



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:07 am BST

PDB ID : 3RQL
Title : Structure of the neuronal nitric oxide synthase heme domain in complex with 6-(((3R,4R)-4-(2-((1S,2R/1R,2S)-2-(3-Clorophenyl)cyclopropylamino)ethoxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine
Authors : Li, H.; Delker, S.L.; Poulos, T.L.
Deposited on : 2011-04-28
Resolution : 1.93 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 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 : 2.11
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) : 2.11

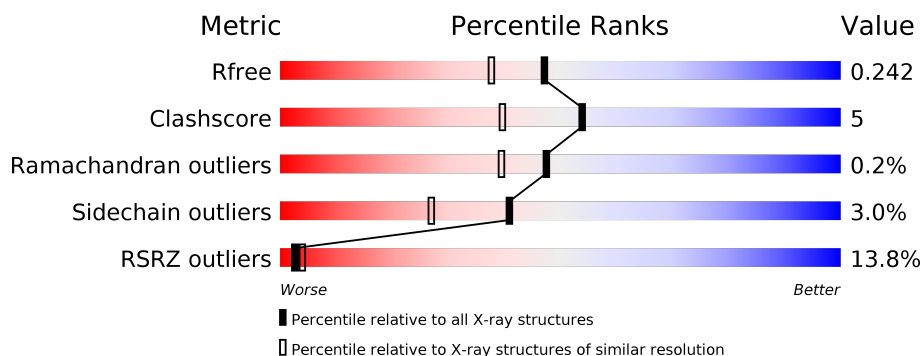
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 on 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	422	<div> <div>18%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>••</div> </div> </div>
1	B	422	<div> <div>9%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>•</div> </div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7193 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.

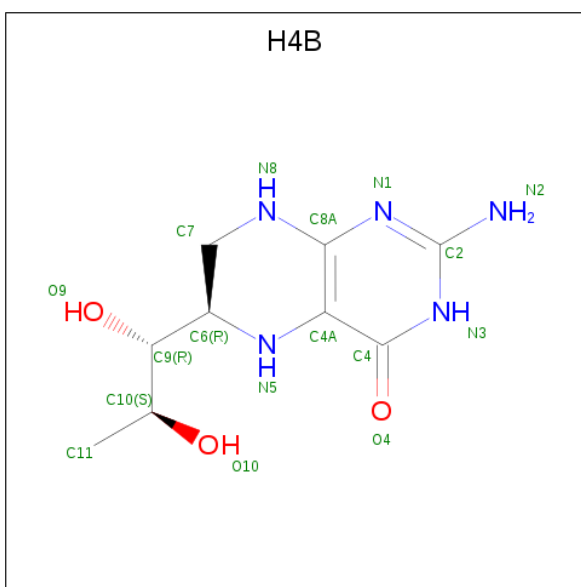
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	2	0
			3337	2136	571	608	22			
1	B	411	Total	C	N	O	S	0	4	0
			3359	2149	575	613	22			

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



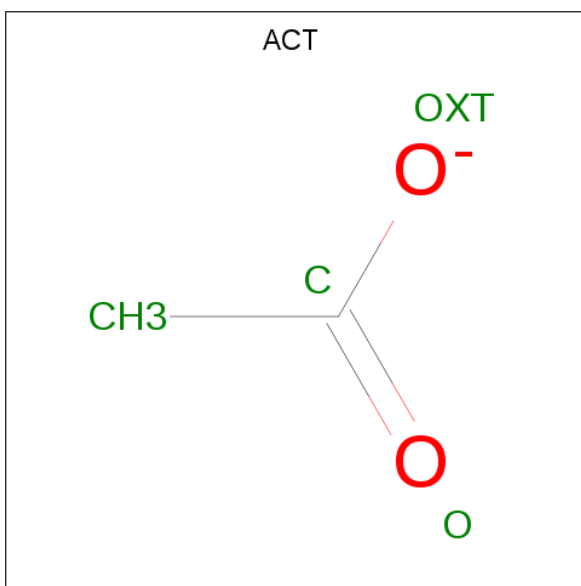
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



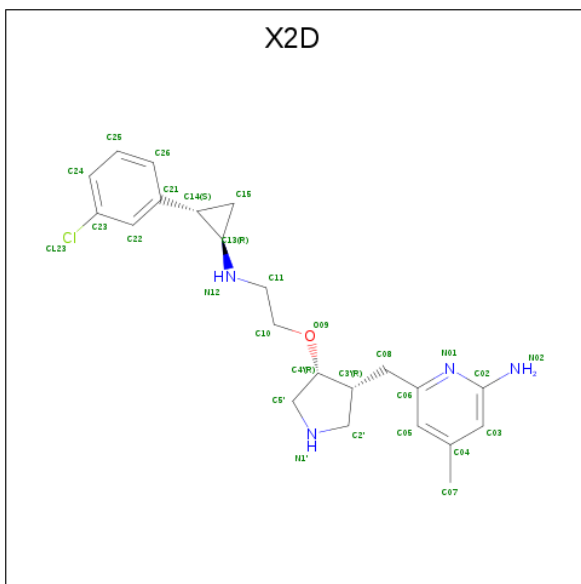
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 17	C 9	N 5	O 3	0	0
3	B	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

- Molecule 5 is 6-{[(3R,4R)-4-(2-{[(1R,2S)-2-(3-chlorophenyl)cyclopropyl]amino}ethoxy)pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine (three-letter code: X2D) (formula: $C_{22}H_{29}ClN_4O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		
5	B	1	Total	C	Cl	N	O	0	0
			28	22	1	4	1		

- 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		

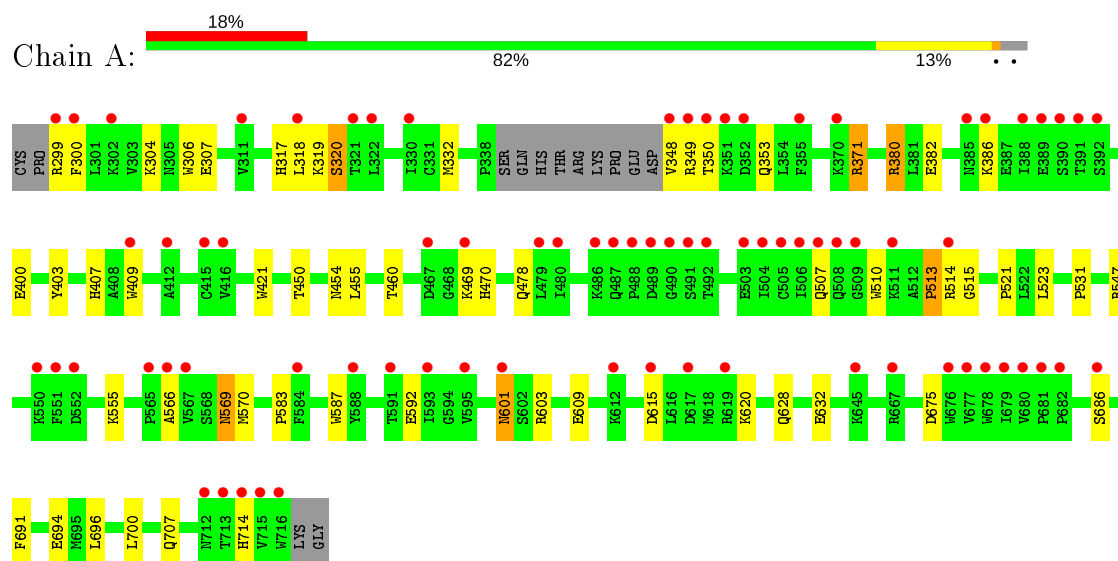
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	131	Total	O	0	0
			131	131		
7	B	181	Total	O	0	0
			181	181		

