



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:42 PM UTC

PDB ID : 7Y0S / pdb_00007y0s
Title : Crystal structure of the P450 BM3 heme domain mutant F87A in complex with N-imidazolyl-hexanoyl-L-tyrosyl-L-tyrosine and hydroxylamine
Authors : Jiang, Y.; Dong, S.; Feng, Y.; Cong, Z.
Deposited on : 2022-06-06
Resolution : 2.06 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

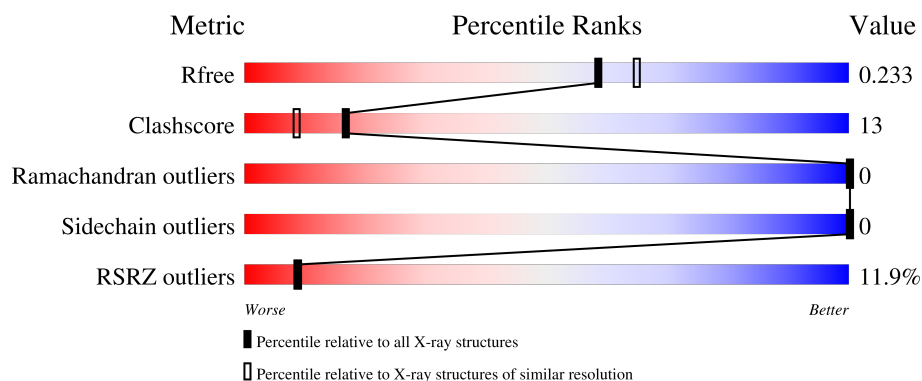
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	465	11% 68% 26% 5%
1	B	465	11% 71% 23% 5%
2	C	3	33% 33% 33%
2	D	3	33% 33% 33%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7506 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	B	441	Total	C	N	O	S	0	1	0
			3458	2210	590	641	17			
1	A	441	Total	C	N	O	S	0	1	0
			3444	2208	590	629	17			

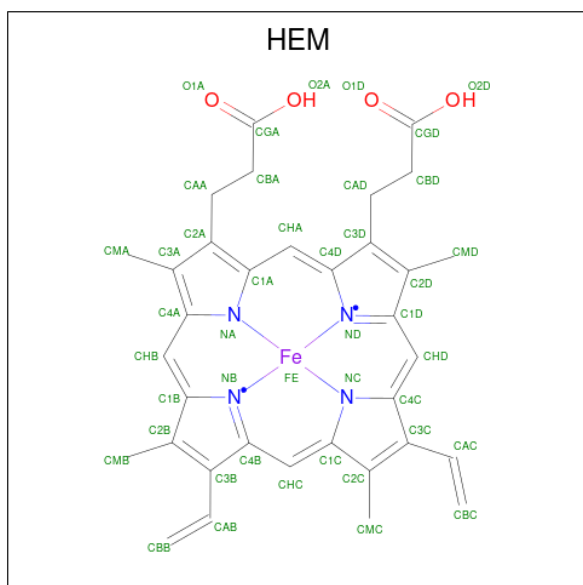
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P14779
B	87	ALA	PHE	engineered mutation	UNP P14779
B	456	LEU	-	expression tag	UNP P14779
B	457	GLU	-	expression tag	UNP P14779
B	458	HIS	-	expression tag	UNP P14779
B	459	HIS	-	expression tag	UNP P14779
B	460	HIS	-	expression tag	UNP P14779
B	461	HIS	-	expression tag	UNP P14779
B	462	HIS	-	expression tag	UNP P14779
B	463	HIS	-	expression tag	UNP P14779
A	-1	GLY	-	expression tag	UNP P14779
A	87	ALA	PHE	engineered mutation	UNP P14779
A	456	LEU	-	expression tag	UNP P14779
A	457	GLU	-	expression tag	UNP P14779
A	458	HIS	-	expression tag	UNP P14779
A	459	HIS	-	expression tag	UNP P14779
A	460	HIS	-	expression tag	UNP P14779
A	461	HIS	-	expression tag	UNP P14779
A	462	HIS	-	expression tag	UNP P14779
A	463	HIS	-	expression tag	UNP P14779

- Molecule 2 is a protein called I7X-TYR-TYR.

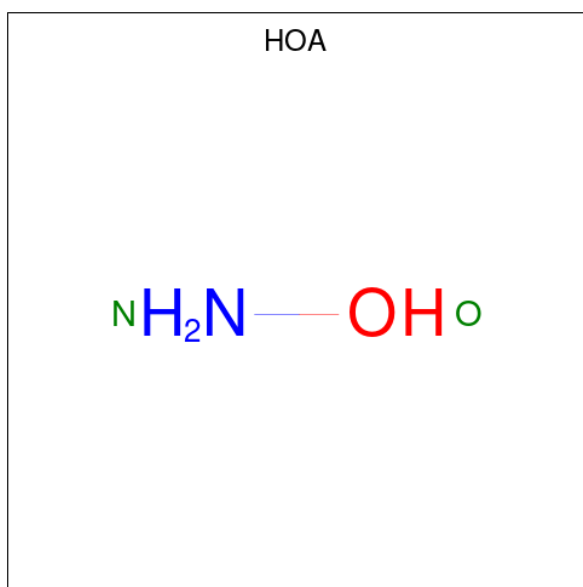
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total 37	C 27	N 4	O 6	0	0	0
2	D	3	Total 37	C 27	N 4	O 6	0	0	0

- Molecule 3 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
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is HYDROXYAMINE (CCD ID: HOA) (formula: H_3NO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	N	O	0	0
			2	1	1		
4	A	1	Total	N	O	0	0
			2	1	1		

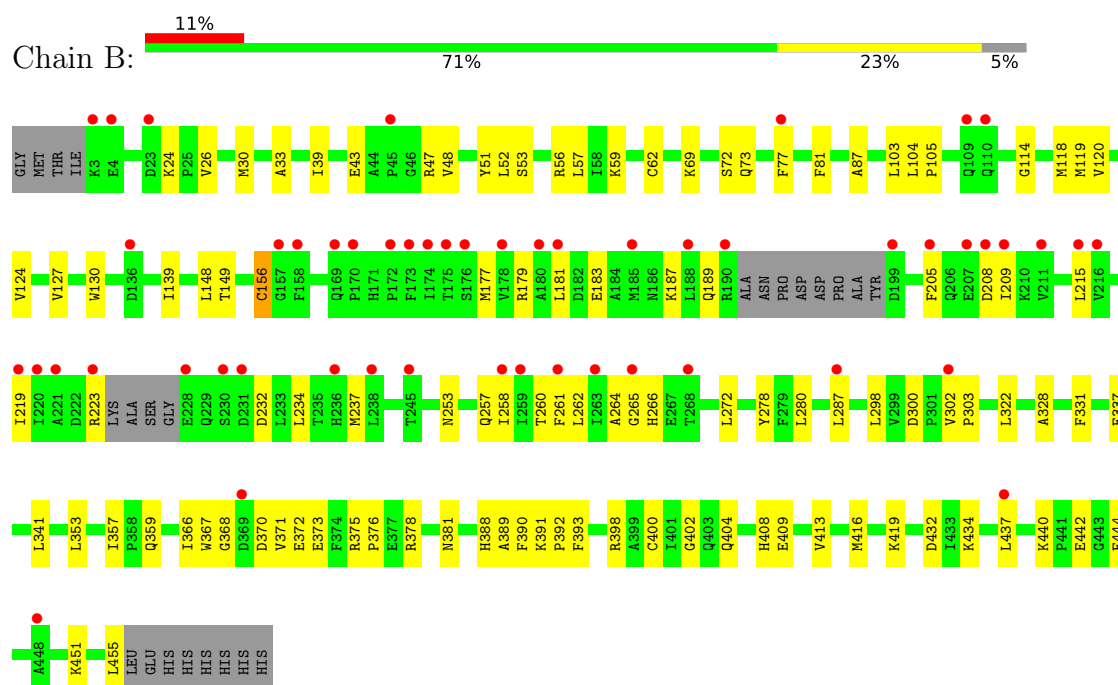
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	209	Total	O	0	0
			209	209		
5	A	227	Total	O	0	0
			227	227		
5	C	2	Total	O	0	0
			2	2		
5	D	2	Total	O	0	0
			2	2		

