



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:12 AM UTC

PDB ID : 5AGL / pdb_00005agl
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with
(S)-2-Amino-5-(2-(methylsulfonyl)acetimidamido)pentanoic acid
Authors : Li, H.; Poulos, T.L.
Deposited on : 2015-02-02
Resolution : 1.94 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

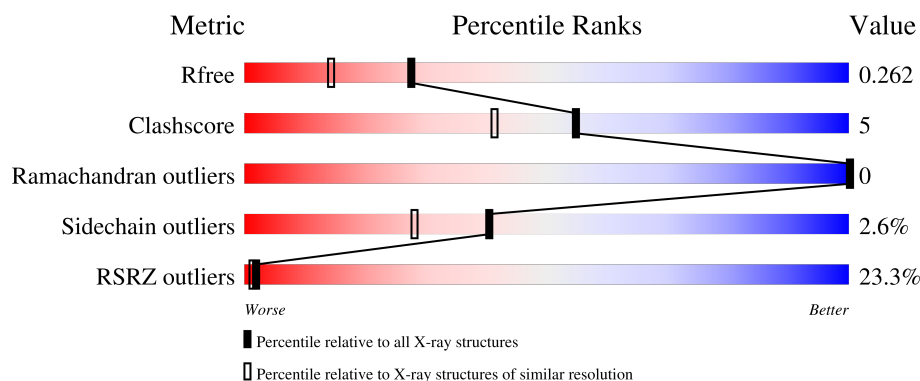
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	422	 39% 83% 12% . .
1	B	422	 6% 88% 9% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

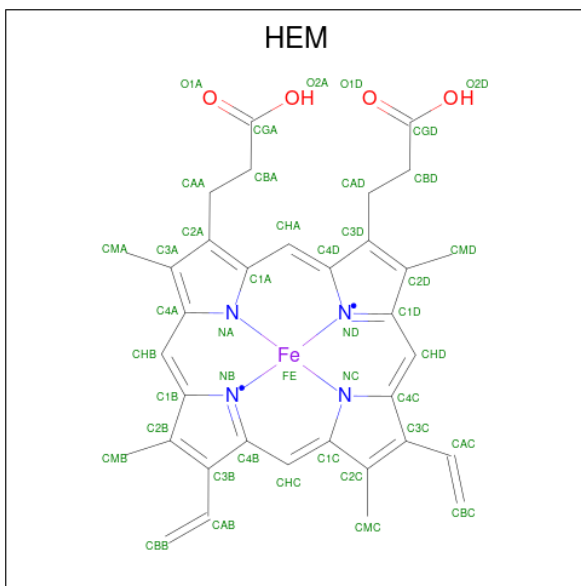
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CCW	B	800	-	-	X	-

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	408	Total 3339	C 2138	N 569	O 610	S 22	0	5	1
1	B	411	Total 3360	C 2150	N 574	O 614	S 22	0	4	0

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



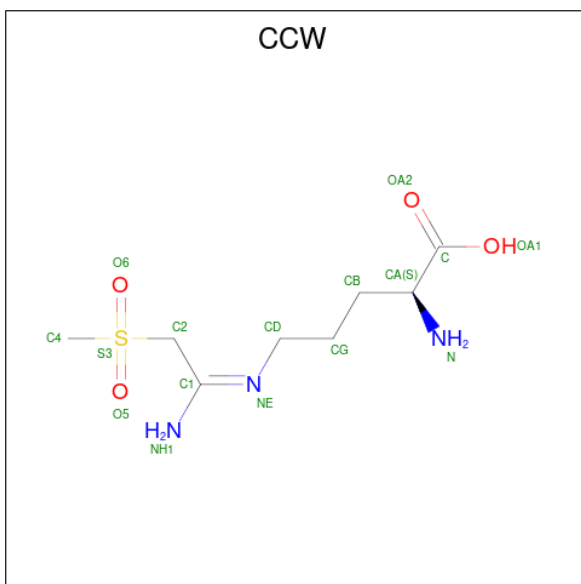
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: $\text{C}_9\text{H}_{15}\text{N}_5\text{O}_3$).



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		

- Molecule 4 is (S)-2-Amino-5-(2-(methylsulfonyl)acetimidamido)pentanoic acid (CCD ID: CCW) (formula: $C_8H_{17}N_3O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			16	8	3	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			16	8	3	4	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	154	Total	O	0	0
			154	154		
7	B	206	Total	O	0	0
			206	206		

- 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	52.01Å 111.34Å 164.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.59 – 1.94 38.59 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.59-1.94) 99.6 (38.59-1.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.179 , 0.210 0.236 , 0.262	Depositor DCC
R_{free} test set	3533 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7220	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ACT, ZN, CCW, H4B

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	0.72	3/3444 (0.1%)	0.86	3/4672 (0.1%)
1	B	0.74	0/3465	0.85	2/4697 (0.0%)
All	All	0.73	3/6909 (0.0%)	0.85	5/9369 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	716	TRP	C-N	-6.56	1.24	1.33
1	A	382	GLU	C-O	5.52	1.30	1.24
1	A	466	THR	CA-C	5.06	1.54	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	707	GLN	CA-C-N	-7.33	112.77	120.03
1	B	707	GLN	C-N-CA	-7.33	112.77	120.03
1	A	680	VAL	CA-C-N	6.09	124.11	119.66
1	A	680	VAL	C-N-CA	6.09	124.11	119.66
1	A	681	PRO	O-C-N	5.21	123.71	121.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3339	0	3256	37	0
1	B	3360	0	3280	27	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	16	0	16	5	0
4	B	16	0	16	7	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	B	1	0	0	0	0
7	A	154	0	0	2	0
7	B	206	0	0	3	0
All	All	7220	0	6664	65	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 5.

