



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 10:36 pm BST

PDB ID : 3DQT
Title : Structure of endothelial NOS heme domain in complex with a inhibitor (+-)-N1-{trans-4'-[(6"-amino-4"-methylpyridin-2"-yl)methyl]pyrrolidin-3'-yl}-N2-(3'-chlorobenzyl)ethane-1,2-diamine
Authors : Igarashi, J.; Li, H.; Poulos, T.L.
Deposited on : 2008-07-09
Resolution : 2.54 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

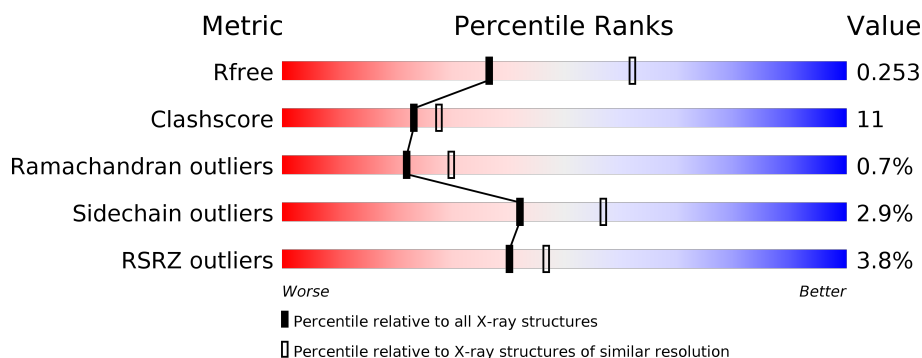
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	416	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	416	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6822 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.

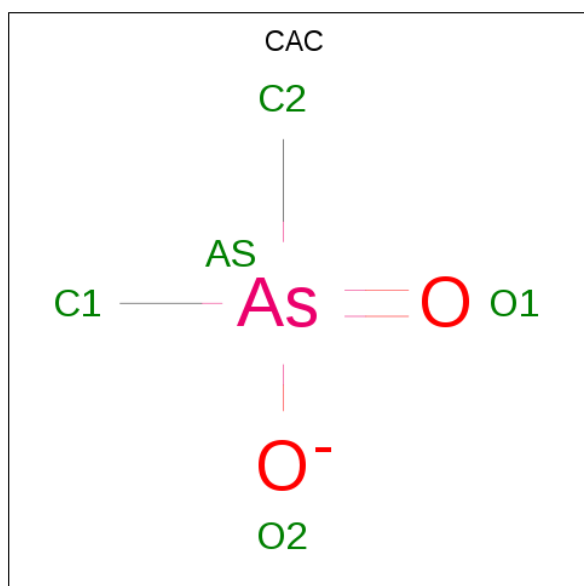
- Molecule 1 is a protein called Nitric oxide synthase, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3216	2046	565	589	16			
1	B	405	Total	C	N	O	S	0	0	0
			3223	2050	568	589	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	VARIANT	UNP P29473
B	100	ARG	CYS	VARIANT	UNP P29473

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



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 (three-letter code: ACT) (formula: $C_2H_3O_2$).



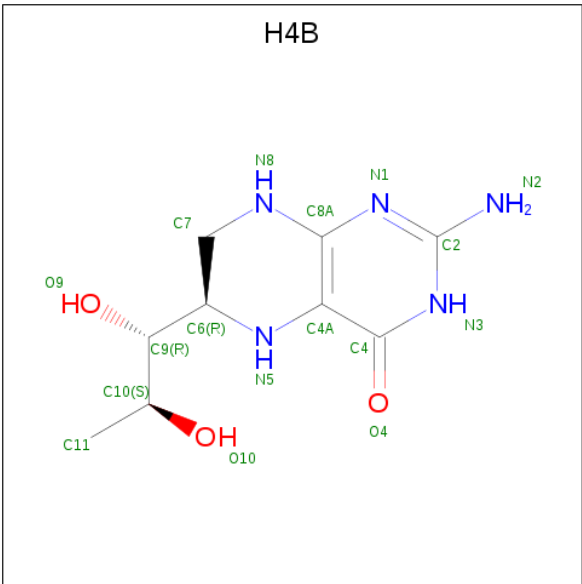
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: C₉H₁₅N₅O₃).