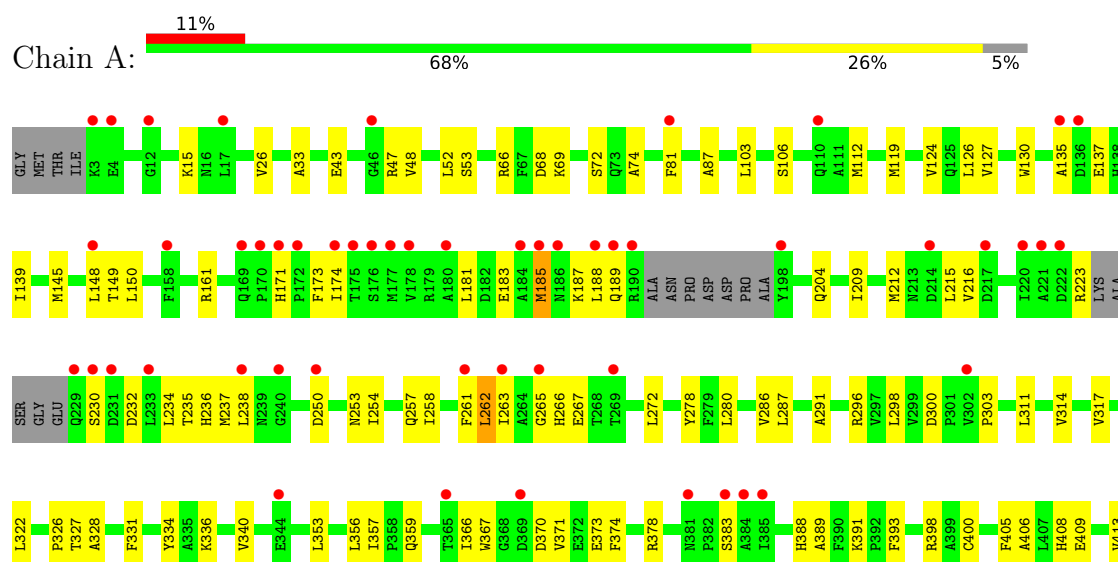
3 Residue-property plots

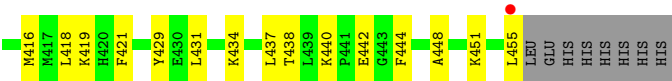
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

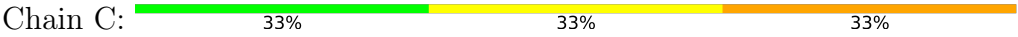


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

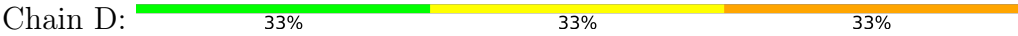




● Molecule 2: I7X-TYR-TYR



● Molecule 2: I7X-TYR-TYR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.43Å 143.78Å 63.04Å 90.00° 99.83° 90.00°	Depositor
Resolution (Å)	52.66 – 2.06 52.66 – 2.06	Depositor EDS
% Data completeness (in resolution range)	97.0 (52.66-2.06) 96.9 (52.66-2.06)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.223 , 0.228 0.230 , 0.233	Depositor DCC
R_{free} test set	2000 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7506	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.11% 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: HOA, HEM, I7X

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	0.40	1/3524 (0.0%)	0.62	2/4770 (0.0%)
1	B	0.47	3/3539 (0.1%)	0.56	0/4793
2	C	2.05	1/26 (3.8%)	1.35	0/33
2	D	1.79	1/26 (3.8%)	0.98	0/33
All	All	0.47	6/7115 (0.1%)	0.60	2/9629 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	TYR	C-N	8.33	1.45	1.33
1	B	376	PRO	C-O	-7.62	1.14	1.24
1	A	262	LEU	C-O	-7.18	1.15	1.24
2	C	2	TYR	C-N	6.60	1.42	1.33
1	B	375	ARG	C-O	-5.76	1.19	1.24
1	B	156	CYS	C-O	-5.61	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	LEU	N-CA-C	-5.92	106.06	113.28
1	A	185	MET	CA-C-O	-5.66	114.42	120.42

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	3444	0	3352	102	0
1	B	3458	0	3345	74	0
2	C	37	0	17	3	0
2	D	37	0	17	5	0
3	A	43	0	30	5	0
3	B	43	0	30	3	0
4	A	2	0	0	1	0
4	B	2	0	0	1	0
5	A	227	0	0	7	0
5	B	209	0	0	10	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
All	All	7506	0	6791	177	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 13.