All (65) 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)
2:B:750:HEM:HMC2	2:B:750:HEM:HBC2	1.58	0.84
1:A:565:PRO:HB2	4:A:800:CCW:H43C	1.62	0.82
1:A:350:THR:N	1:A:353:GLN:HE21	1.79	0.80
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.64	0.79
1:B:565:PRO:HB2	4:B:800:CCW:H43C	1.66	0.78
1:A:567:VAL:HG23	4:A:800:CCW:H42C	1.65	0.77
1:B:567:VAL:HG23	4:B:800:CCW:H42C	1.70	0.72
1:B:706:TYR:OH	2:B:750:HEM:O1D	2.09	0.71
1:A:350:THR:N	1:A:353:GLN:NE2	2.41	0.67
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.78	0.65
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.80	0.62
1:A:322:LEU:HD13	1:A:699:ARG:HH21	1.66	0.61
1:A:565:PRO:HB2	4:A:800:CCW:C4	2.31	0.60
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.85	0.59
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.85	0.58
1:A:380:ARG:HD3	1:A:400:GLU:OE2	2.07	0.55
1:A:300:PHE:HD1	1:A:315:THR:HG22	1.72	0.54
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.91	0.53
1:A:355:PHE:CE1	1:A:385:ASN:HB2	2.45	0.52
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.91	0.52
1:A:609:GLU:HG3	7:A:2119:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:TYR:CE1	1:B:407:HIS:CE1	2.98	0.51
1:A:362:LEU:HD11	1:A:384:VAL:HG21	1.91	0.51
1:B:351:LYS:HE3	1:B:392:SER:OG	2.11	0.51
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.46	0.50
1:A:592:GLU:OE1	4:A:800:CCW:NE	2.45	0.50
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.47	0.49
1:B:565:PRO:HB2	4:B:800:CCW:C4	2.42	0.48
1:B:323:GLU:O	1:B:699:ARG:HD3	2.14	0.48
1:B:445:HIS:C	1:B:445:HIS:CD2	2.93	0.46
1:A:317:HIS:O	1:A:320:SER:HB3	2.16	0.46
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.49	0.46
1:B:595:VAL:O	1:B:599:CYS:HB2	2.16	0.46
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.98	0.46
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.51	0.45
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.98	0.45
1:A:569:ASN:HD22	1:A:569:ASN:H	1.64	0.45
1:A:717:LYS:N	7:A:2096:HOH:O	2.48	0.45
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.50	0.45
1:B:338:PRO:C	7:B:2013:HOH:O	2.60	0.45
1:A:565:PRO:C	4:A:800:CCW:H41C	2.41	0.45
1:A:535:GLN:HE21	1:A:538:PRO:HD3	1.82	0.45
1:B:364:GLN:NE2	7:B:2018:HOH:O	2.47	0.45
1:B:619:ARG:HE	1:B:619:ARG:HB2	1.49	0.44
1:A:423[B]:LYS:O	1:A:457[B]:SER:OG	2.35	0.44
1:B:307[B]:GLU:OE1	7:B:2003:HOH:O	2.21	0.44
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.88	0.44
1:A:525:GLN:HG3	1:A:529:ASN:O	2.18	0.44
1:A:351:LYS:HE2	1:A:392:SER:HB3	2.00	0.43
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.53	0.43
1:B:565:PRO:C	4:B:800:CCW:H41C	2.43	0.43
2:B:750:HEM:HMC2	2:B:750:HEM:CBC	2.39	0.43
1:A:550:LYS:HB2	1:A:550:LYS:HE3	1.73	0.43
1:A:609:GLU:O	1:A:613:LYS:HG2	2.19	0.42
1:A:373:GLY:HA2	1:A:378:MET:HE3	2.01	0.42
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.54	0.42
1:A:445:HIS:CD2	1:A:445:HIS:C	2.97	0.42
1:B:525:GLN:HG3	1:B:529:ASN:O	2.19	0.42
1:A:475:TRP:CE2	1:A:531:PRO:HG3	2.55	0.41
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.89	0.41
4:B:800:CCW:C4	4:B:800:CCW:HD2C	2.49	0.41
1:B:391:THR:O	1:B:392:SER:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:800:CCW:H42C	4:B:800:CCW:HD2C	2.02	0.41
1:A:631:VAL:HG11	1:B:628:GLN:CG	2.51	0.40
1:B:592:GLU:OE1	4:B:800:CCW:NE	2.55	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	409/422 (97%)	398 (97%)	11 (3%)	0	100	100
1	B	411/422 (97%)	405 (98%)	6 (2%)	0	100	100
All	All	820/844 (97%)	803 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/377 (98%)	356 (97%)	12 (3%)	33	20
1	B	370/377 (98%)	361 (98%)	9 (2%)	43	31
All	All	738/754 (98%)	717 (97%)	21 (3%)	40	25

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307[A]	GLU
1	A	307[B]	GLU
1	A	350	THR
1	A	371	ARG
1	A	380	ARG
1	A	507	GLN
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	699	ARG
1	A	715	VAL
1	B	307[A]	GLU
1	B	307[B]	GLU
1	B	337	LEU
1	B	350	THR
1	B	353	GLN
1	B	370	LYS
1	B	390	SER
1	B	486	LYS
1	B	540	LEU

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

Mol	Chain	Res	Type
1	A	425	GLN
1	A	436	HIS
1	A	454	ASN
1	A	508	GLN
1	A	527	ASN
1	A	535	GLN
1	A	569	ASN
1	A	628	GLN
1	A	697	ASN
1	B	385	ASN
1	B	454	ASN
1	B	507	GLN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
1	B	628	GLN
1	B	664	ASN
1	B	697	ASN

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](#)

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	$\# Z > 2$
4	CCW	A	800	-	13,15,15	2.22	4 (30%)	12,20,20	3.24	5 (41%)
4	CCW	B	800	-	13,15,15	2.30	4 (30%)	12,20,20	2.79	7 (58%)
5	ACT	A	860	-	3,3,3	0.86	0	3,3,3	0.69	0
2	HEM	B	750	1	50,50,50	1.72	9 (18%)	67,82,82	1.40	13 (19%)
3	H4B	B	760	-	17,18,18	1.37	2 (11%)	14,26,26	1.69	3 (21%)
2	HEM	A	750	1	50,50,50	1.96	13 (26%)	67,82,82	1.36	7 (10%)
3	H4B	A	760	-	17,18,18	0.91	0	14,26,26	2.05	6 (42%)
5	ACT	B	860	-	3,3,3	0.65	0	3,3,3	1.12	0