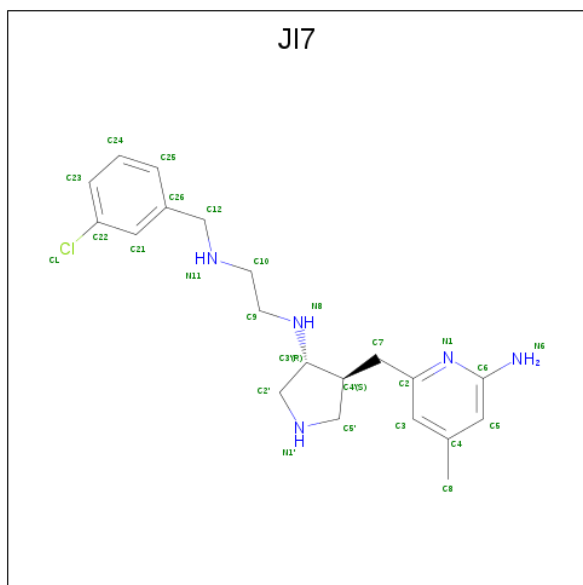
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	9	5	3		

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

- Molecule 6 is N-{(3R,4S)-4-[(6-amino-4-methylpyridin-2-yl)methyl]pyrrolidin-3-yl}-N'-(3-chlorobenzyl)ethane-1,2-diamine (three-letter code: JI7) (formula: C₂₀H₂₈ClN₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	0	0
			26	20	1	5		
6	B	1	Total	C	Cl	N	0	0
			26	20	1	5		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

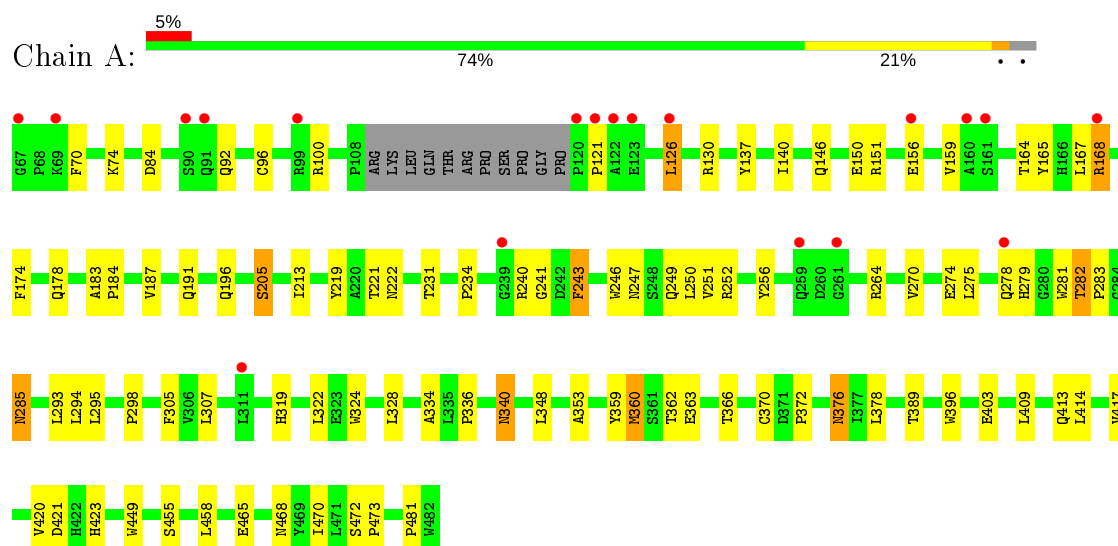
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	102	Total	O	0	0
			102	102		
9	B	82	Total	O	0	0
			82	82		

