



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 5, 2022 – 04:24 PM EDT

PDB ID : 7TS4
Title : Structure of human neuronal nitric oxide synthase R354A/G357D mutant heme domain in complex with 4-methyl-6-(3-(4-methylpiperazin-1-yl)prop-1-yn-1-yl)pyridin-2-amine
Authors : Li, H.; Poulos, T.L.
Deposited on : 2022-01-31
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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

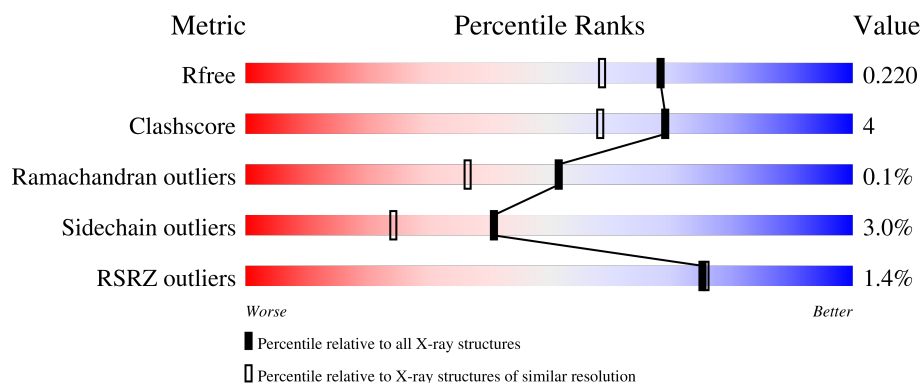
1 Overall quality at a glance

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	423	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 87% 11% .. </div> </div>
1	B	423	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 2% 91% 6% .. </div> </div>
1	C	423	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 2% 89% 8% .. </div> </div>
1	D	423	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 87% 11% .. </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15326 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 Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	5	0
			3435	2197	589	627	22			
1	B	414	Total	C	N	O	S	0	1	0
			3376	2163	575	617	21			
1	C	414	Total	C	N	O	S	0	5	0
			3392	2175	576	620	21			
1	D	418	Total	C	N	O	S	0	4	0
			3425	2191	586	627	21			

There are 16 discrepancies between the modelled and reference sequences:

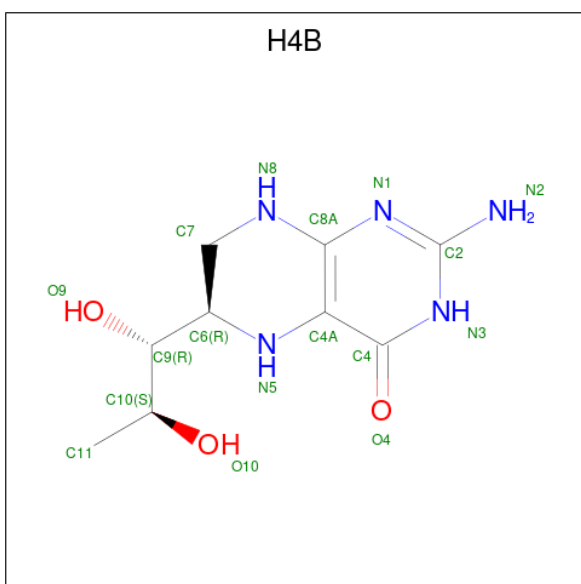
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
A	723	LEU	-	expression tag	UNP P29475
A	724	VAL	-	expression tag	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475
B	723	LEU	-	expression tag	UNP P29475
B	724	VAL	-	expression tag	UNP P29475
C	354	ALA	ARG	engineered mutation	UNP P29475
C	357	ASP	GLY	engineered mutation	UNP P29475
C	723	LEU	-	expression tag	UNP P29475
C	724	VAL	-	expression tag	UNP P29475
D	354	ALA	ARG	engineered mutation	UNP P29475
D	357	ASP	GLY	engineered mutation	UNP P29475
D	723	LEU	-	expression tag	UNP P29475
D	724	VAL	-	expression tag	UNP P29475

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



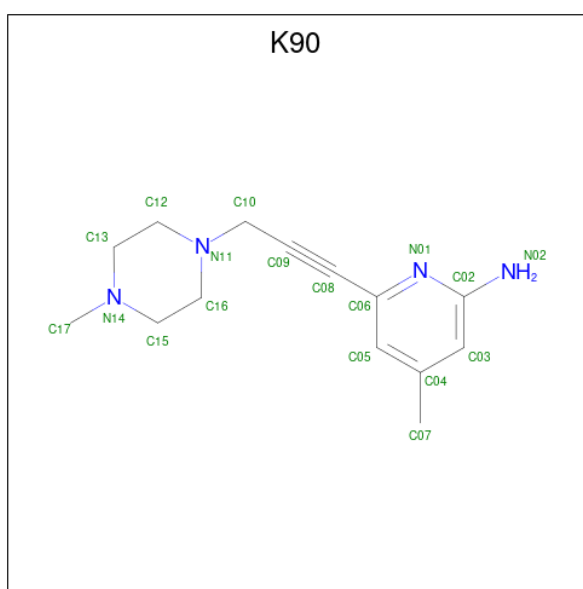
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 4-methyl-6-[3-(4-methylpiperazin-1-yl)prop-1-yn-1-yl]pyridin-2-amine (three-letter code: K90) (formula: C₁₄H₂₀N₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			18	14	4		
4	B	1	Total	C	N	0	0
			18	14	4		
4	C	1	Total	C	N	0	0
			18	14	4		
4	D	1	Total	C	N	0	0
			18	14	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		
6	D	1	Total	Zn	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	328	Total	O	0	0
			328	328		
7	B	327	Total	O	0	0
			327	327		

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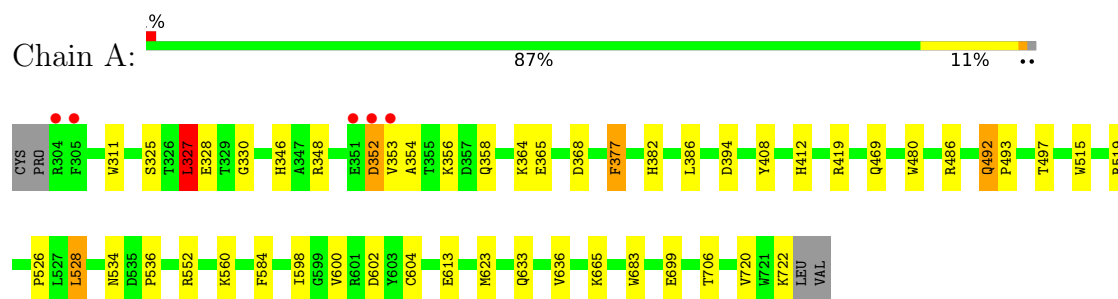
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	348	Total 348	O 348	0	0
7	D	351	Total 351	O 351	0	0

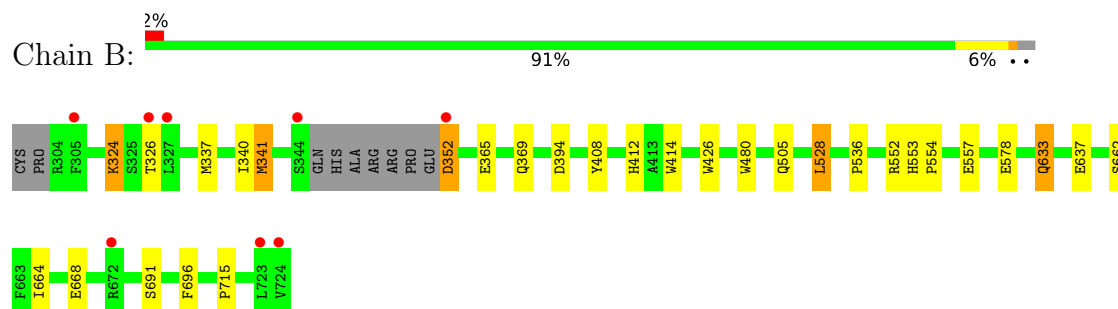
3 Residue-property plots [i](#)

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.

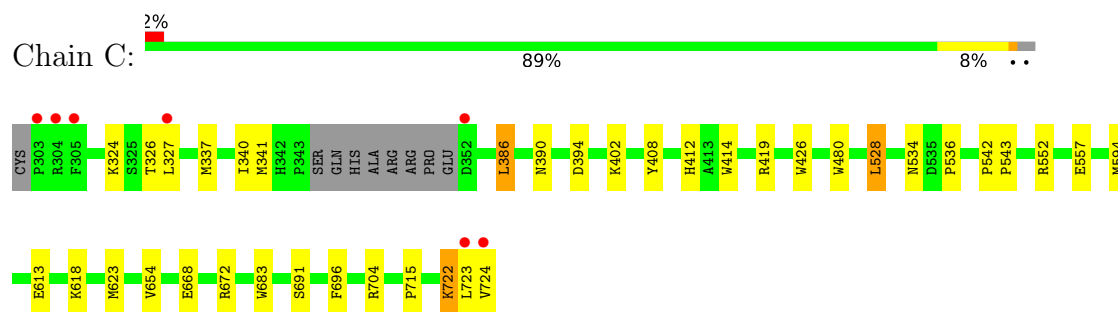
- Molecule 1: Nitric oxide synthase, brain



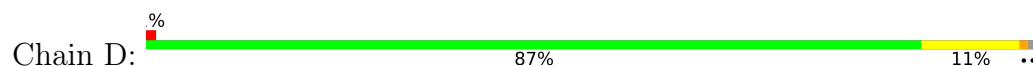
- Molecule 1: Nitric oxide synthase, brain

