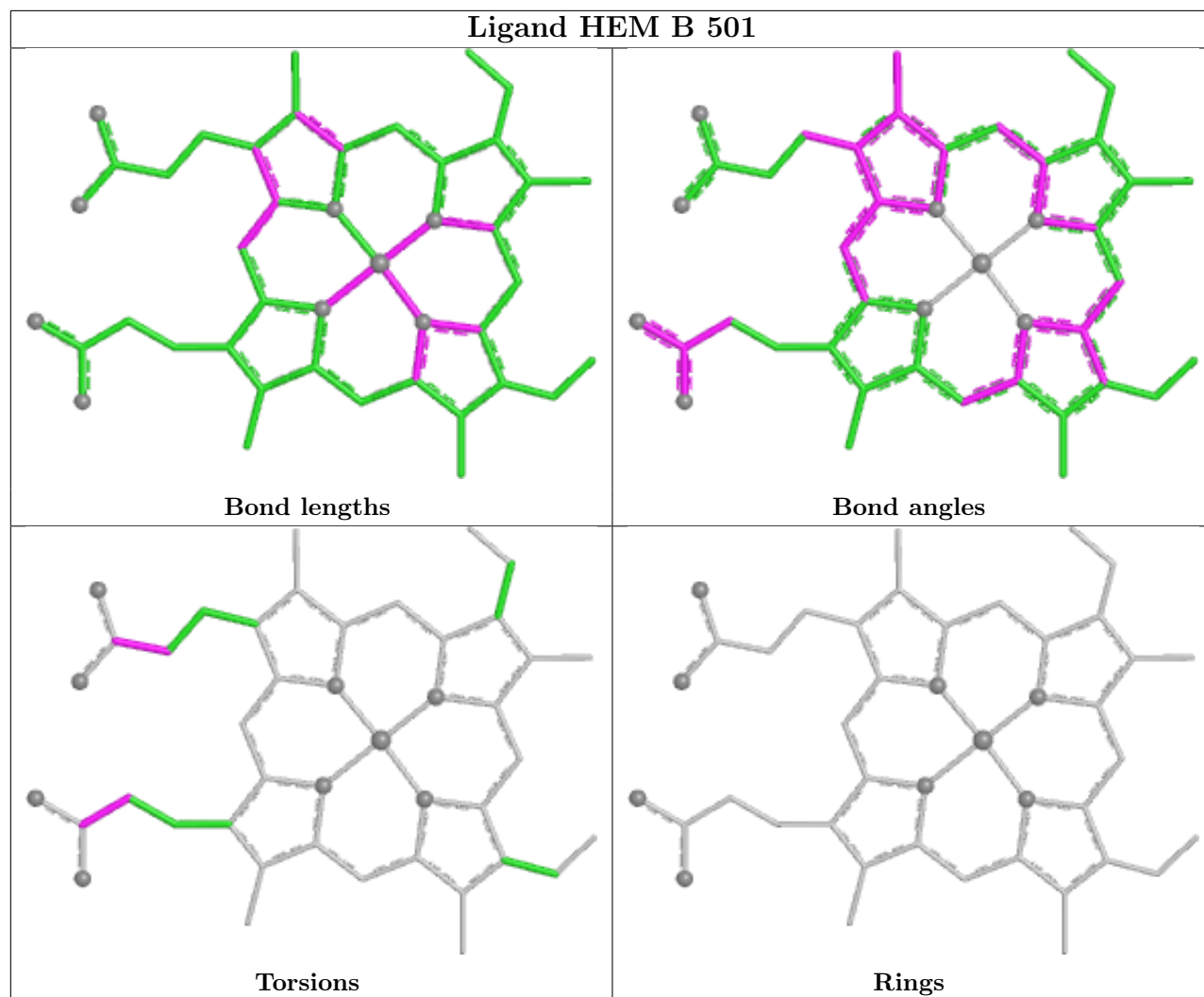
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.