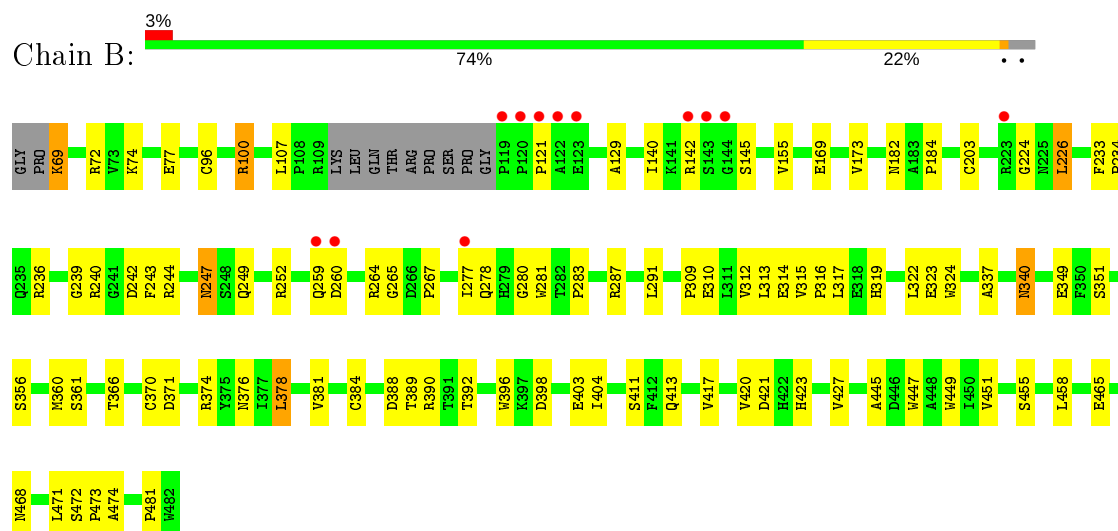
3 Residue-property plots [i](#)

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, endothelial



- Molecule 1: Nitric oxide synthase, endothelial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.25Å 106.49Å 156.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.78 – 2.54 42.78 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.78-2.54) 99.7 (42.78-2.54)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.54Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.197 , 0.258 0.193 , 0.253	Depositor DCC
R_{free} test set	1616 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6822	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: GOL, ZN, H4B, JI7, ACT, CAC, HEM

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	0/3307	0.71	2/4506 (0.0%)
1	B	0.48	0/3314	0.71	1/4515 (0.0%)
All	All	0.49	0/6621	0.71	3/9021 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	MET	N-CA-C	-5.57	95.95	111.00
1	B	280	GLY	N-CA-C	5.16	126.01	113.10
1	A	243	PHE	N-CA-C	-5.14	97.12	111.00

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	3216	0	3121	75	0
1	B	3223	0	3131	66	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	43	0	30	4	0
4	B	43	0	30	5	0
5	A	17	0	15	1	0
5	B	17	0	15	2	0
6	A	26	0	28	3	0
6	B	26	0	28	4	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	B	1	0	0	0	0
9	A	102	0	0	4	0
9	B	82	0	0	2	0
All	All	6822	0	6420	148	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 11.