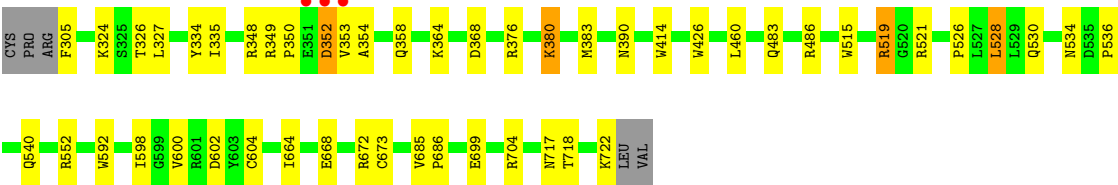


- Molecule 1: Nitric oxide synthase, brain



- Molecule 1: Nitric oxide synthase, brain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.22Å 117.85Å 165.15Å 90.00° 90.40° 90.00°	Depositor
Resolution (Å)	39.09 – 1.85 39.08 – 1.85	Depositor EDS
% Data completeness (in resolution range)	94.5 (39.09-1.85) 94.4 (39.08-1.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.178 , 0.222 0.175 , 0.220	Depositor DCC
R_{free} test set	8222 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.437 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15326	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 3.89% 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: HEM, H4B, GOL, ZN, K90

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	0.37	0/3548	0.53	1/4816 (0.0%)
1	B	0.40	0/3474	0.53	0/4713
1	C	0.40	0/3503	0.53	0/4754
1	D	0.39	0/3535	0.52	0/4798
All	All	0.39	0/14060	0.52	1/19081 (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	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	LEU	CA-CB-CG	6.66	130.61	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	350	PRO	Peptide

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	3435	0	3352	32	0
1	B	3376	0	3290	18	0
1	C	3392	0	3316	21	0
1	D	3425	0	3334	30	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
3	C	17	0	15	1	0
3	D	17	0	15	0	0
4	A	18	0	0	0	0
4	B	18	0	0	0	0
4	C	18	0	0	0	0
4	D	18	0	0	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	12	0	16	0	0
5	D	6	0	8	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	328	0	0	3	0
7	B	327	0	0	3	0
7	C	348	0	0	2	0
7	D	351	0	0	8	0
All	All	15326	0	13512	101	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 (101) 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:C:327:LEU:HB3	1:C:704:ARG:HD3	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:LEU:HD22	1:D:536:PRO:HB2	1.64	0.80
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.71	0.72
1:C:528:LEU:HD22	1:C:536:PRO:HB2	1.71	0.71
1:D:704:ARG:NH1	7:D:901:HOH:O	2.24	0.71
2:D:802:HEM:HBB2	2:D:802:HEM:HHC	1.74	0.70
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.75	0.69
1:A:528:LEU:HD22	1:A:536:PRO:HB2	1.74	0.69
1:D:352:ASP:N	1:D:352:ASP:OD1	2.25	0.68
1:A:560:LYS:NZ	7:A:904:HOH:O	2.27	0.68
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.77	0.67
1:B:578:GLU:OE1	7:B:901:HOH:O	2.12	0.67
2:D:802:HEM:HMC2	2:D:802:HEM:HBC2	1.77	0.65
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.78	0.65
2:B:801:HEM:HMC2	2:B:801:HEM:HBC2	1.78	0.65
2:C:801:HEM:HBC2	2:C:801:HEM:HMC2	1.79	0.64
1:B:664:ILE:O	1:B:668:GLU:HG2	1.98	0.63
1:D:664:ILE:O	1:D:668[B]:GLU:HG2	1.97	0.63
1:A:364:LYS:NZ	1:A:368:ASP:OD2	2.32	0.63
1:C:723:LEU:HD23	1:C:724:VAL:HG22	1.82	0.61
1:A:352:ASP:OD1	1:A:352:ASP:N	2.34	0.60
1:A:328:GLU:H	1:A:346:HIS:HD2	1.48	0.59
1:B:324:LYS:NZ	7:B:904:HOH:O	2.36	0.58
1:D:364:LYS:NZ	1:D:368:ASP:OD2	2.35	0.57
1:D:540:GLN:NE2	7:D:907:HOH:O	2.37	0.56
1:B:352:ASP:N	1:B:352:ASP:OD1	2.39	0.55
2:C:801:HEM:HHC	2:C:801:HEM:HBB2	1.88	0.54
1:D:521:ARG:NH1	7:D:903:HOH:O	2.28	0.54
1:A:356:LYS:HE3	1:D:672:ARG:O	2.08	0.54
1:D:483:GLN:HB2	1:D:486:ARG:HG3	1.90	0.53
1:B:480:TRP:HB2	1:B:528:LEU:HB3	1.91	0.52
1:A:492:GLN:HE21	1:A:493:PRO:HD2	1.74	0.51
1:C:341:MET:HE2	3:C:802:H4B:H9	1.93	0.51
1:C:722:LYS:NZ	7:C:904:HOH:O	2.32	0.50
1:A:327:LEU:HD12	1:A:346:HIS:O	2.12	0.49
1:B:414:TRP:CE3	1:B:426:TRP:HA	2.48	0.49
1:D:327:LEU:HD11	1:D:348:ARG:HD2	1.93	0.49
1:D:515:TRP:CE2	1:D:526:PRO:HD3	2.47	0.49
1:C:480:TRP:HB2	1:C:528:LEU:HB3	1.95	0.49
1:A:330:GLY:O	1:D:380:LYS:HE3	2.14	0.48
1:A:699:GLU:HB3	1:B:340:ILE:HD13	1.95	0.48
1:D:327:LEU:HD21	1:D:348:ARG:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:THR:OG1	7:A:901:HOH:O	2.20	0.48
1:C:414:TRP:CE3	1:C:426:TRP:HA	2.49	0.48
1:A:328:GLU:H	1:A:346:HIS:CD2	2.30	0.47
1:C:408:TYR:CE1	1:C:412:HIS:CE1	3.02	0.47
1:A:356:LYS:HE2	1:A:394:ASP:OD2	2.15	0.47
1:A:519:ARG:NH1	7:A:906:HOH:O	2.42	0.46
1:D:354:ALA:HB1	1:D:358:GLN:HB2	1.97	0.46
1:C:340:ILE:HD13	1:D:699:GLU:HB3	1.96	0.46
1:D:717:ASN:ND2	7:D:908:HOH:O	2.40	0.46
1:A:377:PHE:HA	1:A:382:HIS:ND1	2.30	0.46
1:D:600:VAL:O	1:D:604:CYS:HB2	2.16	0.46
1:B:480:TRP:CE2	1:B:715:PRO:HB2	2.51	0.45
1:D:376:ARG:NH2	7:D:915:HOH:O	2.50	0.45
1:A:534:ASN:HA	1:A:722:LYS:HE3	1.98	0.45
1:A:346:HIS:CE1	1:D:376:ARG:HA	2.52	0.45
1:B:337:MET:HB3	1:B:340:ILE:HG13	1.98	0.45
1:D:414:TRP:CE3	1:D:426:TRP:HA	2.51	0.45
1:D:519:ARG:NH1	7:D:911:HOH:O	2.43	0.45
1:B:553:HIS:CG	1:B:554:PRO:HD2	2.52	0.45
1:A:480:TRP:HB2	1:A:528:LEU:HB3	1.99	0.45
1:A:469:GLN:HB3	1:A:584:PHE:CE2	2.52	0.44
1:A:354:ALA:HB1	1:A:358:GLN:HB2	1.99	0.44
1:C:480:TRP:CE2	1:C:715:PRO:HB2	2.53	0.44
1:C:542:PRO:HA	1:C:543:PRO:HD3	1.91	0.44
1:A:311:TRP:CE2	1:B:341:MET:HE3	2.53	0.44
1:C:402:LYS:HA	1:C:402:LYS:HD3	1.82	0.44
1:D:460:LEU:HD12	1:D:592:TRP:HB3	2.00	0.44
1:A:600:VAL:O	1:A:604:CYS:HB2	2.18	0.43
1:A:633:GLN:NE2	1:B:637:GLU:OE2	2.52	0.43
1:B:341:MET:HE2	1:B:341:MET:HB2	1.75	0.43
1:C:337:MET:HB3	1:C:340:ILE:HG13	2.01	0.43
1:C:534:ASN:HA	1:C:722:LYS:HE2	2.00	0.43
1:A:598:ILE:HA	1:A:602:ASP:HB2	2.01	0.43
1:B:408:TYR:CE1	1:B:412:HIS:CE1	3.07	0.43
1:C:419:ARG:HD3	1:C:683:TRP:CD2	2.53	0.43
1:D:380:LYS:NZ	7:D:921:HOH:O	2.52	0.43
1:C:390:ASN:OD1	7:C:901:HOH:O	2.22	0.42
1:A:348:ARG:CD	1:A:706[B]:THR:HG21	2.49	0.42
1:D:673:CYS:HB3	7:D:1209:HOH:O	2.19	0.42
1:C:691:SER:HA	1:C:696:PHE:CG	2.53	0.42
1:C:668:GLU:O	1:C:672:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:598:ILE:HA	1:D:602:ASP:HB2	2.02	0.42
1:C:386:LEU:HD12	1:C:386:LEU:HA	1.92	0.42
1:D:334:TYR:C	1:D:335:ILE:HG13	2.40	0.42
1:A:613:GLU:HG3	1:A:623:MET:HE3	2.02	0.41
1:A:492:GLN:HE21	1:A:492:GLN:HA	1.86	0.41
1:B:662:SER:HB2	7:B:1077:HOH:O	2.20	0.41
1:D:349:ARG:NH2	1:D:354:ALA:H	2.19	0.41
1:A:636:VAL:HG11	1:B:633:GLN:HG3	2.02	0.41
1:A:408:TYR:CE1	1:A:412:HIS:CE1	3.09	0.41
1:A:515:TRP:CE2	1:A:526:PRO:HD3	2.56	0.41
1:A:665:LYS:HB2	1:A:665:LYS:HE3	1.91	0.40
1:C:594:MET:HA	1:C:654:VAL:O	2.21	0.40
1:D:685:VAL:HA	1:D:686:PRO:HD3	1.96	0.40
1:B:691:SER:HA	1:B:696:PHE:CG	2.56	0.40
1:C:613:GLU:HG3	1:C:623:MET:HE3	2.02	0.40
1:A:419:ARG:HD3	1:A:683:TRP:CD2	2.56	0.40
1:D:460:LEU:HD12	1:D:592:TRP:CB	2.51	0.40
1:D:530:GLN:HG3	1:D:534:ASN:O	2.22	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	422/423 (100%)	410 (97%)	11 (3%)	1 (0%)	47	33
1	B	411/423 (97%)	405 (98%)	6 (2%)	0	100	100
1	C	415/423 (98%)	407 (98%)	8 (2%)	0	100	100
1	D	420/423 (99%)	411 (98%)	9 (2%)	0	100	100
All	All	1668/1692 (99%)	1633 (98%)	34 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	PHE

