



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:37 PM EDT

PDB ID : 2HX2 / pdb_00002hx2
Title : Bovine eNOS heme domain complexed with (4S)-N-{4-Amino-5-[(2-aminoethyl)-hydroxyamino]-pentyl}-N'-nitroguanidine
Authors : Igarashi, J.; Li, H.; Poulos, T.L.
Deposited on : 2006-08-02
Resolution : 1.95 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

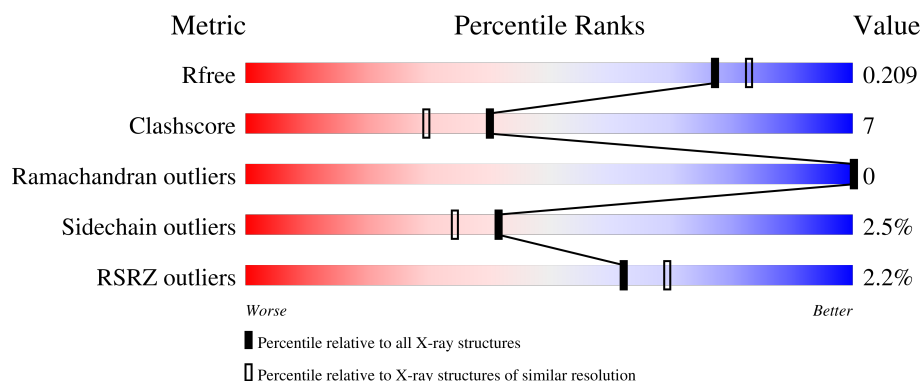
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	416	
1	B	416	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7132 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.

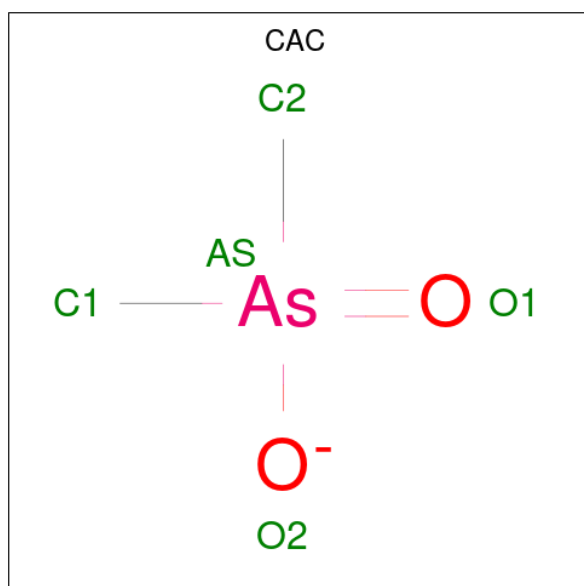
- Molecule 1 is a protein called Nitric-oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3202	2036	563	587	16			
1	B	402	Total	C	N	O	S	0	0	0
			3202	2035	565	586	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

- Molecule 2 is CACODYLATE ION (CCD ID: CAC) (formula: $\text{C}_2\text{H}_6\text{AsO}_2$).



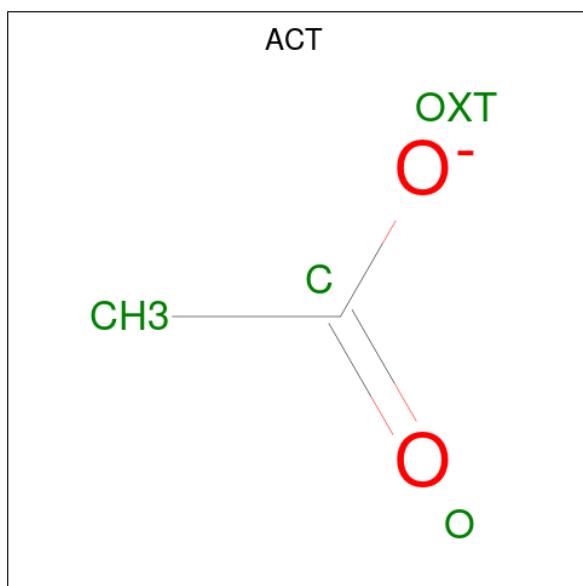
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	As C	0	0
			3	1 2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	As	C	0	0
			3	1	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

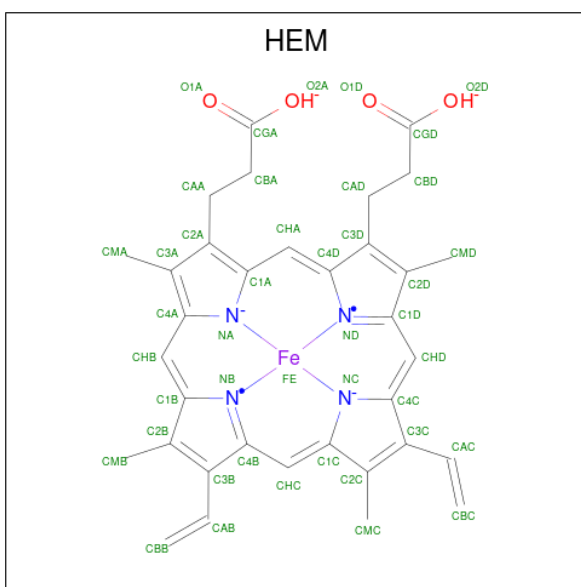


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

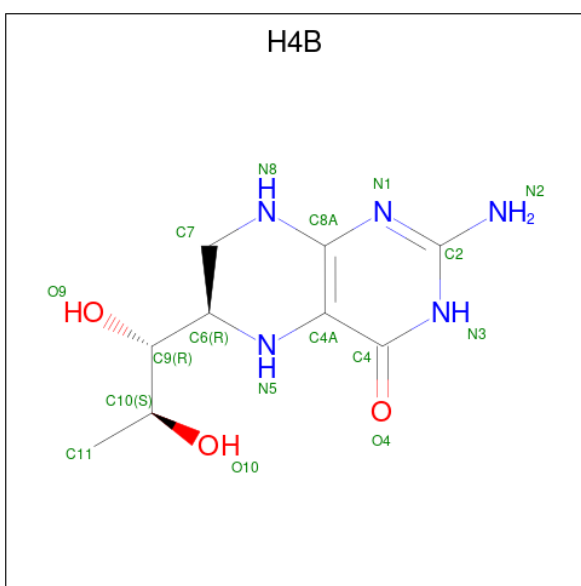
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