All (148) 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:B:249:GLN:HB2	1:B:252:ARG:HD3	1.39	1.00
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.51	0.92
1:B:69:LYS:HE3	1:B:69:LYS:N	1.86	0.90
1:B:107:LEU:HD21	6:B:800:JI7:H24	1.69	0.75
1:A:205:SER:HB3	9:A:930:HOH:O	1.92	0.69
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.28	0.68
4:B:700:HEM:HMC2	4:B:700:HEM:HBC2	1.75	0.68
1:B:323:GLU:CD	1:B:323:GLU:H	1.97	0.68
1:A:249:GLN:HB2	1:A:252:ARG:CG	2.26	0.66
1:A:126:LEU:HD12	1:A:130:ARG:NH2	2.11	0.65
1:B:310:GLU:H	1:B:310:GLU:CD	1.96	0.65
1:A:126:LEU:O	1:A:130:ARG:HG3	1.97	0.64
1:A:126:LEU:HD12	1:A:130:ARG:CZ	2.28	0.63
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.81	0.63
1:B:312:VAL:O	1:B:312:VAL:HG12	1.98	0.62
1:B:310:GLU:OE2	1:B:310:GLU:N	2.31	0.61
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.40	0.61
1:B:278:GLN:HG2	1:B:278:GLN:O	2.02	0.60
1:A:151:ARG:NH2	1:A:168:ARG:HD3	2.17	0.59
1:A:372:PRO:HA	1:A:376:ASN:ND2	2.17	0.59
1:B:277:ILE:HD11	1:B:283:PRO:HB3	1.85	0.59
1:B:236:ARG:HG3	1:B:349:GLU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HG3	1:A:264:ARG:HH11	1.69	0.58
1:A:151:ARG:CZ	1:A:168:ARG:HD3	2.33	0.58
1:B:249:GLN:CB	1:B:252:ARG:HD3	2.26	0.57
1:A:409:LEU:O	1:A:413:GLN:HG3	2.04	0.57
1:A:126:LEU:HD23	1:A:159:VAL:HG11	1.85	0.57
4:B:700:HEM:HHC	4:B:700:HEM:HBB2	1.86	0.57
1:A:378:LEU:HB2	9:A:901:HOH:O	2.04	0.56
1:A:126:LEU:HD12	1:A:130:ARG:NE	2.20	0.56
1:B:361:SER:OG	1:B:421:ASP:HA	2.06	0.56
1:B:140:ILE:HD12	1:B:142:ARG:HD2	1.88	0.55
4:B:700:HEM:HBA1	6:B:800:JI7:H72	1.89	0.55
4:A:700:HEM:HBA2	6:A:800:JI7:H72	1.87	0.55
1:B:244:ARG:NH2	1:B:481:PRO:HD3	2.22	0.55
1:A:472:SER:HA	1:A:473:PRO:O	2.06	0.55
1:A:340:ASN:HD22	1:A:340:ASN:H	1.54	0.54
1:B:324:TRP:CZ3	1:B:384:CYS:HB3	2.43	0.54
1:B:366:THR:O	1:B:370:CYS:HB2	2.08	0.53
1:B:265:GLY:O	1:B:267:PRO:HD3	2.08	0.53
1:B:337:ALA:CB	1:B:356:SER:HB3	2.38	0.52
1:A:472:SER:HA	1:A:473:PRO:C	2.29	0.52
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.90	0.52
9:A:952:HOH:O	1:B:392:THR:HG22	2.09	0.52
1:B:242:ASP:HB3	1:B:351:SER:OG	2.10	0.51
1:A:295:LEU:HD12	1:A:305:PHE:CD1	2.45	0.51
1:B:247:ASN:N	1:B:247:ASN:OD1	2.44	0.51
1:A:246:TRP:CD1	1:A:481:PRO:HG3	2.45	0.50
4:B:700:HEM:CGA	5:B:760:H4B:HN3	2.24	0.50
1:A:414:LEU:HD23	1:A:414:LEU:C	2.32	0.50