All (177) 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:126:LEU:HD22	1:A:148:LEU:HD12	1.52	0.92
1:A:183:GLU:O	1:A:187:LYS:HG3	1.85	0.77
1:A:148:LEU:HD13	1:A:413:VAL:HG11	1.65	0.77
1:A:148:LEU:CD1	1:A:413:VAL:HG11	2.16	0.76
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.68	0.73
1:B:370:ASP:HB2	1:B:373:GLU:HG3	1.71	0.73
1:B:272:LEU:HD13	1:B:322:LEU:HG	1.71	0.72
1:B:59:LYS:NZ	5:B:601:HOH:O	2.21	0.72
1:A:148:LEU:HD23	1:A:148:LEU:C	2.16	0.71
1:B:179:ARG:NH2	1:B:208:ASP:OD1	2.24	0.70
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.73	0.70
1:B:381:ASN:ND2	5:B:607:HOH:O	2.25	0.69
1:A:370:ASP:O	1:A:378:ARG:NH2	2.25	0.69
1:A:173:PHE:CD1	1:A:215:LEU:HD23	2.29	0.68
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.75	0.67
1:A:126:LEU:HD22	1:A:148:LEU:CD1	2.22	0.67
1:B:26:VAL:HG22	2:C:2:TYR:HB3	1.78	0.65
1:B:404:GLN:NE2	5:B:611:HOH:O	2.28	0.65
1:B:124:VAL:HG13	1:B:455:LEU:HD13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HD13	1:A:322:LEU:HG	1.79	0.64
1:B:367:TRP:HB2	1:B:371:VAL:HG12	1.80	0.63
1:A:366:ILE:HG21	1:A:389:ALA:HB1	1.81	0.63
1:B:264:ALA:HB1	4:B:502:HOA:N	2.13	0.63
1:A:230:SER:H	1:A:235:THR:HG21	1.64	0.63
1:B:393:PHE:HB3	1:B:400:CYS:HB3	1.81	0.62
1:B:57:LEU:HD22	1:B:341:LEU:HG	1.81	0.62
1:B:234:LEU:HD13	1:B:258:ILE:HD11	1.82	0.61
1:B:81:PHE:HB3	1:B:209:ILE:HG12	1.82	0.61
1:A:434:LYS:HB2	1:A:442:GLU:HB2	1.82	0.60
1:A:103:LEU:HD13	1:A:261:PHE:HZ	1.66	0.60
1:A:298:LEU:HD22	1:A:303:PRO:HB3	1.83	0.60
1:B:120:VAL:HG11	1:B:302:VAL:HG13	1.84	0.60
1:A:52:LEU:HD11	1:A:353:LEU:HD13	1.84	0.60
1:A:148:LEU:CD1	1:A:413:VAL:CG1	2.79	0.60
1:A:370:ASP:HB2	1:A:373:GLU:HG3	1.83	0.60
1:B:298:LEU:HD22	1:B:303:PRO:HB3	1.85	0.59
1:A:171:HIS:H	1:A:174:ILE:HD12	1.68	0.59
1:A:124:VAL:HG13	1:A:455:LEU:HD13	1.84	0.59
1:A:148:LEU:HD11	1:A:413:VAL:CG1	2.33	0.58
1:B:127:VAL:HG21	1:B:416:MET:HE2	1.84	0.58
1:B:52:LEU:HD11	1:B:353:LEU:HD13	1.84	0.58
1:B:440:LYS:HG2	5:B:710:HOH:O	2.04	0.58
1:B:366:ILE:HG21	1:B:389:ALA:HB1	1.86	0.57
1:A:234:LEU:HD13	1:A:258:ILE:HD11	1.86	0.57
1:A:238:LEU:HD22	1:A:254:ILE:HD13	1.87	0.57
1:A:393:PHE:HB3	1:A:400:CYS:HB3	1.86	0.57
1:A:15:LYS:NZ	5:A:609:HOH:O	2.33	0.56
1:B:181:LEU:HD12	1:B:437:LEU:HD12	1.88	0.55
1:A:15:LYS:HD3	1:A:43:GLU:HB3	1.88	0.54
1:A:173:PHE:CE2	1:A:262:LEU:HD13	2.42	0.54
1:B:215:LEU:O	1:B:219:ILE:HG12	2.08	0.54
1:B:103:LEU:HD13	1:B:261:PHE:HZ	1.74	0.53
1:B:24:LYS:NZ	1:B:432:ASP:OD1	2.36	0.52
1:B:223:ARG:NH2	1:B:232:ASP:OD2	2.27	0.52
1:A:267:GLU:HA	5:A:636:HOH:O	2.09	0.52
1:A:69:LYS:HB3	1:A:398:ARG:HG3	1.91	0.52
1:A:126:LEU:HD21	1:A:145:MET:HE1	1.92	0.52
1:A:149:THR:HA	1:A:409:GLU:OE1	2.09	0.51
1:A:43:GLU:HG2	1:A:48:VAL:HG22	1.92	0.51
1:B:187:LYS:NZ	5:B:609:HOH:O	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.93	0.51
1:B:118:MET:HG3	5:B:657:HOH:O	2.11	0.51
1:A:280:LEU:HB3	1:A:287:LEU:HD12	1.93	0.50
1:A:173:PHE:CZ	1:A:262:LEU:HD13	2.46	0.50
1:B:30:MET:HG2	1:B:359:GLN:HG2	1.93	0.50
1:A:265:GLY:HA2	3:A:501:HEM:C2C	2.45	0.50
1:B:149:THR:HA	1:B:409:GLU:OE1	2.12	0.50
1:A:204:GLN:OE1	1:A:204:GLN:HA	2.10	0.50
1:B:262:LEU:O	1:B:266:HIS:CD2	2.65	0.50
1:B:419:LYS:O	1:B:451:LYS:HD2	2.12	0.49
1:A:253:ASN:O	1:A:257:GLN:HG2	2.12	0.49
1:B:265:GLY:HA2	3:B:501:HEM:C2C	2.48	0.49
1:A:127:VAL:HG21	1:A:416:MET:HE2	1.95	0.49
1:A:150:LEU:HD21	1:A:174:ILE:HG12	1.94	0.49
1:B:368:GLY:O	1:B:371:VAL:HG13	2.13	0.49
1:A:69:LYS:NZ	1:A:87:ALA:O	2.43	0.49
1:A:72:SER:HB2	2:D:3:TYR:C	2.38	0.49
1:A:298:LEU:HB2	1:A:419:LYS:HD2	1.94	0.48
1:A:232:ASP:O	1:A:236:HIS:ND1	2.44	0.48
1:A:300:ASP:O	1:A:419:LYS:NZ	2.46	0.48
1:A:181:LEU:HD11	1:A:263:ILE:HG23	1.96	0.48
1:A:148:LEU:C	1:A:148:LEU:CD2	2.85	0.48
1:B:189:GLN:HA	5:B:704:HOH:O	2.13	0.48
1:A:185:MET:HE3	2:D:2:TYR:CE2	2.49	0.48
1:B:59:LYS:HE3	1:A:296:ARG:HD3	1.96	0.47
1:B:434:LYS:HB2	1:B:442:GLU:HB2	1.95	0.47
1:A:188:LEU:HD12	2:D:2:TYR:CZ	2.50	0.47
1:A:171:HIS:N	1:A:174:ILE:HD12	2.28	0.47
1:B:43:GLU:HG2	1:B:48:VAL:HG22	1.97	0.47
1:B:402:GLY:HA3	3:B:501:HEM:C3C	2.50	0.47
1:A:266:HIS:CE1	1:A:267:GLU:HB3	2.50	0.47
1:B:253:ASN:O	1:B:257:GLN:HG2	2.15	0.47