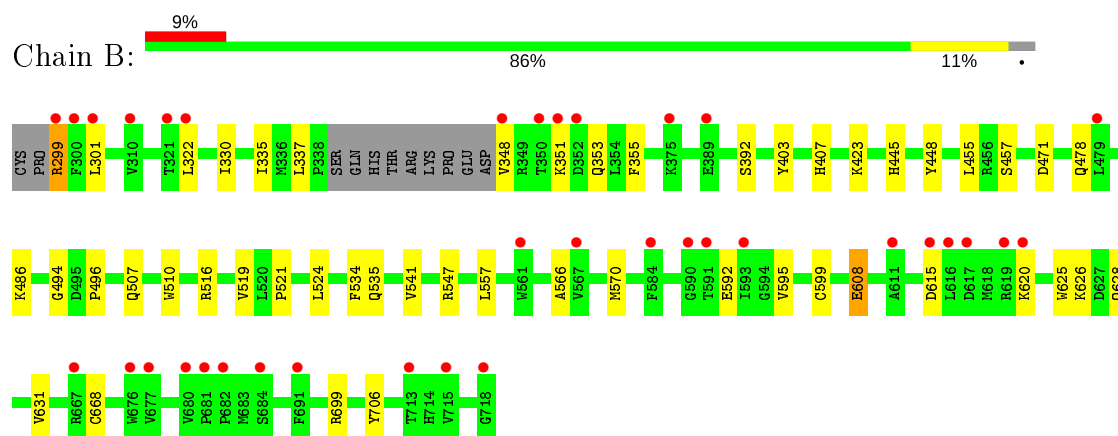
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.70Å 110.78Å 163.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.64 – 1.93 37.80 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.64-1.93) 99.1 (37.80-1.93)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.92Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.190 , 0.235 0.204 , 0.242	Depositor DCC
R_{free} test set	3545 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7193	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: X2D, ZN, H4B, HEM, ACT

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	0.76	0/3436	0.76	2/4661 (0.0%)
1	B	0.83	1/3464 (0.0%)	0.78	2/4696 (0.0%)
All	All	0.80	1/6900 (0.0%)	0.77	4/9357 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	570	MET	CG-SD	-5.89	1.65	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	615	ASP	CB-CG-OD2	-8.48	110.67	118.30
1	B	570	MET	CA-CB-CG	-7.70	100.21	113.30
1	A	570	MET	CA-CB-CG	-6.45	102.33	113.30
1	B	471	ASP	CB-CG-OD2	5.27	123.05	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	513	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	3337	0	3253	43	0
1	B	3359	0	3280	29	1
2	A	43	0	30	1	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	28	0	29	2	0
5	B	28	0	29	2	0
6	A	1	0	0	0	0
7	A	131	0	0	3	0
7	B	181	0	0	9	1
All	All	7193	0	6687	72	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (72) 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:299:ARG:HB2	1:A:318:LEU:HD21	1.53	0.90
1:A:350:THR:H	1:A:353:GLN:NE2	1.67	0.90
1:A:592:GLU:OE2	5:A:800:X2D:H14	1.81	0.80
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.65	0.79
5:A:800:X2D:H26	7:A:1004:HOH:O	1.88	0.72
1:B:592:GLU:OE1	5:B:800:X2D:H14	1.90	0.71
1:B:355:PHE:HB3	7:B:1046:HOH:O	1.90	0.71
1:B:322:LEU:HD22	1:B:699:ARG:HH21	1.58	0.68
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.07	0.67
1:A:382:GLU:HG3	1:A:386:LYS:HE2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:PRO:O	1:A:515:GLY:N	2.28	0.65
1:A:569:ASN:O	1:A:707:GLN:HG2	1.98	0.63
1:B:355:PHE:CB	7:B:1046:HOH:O	2.48	0.59
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.02	0.59
1:A:371:ARG:HG3	1:A:371:ARG:HH21	1.66	0.59
1:A:317:HIS:O	1:A:320:SER:HB3	2.03	0.58
1:A:601:ASN:HB2	7:A:1020:HOH:O	2.02	0.58
1:A:350:THR:N	1:A:353:GLN:NE2	2.45	0.57
5:B:800:X2D:H26	7:B:1004:HOH:O	2.04	0.57
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.66	0.56
1:A:350:THR:H	1:A:353:GLN:HE21	1.53	0.56
1:A:469:LYS:O	1:A:470:HIS:HD2	1.89	0.55
1:B:478:GLN:HA	1:B:566:ALA:O	2.08	0.53
1:B:507:GLN:NE2	7:B:1114:HOH:O	2.36	0.53
1:A:609:GLU:HG3	7:A:1008:HOH:O	2.07	0.53
1:A:694:GLU:HB3	1:B:335:ILE:HD13	1.90	0.53
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.90	0.53
1:B:299:ARG:CZ	1:B:299:ARG:HB3	2.38	0.52
1:B:608:GLU:HB2	7:B:1164:HOH:O	2.11	0.51
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.46	0.51
1:A:332:MET:CE	1:B:301:LEU:HD22	2.41	0.51
1:B:519:VAL:HG21	1:B:541:VAL:HG11	1.93	0.50
1:A:332:MET:HE3	1:B:301:LEU:HD22	1.95	0.48
1:A:460:THR:O	1:A:583:PRO:HD2	2.13	0.48
1:A:632:GLU:OE2	1:B:628:GLN:NE2	2.41	0.48
1:B:615:ASP:HA	7:B:1047:HOH:O	2.14	0.47
1:A:349:ARG:HA	1:A:353:GLN:HE22	1.80	0.47
2:B:750:HEM:CHC	2:B:750:HEM:HBB2	2.39	0.47
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.49	0.47
1:B:348:VAL:HG12	7:B:1013:HOH:O	2.15	0.46
1:B:595:VAL:O	1:B:599:CYS:HB2	2.15	0.46
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.03	0.46
1:A:371:ARG:HG2	1:A:371:ARG:NH2	2.31	0.45
1:A:603:ARG:HH11	1:A:603:ARG:HG3	1.81	0.45
1:A:299:ARG:O	1:A:318:LEU:HD11	2.16	0.45
1:A:350:THR:N	1:A:353:GLN:HE21	2.11	0.45
1:B:337:LEU:HD21	1:B:706:TYR:CD2	2.53	0.44
1:A:675:ASP:OD2	1:A:675:ASP:C	2.56	0.44
1:A:307:GLU:HG3	7:B:1050:HOH:O	2.17	0.44
1:B:445:HIS:C	1:B:445:HIS:CD2	2.92	0.43
1:B:516:ARG:NH2	1:B:557:LEU:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:TRP:CZ3	1:B:626:LYS:HG2	2.54	0.43
1:A:349:ARG:HA	1:A:353:GLN:NE2	2.33	0.43
1:A:628:GLN:HG3	1:B:631:VAL:HG11	2.00	0.42
1:A:696:LEU:HB3	1:B:330:ILE:HD11	2.02	0.42
1:A:320:SER:HA	1:A:700:LEU:HD23	2.00	0.42
1:A:450:THR:HA	1:A:455:LEU:HD22	2.01	0.42
1:B:494:GLY:O	1:B:496:PRO:HD3	2.20	0.42
1:B:535:GLN:HG3	7:B:1090:HOH:O	2.19	0.42
2:B:750:HEM:HHC	2:B:750:HEM:CBB	2.41	0.42
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.02	0.42
1:B:524:LEU:HD12	1:B:534:PHE:CD1	2.55	0.41
1:A:523:LEU:HD22	1:A:531:PRO:HB2	2.01	0.41
1:A:299:ARG:HB2	1:A:318:LEU:CD2	2.35	0.41
1:A:304:LYS:HE2	1:A:306:TRP:CE3	2.54	0.41
1:A:478:GLN:HA	1:A:566:ALA:O	2.20	0.41
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.56	0.41
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.41
1:A:686:SER:HA	1:A:691:PHE:CG	2.55	0.40
1:A:469:LYS:C	1:A:470:HIS:CD2	2.95	0.40
1:B:448:TYR:CD2	1:B:448:TYR:C	2.94	0.40
1:B:423:LYS:O	1:B:457[B]:SER:OG	2.38	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668[B]:CYS:SG	7:B:1012:HOH:O[1_455]	2.07	0.13