Ligand I8F A 502





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	453/456 (99%)	0.63	42 (9%) 14 19	10, 18, 41, 63	2 (0%)
1	B	453/456 (99%)	0.61	39 (8%) 16 21	9, 18, 41, 57	3 (0%)
All	All	906/912 (99%)	0.62	81 (8%) 15 20	9, 18, 41, 63	5 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	437	LEU	7.2
1	A	191	ALA	6.5
1	A	193	PRO	6.3
1	B	193	PRO	5.9
1	B	236	HIS	4.6
1	B	191	ALA	4.2
1	B	197	ALA	4.2
1	B	3	LYS	4.1
1	B	225	ALA	4.0
1	A	135	ALA	3.8
1	B	437	LEU	3.7
1	B	268	THR	3.7
1	A	198	TYR	3.7
1	A	197	ALA	3.7
1	A	385	ILE	3.7
1	A	192	ASN	3.6
1	A	158	PHE	3.4
1	A	195	ASP	3.4
1	B	231	ASP	3.4
1	B	188	LEU	3.4
1	B	170	PRO	3.3
1	B	227	GLY	3.3
1	A	455	LEU	3.2
1	A	182	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	225	ALA	3.2
1	B	198	TYR	3.2
1	A	229	GLN	3.2
1	B	182	ASP	3.2
1	B	158	PHE	3.1
1	A	3	LYS	3.1
1	A	4	GLU	3.1
1	A	236	HIS	3.1
1	A	268	THR	3.0
1	B	194	ASP	3.0
1	B	136	ASP	2.9
1	A	189	GLN	2.9
1	B	185	MET	2.9
1	A	170	PRO	2.9
1	A	231	ASP	2.8
1	A	238	LEU	2.8
1	A	215	LEU	2.8
1	B	105	PRO	2.8
1	A	380	GLU	2.8
1	B	196	PRO	2.8
1	A	194	ASP	2.7
1	B	235	THR	2.7
1	A	136	ASP	2.7
1	A	196	PRO	2.6
1	B	230	SER	2.6
1	A	381	ASN	2.5
1	B	135	ALA	2.4
1	A	230	SER	2.4
1	A	219	ILE	2.4
1	A	188	LEU	2.4
1	A	438	THR	2.4
1	A	185	MET	2.4
1	B	13	GLU	2.4
1	A	383[A]	SER	2.4
1	B	187	LYS	2.3
1	A	436	THR	2.3
1	B	200	GLU	2.3
1	B	226	SER	2.3
1	B	228	GLU	2.3
1	B	370	ASP	2.2
1	A	211	VAL	2.2
1	B	173	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	209	ILE	2.2
1	B	205	PHE	2.2
1	A	13	GLU	2.2
1	A	267	GLU	2.2
1	A	227	GLY	2.1
1	A	169	GLN	2.1
1	B	190	ARG	2.1
1	A	341	LEU	2.1
1	A	202	LYS	2.1
1	B	33	ALA	2.0
1	B	238	LEU	2.0
1	B	192	ASN	2.0
1	B	45	PRO	2.0
1	B	181	LEU	2.0
1	B	369	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

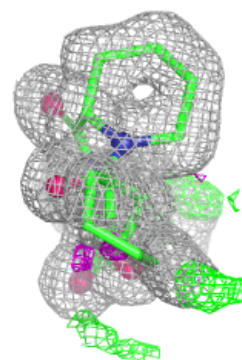
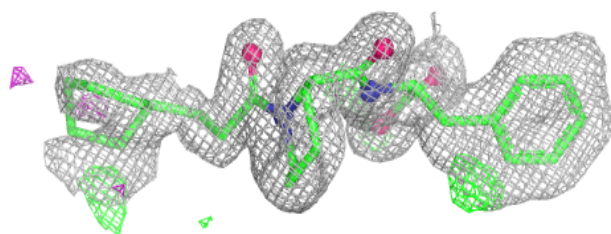
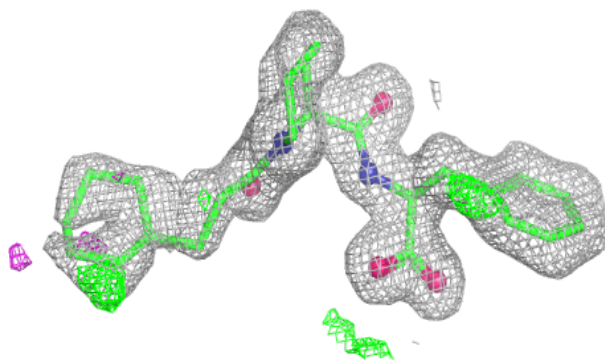
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	I8F	A	502	30/30	0.91	0.12	17,21,37,39	0
3	I8F	B	502	30/30	0.92	0.11	18,24,39,39	0
2	HEM	A	501	43/43	0.98	0.06	9,11,13,20	0
2	HEM	B	501	43/43	0.98	0.07	9,10,13,19	0

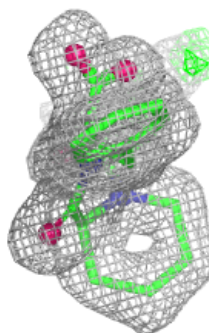
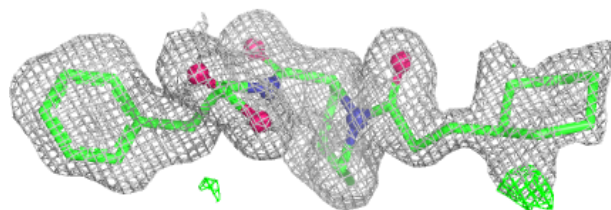
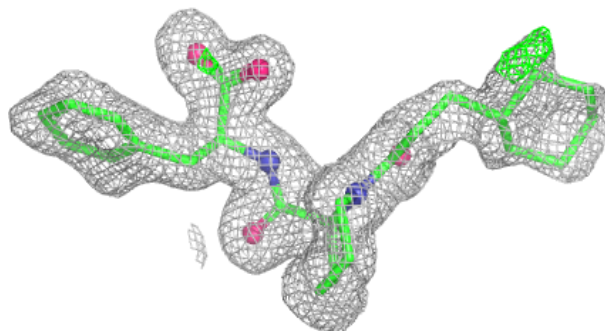
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around I8F 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)