1:A:372:PRO:HG2	1:B:77:GLU:HG3	1.94	0.50
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.42	0.49
1:B:313:LEU:HD12	1:B:314:GLU:H	1.78	0.49
1:A:184:PRO:HB3	1:A:468:ASN:ND2	2.28	0.49
1:B:281:TRP:O	1:B:283:PRO:HD3	2.13	0.49
1:A:389:THR:HA	1:A:396:TRP:CD1	2.48	0.49
1:B:447:TRP:CZ2	1:B:451:VAL:HG21	2.48	0.48
1:A:246:TRP:HB2	1:A:294:LEU:HB2	1.95	0.48
1:A:340:ASN:HD22	1:A:340:ASN:N	2.11	0.48
1:A:146:GLN:O	1:A:150:GLU:HG3	2.14	0.48
1:A:274:GLU:O	1:A:278:GLN:HG3	2.12	0.48
1:A:360:MET:HA	1:A:420:VAL:O	2.13	0.48
1:B:423:HIS:O	1:B:427:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:700:HEM:C1C	6:B:800:JI7:H83	2.49	0.47
1:B:472:SER:HA	1:B:473:PRO:C	2.35	0.47
1:A:168:ARG:HD2	1:A:168:ARG:N	2.29	0.47
1:A:241:GLY:O	1:A:298:PRO:HB3	2.15	0.47
1:A:247:ASN:OD1	1:A:247:ASN:N	2.48	0.47
1:B:234:PRO:HB2	1:B:243:PHE:CE1	2.50	0.47
1:A:174:PHE:CZ	1:A:178:GLN:HG3	2.49	0.47
1:A:275:LEU:O	1:A:279:HIS:HD2	1.97	0.47
1:B:340:ASN:HD22	1:B:340:ASN:H	1.63	0.47
1:B:389:THR:HA	1:B:396:TRP:CD1	2.50	0.47
1:B:313:LEU:HD12	1:B:314:GLU:N	2.30	0.46
6:B:800:JI7:H121	6:B:800:JI7:H91	1.82	0.46
1:A:70:PHE:HB3	1:A:84:ASP:O	2.16	0.46
1:A:126:LEU:HA	1:A:126:LEU:HD22	1.66	0.46
1:A:168:ARG:CZ	9:A:957:HOH:O	2.64	0.46
1:A:256:TYR:CE1	1:A:285:ASN:HA	2.51	0.46
4:A:700:HEM:O2D	6:A:800:JI7:H92	2.15	0.46
1:A:231:THR:O	1:A:353:ALA:HA	2.16	0.46
1:A:74:LYS:O	1:A:465:GLU:HG3	2.15	0.46
1:A:187:VAL:O	1:A:187:VAL:HG22	2.15	0.45
1:B:224:GLY:O	1:B:417:VAL:HA	2.16	0.45
1:A:240:ARG:HG2	1:A:241:GLY:N	2.30	0.45
1:B:72:ARG:NH2	9:B:957:HOH:O	2.42	0.45
1:A:366:THR:O	1:A:370:CYS:HB2	2.17	0.45
1:B:319:HIS:NE2	1:B:403:GLU:OE2	2.44	0.45
1:B:340:ASN:N	1:B:340:ASN:HD22	2.14	0.45
1:A:319:HIS:NE2	1:A:403:GLU:OE1	2.49	0.45
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.97	0.44
1:A:92:GLN:HG2	1:A:470:ILE:HD12	2.00	0.44
1:B:129:ALA:HB1	1:B:155:VAL:HG11	1.98	0.44
1:A:449:TRP:HA	5:A:760:H4B:N1	2.33	0.44
1:A:340:ASN:ND2	1:A:340:ASN:H	2.15	0.44
1:A:363:GLU:OE2	6:A:800:JI7:N1	2.50	0.44
1:B:226:LEU:N	1:B:226:LEU:CD1	2.81	0.43
1:A:455:SER:HB3	1:A:458:LEU:HD12	2.00	0.43
1:B:360:MET:HA	1:B:420:VAL:O	2.17	0.43
1:B:100:ARG:HG2	1:B:100:ARG:HH11	1.82	0.43
1:B:74:LYS:O	1:B:465:GLU:HG3	2.18	0.43
1:A:389:THR:HG22	1:A:396:TRP:CD2	2.54	0.43
1:B:371:ASP:HB2	1:B:374:ARG:CG	2.48	0.43