1:B:298:LEU:HB2	1:B:419:LYS:HD2	1.96	0.47
1:A:106:SER:HB3	1:A:236:HIS:CD2	2.49	0.47
1:A:126:LEU:CD2	1:A:148:LEU:HD12	2.35	0.47
1:B:179:ARG:HB3	1:B:208:ASP:OD2	2.15	0.47
3:B:501:HEM:HBC2	3:B:501:HEM:HMC2	1.95	0.47
1:B:69:LYS:HB3	1:B:398:ARG:HG3	1.98	0.47
1:B:261:PHE:O	1:B:265:GLY:N	2.46	0.47
1:A:119:MET:SD	1:A:408:HIS:HD2	2.38	0.47
1:A:331:PHE:HD1	1:A:357:ILE:HD11	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:LYS:O	1:A:451:LYS:HD2	2.15	0.46
1:B:331:PHE:HD1	1:B:357:ILE:HD11	1.79	0.46
1:A:53:SER:HB3	1:A:359:GLN:HB3	1.98	0.46
1:A:336:LYS:HD3	5:A:793:HOH:O	2.15	0.46
1:B:118:MET:CE	1:B:156:CYS:HA	2.46	0.46
1:A:212:MET:O	1:A:216:VAL:HG23	2.16	0.46
1:B:328:ALA:O	1:B:357:ILE:HD12	2.15	0.46
1:B:300:ASP:O	1:B:419:LYS:NZ	2.49	0.46
1:A:68:ASP:HB3	1:A:334:TYR:CZ	2.51	0.46
1:A:250:ASP:N	1:A:250:ASP:OD1	2.49	0.46
1:B:73:GLN:HG3	1:B:77:PHE:CE2	2.51	0.45
1:B:119:MET:SD	1:B:408:HIS:HD2	2.39	0.45
1:A:317:VAL:HG13	1:A:374:PHE:HZ	1.80	0.45
1:A:26:VAL:HG22	2:D:2:TYR:HB3	1.98	0.45
1:A:223:ARG:NH1	1:A:235:THR:HG23	2.32	0.45
1:B:33:ALA:HB3	1:B:359:GLN:HG3	1.99	0.45
1:A:173:PHE:HB2	1:A:215:LEU:HD22	1.99	0.45
3:A:501:HEM:HMC2	3:A:501:HEM:HBC2	1.98	0.45
1:A:278:TYR:HA	1:A:444:PHE:CZ	2.52	0.44
1:B:370:ASP:O	1:B:378:ARG:NH2	2.46	0.44
1:B:260:THR:O	1:B:264:ALA:N	2.39	0.44
1:A:359:GLN:OE1	5:A:601:HOH:O	2.21	0.44
1:A:328:ALA:O	1:A:357:ILE:HD12	2.18	0.44
1:B:62:CYS:SG	1:B:391:LYS:HE2	2.58	0.44
1:B:237:MET:HE1	1:B:258:ILE:HG13	1.98	0.44
1:A:66:ARG:NH2	1:A:340:VAL:O	2.51	0.43
1:B:53:SER:HB3	1:B:359:GLN:HB3	2.00	0.43
1:A:286:VAL:HG11	1:A:374:PHE:HE2	1.83	0.43
1:B:177:MET:HE1	1:B:266:HIS:NE2	2.33	0.43
1:A:148:LEU:HD23	1:A:148:LEU:O	2.18	0.43
1:A:356:LEU:HD12	1:A:356:LEU:HA	1.89	0.43
1:A:406:ALA:HB2	3:A:501:HEM:HHC	2.00	0.43
1:B:104:LEU:HD21	1:A:383:SER:CB	2.49	0.43
1:B:183:GLU:HG2	1:B:205:PHE:HB2	2.00	0.43
1:A:440:LYS:HG2	5:A:708:HOH:O	2.18	0.43
1:B:372:GLU:OE2	5:B:602:HOH:O	2.22	0.43
1:B:56:ARG:HA	1:B:59:LYS:HE2	2.01	0.43
1:B:130:TRP:CZ2	1:B:139:ILE:HG21	2.54	0.43
1:A:267:GLU:HG3	1:A:438:THR:HG21	2.00	0.42
1:B:114:GLY:HA3	5:B:735:HOH:O	2.19	0.42
1:A:367:TRP:HB2	1:A:371:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:HB3	1:B:105:PRO:HD3	2.01	0.42
1:A:112:MET:SD	1:A:405:PHE:HA	2.60	0.42
1:A:189:GLN:H	1:A:189:GLN:HG3	1.57	0.42
1:B:390:PHE:CZ	1:B:392:PRO:HG3	2.55	0.42
1:B:337:GLU:HB3	5:B:617:HOH:O	2.20	0.42
1:A:280:LEU:HD13	1:A:418:LEU:HD21	2.00	0.42
1:A:421:PHE:HB3	1:A:448:ALA:HB1	2.01	0.42
1:B:69:LYS:NZ	1:B:87:ALA:O	2.51	0.42
1:B:72:SER:HB2	2:C:3:TYR:C	2.45	0.42
1:A:237:MET:HE1	1:A:258:ILE:HG13	2.01	0.42
1:A:326:PRO:HB2	5:A:705:HOH:O	2.20	0.42
1:A:103:LEU:HD13	1:A:261:PHE:CZ	2.51	0.42
1:A:161:ARG:HA	5:A:685:HOH:O	2.19	0.42
1:A:74:ALA:HB2	1:A:188:LEU:HD11	2.01	0.42
1:A:258:ILE:O	1:A:262:LEU:HG	2.20	0.42
1:A:291:ALA:HA	1:A:418:LEU:HB3	2.01	0.42
1:B:280:LEU:HD22	1:B:287:LEU:HA	2.02	0.41
1:A:173:PHE:CZ	1:A:262:LEU:CD1	3.02	0.41
1:A:69:LYS:CB	1:A:398:ARG:HG3	2.50	0.41
1:A:33:ALA:HB3	1:A:359:GLN:HG3	2.02	0.41
1:A:130:TRP:CZ2	1:A:139:ILE:HG21	2.55	0.41
1:B:47:ARG:HG2	2:C:3:TYR:OH	2.21	0.41
1:A:47:ARG:HG2	2:D:3:TYR:OH	2.20	0.41
1:A:135:ALA:C	1:A:137:GLU:H	2.28	0.41
1:A:185:MET:HE2	1:A:189:GLN:NE2	2.35	0.41
1:A:69:LYS:HD3	1:A:398:ARG:CZ	2.51	0.41
1:A:400:CYS:HB2	3:A:501:HEM:NA	2.35	0.41
1:A:81:PHE:HB3	1:A:209:ILE:HG12	2.03	0.41
1:A:272:LEU:N	1:A:327:THR:HG21	2.36	0.41
3:A:501:HEM:NB	4:A:502:HOA:O	2.54	0.40
1:B:183:GLU:O	1:B:187:LYS:HG3	2.21	0.40
1:B:278:TYR:HA	1:B:444:PHE:CZ	2.56	0.40
1:A:311:LEU:HB3	1:A:314:VAL:HB	2.03	0.40
1:B:39:ILE:HA	1:B:51:TYR:O	2.22	0.40
1:A:429:TYR:CE2	1:A:431:LEU:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	436/465 (94%)	418 (96%)	18 (4%)	0	100	100
1	B	436/465 (94%)	419 (96%)	17 (4%)	0	100	100
All	All	872/930 (94%)	837 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	356/407 (88%)	356 (100%)	0	100	100
1	B	360/407 (88%)	360 (100%)	0	100	100
2	C	2/2 (100%)	2 (100%)	0	100	100
2	D	2/2 (100%)	2 (100%)	0	100	100
All	All	720/818 (88%)	720 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	163	ASN
1	B	186	ASN
1	B	229	GLN