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
4	CCW	A	800	-	-	2/12/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CCW	B	800	-	-	2/12/16/16	-
2	HEM	B	750	1	-	0/14/54/54	-
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
2	HEM	A	750	1	-	1/14/54/54	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C2D	6.95	1.51	1.36
2	B	750	HEM	C3D-C2D	6.49	1.50	1.36
4	B	800	CCW	C2-S3	-5.90	1.69	1.79
4	A	800	CCW	C2-S3	-5.87	1.69	1.79
2	A	750	HEM	FE-NC	4.45	2.09	1.95
2	A	750	HEM	FE-ND	4.44	2.08	1.94
2	A	750	HEM	FE-NB	4.19	2.07	1.94
2	B	750	HEM	FE-NA	3.64	2.07	1.95
2	A	750	HEM	FE-NA	3.52	2.06	1.95
3	B	760	H4B	C7-C6	3.39	1.55	1.52
4	B	800	CCW	C1-NH1	-3.31	1.28	1.33
4	B	800	CCW	C4-S3	-3.12	1.65	1.75
2	B	750	HEM	FE-ND	3.09	2.04	1.94
4	A	800	CCW	C1-NH1	-2.96	1.28	1.33
4	A	800	CCW	C1-NE	2.95	1.35	1.28
2	A	750	HEM	CAB-C3B	2.92	1.55	1.47
2	A	750	HEM	CMC-C2C	2.84	1.56	1.50
2	B	750	HEM	CMC-C2C	2.76	1.56	1.50
2	B	750	HEM	FE-NC	2.71	2.04	1.95
2	B	750	HEM	CAB-C3B	2.70	1.54	1.47
2	A	750	HEM	CMD-C2D	2.69	1.56	1.50
4	A	800	CCW	C4-S3	-2.66	1.66	1.75
2	A	750	HEM	CAC-C3C	2.62	1.54	1.47
2	B	750	HEM	CMD-C2D	2.60	1.56	1.50
4	B	800	CCW	C1-NE	2.51	1.34	1.28
2	B	750	HEM	CAC-C3C	2.41	1.53	1.47
2	A	750	HEM	CMB-C2B	2.35	1.55	1.50
2	B	750	HEM	CMB-C2B	2.35	1.55	1.50
2	A	750	HEM	C3B-C2B	-2.32	1.32	1.37
3	B	760	H4B	C7-N8	2.25	1.48	1.46
2	A	750	HEM	CMA-C3A	2.09	1.55	1.50
2	A	750	HEM	C2A-C3A	-2.02	1.33	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	CCW	O6-S3-C4	7.81	116.14	108.87
4	B	800	CCW	O6-S3-C4	6.35	114.77	108.87
2	B	750	HEM	CBA-CAA-C2A	-4.72	99.48	112.53
3	A	760	H4B	C2-N1-C8A	4.57	121.42	113.36
2	A	750	HEM	CBA-CAA-C2A	-4.46	100.21	112.53
2	A	750	HEM	C4D-ND-C1D	4.33	110.34	105.21
4	A	800	CCW	O5-S3-C4	-4.26	104.91	108.87
4	A	800	CCW	O5-S3-O6	-3.79	110.11	117.22
4	A	800	CCW	CG-CD-NE	3.70	117.22	110.67
4	B	800	CCW	O5-S3-C4	-3.43	105.68	108.87
3	B	760	H4B	C2-N1-C8A	3.26	119.10	113.36
4	B	800	CCW	O5-S3-C2	-3.03	104.19	107.76
2	B	750	HEM	CHB-C1B-NB	2.99	128.07	124.37
2	B	750	HEM	C4D-ND-C1D	2.96	108.71	105.21
4	B	800	CCW	CG-CD-NE	2.93	115.87	110.67
2	B	750	HEM	C4C-C3C-C2C	2.90	109.33	106.81
2	B	750	HEM	CBD-CAD-C3D	-2.78	104.84	112.53
2	A	750	HEM	CBD-CAD-C3D	-2.69	105.08	112.53
3	B	760	H4B	O4-C4-C4A	-2.69	120.78	127.26
3	B	760	H4B	C4A-C4-N3	2.57	119.17	112.13
2	A	750	HEM	C4C-C3C-C2C	2.55	109.03	106.81
3	A	760	H4B	C4A-C4-N3	2.47	118.90	112.13
4	B	800	CCW	C2-C1-NH1	2.45	120.69	117.31
3	A	760	H4B	O4-C4-C4A	-2.42	121.42	127.26
2	B	750	HEM	CHC-C4B-NB	2.40	127.01	124.42
3	A	760	H4B	N3-C2-N1	-2.38	118.97	123.32
4	B	800	CCW	OA1-C-OA2	-2.34	118.77	124.08
4	A	800	CCW	C2-C1-NH1	2.33	120.53	117.31
3	A	760	H4B	N2-C2-N3	2.33	121.67	116.76
4	B	800	CCW	O5-S3-O6	-2.30	112.90	117.22
2	A	750	HEM	C3B-C2B-C1B	2.28	108.12	106.41
2	B	750	HEM	C3B-C4B-NB	-2.27	107.84	109.47
2	A	750	HEM	CMD-C2D-C1D	2.26	128.57	125.03
2	B	750	HEM	CAD-C3D-C4D	2.22	128.56	124.70
2	B	750	HEM	CMD-C2D-C1D	2.21	128.49	125.03
2	B	750	HEM	CHA-C4D-ND	2.18	127.07	124.37
2	B	750	HEM	C1D-C2D-C3D	-2.14	104.73	106.98
2	B	750	HEM	C4A-CHB-C1B	-2.10	121.31	126.25
3	A	760	H4B	C4-C4A-N5	2.07	121.91	116.27
2	B	750	HEM	CAB-C3B-C2B	-2.02	121.88	128.43
2	A	750	HEM	CAB-C3B-C2B	-2.02	121.88	128.43

There are no chirality outliers.