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	379/378 (100%)	368 (97%)	11 (3%)	42	26
1	B	371/378 (98%)	359 (97%)	12 (3%)	39	22
1	C	375/378 (99%)	366 (98%)	9 (2%)	49	33
1	D	377/378 (100%)	364 (97%)	13 (3%)	37	19
All	All	1502/1512 (99%)	1457 (97%)	45 (3%)	41	24

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	SER
1	A	327	LEU
1	A	352	ASP
1	A	353	VAL
1	A	365	GLU
1	A	386	LEU
1	A	486	ARG
1	A	492	GLN
1	A	528	LEU
1	A	552	ARG
1	A	720	VAL
1	B	324	LYS
1	B	326	THR
1	B	341	MET
1	B	352	ASP
1	B	365	GLU
1	B	369	GLN
1	B	394	ASP
1	B	505	GLN
1	B	528	LEU
1	B	552	ARG

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Mol	Chain	Res	Type
1	B	557	GLU
1	B	633	GLN
1	C	324	LYS
1	C	326	THR
1	C	386	LEU
1	C	394	ASP
1	C	528	LEU
1	C	552	ARG
1	C	557	GLU
1	C	618	LYS
1	C	722	LYS
1	D	305	PHE
1	D	324	LYS
1	D	326	THR
1	D	352	ASP
1	D	353	VAL
1	D	380	LYS
1	D	383	MET
1	D	390	ASN
1	D	519	ARG
1	D	528	LEU
1	D	552	ARG
1	D	718	THR
1	D	722	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	HIS
1	A	492	GLN
1	D	540	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

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	H4B	C	802	-	16,18,18	0.99	1 (6%)	11,26,26	2.53	5 (45%)
2	HEM	A	801	1	41,50,50	1.53	7 (17%)	45,82,82	1.61	7 (15%)
4	K90	C	803	-	19,19,19	2.05	1 (5%)	25,25,25	1.42	3 (12%)
4	K90	B	803	-	19,19,19	2.01	1 (5%)	25,25,25	1.54	4 (16%)
4	K90	D	804	-	19,19,19	2.10	1 (5%)	25,25,25	1.41	3 (12%)
5	GOL	A	804	-	5,5,5	0.26	0	5,5,5	0.69	0
5	GOL	D	805	-	5,5,5	0.42	0	5,5,5	0.10	0
3	H4B	D	803	-	16,18,18	0.86	0	11,26,26	2.50	5 (45%)
3	H4B	B	802	-	16,18,18	0.85	0	11,26,26	2.58	6 (54%)
5	GOL	C	805	-	5,5,5	0.37	0	5,5,5	0.39	0
4	K90	A	803	-	19,19,19	2.16	1 (5%)	25,25,25	1.41	5 (20%)
5	GOL	B	804	-	5,5,5	0.34	0	5,5,5	0.29	0
2	HEM	D	802	1	41,50,50	1.51	6 (14%)	45,82,82	1.84	11 (24%)
2	HEM	C	801	1	41,50,50	1.46	4 (9%)	45,82,82	1.59	7 (15%)
2	HEM	B	801	1	41,50,50	1.51	8 (19%)	45,82,82	1.56	8 (17%)
5	GOL	C	804	-	5,5,5	0.35	0	5,5,5	0.33	0
3	H4B	A	802	-	16,18,18	0.85	0	11,26,26	2.58	6 (54%)

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	H4B	C	802	-	-	0/8/17/17	0/2/2/2
2	HEM	A	801	1	-	1/12/54/54	-
4	K90	C	803	-	-	3/5/16/16	0/2/2/2
4	K90	B	803	-	-	3/5/16/16	0/2/2/2
4	K90	D	804	-	-	2/5/16/16	0/2/2/2
5	GOL	A	804	-	-	0/4/4/4	-
5	GOL	D	805	-	-	4/4/4/4	-
3	H4B	D	803	-	-	0/8/17/17	0/2/2/2
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
5	GOL	C	805	-	-	2/4/4/4	-
4	K90	A	803	-	-	2/5/16/16	0/2/2/2
5	GOL	B	804	-	-	2/4/4/4	-
2	HEM	D	802	1	-	3/12/54/54	-
2	HEM	C	801	1	-	2/12/54/54	-
2	HEM	B	801	1	-	1/12/54/54	-
5	GOL	C	804	-	-	0/4/4/4	-
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	K90	C06-C08	-9.17	1.29	1.44
4	D	804	K90	C06-C08	-8.93	1.29	1.44
4	C	803	K90	C06-C08	-8.72	1.29	1.44
4	B	803	K90	C06-C08	-8.59	1.30	1.44
2	C	801	HEM	C3C-CAC	3.79	1.55	1.47
2	A	801	HEM	C3C-C2C	-3.67	1.35	1.40
2	A	801	HEM	C3C-CAC	3.58	1.55	1.47
2	B	801	HEM	C3C-CAC	3.48	1.54	1.47
2	C	801	HEM	C3C-C2C	-3.40	1.35	1.40
2	D	802	HEM	C3C-CAC	3.33	1.54	1.47
2	B	801	HEM	C3C-C2C	-3.20	1.35	1.40
2	B	801	HEM	CAB-C3B	3.14	1.56	1.47
2	C	801	HEM	CAB-C3B	3.12	1.55	1.47
2	D	802	HEM	CAB-C3B	3.00	1.55	1.47
2	D	802	HEM	C3C-C2C	-2.96	1.36	1.40
2	A	801	HEM	CAB-C3B	2.93	1.55	1.47
3	C	802	H4B	C4A-C4	-2.57	1.38	1.41
2	A	801	HEM	FE-NB	2.54	2.09	1.96
2	B	801	HEM	FE-NB	2.46	2.09	1.96
2	D	802	HEM	FE-NB	2.44	2.08	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	CMD-C2D	2.25	1.55	1.50
2	D	802	HEM	CAD-C3D	2.23	1.57	1.51
2	A	801	HEM	CMB-C2B	2.22	1.55	1.50
2	C	801	HEM	CMB-C2B	2.20	1.55	1.50
2	D	802	HEM	CMB-C2B	2.18	1.55	1.50
2	B	801	HEM	CMB-C2B	2.17	1.55	1.50
2	B	801	HEM	CMA-C3A	2.16	1.56	1.51
2	A	801	HEM	C3B-C2B	-2.09	1.33	1.37
2	B	801	HEM	CMD-C2D	2.08	1.55	1.50
2	B	801	HEM	FE-ND	2.03	2.06	1.96