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Mol	Chain	Res	Type
1	A	70	ASN
1	A	134	ASN
1	A	163	ASN
1	A	189	GLN
1	A	359	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	HEM	A	501	4,1	50,50,50	1.38	9 (18%)	67,82,82	1.15	4 (5%)
4	HOA	A	502	3	0,1,1	-	-	-		
4	HOA	B	502	3	0,1,1	-	-	-		
3	HEM	B	501	4,1	50,50,50	1.43	7 (14%)	67,82,82	1.18	5 (7%)

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	HEM	A	501	4,1	-	0/14/54/54	-
3	HEM	B	501	4,1	-	0/14/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	HEM	FE-NC	3.98	2.08	1.95
3	B	501	HEM	FE-NB	3.66	2.06	1.94
3	A	501	HEM	FE-NA	3.54	2.06	1.95
3	A	501	HEM	FE-NB	3.12	2.04	1.94
3	B	501	HEM	FE-NA	2.95	2.04	1.95
3	B	501	HEM	CAB-C3B	2.94	1.55	1.47
3	B	501	HEM	CAC-C3C	2.93	1.55	1.47
3	A	501	HEM	CAB-C3B	2.86	1.55	1.47
3	A	501	HEM	CAC-C3C	2.86	1.55	1.47
3	A	501	HEM	FE-NC	2.73	2.04	1.95
3	A	501	HEM	FE-ND	2.24	2.01	1.94
3	B	501	HEM	CMB-C2B	2.14	1.55	1.50
3	A	501	HEM	CMC-C2C	2.13	1.55	1.50
3	B	501	HEM	CMC-C2C	2.11	1.55	1.50
3	A	501	HEM	CMB-C2B	2.01	1.54	1.50
3	A	501	HEM	CMA-C3A	2.01	1.54	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	HEM	C4D-ND-C1D	2.60	108.28	105.21
3	A	501	HEM	C4D-ND-C1D	2.51	108.19	105.21
3	B	501	HEM	C2A-C1A-NA	-2.42	107.46	110.15
3	B	501	HEM	C1B-NB-C4B	2.41	108.06	105.21
3	A	501	HEM	C3D-C4D-ND	-2.34	107.61	110.17
3	A	501	HEM	C1B-NB-C4B	2.33	107.97	105.21
3	A	501	HEM	C2A-C1A-NA	-2.26	107.64	110.15
3	B	501	HEM	C3D-C4D-ND	-2.24	107.71	110.17
3	B	501	HEM	CBA-CAA-C2A	-2.09	106.74	112.53

There are no chirality outliers.

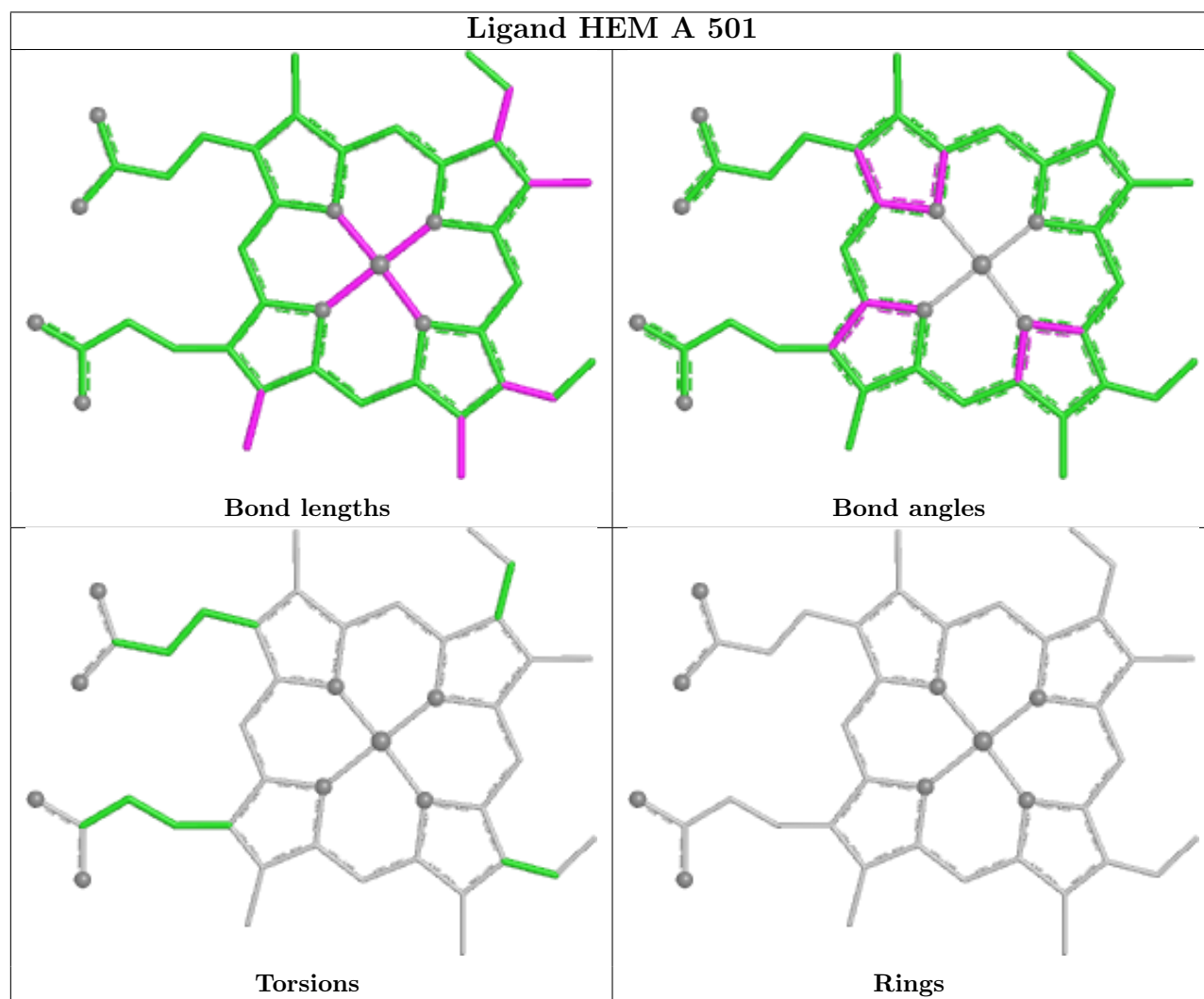
There are no torsion outliers.