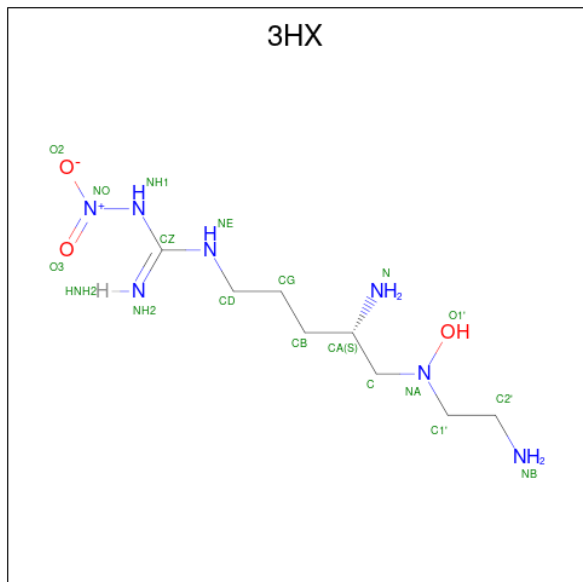
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



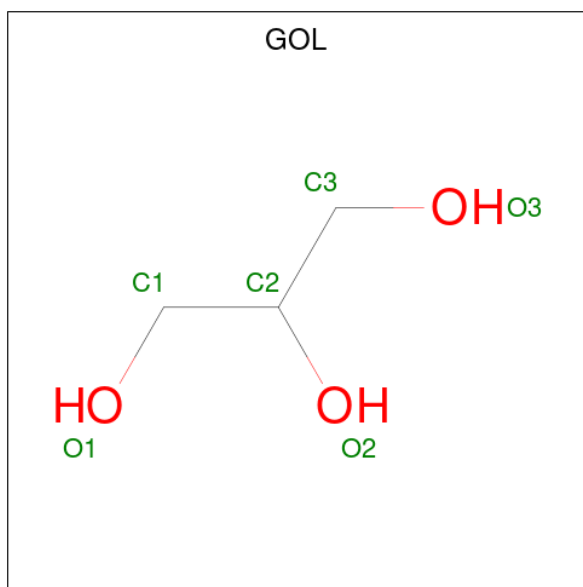
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 17	C 9	N 5	O 3	0	0
6	B	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 7 is (4S)-N-{4-AMINO-5-[(2-AMINOETHYL)(HYDROXYAMINO)-PENTYL]-N²-NITROGUANIDINE (CCD ID: 3HX) (formula: C₈H₂₁N₇O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			18	8	7	3		
7	B	1	Total	C	N	O	0	0
			18	8	7	3		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

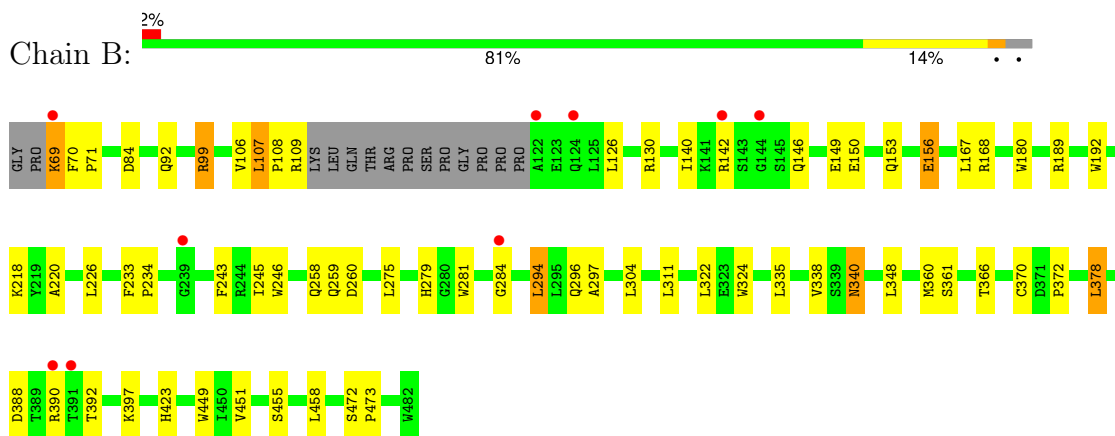
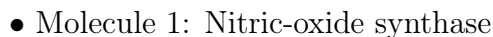


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 6	C 3	O 3	0	0
8	B	1	Total 6	C 3	O 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	269	Total 269	O 269	0	0
9	B	268	Total 268	O 268	0	0

- Molecule 1: Nitric-oxide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.82Å 106.85Å 156.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.36 – 1.95 48.36 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.36-1.95) 98.3 (48.36-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.213 0.177 , 0.209	Depositor DCC
R_{free} test set	3472 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7132	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, GOL, ZN, CAC, H4B, 3HX, 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	0.50	0/3291	0.96	8/4483 (0.2%)
1	B	0.49	0/3290	0.97	12/4480 (0.3%)
All	All	0.49	0/6581	0.96	20/8963 (0.2%)