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	407/422 (96%)	393 (97%)	12 (3%)	2 (0%)	29	17
1	B	411/422 (97%)	405 (98%)	6 (2%)	0	100	100
All	All	818/844 (97%)	798 (98%)	18 (2%)	2 (0%)	47	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	ARG
1	A	714	HIS

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	367/377 (97%)	354 (96%)	13 (4%)	36	21
1	B	370/377 (98%)	361 (98%)	9 (2%)	49	36
All	All	737/754 (98%)	715 (97%)	22 (3%)	41	27

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	300	PHE
1	A	319	LYS
1	A	320	SER
1	A	348	VAL
1	A	371	ARG
1	A	380	ARG
1	A	454	ASN
1	A	507	GLN
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	601	ASN
1	A	620	LYS
1	B	299	ARG

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Mol	Chain	Res	Type
1	B	351	LYS
1	B	353	GLN
1	B	392	SER
1	B	455	LEU
1	B	486	LYS
1	B	547	ARG
1	B	608	GLU
1	B	620	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	454	ASN
1	A	470	HIS
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN
1	A	601	ASN
1	A	605	ASN
1	A	697	ASN
1	B	364	GLN
1	B	385	ASN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN
1	B	697	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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
5	X2D	A	800	-	29,31,31	1.16	4 (13%)	33,43,43	2.42	9 (27%)
2	HEM	A	750	1	27,50,50	2.07	6 (22%)	17,82,82	2.09	6 (35%)
2	HEM	B	750	1	27,50,50	1.98	8 (29%)	17,82,82	2.45	6 (35%)
4	ACT	A	860	-	1,3,3	1.42	0	0,3,3	0.00	-
5	X2D	B	800	-	29,31,31	1.00	3 (10%)	33,43,43	2.07	9 (27%)
3	H4B	B	760	-	16,18,18	1.06	1 (6%)	11,26,26	2.65	4 (36%)
4	ACT	B	860	-	1,3,3	1.97	0	0,3,3	0.00	-
3	H4B	A	760	-	16,18,18	0.80	0	11,26,26	2.51	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
5	X2D	A	800	-	-	1/13/30/30	0/4/4/4
2	HEM	A	750	1	-	0/6/54/54	-
2	HEM	B	750	1	-	0/6/54/54	-
5	X2D	B	800	-	-	2/13/30/30	0/4/4/4
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C2D	5.14	1.52	1.37
2	A	750	HEM	C3B-C2B	-5.13	1.33	1.40
2	B	750	HEM	C3D-C2D	4.06	1.49	1.37
2	B	750	HEM	C3B-C2B	-3.93	1.34	1.40
2	B	750	HEM	C3C-C2C	-3.70	1.35	1.40
2	A	750	HEM	C3B-CAB	3.18	1.54	1.47
2	A	750	HEM	C3C-C2C	-3.05	1.36	1.40
2	B	750	HEM	C4A-NA	3.02	1.42	1.36
5	A	800	X2D	C15-C13	3.02	1.53	1.49
2	A	750	HEM	C3C-CAC	3.01	1.54	1.47
5	B	800	X2D	C15-C13	2.98	1.53	1.49
2	B	750	HEM	C3C-CAC	2.81	1.53	1.47
5	A	800	X2D	C23-CL23	2.56	1.80	1.74
2	B	750	HEM	CMA-C3A	2.37	1.56	1.51