1:A:294:LEU:HD23	1:A:294:LEU:HA	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ALA:O	1:B:468:ASN:HB2	2.19	0.43
1:A:334:ALA:CB	1:A:417:VAL:HG11	2.49	0.43
4:A:700:HEM:HMC1	4:A:700:HEM:HBC2	2.01	0.43
1:A:234:PRO:HB2	1:A:243:PHE:CE1	2.53	0.43
1:A:270:VAL:O	1:A:274:GLU:HG3	2.19	0.43
1:A:360:MET:CE	1:A:362:THR:OG1	2.67	0.43
1:B:169:GLU:O	1:B:173:VAL:HG23	2.18	0.42
1:B:264:ARG:NH1	1:B:287:ARG:HG3	2.35	0.42
1:A:191:GLN:HE21	1:A:191:GLN:HB3	1.67	0.42
1:A:282:THR:HG22	1:A:282:THR:O	2.18	0.42
1:B:233:PHE:HB3	1:B:234:PRO:HD2	2.01	0.42
1:A:213:ILE:HG23	1:A:250:LEU:HD13	2.02	0.42
4:A:700:HEM:HBB2	4:A:700:HEM:HHC	2.01	0.42
1:B:100:ARG:HG2	1:B:100:ARG:NH1	2.35	0.42
1:B:381:VAL:HG21	1:B:404:ILE:HD11	2.00	0.42
1:A:293:LEU:HD11	1:A:307:LEU:HD21	2.01	0.42
1:B:471:LEU:O	1:B:474:ALA:HB2	2.20	0.42
1:A:159:VAL:HA	1:A:164:THR:O	2.20	0.42
1:B:226:LEU:HD13	1:B:226:LEU:H	1.85	0.42
1:B:376:ASN:HA	9:B:928:HOH:O	2.20	0.42
1:B:323:GLU:N	1:B:323:GLU:CD	2.70	0.42
1:B:340:ASN:ND2	1:B:340:ASN:H	2.16	0.42
1:A:458:LEU:HD22	1:B:378:LEU:HD21	2.02	0.42
1:B:182:ASN:O	1:B:184:PRO:HD3	2.20	0.41
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.94	0.41
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.55	0.41
1:A:336:PRO:HB3	1:A:359:TYR:CZ	2.55	0.41
1:A:421:ASP:OD2	1:A:423:HIS:HB2	2.20	0.41
1:B:317:LEU:HA	1:B:411:SER:OG	2.20	0.41
1:A:96:CYS:HB3	1:B:96:CYS:HB3	2.03	0.41
1:A:251:VAL:O	1:A:252:ARG:HG2	2.20	0.41
1:A:281:TRP:O	1:A:283:PRO:HD3	2.21	0.41
1:A:196:GLN:HG2	1:A:219:TYR:CZ	2.56	0.40
1:B:315:VAL:HA	1:B:316:PRO:HD3	1.86	0.40
1:B:324:TRP:CZ3	1:B:384:CYS:CB	3.03	0.40
1:A:221:THR:O	1:A:222:ASN:C	2.59	0.40
1:B:252:ARG:HB2	1:B:291:LEU:HD12	2.03	0.40
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.96	0.40
1:A:167:LEU:HG	1:A:348:LEU:HD12	2.03	0.40
1:A:184:PRO:CB	1:A:468:ASN:HD21	2.34	0.40
1:B:388:ASP:OD2	1:B:390:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:HA	1:A:140:ILE:HG12	2.03	0.40
1:A:164:THR:HG23	1:A:165:TYR:N	2.37	0.40
1:B:449:TRP:HA	5:B:760:H4B:N1	2.36	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	401/416 (96%)	375 (94%)	25 (6%)	1 (0%)	47	60
1	B	401/416 (96%)	367 (92%)	29 (7%)	5 (1%)	13	17
All	All	802/832 (96%)	742 (92%)	54 (7%)	6 (1%)	22	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	SER
1	B	240	ARG
1	A	121	PRO
1	B	239	GLY
1	B	309	PRO
1	B	121	PRO