All (5) torsion outliers are listed below:

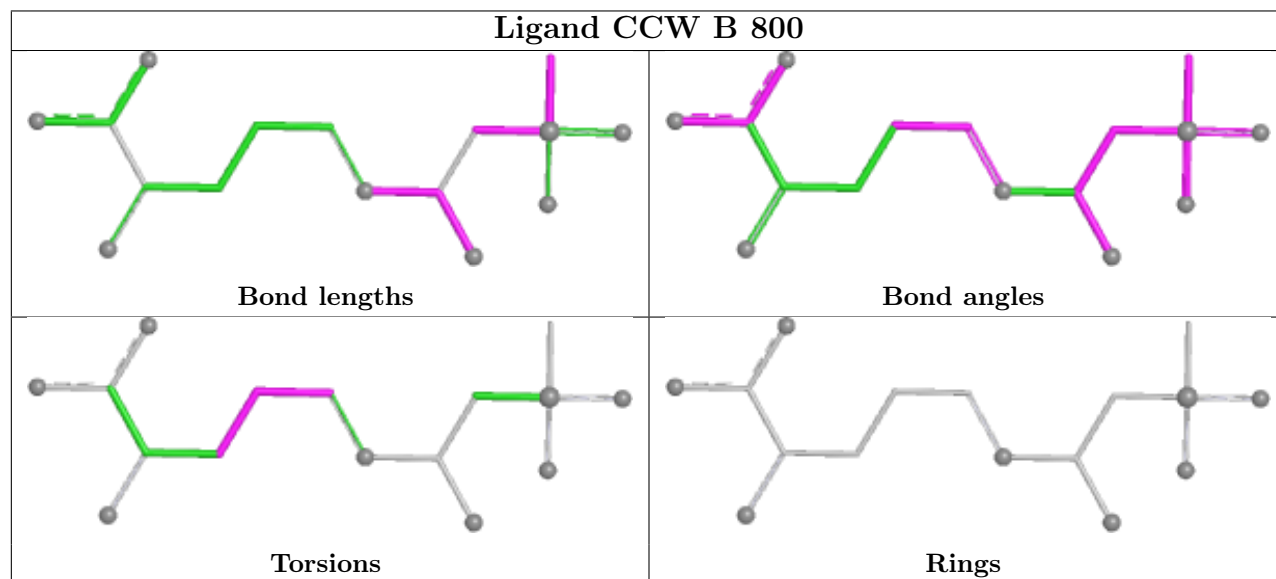
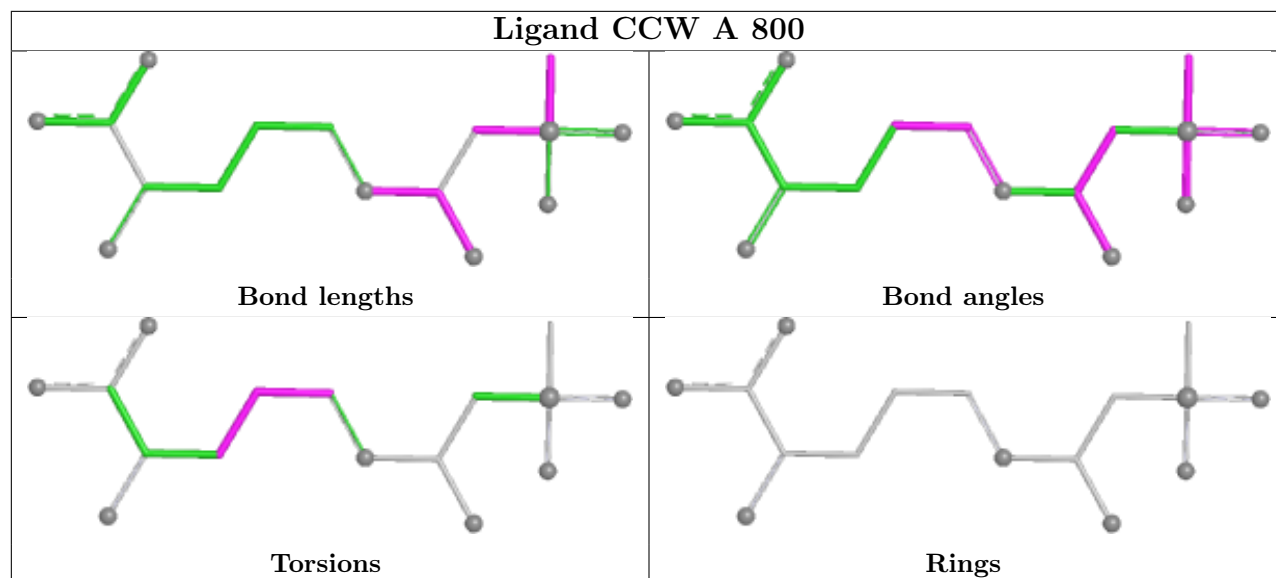
Mol	Chain	Res	Type	Atoms
4	B	800	CCW	NE-CD-CG-CB
4	A	800	CCW	NE-CD-CG-CB
2	A	750	HEM	C4B-C3B-CAB-CBB
4	A	800	CCW	CA-CB-CG-CD
4	B	800	CCW	CA-CB-CG-CD