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	H4B	C8A-C4A-C4	4.70	118.75	114.57
3	A	802	H4B	C8A-C4A-C4	4.62	118.68	114.57
3	D	803	H4B	C8A-C4A-C4	4.61	118.66	114.57
4	B	803	K90	C05-C06-N01	-4.51	118.99	123.61
3	C	802	H4B	C8A-C4A-C4	4.49	118.55	114.57
4	C	803	K90	C05-C06-N01	-4.25	119.26	123.61
2	A	801	HEM	CBA-CAA-C2A	-4.14	105.56	112.62
2	D	802	HEM	CBA-CAA-C2A	-3.99	105.81	112.62
2	A	801	HEM	C4B-CHC-C1C	3.88	127.68	122.56
4	D	804	K90	C05-C06-N01	-3.84	119.67	123.61
2	C	801	HEM	C4B-CHC-C1C	3.77	127.53	122.56
3	B	802	H4B	C2-N3-C4	3.76	121.90	115.93
3	C	802	H4B	C2-N3-C4	3.68	121.78	115.93
3	D	803	H4B	C2-N3-C4	3.64	121.71	115.93
2	D	802	HEM	C4B-CHC-C1C	3.63	127.35	122.56
3	C	802	H4B	N1-C2-N3	-3.61	119.75	125.42
2	C	801	HEM	CBA-CAA-C2A	-3.61	106.47	112.62
3	A	802	H4B	C2-N3-C4	3.60	121.64	115.93
2	B	801	HEM	C4B-CHC-C1C	3.59	127.30	122.56
2	D	802	HEM	C4D-ND-C1D	3.54	108.73	105.07
2	D	802	HEM	C1B-NB-C4B	3.49	108.68	105.07
3	B	802	H4B	N1-C2-N3	-3.47	119.98	125.42
3	A	802	H4B	N1-C2-N3	-3.44	120.02	125.42
2	B	801	HEM	CBA-CAA-C2A	-3.38	106.85	112.62
3	D	803	H4B	N1-C2-N3	-3.37	120.13	125.42
4	A	803	K90	C05-C06-N01	-3.29	120.24	123.61
4	D	804	K90	C06-N01-C02	3.23	122.15	116.90
4	B	803	K90	C06-C05-C04	2.86	121.36	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	802	HEM	C4C-CHD-C1D	2.85	126.32	122.56
3	A	802	H4B	N2-C2-N1	2.83	121.65	117.25
4	A	803	K90	C06-N01-C02	2.78	121.42	116.90
2	D	802	HEM	CMA-C3A-C4A	-2.76	124.22	128.46
2	A	801	HEM	C1B-NB-C4B	2.76	107.92	105.07
2	B	801	HEM	C4D-ND-C1D	2.76	107.92	105.07
4	C	803	K90	C06-N01-C02	2.73	121.35	116.90
2	A	801	HEM	C3B-C2B-C1B	2.73	108.51	106.49
4	B	803	K90	C08-C06-N01	2.70	120.91	116.55
2	B	801	HEM	C1B-NB-C4B	2.69	107.86	105.07
2	C	801	HEM	C1B-NB-C4B	2.69	107.85	105.07
3	D	803	H4B	N2-C2-N1	2.66	121.39	117.25
2	C	801	HEM	C4D-ND-C1D	2.66	107.82	105.07
2	A	801	HEM	C4D-ND-C1D	2.63	107.78	105.07
3	C	802	H4B	N2-C2-N1	2.61	121.31	117.25
2	D	802	HEM	CMC-C2C-C3C	2.58	129.50	124.68
3	A	802	H4B	C2-N1-C8A	2.55	120.25	114.54
2	D	802	HEM	C3B-C2B-C1B	2.50	108.34	106.49
2	D	802	HEM	C2D-C1D-ND	-2.49	106.91	109.88
3	B	802	H4B	C2-N1-C8A	2.48	120.10	114.54
2	A	801	HEM	CMA-C3A-C4A	-2.40	124.78	128.46
2	C	801	HEM	C3B-C2B-C1B	2.39	108.26	106.49
2	B	801	HEM	CMC-C2C-C3C	2.38	129.14	124.68
3	D	803	H4B	C2-N1-C8A	2.37	119.84	114.54
3	A	802	H4B	C4-C4A-N5	2.34	121.09	119.12
3	C	802	H4B	C2-N1-C8A	2.33	119.77	114.54
2	B	801	HEM	CBD-CAD-C3D	-2.33	106.16	112.63
3	B	802	H4B	N2-C2-N1	2.32	120.86	117.25
2	D	802	HEM	C2C-C3C-C4C	2.32	108.52	106.90
2	C	801	HEM	C3D-C4D-ND	-2.32	107.59	110.17
4	B	803	K90	C06-N01-C02	2.31	120.66	116.90
2	B	801	HEM	C3B-C2B-C1B	2.30	108.19	106.49
4	D	804	K90	C05-C06-C08	2.26	122.25	119.83
2	B	801	HEM	C3D-C4D-ND	-2.26	107.66	110.17
4	C	803	K90	C08-C06-N01	2.24	120.17	116.55
2	C	801	HEM	CMC-C2C-C3C	2.23	128.85	124.68
4	A	803	K90	N02-C02-N01	2.22	120.00	116.49
2	A	801	HEM	C3D-C4D-ND	-2.21	107.71	110.17
3	B	802	H4B	C4A-N5-C6	-2.12	115.38	121.16
4	A	803	K90	C08-C06-N01	2.12	119.98	116.55
4	A	803	K90	C10-N11-C12	-2.10	109.27	111.71
2	D	802	HEM	C3D-C4D-ND	-2.04	107.89	110.17

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	K90	C05-C06-C08-C09
4	A	803	K90	N01-C06-C08-C09
4	B	803	K90	C08-C09-C10-N11
4	B	803	K90	C05-C06-C08-C09
4	B	803	K90	N01-C06-C08-C09
4	C	803	K90	C08-C09-C10-N11
4	C	803	K90	N01-C06-C08-C09
4	D	804	K90	C08-C09-C10-N11
5	B	804	GOL	O1-C1-C2-C3
5	C	805	GOL	O1-C1-C2-C3
5	D	805	GOL	O1-C1-C2-C3
5	D	805	GOL	C1-C2-C3-O3
5	C	805	GOL	O1-C1-C2-O2
5	D	805	GOL	O1-C1-C2-O2
5	B	804	GOL	O1-C1-C2-O2
5	D	805	GOL	O2-C2-C3-O3
2	A	801	HEM	C4B-C3B-CAB-CBB
2	B	801	HEM	C4B-C3B-CAB-CBB
2	D	802	HEM	C4B-C3B-CAB-CBB
4	C	803	K90	C05-C06-C08-C09
2	D	802	HEM	CAA-CBA-CGA-O2A
2	D	802	HEM	CAA-CBA-CGA-O1A
2	C	801	HEM	CAA-CBA-CGA-O2A
4	D	804	K90	N01-C06-C08-C09
2	C	801	HEM	CAA-CBA-CGA-O1A

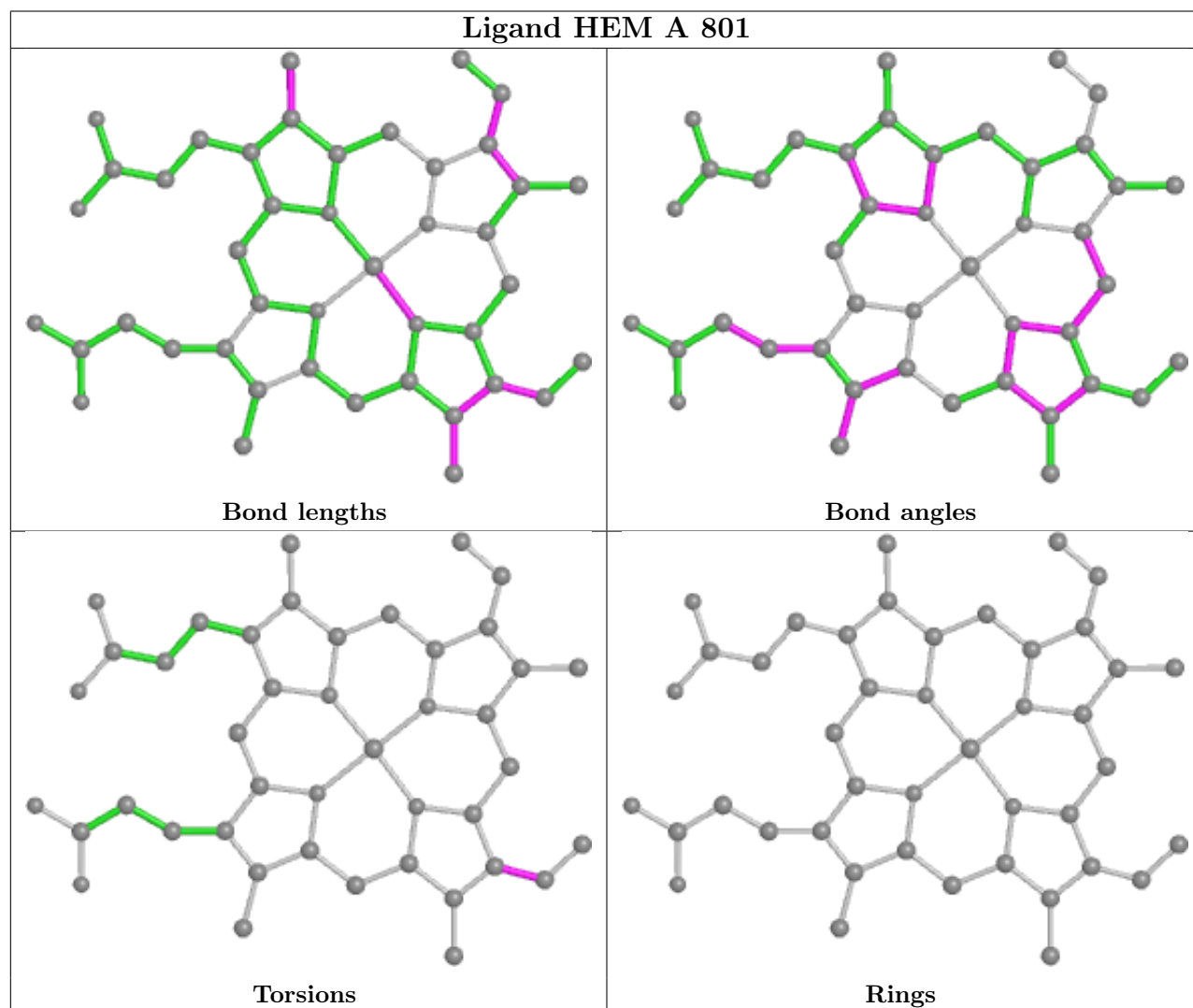
There are no ring outliers.