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

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	MET	N-CA-C	-8.51	95.37	109.24
1	A	360	MET	N-CA-C	-7.65	96.77	109.24
1	B	243	PHE	N-CA-C	-7.24	98.24	109.76
1	B	451	VAL	CA-C-N	7.22	124.93	119.66
1	B	451	VAL	C-N-CA	7.22	124.93	119.66
1	B	245	ILE	N-CA-C	-6.98	97.68	107.80
1	A	192	TRP	N-CA-C	6.88	119.66	111.33
1	A	335	LEU	N-CA-C	6.31	120.06	108.69
1	A	361	SER	N-CA-C	6.26	119.77	111.75
1	A	243	PHE	N-CA-C	-6.11	100.55	110.20
1	B	189	ARG	N-CA-C	6.08	120.16	112.87
1	B	168	ARG	N-CA-C	-6.06	102.37	110.55
1	A	359	TYR	N-CA-C	6.05	119.03	110.50
1	B	361	SER	N-CA-C	6.04	119.47	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	335	LEU	N-CA-C	5.84	119.19	108.69
1	B	296	GLN	N-CA-C	5.66	117.64	108.41
1	A	189	ARG	N-CA-C	5.59	119.57	112.87
1	B	284	GLY	N-CA-C	-5.13	105.27	112.60
1	A	475	PHE	N-CA-C	-5.06	101.00	109.24
1	B	297	ALA	N-CA-C	-5.05	103.60	110.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3202	0	3106	41	0
1	B	3202	0	3109	45	0
2	A	3	0	0	0	0
2	B	3	0	0	1	0
3	A	8	0	6	0	0
3	B	8	0	6	0	0
4	A	1	0	0	0	0
5	A	43	0	30	1	0
5	B	43	0	30	1	0
6	A	17	0	15	1	0
6	B	17	0	15	1	0
7	A	18	0	21	4	0
7	B	18	0	21	3	0
8	A	6	0	8	1	0
8	B	6	0	8	0	0
9	A	269	0	0	6	0
9	B	268	0	0	2	0
All	All	7132	0	6375	85	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 7.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.49	0.93
1:A:92:GLN:HE22	1:A:476:ARG:HH22	0.97	0.90
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.57	0.85
1:A:92:GLN:NE2	1:A:476:ARG:HH22	1.76	0.83
1:B:130:ARG:HH11	1:B:130:ARG:HB3	1.42	0.82
1:B:69:LYS:HD2	1:B:70:PHE:H	1.48	0.78
1:A:99:ARG:HB2	1:A:99:ARG:HH11	1.49	0.77
1:B:338:VAL:HG22	7:B:793:3HX:H1	1.66	0.75
1:A:243:PHE:O	1:A:244:ARG:HG2	1.87	0.75
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.49	0.74
1:B:106:VAL:HG12	1:B:107:LEU:HD13	1.72	0.71
1:A:149:GLU:O	1:A:153:GLN:HG2	1.93	0.69
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.24	0.67
1:B:388:ASP:OD1	1:B:390:ARG:HB3	1.95	0.66
1:B:130:ARG:HB3	1:B:130:ARG:NH1	2.10	0.66
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.36	0.65
1:B:126:LEU:O	1:B:130:ARG:HG3	1.96	0.65
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.78	0.64
1:A:99:ARG:HB2	1:A:99:ARG:NH1	2.13	0.63
8:A:880:GOL:H2	9:A:906:HOH:O	1.98	0.62
1:B:126:LEU:HD21	1:B:156:GLU:OE2	2.00	0.61
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.43	0.59
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.85	0.59
1:A:152:LEU:O	1:A:156:GLU:HG3	2.05	0.56
1:B:140:ILE:HD12	1:B:142:ARG:HD2	1.86	0.56
1:B:338:VAL:CG2	7:B:793:3HX:H1	2.35	0.56
1:A:270:VAL:O	1:A:274:GLU:HG3	2.06	0.55
1:B:69:LYS:HD2	1:B:70:PHE:N	2.21	0.54
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.89	0.54
5:B:700:HEM:O2D	7:B:793:3HX:H1'2	2.08	0.54
1:A:126:LEU:HD12	1:A:130:ARG:CZ	2.39	0.53
1:B:259:GLN:H	1:B:259:GLN:CD	2.17	0.53
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.91	0.52
1:B:146:GLN:O	1:B:150:GLU:HG3	2.10	0.52
1:A:240:ARG:HD2	1:A:241:GLY:O	2.09	0.52
1:B:149:GLU:O	1:B:153:GLN:HG3	2.10	0.51
1:A:218:LYS:HG2	1:A:311:LEU:HD22	1.92	0.51
1:B:246:TRP:HB2	1:B:294:LEU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ASN:HD22	1:B:340:ASN:H	1.58	0.50
1:A:95:PRO:HB3	1:A:108:PRO:HB2	1.95	0.49
5:A:700:HEM:O2D	7:A:793:3HX:H2	2.12	0.49
1:A:214:CYS:SG	9:A:1168:HOH:O	2.60	0.49
1:A:340:ASN:HD21	7:A:793:3HX:H2'1	1.78	0.49
1:A:240:ARG:NH2	9:A:1071:HOH:O	2.42	0.49
1:A:378:LEU:HB2	9:A:905:HOH:O	2.13	0.49
1:A:151:ARG:HD3	1:A:168:ARG:CZ	2.43	0.49
1:A:338:VAL:CG2	7:A:793:3HX:H1	2.43	0.49
1:B:69:LYS:HD2	1:B:69:LYS:N	2.28	0.48
1:A:310:GLU:HG2	9:A:1159:HOH:O	2.13	0.48
1:A:449:TRP:HA	6:A:760:H4B:N1	2.28	0.48
1:B:472:SER:HA	1:B:473:PRO:C	2.39	0.47
1:A:472:SER:HA	1:A:473:PRO:C	2.39	0.47
1:B:449:TRP:HA	6:B:760:H4B:N1	2.29	0.47
1:B:378:LEU:HB2	9:B:1076:HOH:O	2.15	0.47
1:A:423:HIS:HB2	1:B:392:THR:HB	1.96	0.46
1:A:99:ARG:CZ	1:A:99:ARG:HA	2.46	0.45
1:A:70:PHE:O	1:B:109:ARG:NH1	2.50	0.45
1:A:338:VAL:HG22	7:A:793:3HX:H1	1.99	0.45
1:A:218:LYS:HE2	1:A:311:LEU:HD21	1.98	0.44
1:B:340:ASN:HD22	1:B:340:ASN:N	2.13	0.44
1:A:158:GLU:HG2	1:A:165:TYR:HA	2.00	0.43
1:A:279:HIS:HE1	9:A:1092:HOH:O	2.00	0.43
1:B:259:GLN:CD	1:B:259:GLN:N	2.75	0.43
1:B:218:LYS:HE3	1:B:311:LEU:HD11	2.00	0.43
1:B:366:THR:O	1:B:370:CYS:HB2	2.19	0.43
1:A:126:LEU:HD23	1:A:159:VAL:HG11	2.01	0.43
1:A:99:ARG:NH1	1:A:99:ARG:CB	2.80	0.43
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.49	0.43
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.54	0.42
1:B:340:ASN:H	1:B:340:ASN:ND2	2.17	0.42
1:B:71:PRO:HG2	1:B:84:ASP:HB3	2.01	0.42
1:A:126:LEU:HD12	1:A:130:ARG:NH1	2.34	0.41
1:B:108:PRO:HA	9:B:1019:HOH:O	2.20	0.41
1:A:126:LEU:HD21	1:A:156:GLU:HA	2.02	0.41
1:A:344:GLU:OE1	1:A:476:ARG:NH2	2.53	0.41
1:B:259:GLN:NE2	1:B:260:ASP:OD1	2.54	0.41
1:B:130:ARG:HH11	1:B:130:ARG:CB	2.21	0.41
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.96	0.41
1:A:392:THR:HB	1:B:423:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:SER:HB3	1:B:458:LEU:HD12	2.01	0.41
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.56	0.41
1:B:99:ARG:HH11	1:B:99:ARG:CB	2.26	0.40
1:B:220:ALA:O	1:B:226:LEU:HA	2.22	0.40
1:B:324:TRP:HB2	2:B:850:CAC:C2	2.52	0.40
1:B:275:LEU:O	1:B:279:HIS:HD2	2.04	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	399/416 (96%)	392 (98%)	7 (2%)	0	100	100
1	B	398/416 (96%)	382 (96%)	16 (4%)	0	100	100
All	All	797/832 (96%)	774 (97%)	23 (3%)	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	342/354 (97%)	335 (98%)	7 (2%)	48	43
1	B	342/354 (97%)	332 (97%)	10 (3%)	37	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	684/708 (97%)	667 (98%)	17 (2%)	42	34