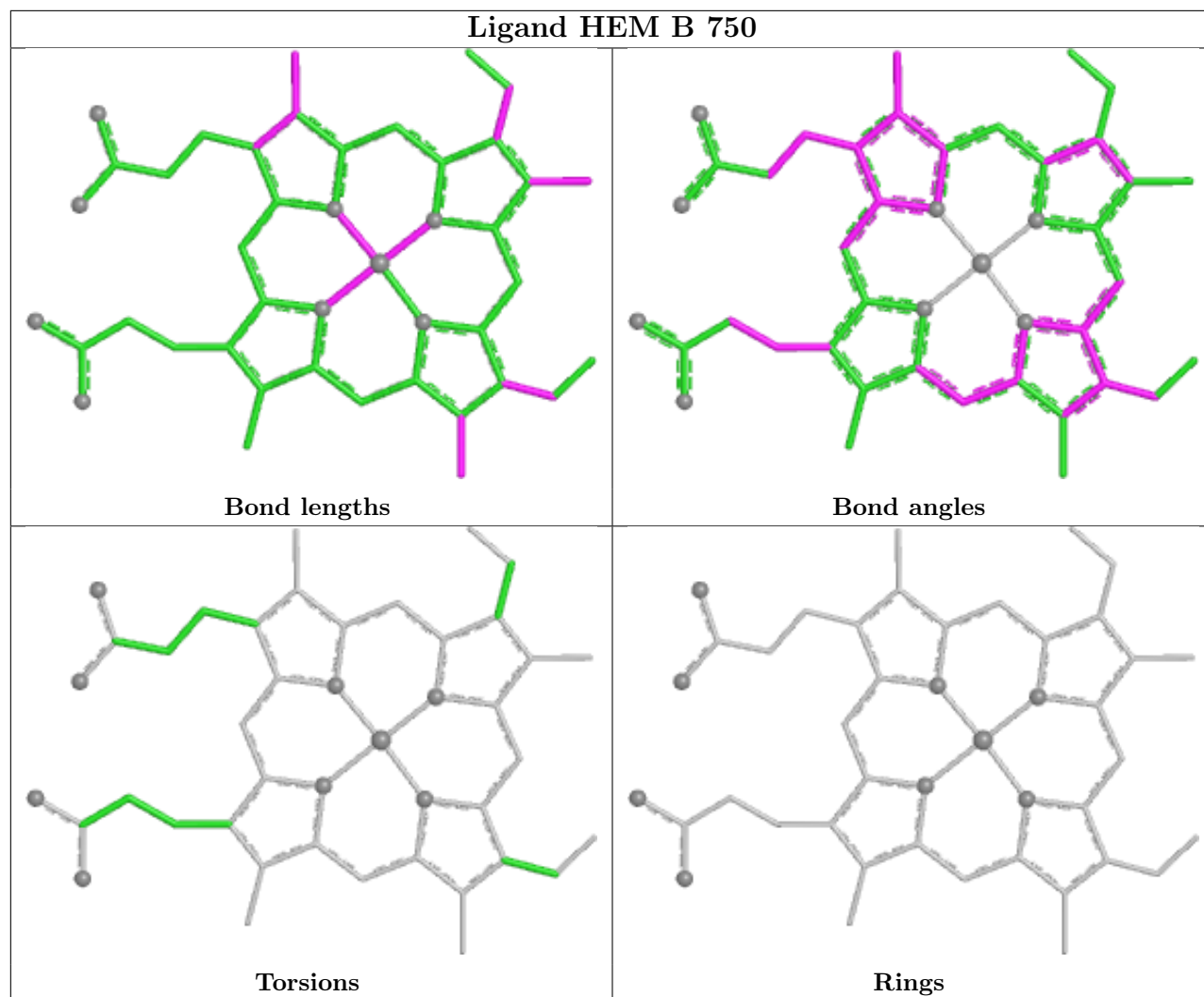
There are no ring outliers.

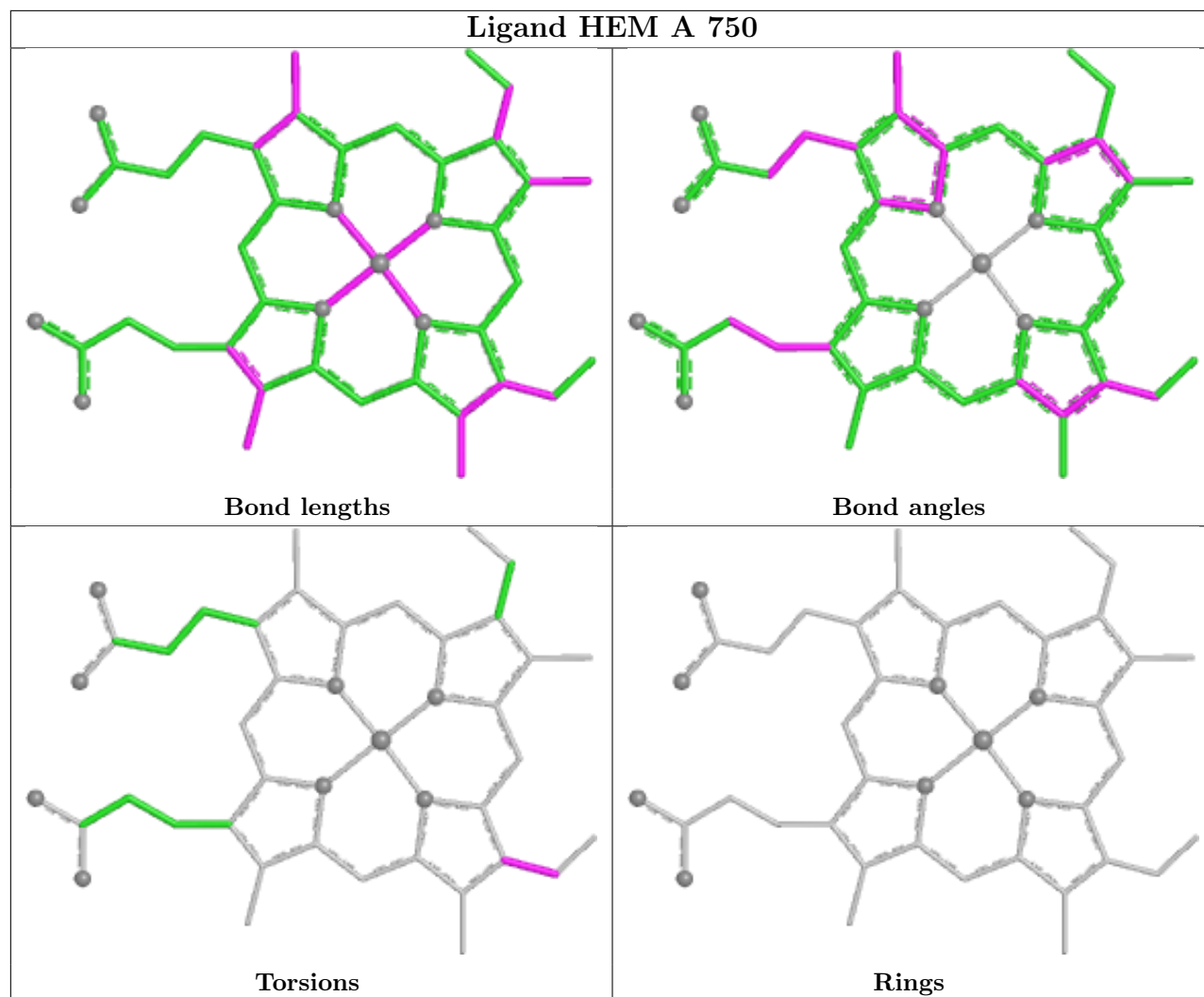
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	CCW	5	0
4	B	800	CCW	7	0
2	B	750	HEM	4	0
2	A	750	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.