5 monomers are involved in 9 short contacts:

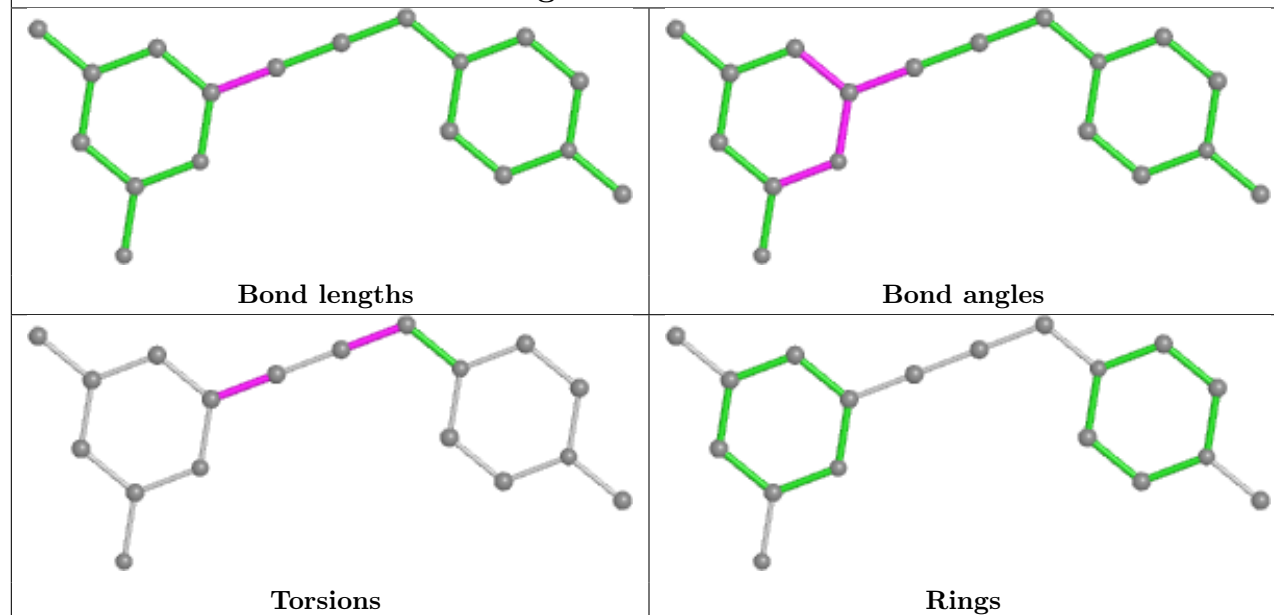
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	H4B	1	0
2	A	801	HEM	2	0
2	D	802	HEM	2	0
2	C	801	HEM	2	0
2	B	801	HEM	2	0

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

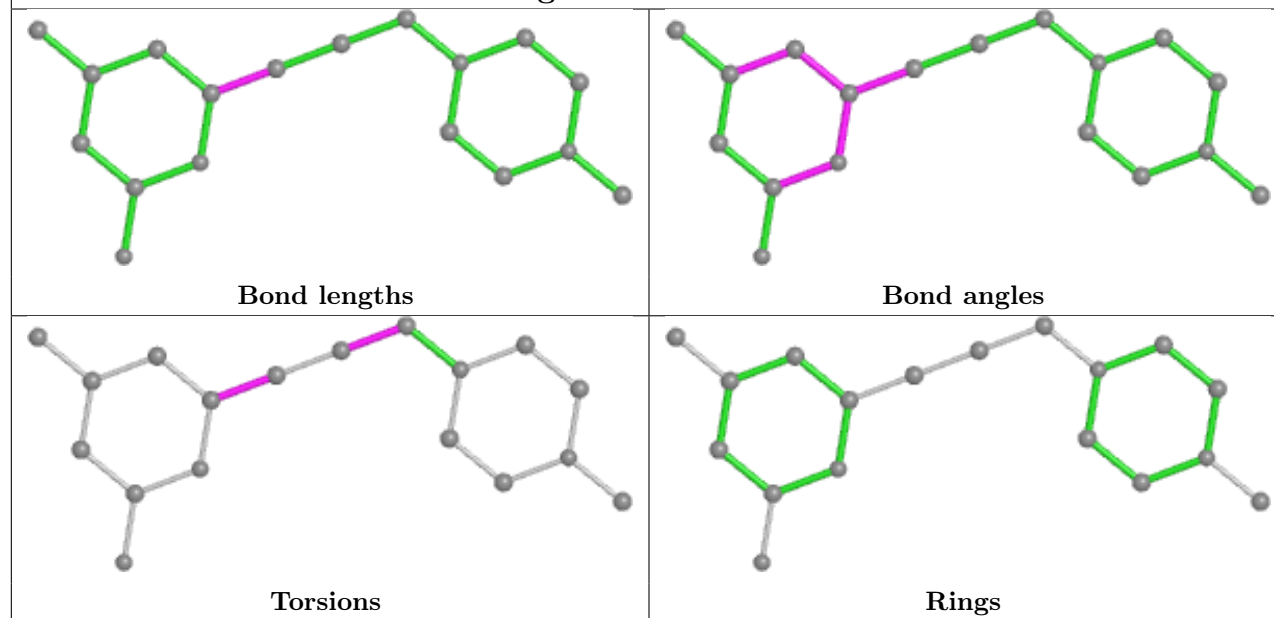
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