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	PRO
1	A	99	ARG
1	A	126	LEU
1	A	194	LYS
1	A	306	VAL
1	A	340	ASN
1	A	378	LEU
1	B	69	LYS
1	B	92	GLN
1	B	99	ARG
1	B	107	LEU
1	B	156	GLU
1	B	258	GLN
1	B	294	LEU
1	B	340	ASN
1	B	378	LEU
1	B	397	LYS

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

Mol	Chain	Res	Type
1	A	91	GLN
1	A	92	GLN
1	A	191	GLN
1	A	278	GLN
1	A	279	HIS
1	A	340	ASN
1	A	413	GLN
1	A	468	ASN
1	B	89	GLN
1	B	191	GLN
1	B	279	HIS
1	B	340	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	HEM	B	700	1	50,50,50	1.26	6 (12%)	67,82,82	1.06	5 (7%)
3	ACT	A	861	-	3,3,3	0.95	0	3,3,3	0.97	0
2	CAC	B	850	1	0,2,4	-	-	0,1,6	-	-
7	3HX	B	793	-	10,17,17	2.14	3 (30%)	11,20,20	1.11	0
3	ACT	B	860	-	3,3,3	0.98	0	3,3,3	0.71	0
5	HEM	A	700	1	50,50,50	1.15	4 (8%)	67,82,82	0.93	2 (2%)
8	GOL	A	880	-	5,5,5	0.22	0	5,5,5	0.20	0
3	ACT	A	860	-	3,3,3	0.94	0	3,3,3	0.79	0
6	H4B	A	760	-	17,18,18	1.71	4 (23%)	14,26,26	1.92	3 (21%)
8	GOL	B	880	-	5,5,5	0.19	0	5,5,5	0.24	0
6	H4B	B	760	-	17,18,18	1.65	2 (11%)	14,26,26	1.81	3 (21%)
3	ACT	B	861	-	3,3,3	0.90	0	3,3,3	0.81	0
2	CAC	A	850	1	0,2,4	-	-	0,1,6	-	-
7	3HX	A	793	-	10,17,17	1.98	3 (30%)	11,20,20	0.94	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
5	HEM	B	700	1	-	0/14/54/54	-
7	3HX	B	793	-	-	9/14/18/18	-
5	HEM	A	700	1	-	0/14/54/54	-
8	GOL	A	880	-	-	0/4/4/4	-
6	H4B	A	760	-	-	0/8/17/17	0/2/2/2
8	GOL	B	880	-	-	2/4/4/4	-
6	H4B	B	760	-	-	0/8/17/17	0/2/2/2
7	3HX	A	793	-	-	5/14/18/18	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	793	3HX	CB-CA	4.09	1.59	1.53
6	B	760	H4B	C4A-N5	4.08	1.47	1.37
6	A	760	H4B	C6-N5	3.77	1.54	1.47
6	A	760	H4B	C4A-N5	3.76	1.46	1.37
6	B	760	H4B	C6-N5	3.63	1.54	1.47
7	B	793	3HX	C-CA	3.51	1.58	1.53
7	A	793	3HX	C-CA	3.46	1.57	1.53
7	A	793	3HX	CB-CA	3.23	1.57	1.53
7	B	793	3HX	CD-NE	2.81	1.52	1.46
7	A	793	3HX	CD-NE	2.79	1.52	1.46
5	B	700	HEM	FE-NB	2.67	2.03	1.94
5	B	700	HEM	FE-ND	2.65	2.03	1.94
5	A	700	HEM	FE-NA	2.57	2.03	1.95
5	B	700	HEM	FE-NC	2.57	2.03	1.95
5	B	700	HEM	FE-NA	2.51	2.03	1.95
5	A	700	HEM	FE-NC	2.50	2.03	1.95
5	A	700	HEM	CAB-C3B	-2.45	1.40	1.47
5	B	700	HEM	C1B-NB	-2.40	1.36	1.40
6	A	760	H4B	C7-C6	2.17	1.54	1.52
5	A	700	HEM	CAC-C3C	-2.16	1.41	1.47
6	A	760	H4B	C7-N8	2.07	1.48	1.46
5	B	700	HEM	CAB-C3B	-2.00	1.42	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	760	H4B	C2-N1-C8A	5.33	122.76	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	760	H4B	C2-N1-C8A	4.92	122.05	113.36
5	B	700	HEM	CBA-CAA-C2A	-3.70	102.31	112.53
6	A	760	H4B	N3-C2-N1	-3.05	117.75	123.32
5	B	700	HEM	C4C-C3C-C2C	-2.88	104.32	106.81
6	B	760	H4B	N3-C2-N1	-2.85	118.10	123.32
6	B	760	H4B	O10-C10-C9	-2.72	105.27	109.77
6	A	760	H4B	O10-C10-C9	-2.60	105.47	109.77
5	A	700	HEM	CBA-CAA-C2A	-2.55	105.49	112.53
5	B	700	HEM	C3B-C2B-C1B	2.21	108.07	106.41
5	B	700	HEM	C4B-C3B-C2B	-2.14	105.31	107.28
5	B	700	HEM	C3B-C4B-NB	2.10	110.98	109.47
5	A	700	HEM	C3B-C4B-NB	2.07	110.95	109.47

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	793	3HX	N-CA-CB-CG
7	A	793	3HX	C2'-C1'-NA-O1'
7	B	793	3HX	CZ-NH1-NO-O3
7	B	793	3HX	NA-C-CA-N
7	B	793	3HX	CA-CB-CG-CD
7	B	793	3HX	C2'-C1'-NA-O1'
7	B	793	3HX	NA-C1'-C2'-NB
7	B	793	3HX	NE-CD-CG-CB
8	B	880	GOL	O1-C1-C2-C3
7	A	793	3HX	NA-C1'-C2'-NB
8	B	880	GOL	O1-C1-C2-O2
7	B	793	3HX	NA-C-CA-CB
7	A	793	3HX	CA-C-NA-C1'
7	B	793	3HX	CA-C-NA-C1'
7	B	793	3HX	CG-CD-NE-CZ
7	A	793	3HX	C-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 11 short contacts:

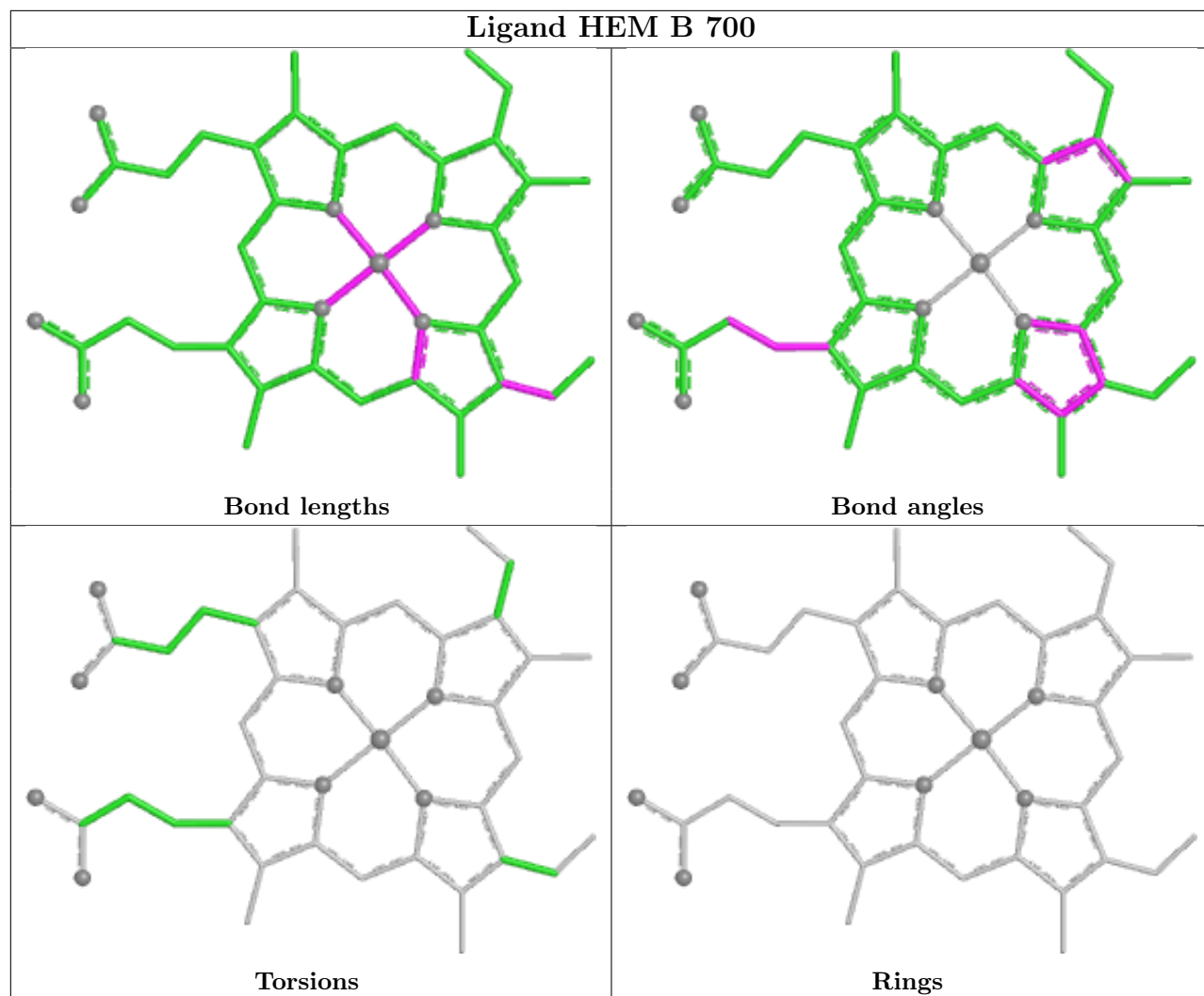
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	700	HEM	1	0
2	B	850	CAC	1	0
7	B	793	3HX	3	0