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	408/422 (96%)	1.67	165 (40%) 0 0	18, 47, 93, 117	5 (1%)
1	B	411/422 (97%)	0.50	26 (6%) 26 29	20, 35, 60, 81	4 (0%)
All	All	819/844 (97%)	1.08	191 (23%) 2 1	18, 40, 85, 117	9 (1%)

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	715	VAL	7.5
1	A	384	VAL	7.0
1	A	551	PHE	6.7
1	A	493	LEU	6.1
1	A	355	PHE	5.9
1	A	553	TRP	5.8
1	A	528	GLY	5.4
1	A	376	ALA	5.4
1	A	616	LEU	5.3
1	A	716	TRP	5.2
1	A	509	GLY	5.1
1	A	554	PHE	5.0
1	A	513	PRO	5.0
1	A	373	GLY	5.0
1	A	372	PHE	4.9
1	A	300	PHE	4.9
1	A	559	LEU	4.9
1	A	533	LEU	4.8
1	A	512	ALA	4.8
1	B	348	VAL	4.7
1	A	625	TRP	4.7
1	A	381	LEU	4.7
1	A	506	ILE	4.7
1	A	378	MET	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	485	TYR	4.5
1	A	488	PRO	4.4
1	A	546	ILE	4.3
1	A	618	MET	4.2
1	A	377	HIS	4.1
1	A	557	LEU	4.1
1	A	505	CYS	4.1
1	A	487	GLN	4.0
1	A	363	ASP	4.0
1	A	338	PRO	4.0
1	B	300	PHE	4.0
1	A	510	TRP	3.9
1	B	350	THR	3.9
1	A	494	GLY	3.9
1	A	504	ILE	3.9
1	A	486	LYS	3.8
1	A	356	PRO	3.8
1	A	501	PHE	3.8
1	A	483	ALA	3.8
1	A	383	GLU	3.8
1	A	388	ILE	3.8
1	A	385	ASN	3.7
1	A	517	PHE	3.7
1	A	514	ARG	3.7
1	B	355	PHE	3.7
1	A	321	THR	3.7
1	A	362	LEU	3.7
1	A	712	ASN	3.7
1	A	350	THR	3.7
1	A	374	SER	3.6
1	A	640	SER	3.6
1	A	318	LEU	3.6
1	A	322	LEU	3.6
1	A	354	LEU	3.6
1	A	550	LYS	3.6
1	A	466	THR	3.6
1	A	499	VAL	3.5
1	A	548	HIS	3.5
1	A	545	PRO	3.5
1	A	299	ARG	3.4
1	A	361	PHE	3.4
1	A	714	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	358	ALA	3.3
1	A	470	HIS	3.3
1	A	711	TRP	3.3
1	B	553	TRP	3.3
1	A	319	LYS	3.3
1	A	549	PRO	3.3
1	A	639	TYR	3.2
1	A	610	VAL	3.2
1	A	490	GLY	3.2
1	A	552	ASP	3.2
1	A	503	GLU	3.2
1	A	531	PRO	3.1
1	A	357	LEU	3.1
1	A	713	THR	3.1
1	A	529	ASN	3.1
1	A	629	ALA	3.1
1	A	382	GLU	3.1
1	A	468	GLY	3.1
1	A	366	TYR	3.0
1	A	706	TYR	3.0
1	A	515	GLY	3.0
1	B	392	SER	3.0
1	A	508	GLN	3.0
1	A	484	GLY	3.0
1	A	614	MET	3.0
1	B	322	LEU	2.9
1	A	301	LEU	2.9
1	A	472	PHE	2.9
1	A	380	ARG	2.9
1	A	612	LYS	2.9
1	A	613	LYS	2.9
1	A	393	THR	2.8
1	A	544	VAL	2.8
1	A	518	ASP	2.8
1	B	618	MET	2.8
1	B	389	GLU	2.8
1	A	558	GLY	2.8
1	A	577	LEU	2.8
1	A	633	ILE	2.8
1	B	616	LEU	2.8
1	A	434	THR	2.8
1	A	489	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	369	ILE	2.8
1	A	392	SER	2.7
1	A	375	LYS	2.7
1	A	670	GLY	2.7
1	A	311	VAL	2.7
1	A	482	TYR	2.7
1	A	611	ALA	2.7
1	A	520	LEU	2.7
1	A	330	ILE	2.7
1	A	555	LYS	2.7
1	A	534	PHE	2.7
1	A	492	THR	2.7
1	A	710	PRO	2.7
1	A	394	TYR	2.6
1	B	551	PHE	2.6
1	A	617	ASP	2.6
1	A	643	SER	2.6
1	B	321	THR	2.6
1	B	338	PRO	2.6
1	A	475	TRP	2.6
1	A	606	ILE	2.6
1	A	620	LYS	2.6
1	A	601	ASN	2.6
1	A	621	THR	2.6
1	A	435	ALA	2.5
1	A	390	SER	2.5
1	A	328	GLU	2.5
1	A	467	ASP	2.5
1	A	511	LYS	2.5
1	A	379	ASP	2.5
1	B	352	ASP	2.5
1	A	667	ARG	2.4
1	A	367	SER	2.4
1	A	502[A]	THR	2.4
1	A	365	TYR	2.4
1	A	469	LYS	2.4
1	A	556	ASP	2.4
1	A	523	LEU	2.4
1	B	493	LEU	2.4
1	A	609	GLU	2.4
1	A	496	PRO	2.4
1	A	351	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	396	LEU	2.3
1	A	387	GLU	2.3
1	A	353	GLN	2.3
1	A	315	THR	2.3
1	B	356	PRO	2.3
1	A	516	ARG	2.3
1	B	615	ASP	2.3
1	A	519	VAL	2.3
1	A	436	HIS	2.3
1	A	439	PHE	2.2
1	A	526	ALA	2.2
1	A	605	ASN	2.2
1	B	337	LEU	2.2
1	A	576	GLY	2.2
1	A	370	LYS	2.2
1	A	310	VAL	2.2
1	A	433	THR	2.2
1	A	364	GLN	2.2
1	B	310	VAL	2.2
1	A	313	THR	2.2
1	B	611	ALA	2.2
1	A	527	ASN	2.1
1	A	530	ASP	2.1
1	A	359	LYS	2.1
1	A	386	LYS	2.1
1	A	538	PRO	2.1
1	B	299	ARG	2.1
1	B	535	GLN	2.1
1	A	644	ASP	2.1
1	A	619	ARG	2.1
1	A	320	SER	2.1
1	A	371	ARG	2.1
1	A	389	GLU	2.1
1	B	329	HIS	2.1
1	B	610	VAL	2.1
1	B	552	ASP	2.1
1	A	575	GLY	2.0
1	A	500	GLN	2.0
1	A	303	VAL	2.0
1	A	352	ASP	2.0
1	B	311	VAL	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](#)