5	B	800	X2D	C15-C14	2.32	1.54	1.50
2	B	750	HEM	C3B-CAB	2.30	1.52	1.47
5	A	800	X2D	C15-C14	2.21	1.54	1.50
3	B	760	H4B	C7-N8	2.21	1.48	1.44
2	A	750	HEM	CMA-C3A	2.07	1.55	1.51
2	B	750	HEM	CAD-C3D	2.04	1.55	1.52
5	B	800	X2D	C23-CL23	2.01	1.78	1.74
5	A	800	X2D	C06-N01	2.01	1.38	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	X2D	C15-C13-N12	-7.19	103.48	117.50
3	B	760	H4B	C4-C4A-C8A	7.09	120.87	114.57
5	A	800	X2D	C15-C14-C21	-7.02	108.73	122.24
5	B	800	X2D	C15-C14-C21	-6.40	109.94	122.24
2	B	750	HEM	CBD-CAD-C3D	-5.85	101.70	112.48
3	A	760	H4B	C4-C4A-C8A	5.39	119.36	114.57
5	A	800	X2D	C02-N01-C06	5.18	122.03	118.10
2	B	750	HEM	CBA-CAA-C2A	-5.12	103.05	112.49
5	B	800	X2D	C15-C13-N12	-4.97	107.82	117.50
2	A	750	HEM	CBA-CAA-C2A	-4.47	104.25	112.49
5	B	800	X2D	C02-N01-C06	4.10	121.21	118.10
2	A	750	HEM	CBD-CAD-C3D	-3.83	105.42	112.48
2	B	750	HEM	C3B-C4B-NB	-3.25	105.01	109.21
2	A	750	HEM	C4C-C3C-C2C	3.22	109.15	106.90
5	A	800	X2D	N02-C02-N01	3.10	121.39	116.49
3	B	760	H4B	C4-N3-C2	3.06	120.80	115.93
2	B	750	HEM	C4C-C3C-C2C	2.84	108.88	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	C2-N1-C8A	2.74	120.68	114.54
3	A	760	H4B	N3-C2-N1	-2.65	121.26	125.42
3	A	760	H4B	C4-C4A-N5	2.64	121.34	119.12
5	A	800	X2D	C05-C06-N01	-2.63	120.11	122.90
2	A	750	HEM	CAA-CBA-CGA	-2.61	108.30	112.67
5	A	800	X2D	C22-C23-CL23	-2.57	115.93	119.15
5	B	800	X2D	C5'-N1'-C2'	2.56	111.46	105.42
3	A	760	H4B	C4-N3-C2	2.53	119.95	115.93
3	A	760	H4B	N2-C2-N1	2.48	121.11	117.25
2	B	750	HEM	CMB-C2B-C3B	2.46	129.28	124.68
5	B	800	X2D	C11-N12-C13	2.41	117.61	114.20
5	B	800	X2D	C05-C06-N01	-2.40	120.35	122.90
2	A	750	HEM	C3C-C4C-NC	-2.38	106.45	110.94
5	A	800	X2D	O09-C4'-C5'	-2.34	105.19	111.42
5	B	800	X2D	C10-C11-N12	2.17	116.97	111.54
5	B	800	X2D	N02-C02-N01	2.16	119.90	116.49
2	B	750	HEM	CAA-CBA-CGA	-2.12	109.12	112.67
3	B	760	H4B	C4A-N5-C6	-2.11	115.42	121.16
2	A	750	HEM	CMC-C2C-C3C	2.11	128.62	124.68
5	A	800	X2D	C06-C08-C3'	-2.09	108.67	115.55
3	B	760	H4B	C4A-C4-N3	-2.07	118.13	124.01
5	A	800	X2D	C5'-N1'-C2'	2.03	110.21	105.42
5	B	800	X2D	C06-C08-C3'	-2.02	108.91	115.55

There are no chirality outliers.

All (3) torsion outliers are listed below:

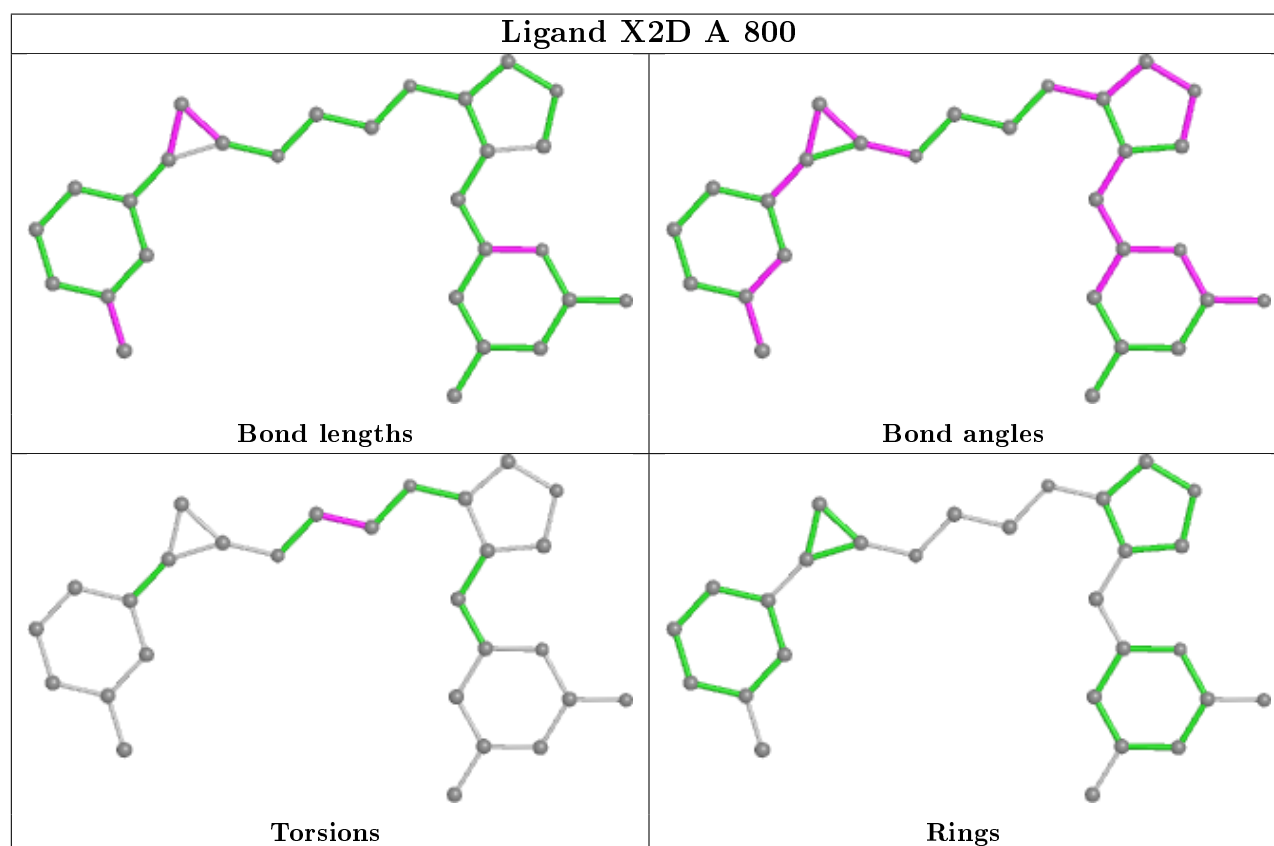
Mol	Chain	Res	Type	Atoms
5	B	800	X2D	C15-C14-C21-C26
5	B	800	X2D	C15-C14-C21-C22
5	A	800	X2D	O09-C10-C11-N12