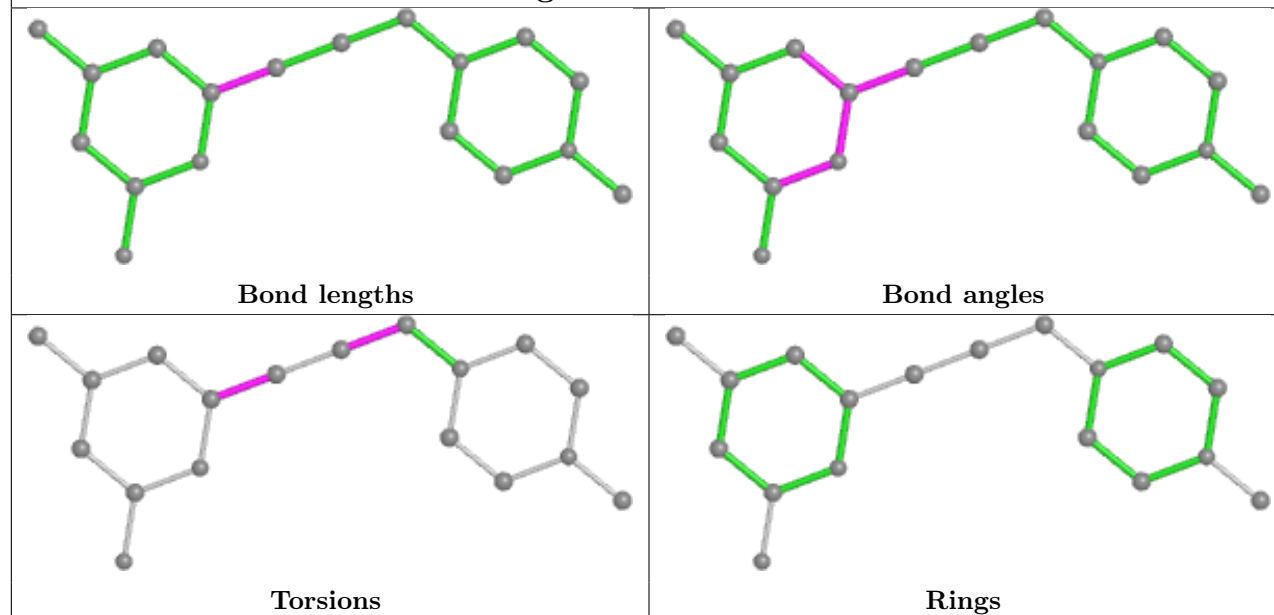
Ligand K90 C 803



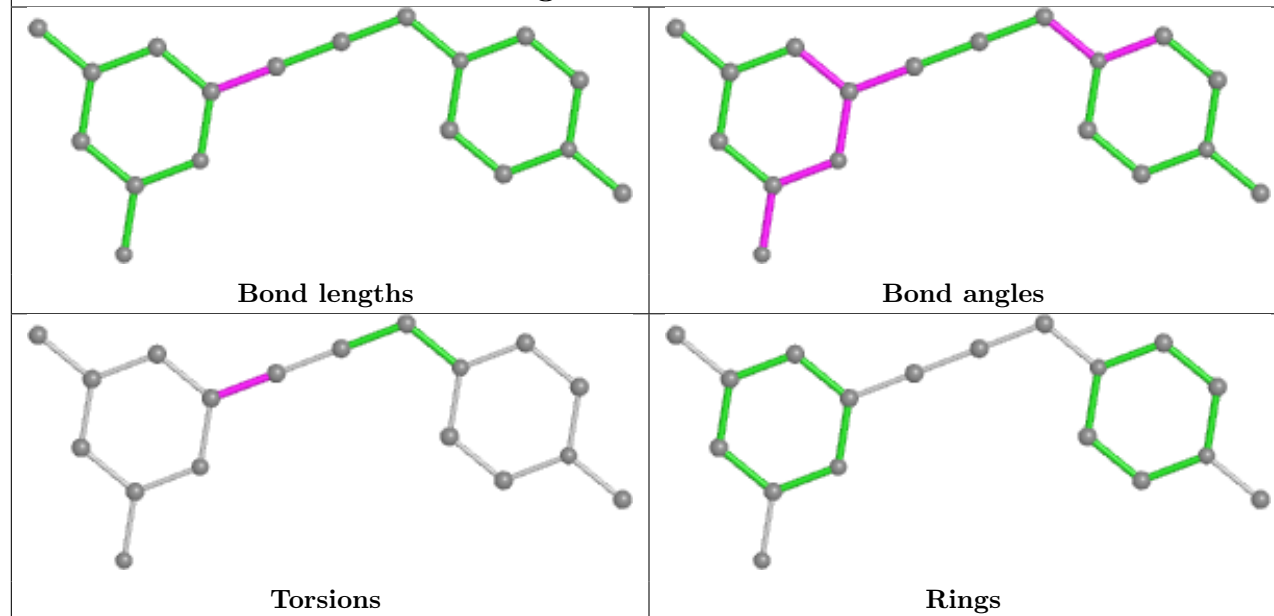
Ligand K90 B 803

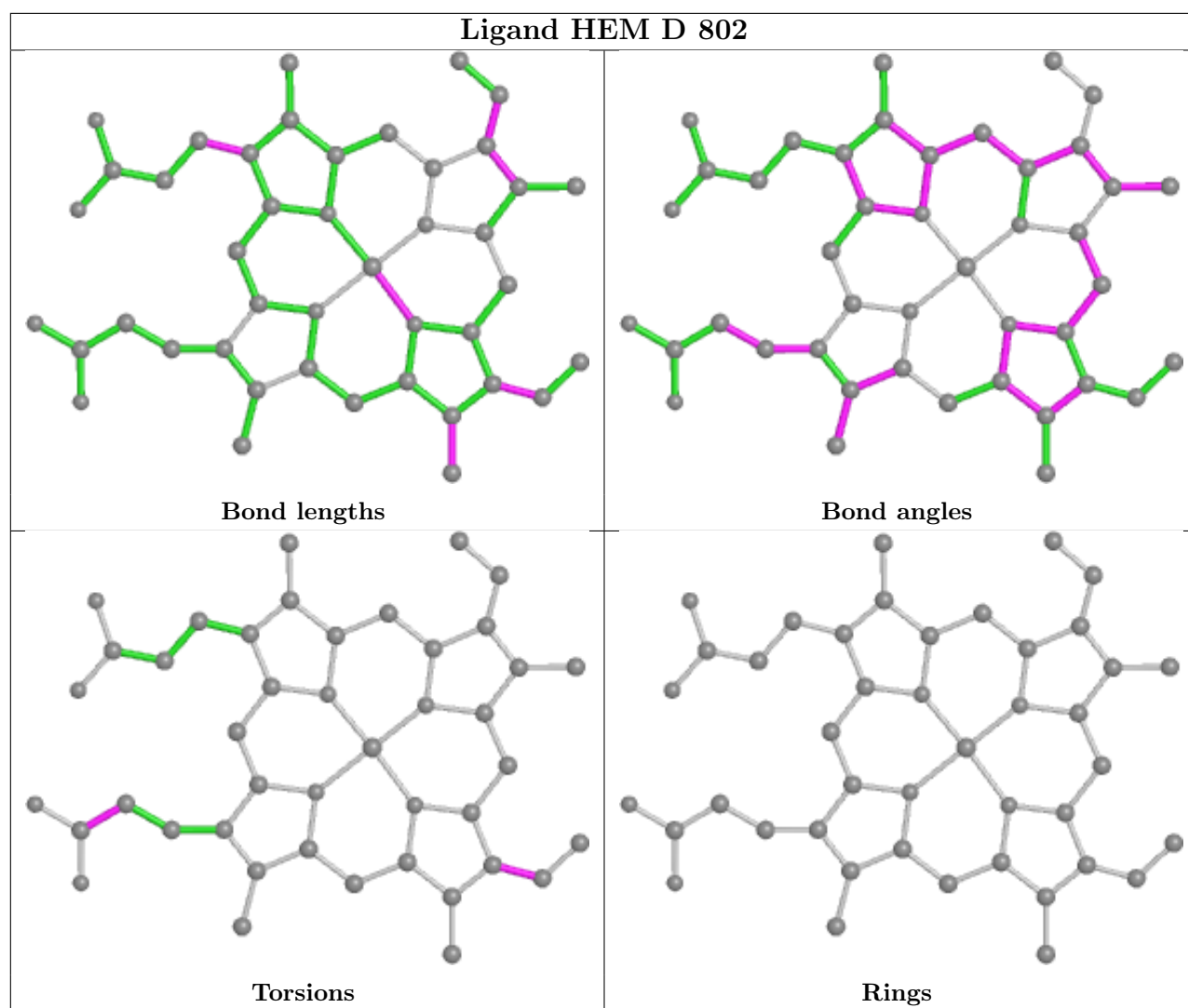


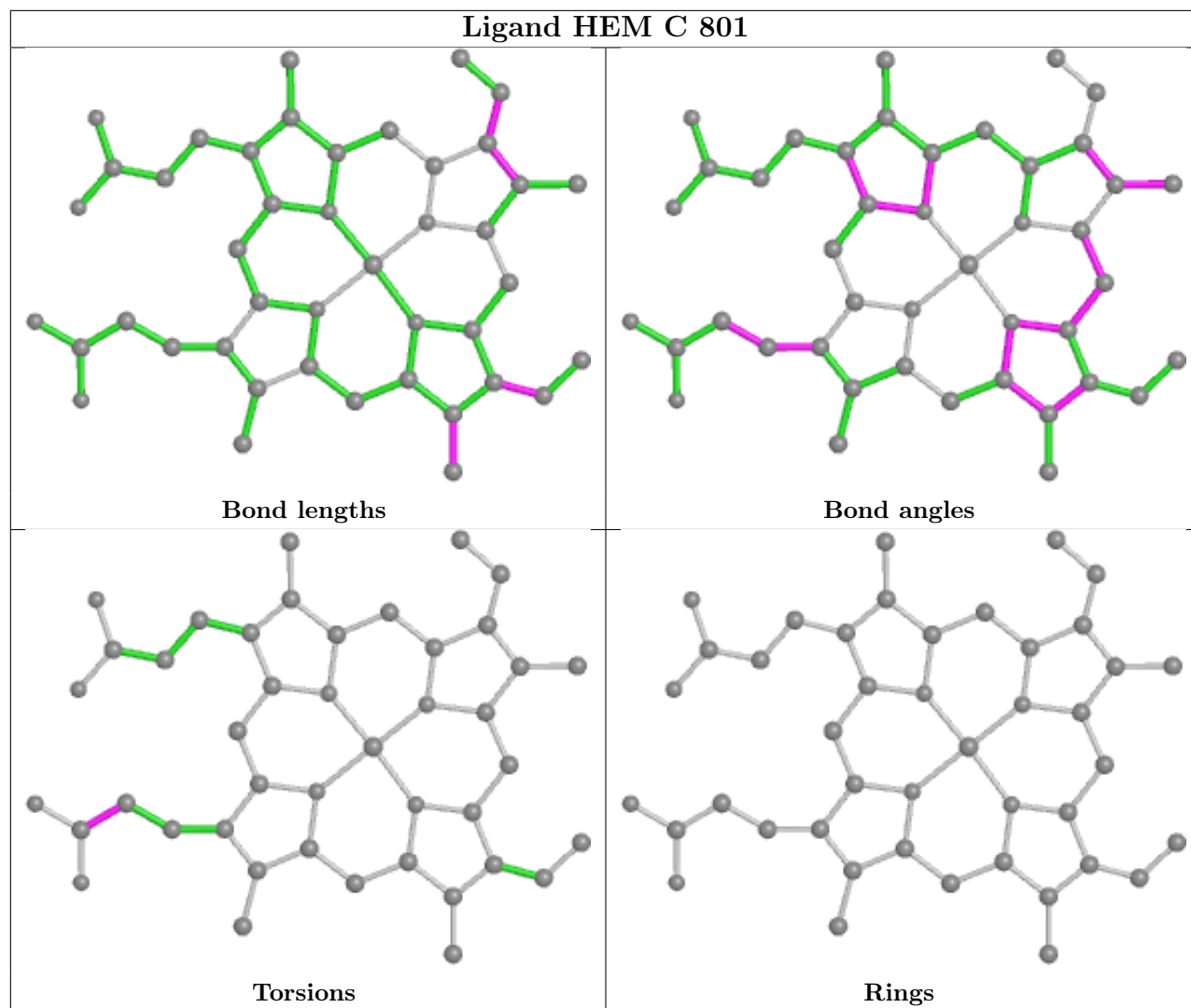
Ligand K90 D 804

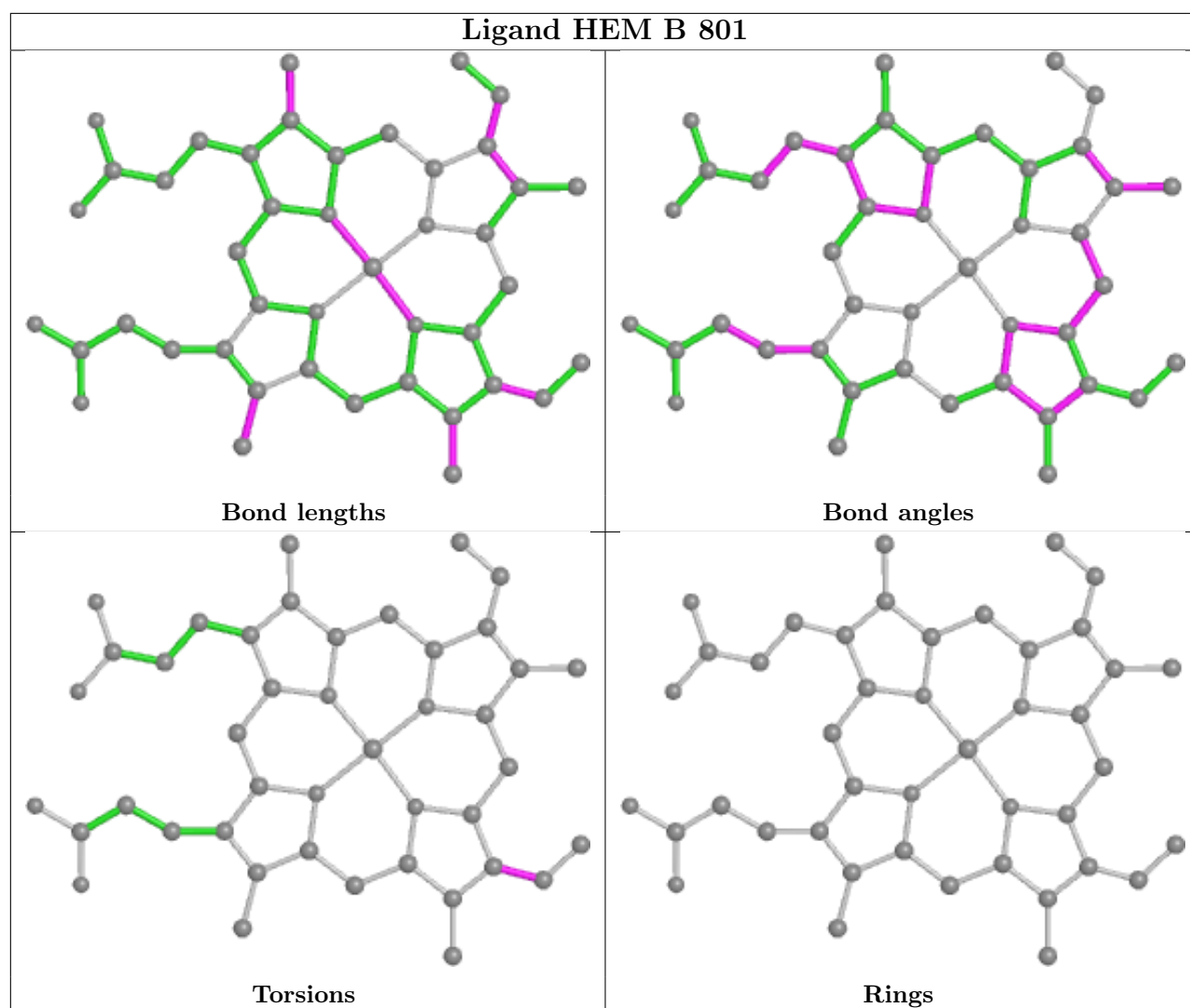


Ligand K90 A 803









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	419/423 (99%)	-0.47	5 (1%) 79 79	22, 37, 69, 100	0
1	B	414/423 (97%)	-0.51	8 (1%) 66 66	20, 34, 62, 91	0
1	C	414/423 (97%)	-0.50	7 (1%) 70 70	21, 33, 61, 89	0
1	D	418/423 (98%)	-0.52	3 (0%) 87 88	22, 37, 67, 95	0
All	All	1665/1692 (98%)	-0.50	23 (1%) 75 76	20, 35, 66, 100	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	724	VAL	5.6
1	A	351	GLU	4.7
1	C	724	VAL	4.5
1	A	353	VAL	4.4
1	A	352	ASP	4.3
1	C	327	LEU	4.2
1	D	351	GLU	3.8
1	C	723	LEU	3.8
1	B	352	ASP	3.7
1	C	304	ARG	3.5
1	A	305	PHE	3.4
1	C	303	PRO	3.1
1	C	352	ASP	3.1
1	B	305	PHE	3.0
1	D	352	ASP	3.0
1	C	305	PHE	2.7
1	B	723	LEU	2.6
1	B	326	THR	2.5
1	B	672	ARG	2.4
1	B	344	SER	2.3
1	D	353	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	327	LEU	2.3
1	A	304	ARG	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 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.

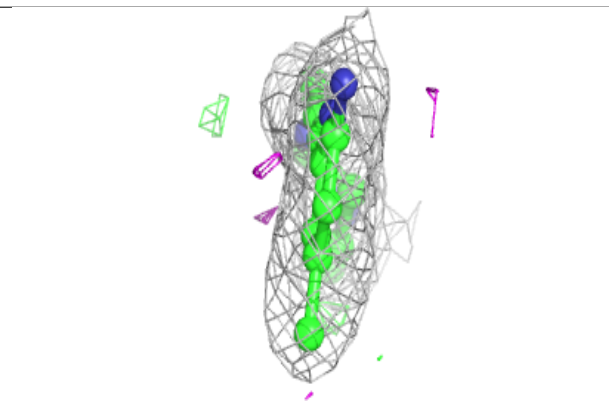
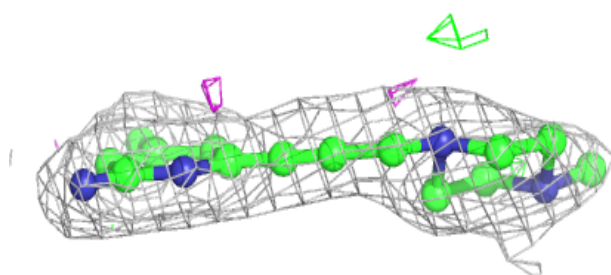