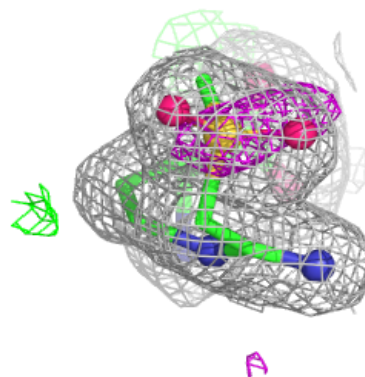
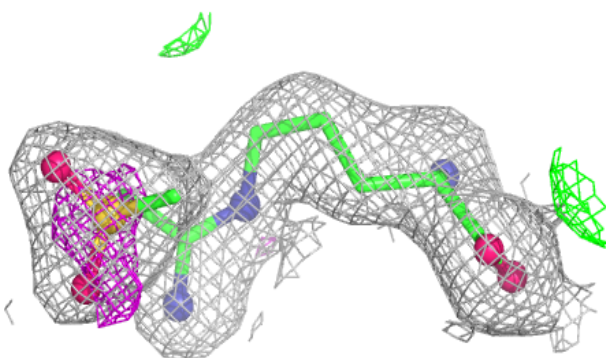
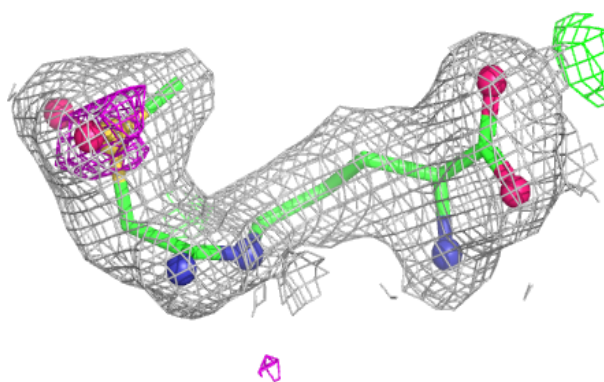
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CCW	A	800	16/16	0.91	0.11	36,39,41,42	0
4	CCW	B	800	16/16	0.91	0.11	32,35,41,44	0
3	H4B	A	760	17/17	0.93	0.07	23,27,30,31	0
5	ACT	A	860	4/4	0.94	0.12	52,52,53,53	0
5	ACT	B	860	4/4	0.96	0.09	39,40,41,43	0
3	H4B	B	760	17/17	0.97	0.05	21,24,28,30	0
2	HEM	A	750	43/43	0.98	0.07	24,27,34,39	0
2	HEM	B	750	43/43	0.98	0.07	22,25,30,40	0
6	ZN	B	900	1/1	0.99	0.02	31,31,31,31	0

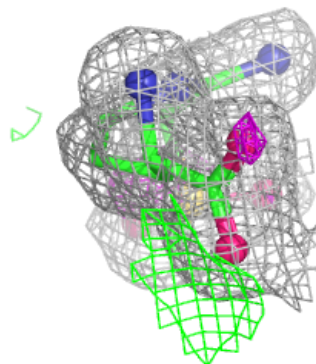
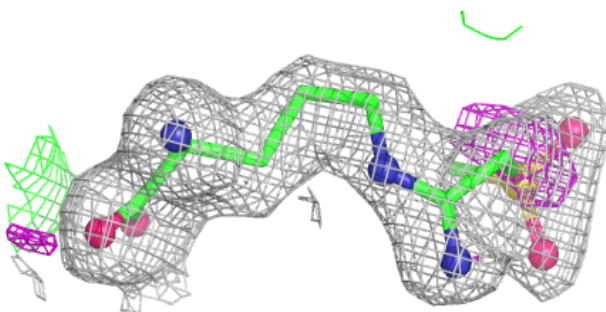
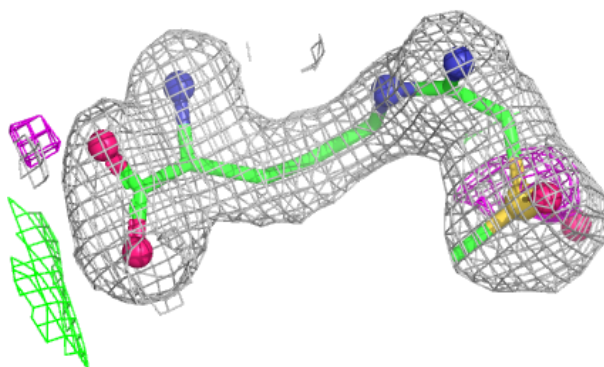
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CCW 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)