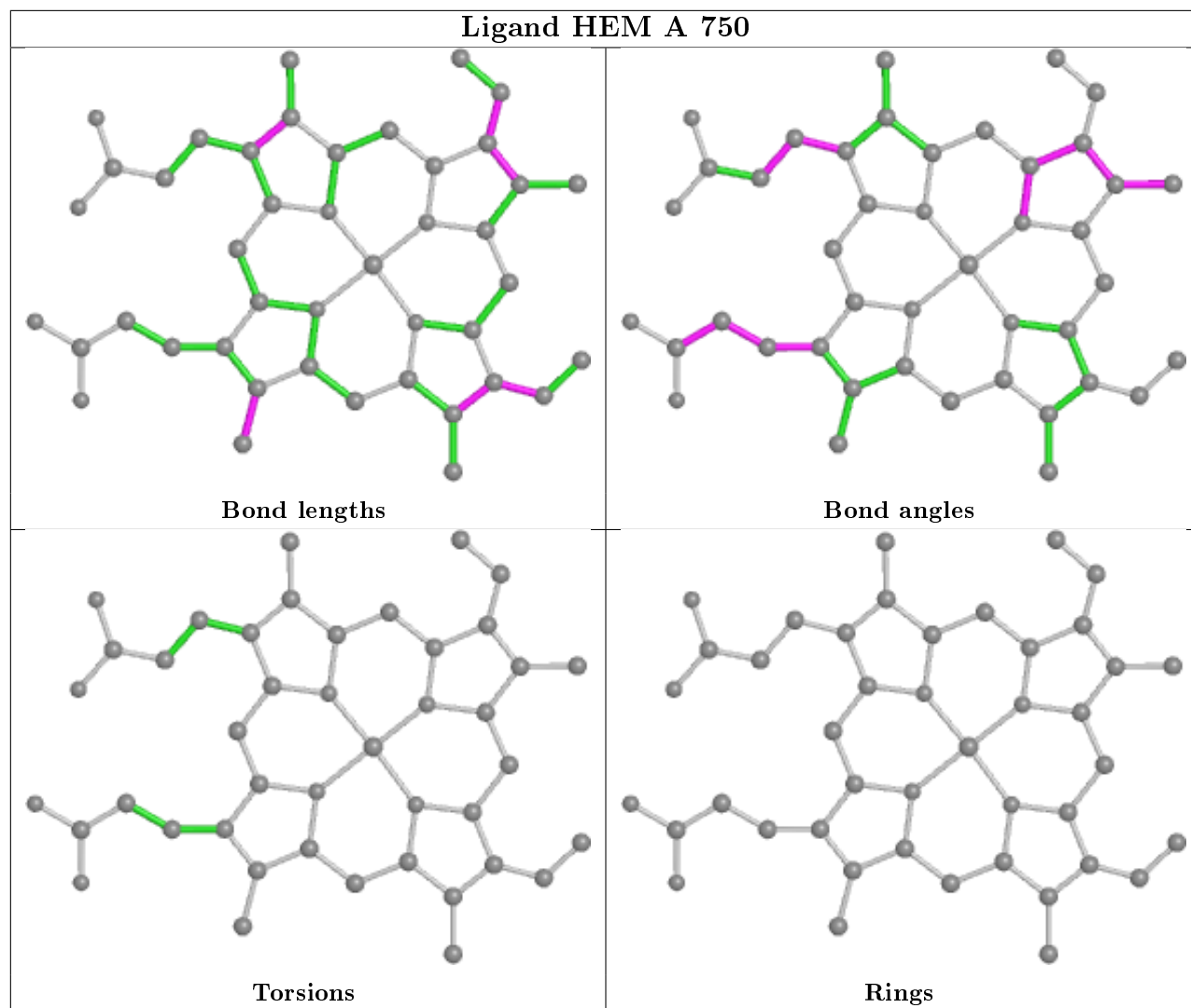
There are no ring outliers.

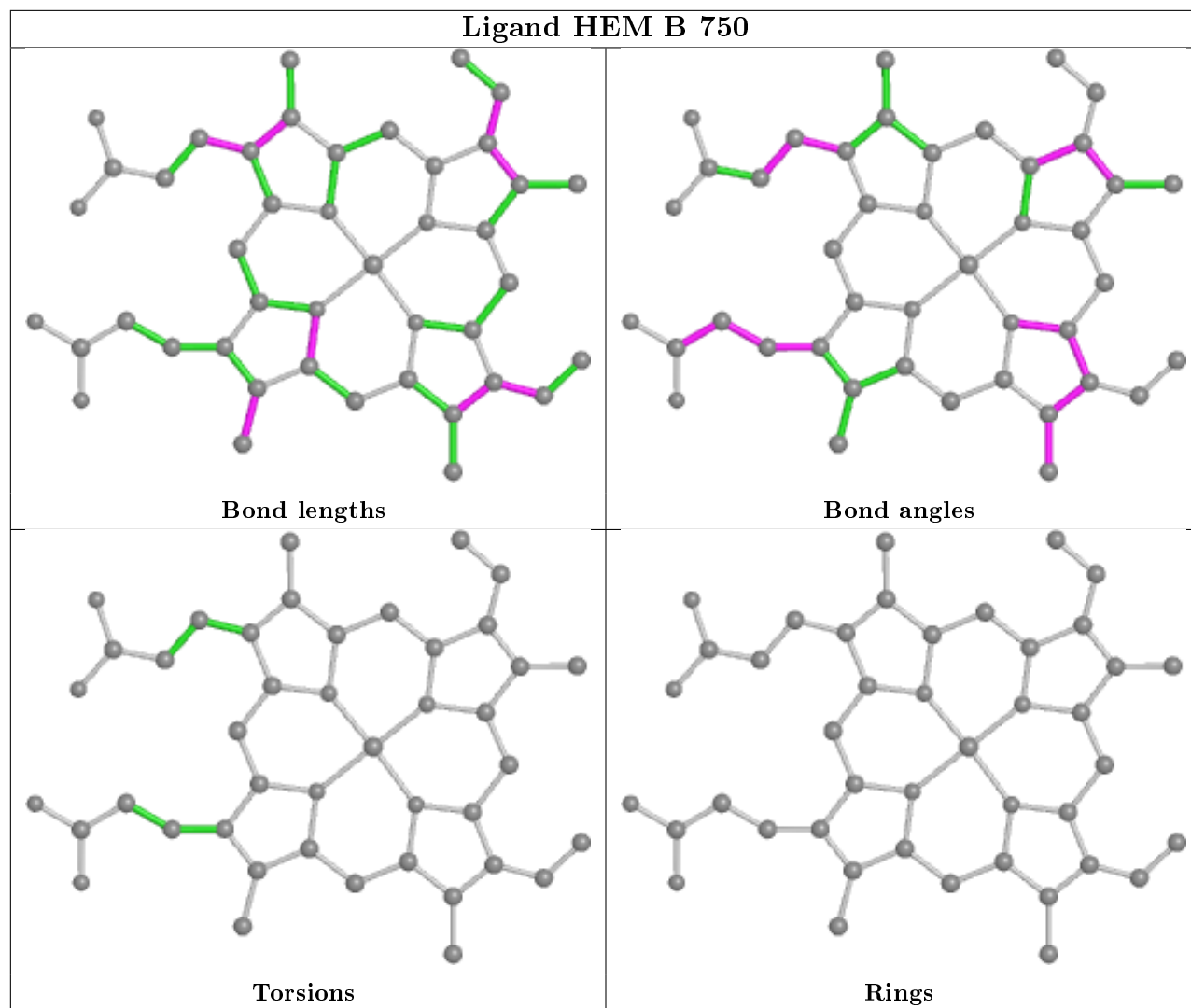
4 monomers are involved in 8 short contacts:

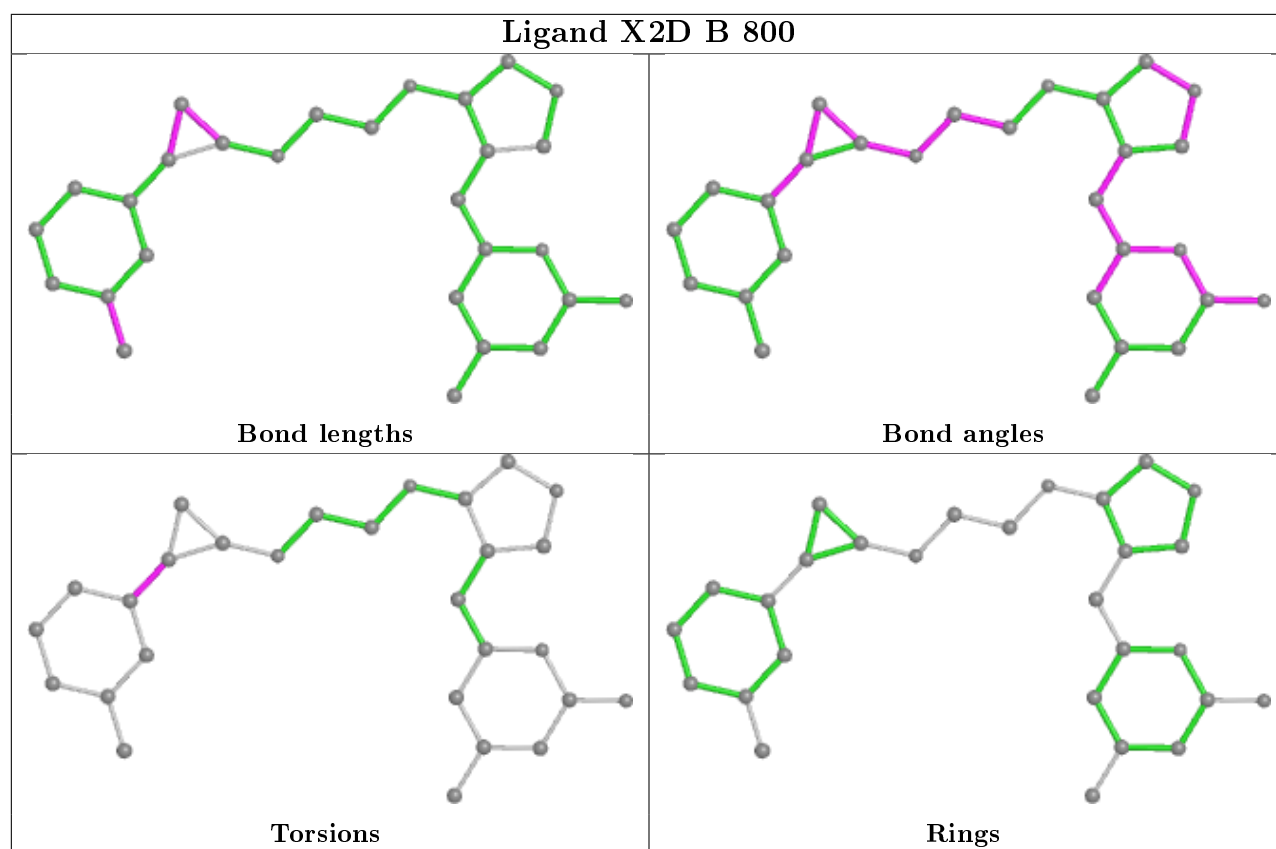
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	X2D	2	0
2	A	750	HEM	1	0
2	B	750	HEM	3	0
5	B	800	X2D	2	0

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.