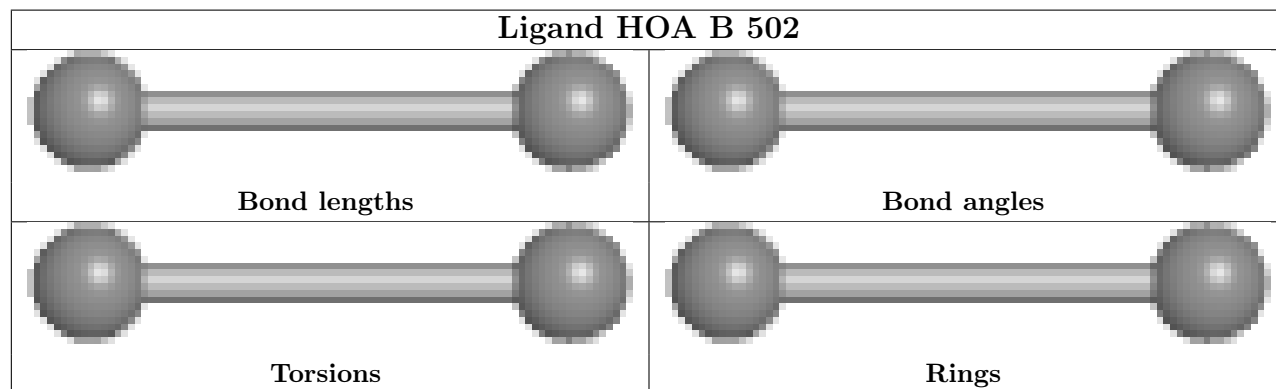
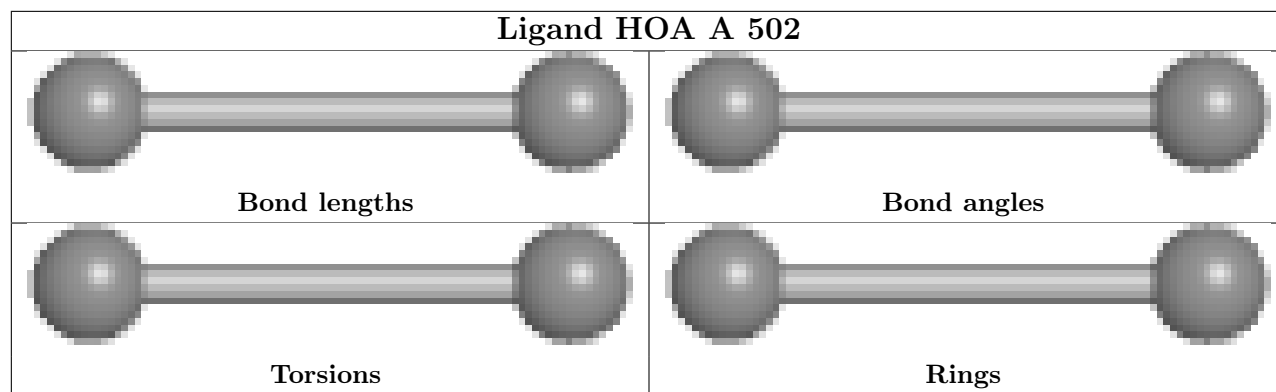
There are no ring outliers.

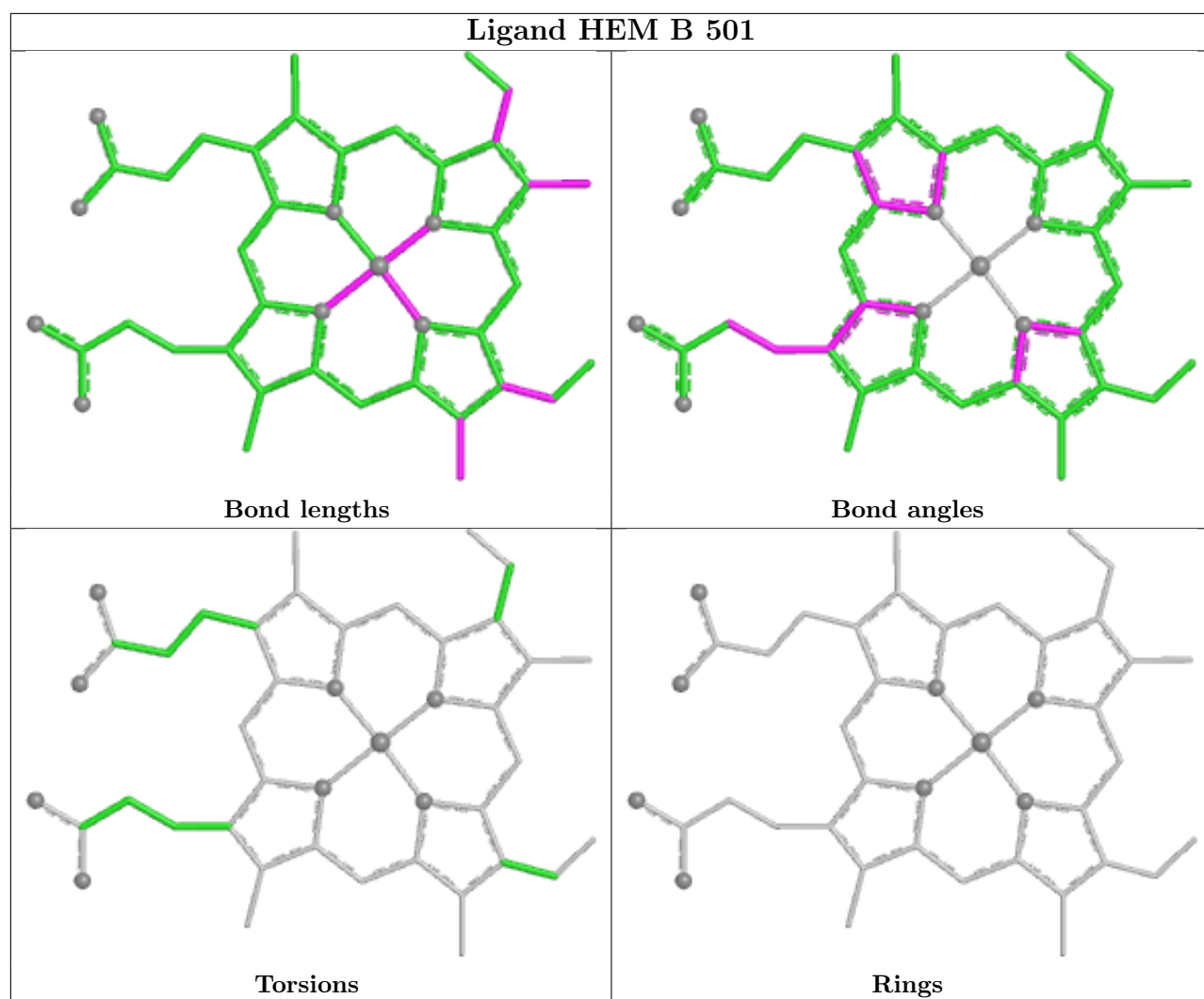
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	HEM	5	0
4	A	502	HOA	1	0
4	B	502	HOA	1	0
3	B	501	HEM	3	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	441/465 (94%)	0.98	53 (12%) 9 8	21, 37, 62, 88	1 (0%)
1	B	441/465 (94%)	0.91	52 (11%) 9 9	21, 36, 67, 74	1 (0%)
2	C	2/3 (66%)	0.56	0 100 100	34, 34, 34, 37	0
2	D	2/3 (66%)	0.86	0 100 100	34, 34, 34, 36	0
All	All	886/936 (94%)	0.95	105 (11%) 9 9	21, 37, 65, 88	2 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	TYR	5.6
1	A	231	ASP	5.6
1	B	220	ILE	4.7
1	A	220	ILE	4.7
1	B	215	LEU	4.4
1	A	383	SER	4.3
1	B	199	ASP	4.1
1	B	110	GLN	4.1
1	B	173	PHE	3.9
1	A	190	ARG	3.9
1	B	265	GLY	3.9
1	B	216	VAL	3.8
1	B	221	ALA	3.7
1	B	211	VAL	3.6
1	B	231	ASP	3.5
1	A	180	ALA	3.3
1	A	172	PRO	3.2
1	A	229	GLN	3.2
1	A	136	ASP	3.1
1	A	217	ASP	3.1
1	B	3	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	265	GLY	3.1
1	A	184	ALA	3.1
1	B	188	LEU	3.1
1	A	175	THR	3.1
1	A	263	ILE	3.1
1	A	158	PHE	3.0
1	B	238	LEU	3.0
1	A	185	MET	3.0
1	A	230	SER	3.0
1	B	172	PRO	3.0
1	A	188	LEU	2.9
1	A	369	ASP	2.9
1	A	261	PHE	2.9
1	A	221	ALA	2.9
1	A	189	GLN	2.9
1	B	219	ILE	2.9
1	B	263	ILE	2.9
1	A	177	MET	2.9
1	B	228	GLU	2.9
1	A	344	GLU	2.9
1	A	385	ILE	2.8
1	B	190	ARG	2.8
1	B	208	ASP	2.8
1	B	157	GLY	2.8
1	A	186	ASN	2.8
1	B	77	PHE	2.8
1	A	81	PHE	2.7
1	B	175	THR	2.7
1	B	437	LEU	2.7
1	B	23	ASP	2.7
1	A	384	ALA	2.6
1	A	222	ASP	2.6
1	A	176	SER	2.6
1	B	158	PHE	2.5
1	A	174	ILE	2.5
1	B	45	PRO	2.5
1	B	170	PRO	2.5
1	B	178	VAL	2.5
1	B	223	ARG	2.5
1	B	230	SER	2.5
1	A	214	ASP	2.5
1	B	258	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	207	GLU	2.4
1	A	170	PRO	2.4
1	A	148	LEU	2.4
1	B	176	SER	2.4
1	B	185	MET	2.4
1	A	169	GLN	2.4
1	B	209	ILE	2.4
1	A	302	VAL	2.4
1	A	46	GLY	2.4
1	B	4	GLU	2.3
1	B	236	HIS	2.3
1	A	17	LEU	2.3
1	B	136	ASP	2.3
1	B	174	ILE	2.3
1	A	250	ASP	2.3
1	A	178	VAL	2.3
1	A	269	THR	2.3
1	A	3	LYS	2.3
1	B	181	LEU	2.3
1	A	4	GLU	2.2
1	A	171	HIS	2.2
1	A	365	THR	2.2
1	A	240	GLY	2.2
1	B	287	LEU	2.2
1	B	369	ASP	2.2
1	B	448	ALA	2.2
1	A	135	ALA	2.2
1	A	12	GLY	2.2
1	A	233	LEU	2.2
1	A	455	LEU	2.2
1	A	238	LEU	2.1
1	A	381	ASN	2.1
1	B	302	VAL	2.1
1	B	169	GLN	2.1
1	B	245	THR	2.1
1	B	268	THR	2.1
1	B	261	PHE	2.1
1	B	180	ALA	2.1
1	A	110	GLN	2.0
1	B	259	ILE	2.0
1	B	205	PHE	2.0
1	B	109	GLN	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](#)