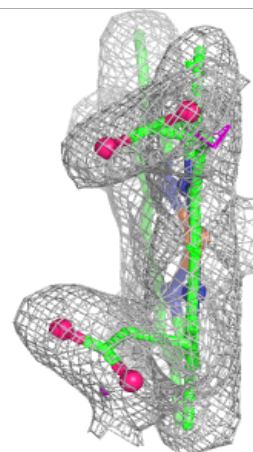
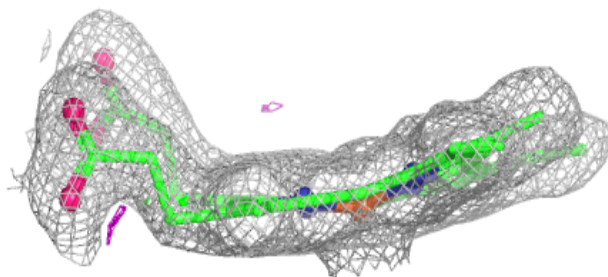
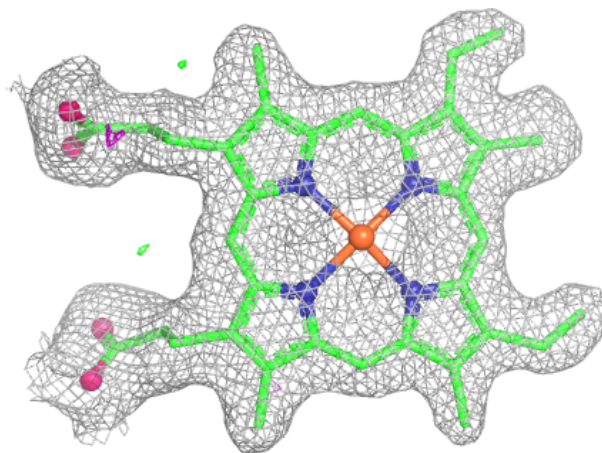
**Electron density around CCW B 800:**

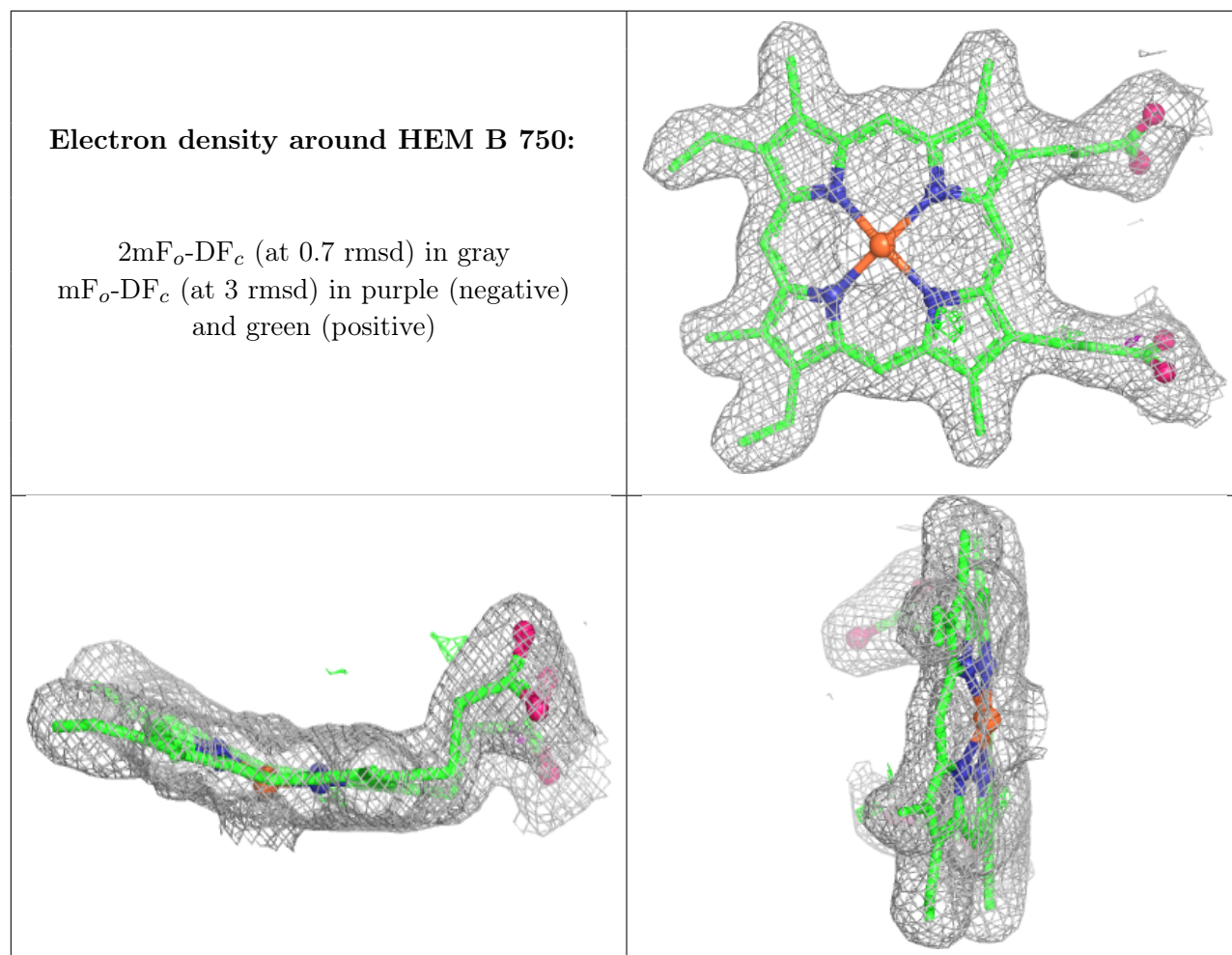
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

There are no such residues in this entry.