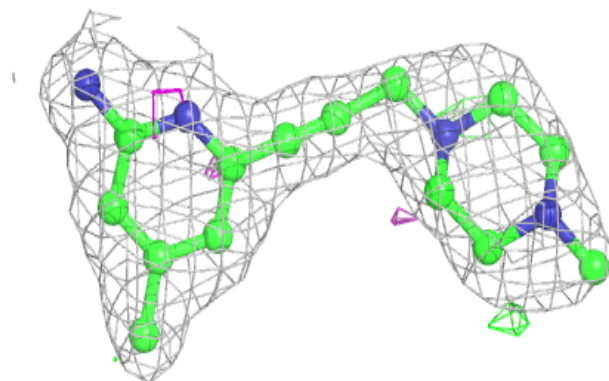
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	C	804	6/6	0.74	0.19	68,69,74,77	0
5	GOL	D	805	6/6	0.86	0.19	58,70,75,77	0
5	GOL	C	805	6/6	0.87	0.16	42,58,61,62	0
5	GOL	B	804	6/6	0.88	0.20	58,66,72,74	0
5	GOL	A	804	6/6	0.91	0.14	42,55,61,66	0
4	K90	D	804	18/18	0.95	0.11	21,36,60,60	0
4	K90	B	803	18/18	0.95	0.13	21,43,66,70	0
4	K90	C	803	18/18	0.95	0.12	26,39,68,70	0
3	H4B	C	802	17/17	0.96	0.07	23,29,32,34	0
4	K90	A	803	18/18	0.96	0.10	23,41,57,59	0
3	H4B	A	802	17/17	0.97	0.06	22,32,37,38	0
3	H4B	B	802	17/17	0.97	0.07	22,28,31,31	0
3	H4B	D	803	17/17	0.98	0.06	25,31,35,37	0
2	HEM	B	801	43/43	0.98	0.08	19,27,35,42	0
2	HEM	C	801	43/43	0.99	0.08	19,27,34,38	0
2	HEM	D	802	43/43	0.99	0.08	17,25,35,40	0
2	HEM	A	801	43/43	0.99	0.08	19,27,37,43	0
6	ZN	A	805	1/1	1.00	0.06	29,29,29,29	0
6	ZN	D	801	1/1	1.00	0.08	29,29,29,29	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.

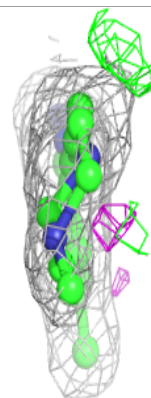
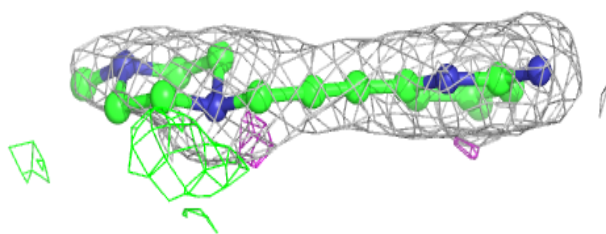
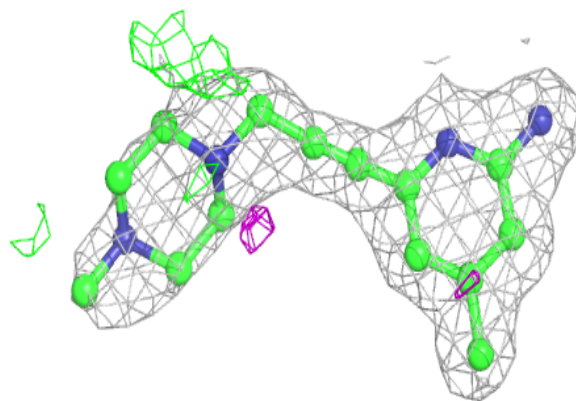
Electron density around K90 D 804:

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

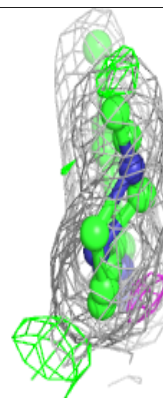
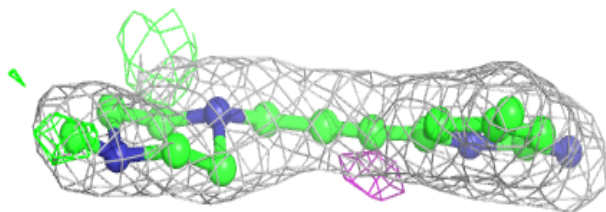
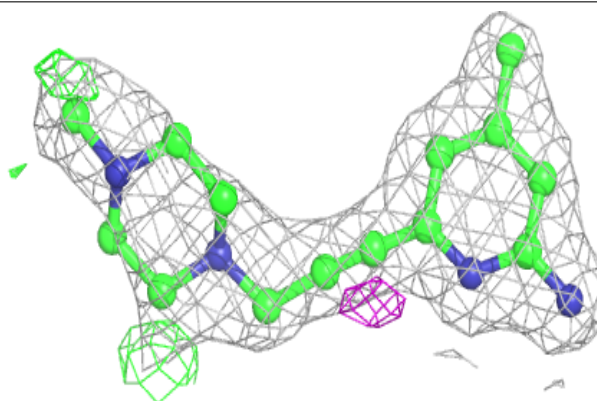