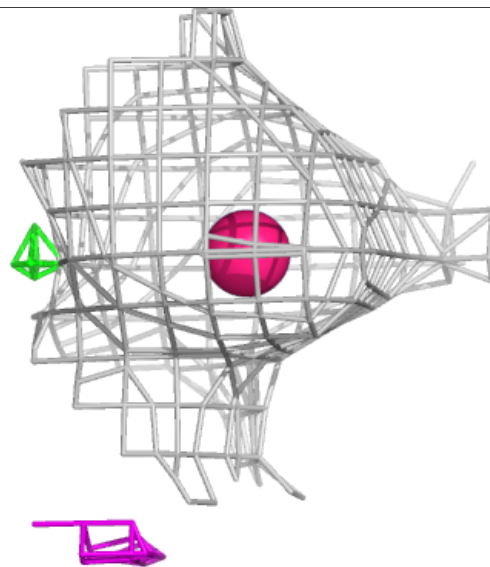
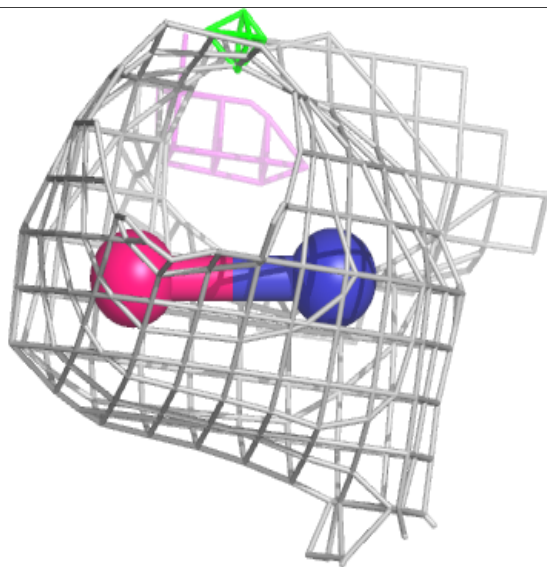
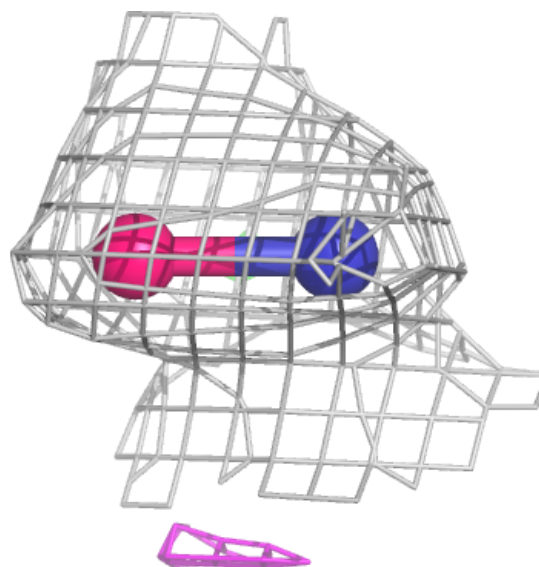
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	HOA	B	502	2/2	0.87	0.12	37,37,37,45	0
4	HOA	A	502	2/2	0.88	0.12	38,38,38,44	0
3	HEM	B	501	43/43	0.95	0.09	25,30,33,41	0
3	HEM	A	501	43/43	0.96	0.10	24,29,34,45	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.

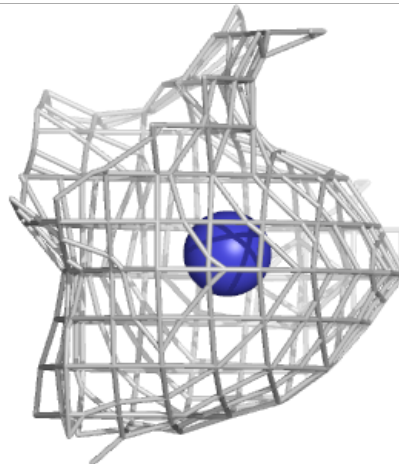
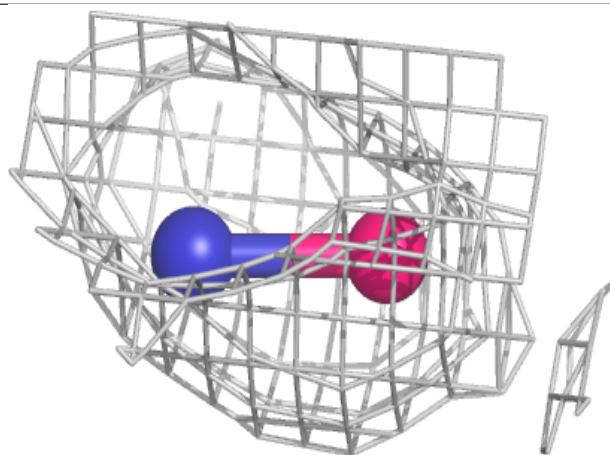
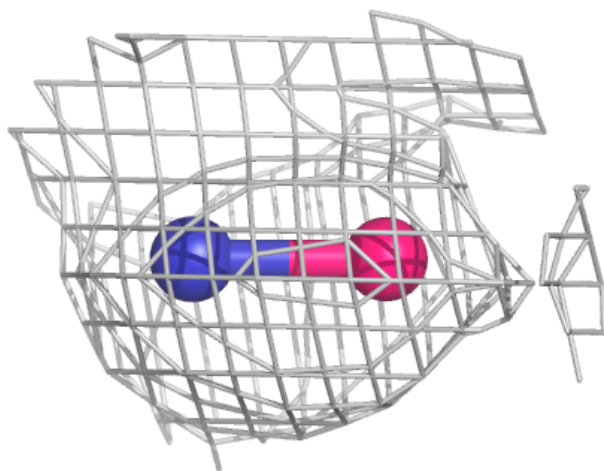
Electron density around HOA B 502:

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



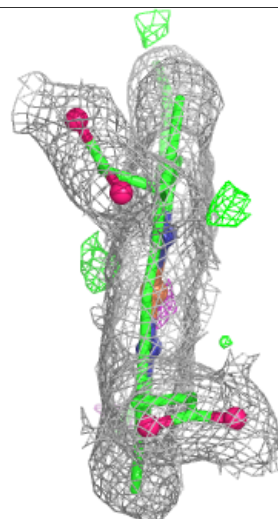
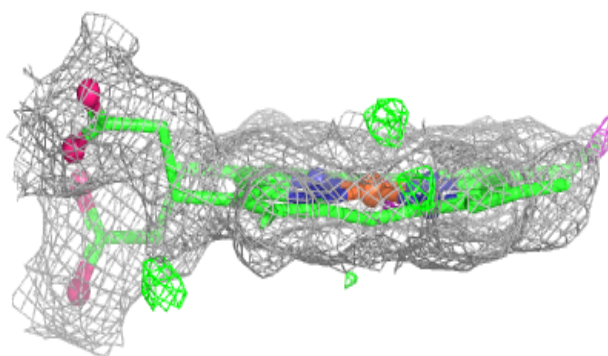
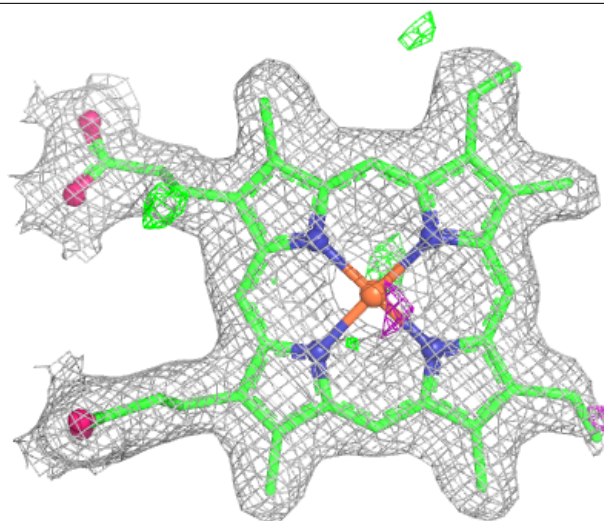
Electron density around HOA A 502:

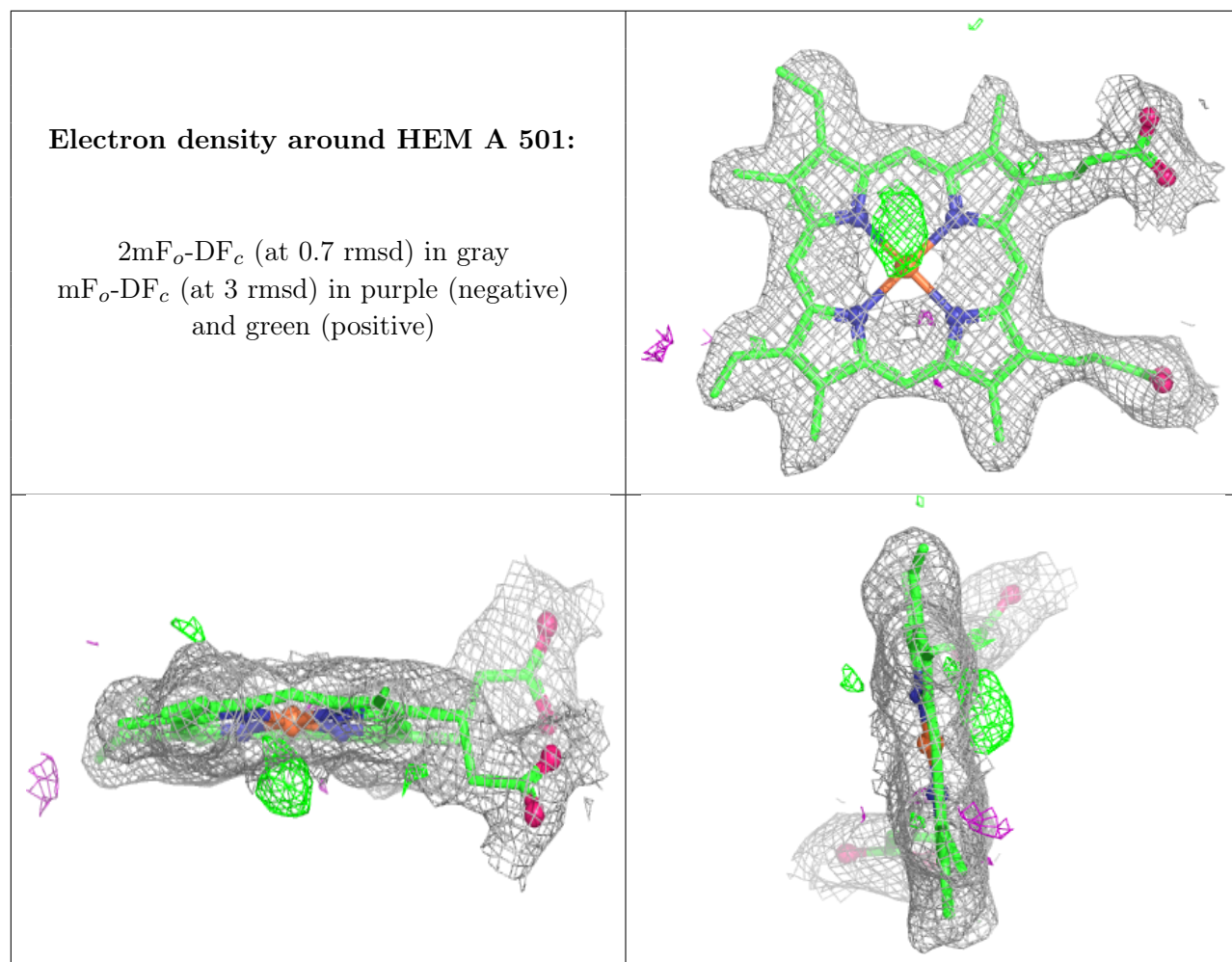
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.