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	409/422 (96%)	1.01	77 (18%) 1 1	27, 52, 90, 117	0
1	B	411/422 (97%)	0.47	36 (8%) 10 15	27, 42, 66, 83	0
All	All	820/844 (97%)	0.74	113 (13%) 2 4	27, 47, 83, 117	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	10.0
1	A	488	PRO	7.6
1	A	716	TRP	6.3
1	A	300	PHE	6.3
1	A	348	VAL	6.0
1	A	713	THR	5.9
1	A	355	PHE	5.7
1	A	486	LYS	5.6
1	A	715	VAL	5.6
1	B	348	VAL	5.0
1	A	352	ASP	5.0
1	B	619	ARG	4.6
1	A	712	ASN	4.4
1	A	299	ARG	4.2
1	A	552	ASP	4.2
1	A	321	THR	4.1
1	A	506	ILE	4.0
1	A	619	ARG	4.0
1	A	351	LYS	4.0
1	A	386	LYS	3.8
1	A	388	ILE	3.8
1	A	503	GLU	3.8
1	A	322	LEU	3.8
1	B	310	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	350	THR	3.6
1	A	678	TRP	3.6
1	A	551	PHE	3.6
1	A	487	GLN	3.6
1	B	715	VAL	3.5
1	A	349	ARG	3.5
1	A	593	ILE	3.5
1	B	301	LEU	3.5
1	A	507	GLN	3.4
1	A	415	CYS	3.4
1	A	390	SER	3.3
1	A	491	SER	3.3
1	A	679	ILE	3.3
1	A	682	PRO	3.3
1	A	567	VAL	3.2
1	A	492	THR	3.2
1	A	514	ARG	3.1
1	B	667	ARG	3.1
1	B	680	VAL	3.1
1	A	490	GLY	3.1
1	A	714	HIS	3.0
1	A	385	ASN	3.0
1	A	392	SER	3.0
1	B	299	ARG	3.0
1	A	416	VAL	3.0
1	B	351	LYS	3.0
1	B	616	LEU	2.9
1	A	479	LEU	2.9
1	A	591	THR	2.9
1	A	511	LYS	2.9
1	B	561	TRP	2.9
1	A	489	ASP	2.9
1	A	389	GLU	2.8
1	A	480	ILE	2.8
1	A	588	TYR	2.8
1	A	677	VAL	2.8
1	A	469	LYS	2.8
1	A	330	ILE	2.8
1	B	691	PHE	2.8
1	A	391	THR	2.7
1	A	504	ILE	2.7
1	A	595	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	508	GLN	2.7
1	A	615	ASP	2.7
1	A	311	VAL	2.6
1	A	550	LYS	2.6
1	A	681	PRO	2.6
1	A	350	THR	2.6
1	A	676	TRP	2.6
1	A	680	VAL	2.6
1	A	584	PHE	2.5
1	B	620	LYS	2.5
1	B	611	ALA	2.5
1	A	667	ARG	2.5
1	B	677	VAL	2.5
1	A	617	ASP	2.5
1	A	565	PRO	2.4
1	A	509	GLY	2.4
1	A	302	LYS	2.4
1	B	375	LYS	2.4
1	A	412	ALA	2.4
1	A	505	CYS	2.4
1	B	682	PRO	2.4
1	B	567	VAL	2.4
1	B	352	ASP	2.3
1	B	322	LEU	2.3
1	B	584	PHE	2.3
1	A	612	LYS	2.3
1	B	591	THR	2.3
1	B	713	THR	2.3
1	A	318	LEU	2.3
1	A	645	LYS	2.3
1	B	593	ILE	2.2
1	B	389	GLU	2.2
1	B	321	THR	2.2
1	B	718	GLY	2.2
1	A	370	LYS	2.2
1	A	601	ASN	2.1
1	A	686	SER	2.1
1	B	681	PRO	2.1
1	B	590	GLY	2.1
1	B	479	LEU	2.1
1	B	617	ASP	2.1
1	B	676	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	615	ASP	2.0
1	A	467	ASP	2.0
1	A	566	ALA	2.0
1	A	409	TRP	2.0
1	B	684	SER	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 carbohydrates in this entry.

6.4 Ligands [i](#)

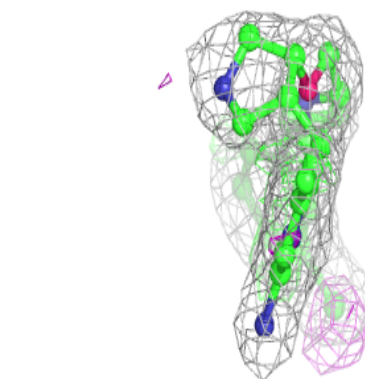
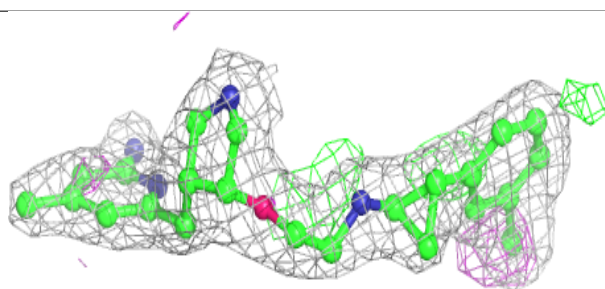
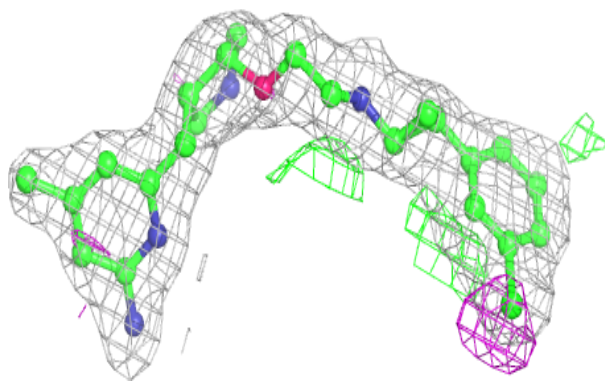
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	X2D	A	800	28/28	0.90	0.16	27,33,36,46	0
4	ACT	A	860	4/4	0.92	0.33	59,60,62,64	0
5	X2D	B	800	28/28	0.93	0.20	35,41,45,52	0
4	ACT	B	860	4/4	0.94	0.13	48,50,51,52	0
3	H4B	A	760	17/17	0.94	0.19	30,33,40,40	0
2	HEM	A	750	43/43	0.97	0.23	29,34,38,39	0
3	H4B	B	760	17/17	0.97	0.18	28,33,38,40	0
2	HEM	B	750	43/43	0.98	0.18	25,32,39,44	0
6	ZN	A	900	1/1	1.00	0.06	38,38,38,38	0

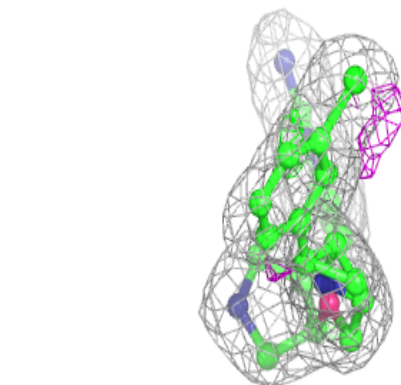
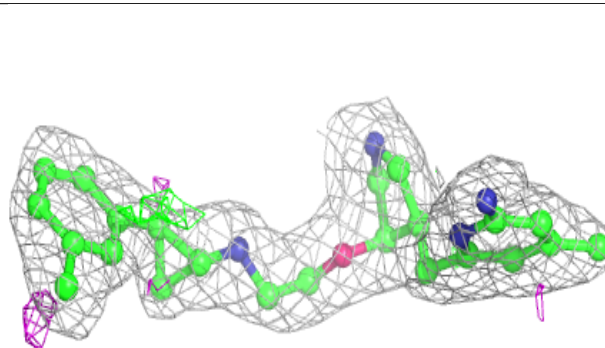
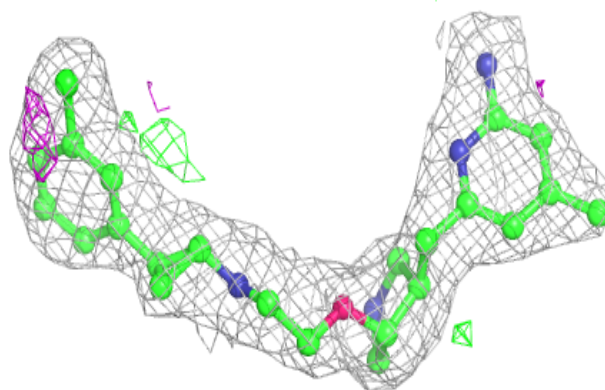
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around X2D A 800:

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

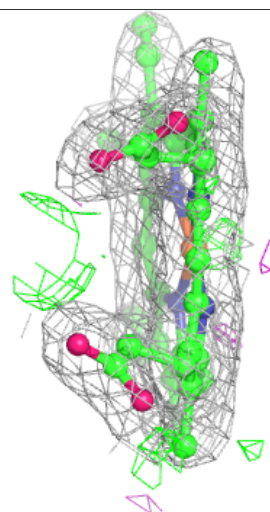
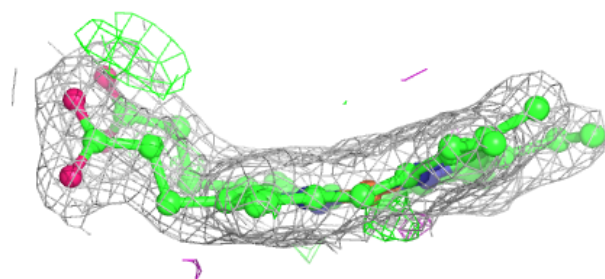
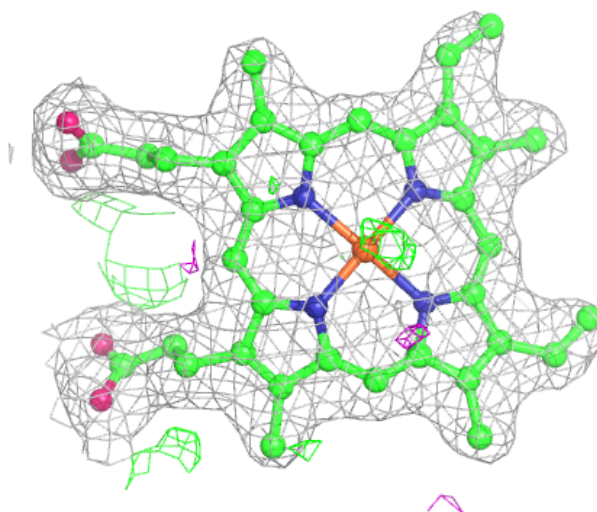
**Electron density around X2D B 800:**

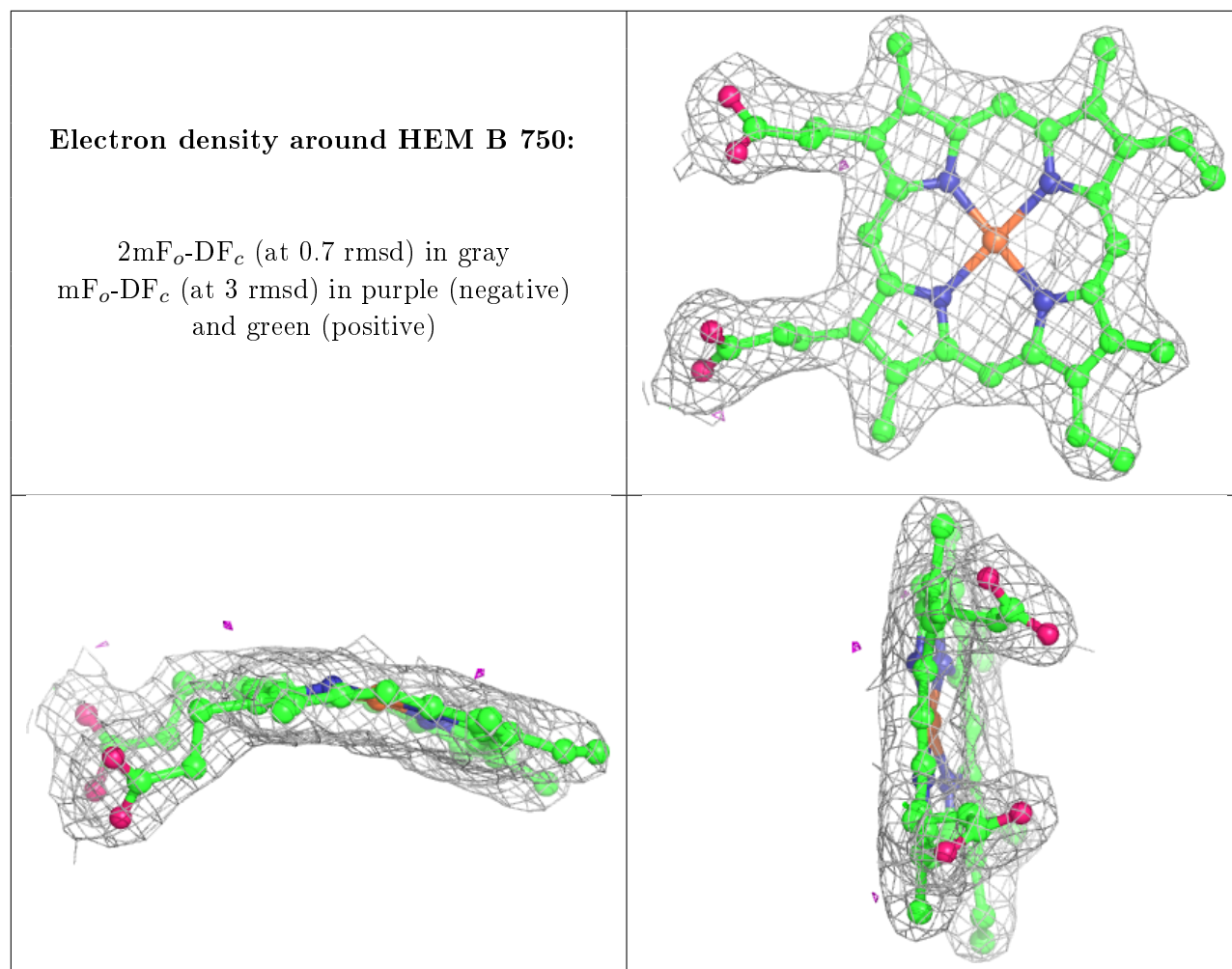
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 750:

$2mF_o-DF_c$ (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.