Electron density around K90 B 803:

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

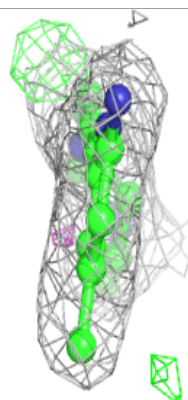
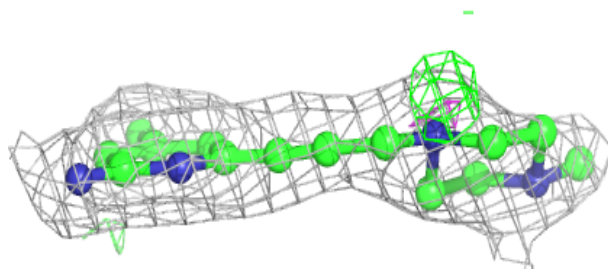
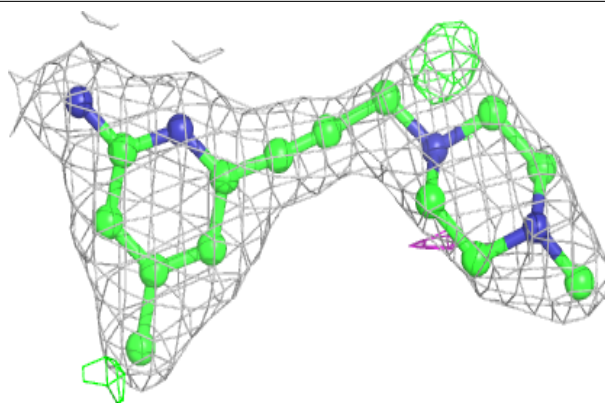
**Electron density around K90 C 803:**

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



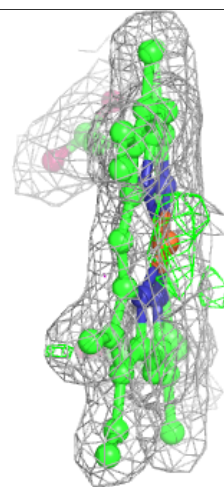
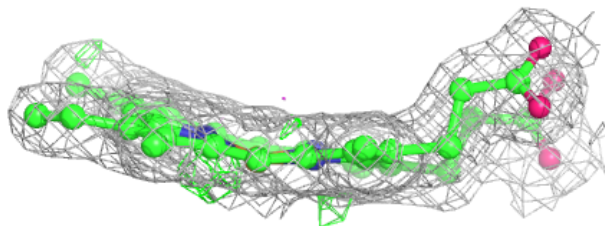
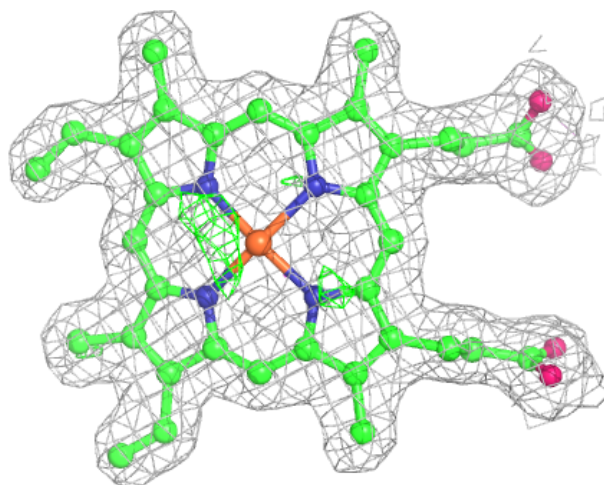
Electron density around K90 A 803:

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



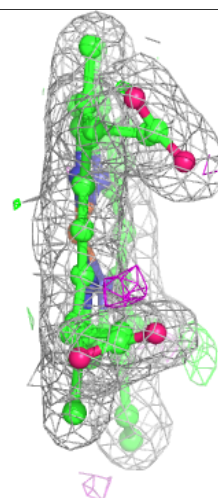
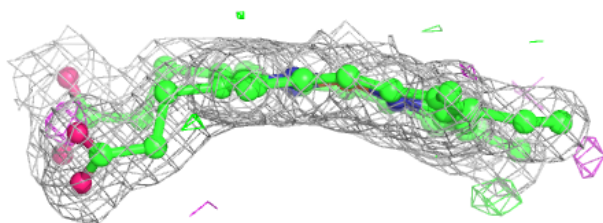
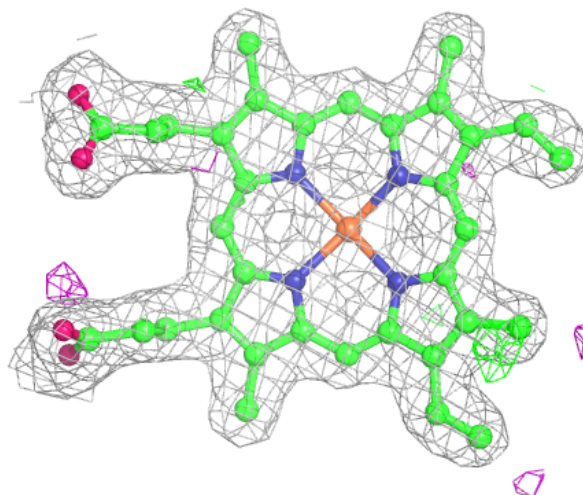
Electron density around HEM B 801:

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



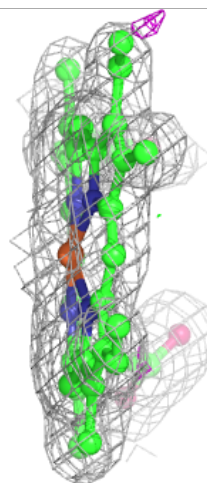
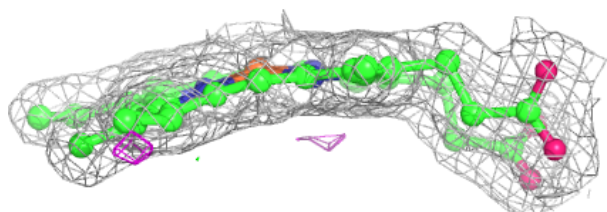
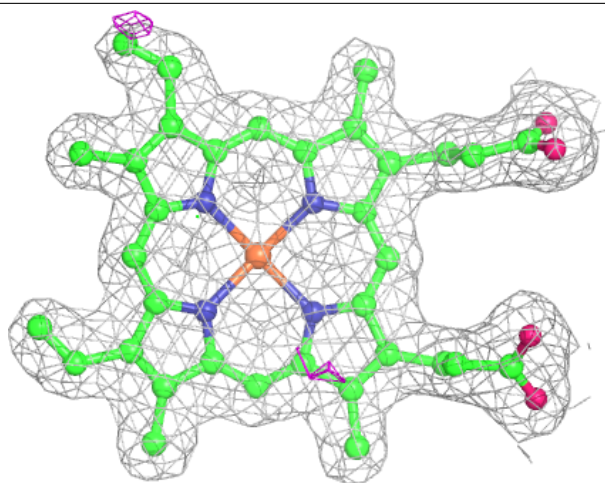
Electron density around HEM C 801:

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



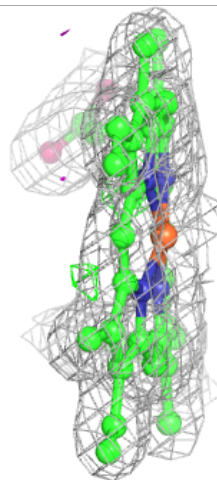
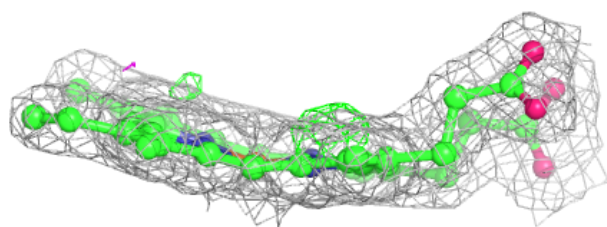
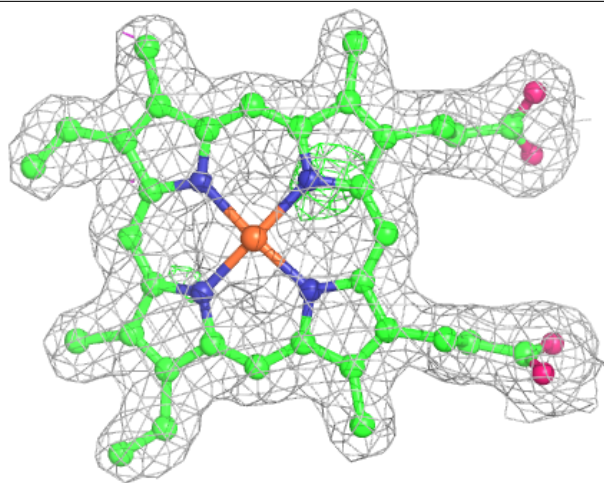
Electron density around HEM D 802:

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



Electron density around HEM A 801:

$2mF_o-DF_c$ (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.