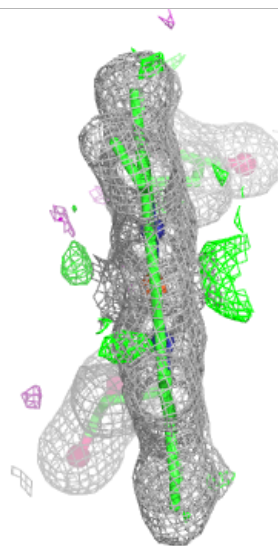
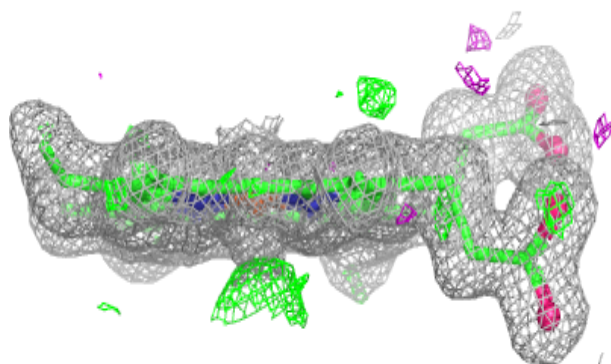
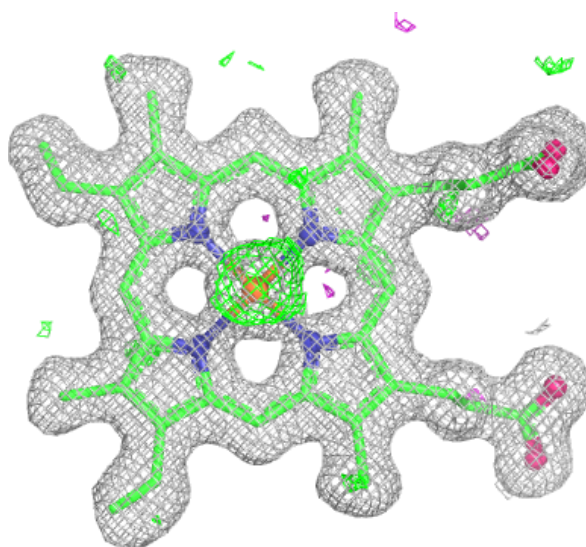
**Electron density around I8F B 502:**

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



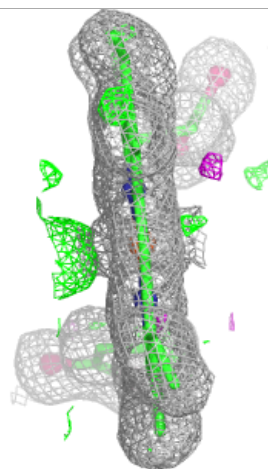
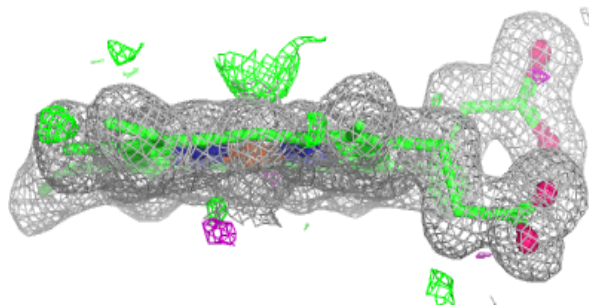
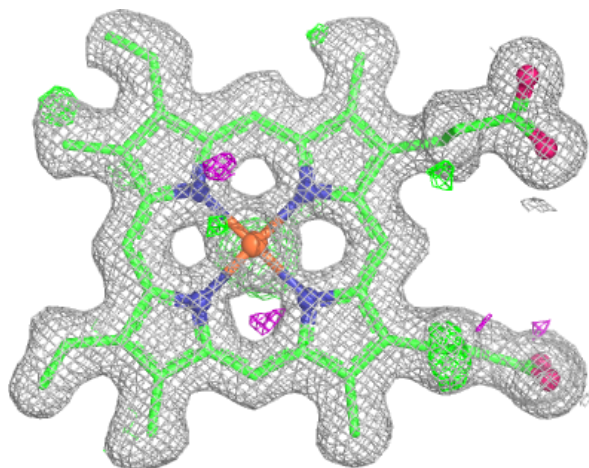
Electron density around HEM A 501:

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



Electron density around HEM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.