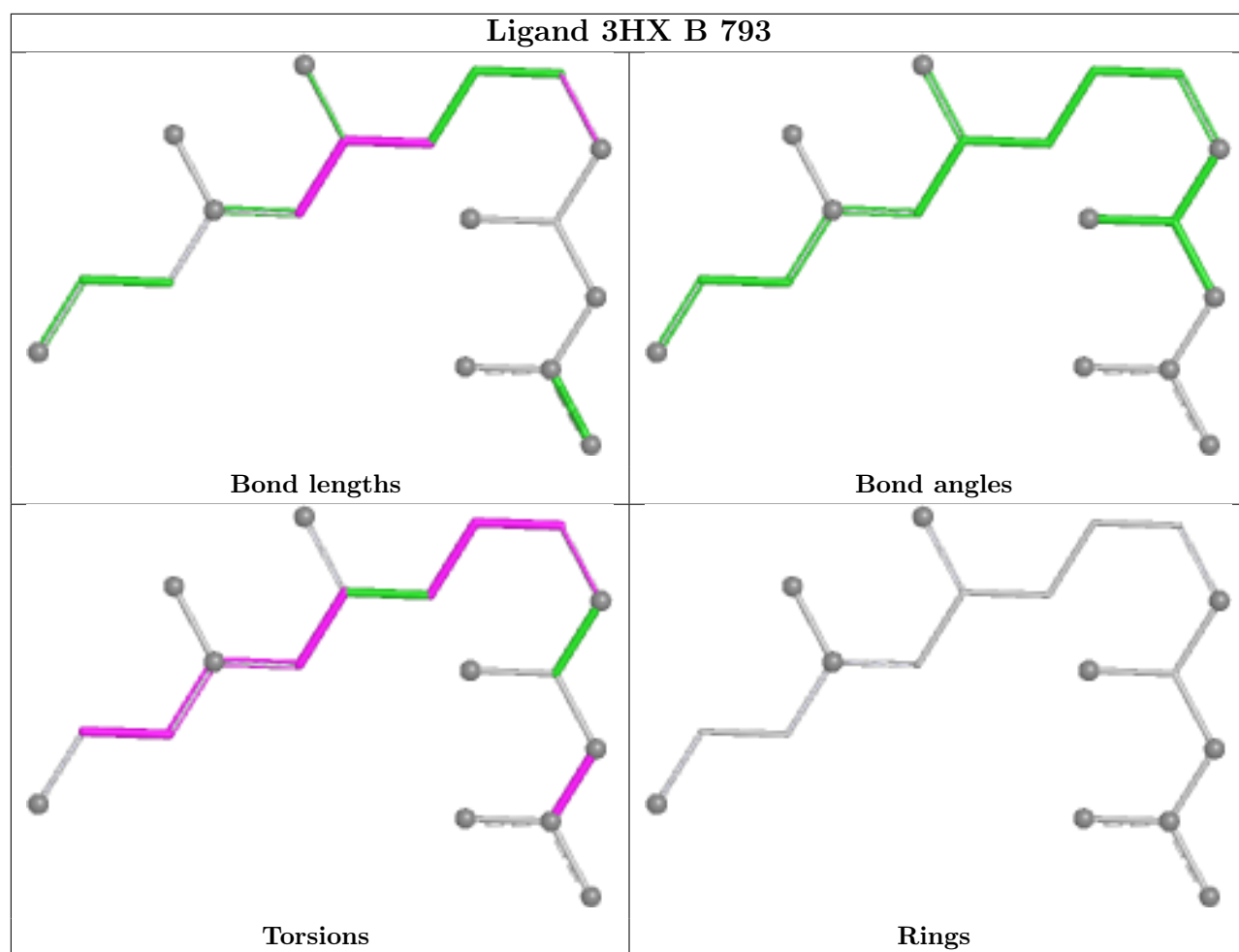
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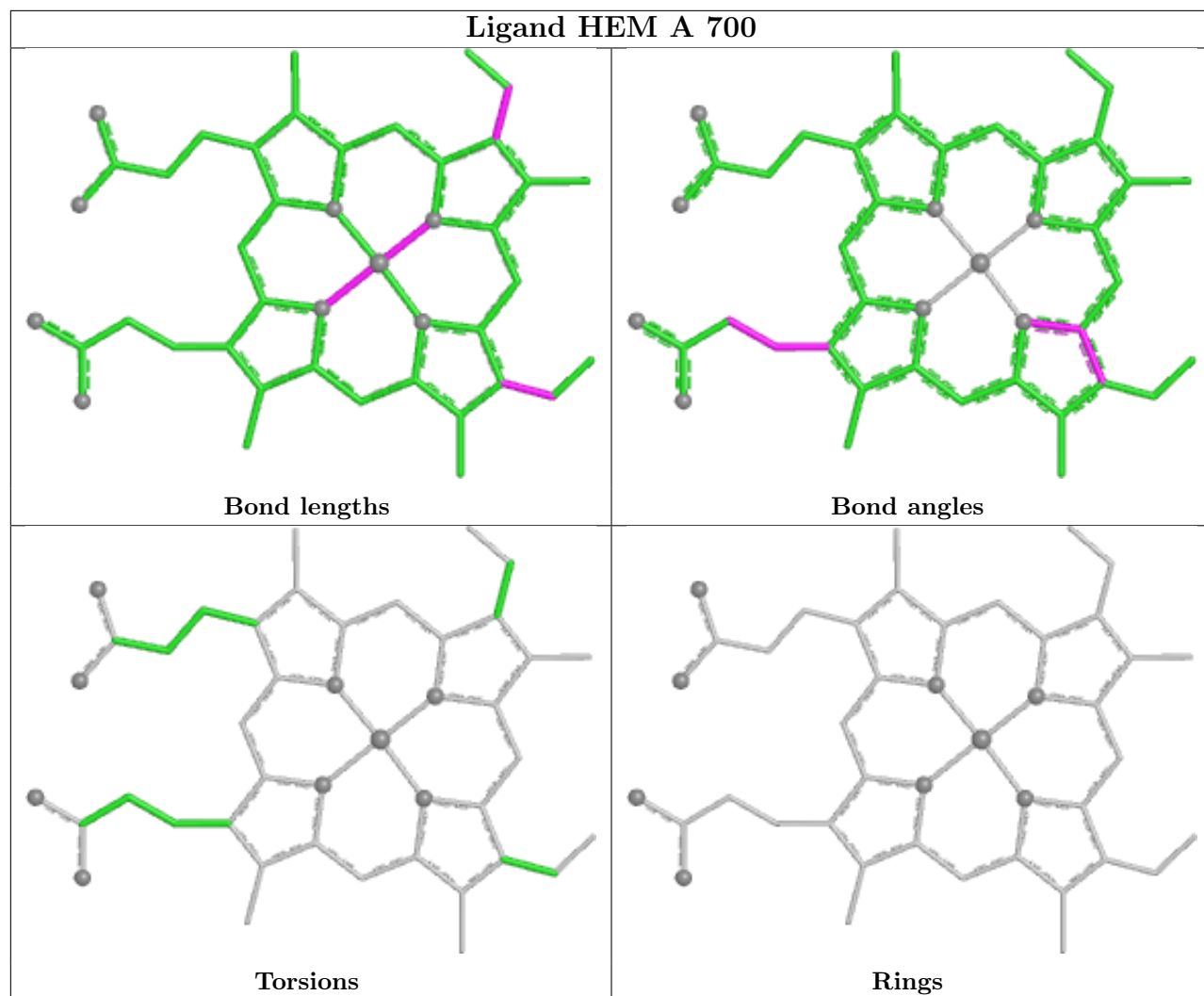
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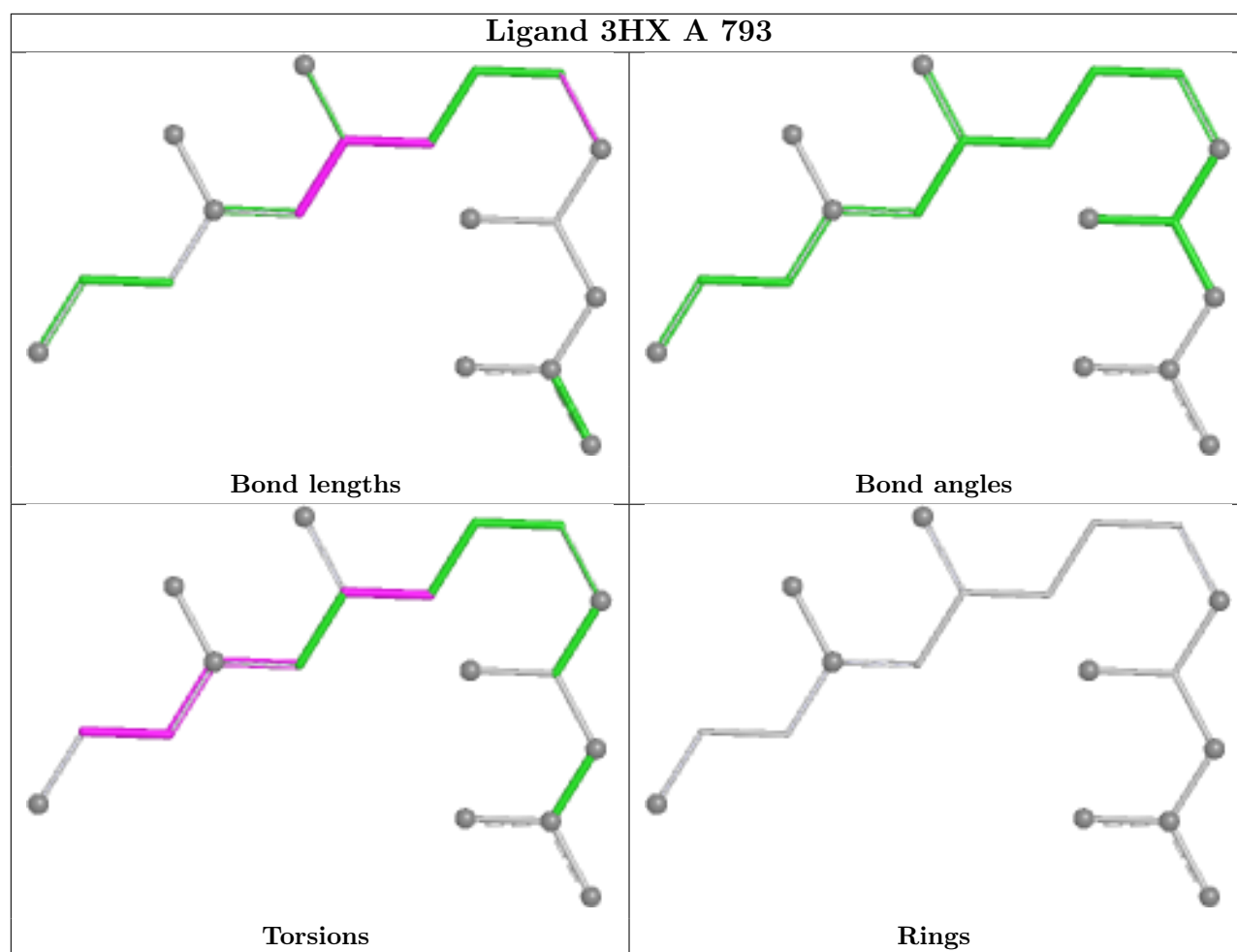
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	700	HEM	1	0
8	A	880	GOL	1	0
6	A	760	H4B	1	0
6	B	760	H4B	1	0
7	A	793	3HX	4	0

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









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	403/416 (96%)	0.02	9 (2%) 62 69	20, 30, 54, 73	0
1	B	402/416 (96%)	0.12	9 (2%) 62 69	21, 32, 53, 73	0
All	All	805/832 (96%)	0.07	18 (2%) 62 69	20, 31, 54, 73	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	ALA	3.5
1	A	239	GLY	3.1
1	B	144	GLY	2.9
1	B	390	ARG	2.8
1	A	108	PRO	2.8
1	A	99	ARG	2.7
1	B	239	GLY	2.6
1	A	107	LEU	2.6
1	B	122	ALA	2.5
1	B	142	ARG	2.3
1	A	92	GLN	2.3
1	B	69	LYS	2.3
1	A	238	PRO	2.3
1	A	123	GLU	2.2
1	A	127	SER	2.1
1	B	391	THR	2.1
1	B	284	GLY	2.1
1	B	124	GLN	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

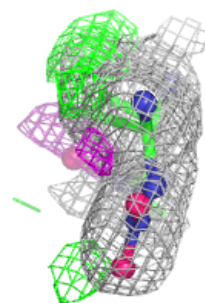
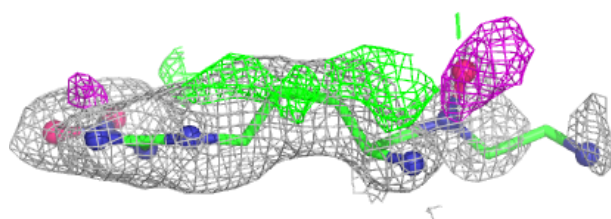
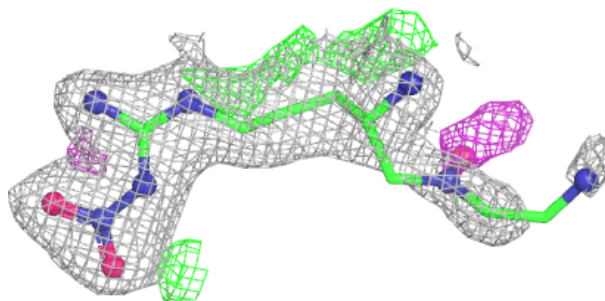
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	A	860	4/4	0.75	0.19	41,42,45,45	0
8	GOL	A	880	6/6	0.80	0.22	61,61,62,63	0
7	3HX	B	793	18/18	0.85	0.16	31,47,63,63	0
3	ACT	B	860	4/4	0.85	0.15	46,47,47,48	0
3	ACT	A	861	4/4	0.86	0.15	40,41,41,42	0
7	3HX	A	793	18/18	0.87	0.14	30,46,55,56	0
3	ACT	B	861	4/4	0.89	0.18	43,44,44,45	0
8	GOL	B	880	6/6	0.91	0.13	40,45,46,47	0
6	H4B	A	760	17/17	0.97	0.05	21,22,25,26	0
6	H4B	B	760	17/17	0.97	0.05	20,23,25,26	0
2	CAC	A	850	3/5	0.98	0.10	42,42,43,46	0
2	CAC	B	850	3/5	0.98	0.10	47,47,48,49	0
5	HEM	A	700	43/43	0.99	0.05	20,22,30,32	0
5	HEM	B	700	43/43	0.99	0.04	19,23,29,30	0
4	ZN	A	900	1/1	1.00	0.01	24,24,24,24	0

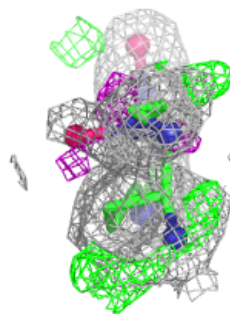
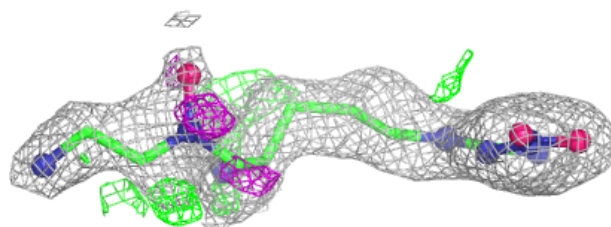
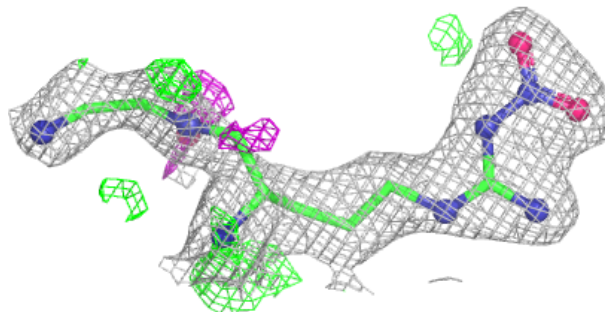
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3HX B 793:

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

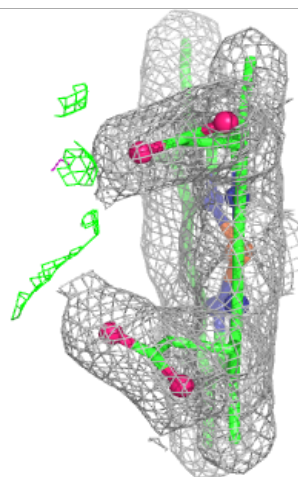
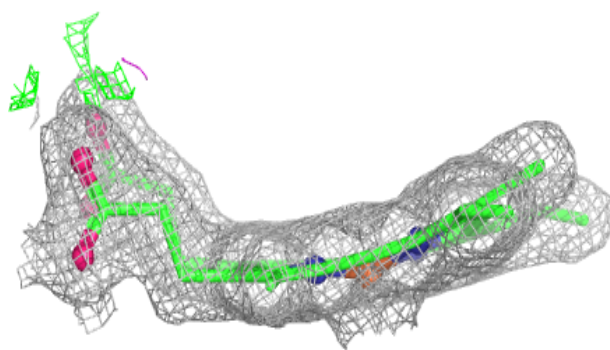
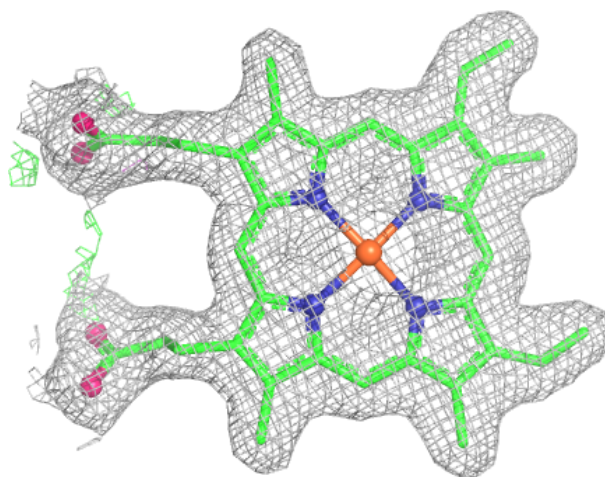
**Electron density around 3HX A 793:**

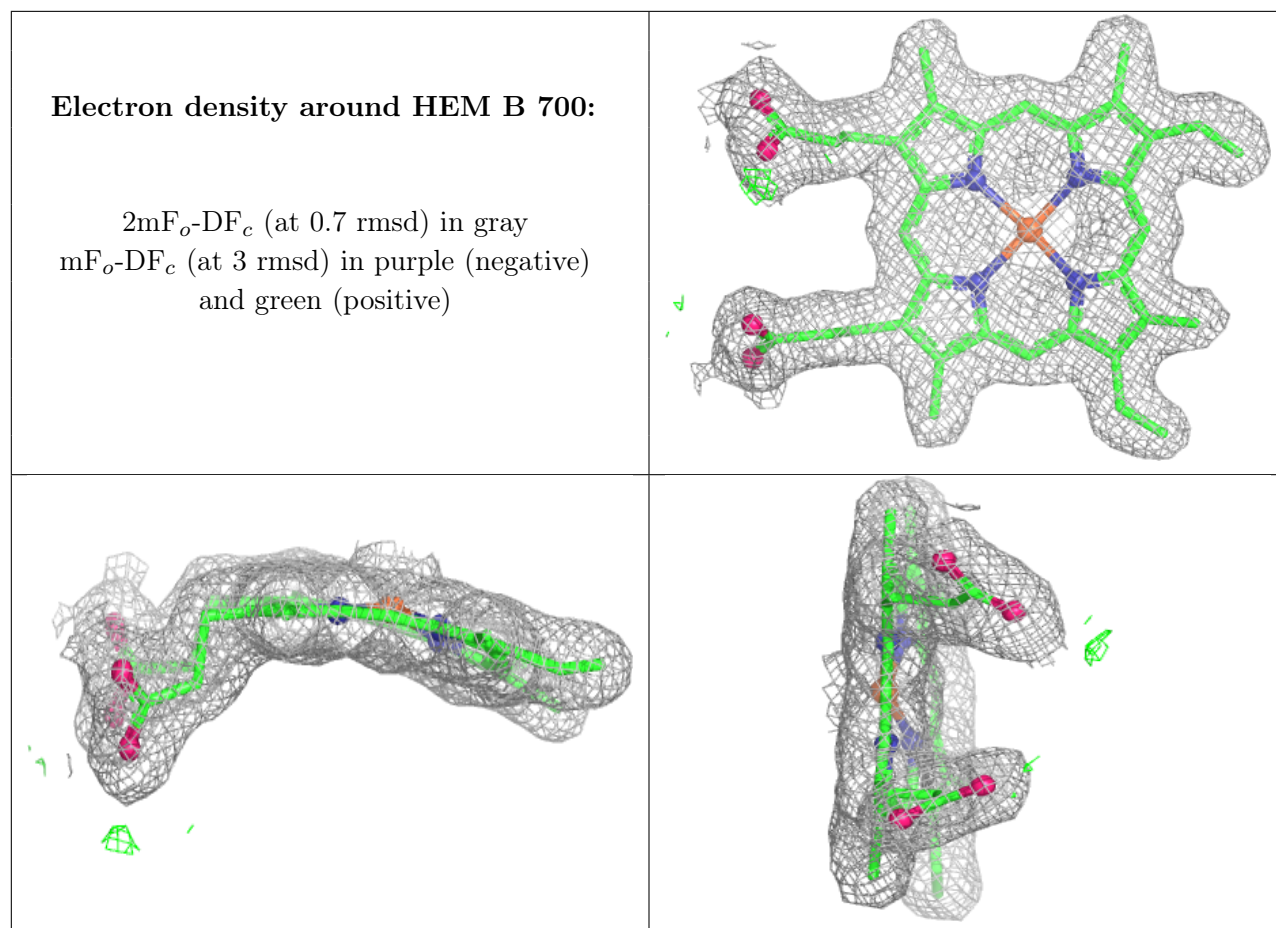
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 700:

$2mF_o-DF_c$ (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.