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	344/354 (97%)	335 (97%)	9 (3%)	46	61
1	B	345/354 (98%)	334 (97%)	11 (3%)	39	53
All	All	689/708 (97%)	669 (97%)	20 (3%)	42	57

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	126	LEU
1	A	168	ARG
1	A	205	SER
1	A	282	THR
1	A	285	ASN
1	A	328	LEU
1	A	340	ASN
1	A	376	ASN
1	B	69	LYS
1	B	100	ARG
1	B	203	CYS
1	B	226	LEU
1	B	247	ASN
1	B	259	GLN
1	B	260	ASP
1	B	340	ASN
1	B	378	LEU
1	B	398	ASP
1	B	413	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	153	GLN
1	A	191	GLN
1	A	207	GLN
1	A	259	GLN
1	A	279	HIS
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN

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Mol	Chain	Res	Type
1	B	124	GLN
1	B	146	GLN
1	B	222	ASN
1	B	279	HIS
1	B	340	ASN
1	B	405	ASN
1	B	413	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\# Z > 2$
7	GOL	B	880	-	5,5,5	0.18	0	5,5,5	0.29	0
5	H4B	A	760	-	16,18,18	1.99	4 (25%)	11,26,26	4.33	8 (72%)
6	JI7	B	800	-	26,28,28	1.43	3 (11%)	30,37,37	1.37	3 (10%)
3	ACT	A	860	-	1,3,3	2.83	1 (100%)	0,3,3	0.00	-
3	ACT	B	860	-	1,3,3	2.24	1 (100%)	0,3,3	0.00	-
2	CAC	A	850	-	0,2,4	0.00	-	0,1,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	A	700	1	27,50,50	1.54	4 (14%)	17,82,82	2.47	4 (23%)
5	H4B	B	760	-	16,18,18	2.14	5 (31%)	11,26,26	4.31	8 (72%)
7	GOL	A	880	-	5,5,5	0.17	0	5,5,5	0.29	0
6	JI7	A	800	-	26,28,28	1.53	4 (15%)	30,37,37	1.17	2 (6%)
4	HEM	B	700	1	27,50,50	1.68	6 (22%)	17,82,82	1.45	3 (17%)
2	CAC	B	850	-	0,2,4	0.00	-	0,1,6	0.00	-

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
7	GOL	B	880	-	-	2/4/4/4	-
5	H4B	A	760	-	-	0/8/17/17	0/2/2/2
7	GOL	A	880	-	-	0/4/4/4	-
4	HEM	A	700	1	-	0/6/54/54	-
5	H4B	B	760	-	-	3/8/17/17	0/2/2/2
6	JI7	A	800	-	-	5/12/22/22	0/3/3/3
4	HEM	B	700	1	-	0/6/54/54	-
6	JI7	B	800	-	-	5/12/22/22	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	760	H4B	C4-N3	5.26	1.42	1.33
5	A	760	H4B	C4-N3	5.18	1.42	1.33
5	B	760	H4B	C4A-N5	4.06	1.46	1.38
4	A	700	HEM	C3B-CAB	-3.91	1.40	1.47
4	B	700	HEM	C3C-C2C	-3.89	1.35	1.40
5	A	760	H4B	C4A-N5	3.86	1.45	1.38
4	B	700	HEM	C3B-CAB	-3.83	1.40	1.47
6	A	800	JI7	C21-C26	3.78	1.45	1.39
4	B	700	HEM	C3C-CAC	-3.77	1.40	1.47
5	B	760	H4B	C6-N5	3.29	1.52	1.45
6	B	800	JI7	C21-C26	3.29	1.44	1.39
6	A	800	JI7	C21-C22	3.27	1.43	1.38
4	A	700	HEM	C4A-NA	3.18	1.42	1.36
5	A	760	H4B	C6-N5	3.16	1.52	1.45
4	A	700	HEM	C3B-C2B	-3.10	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	HEM	C3C-CAC	-3.04	1.41	1.47
6	B	800	JI7	C21-C22	2.84	1.43	1.38
3	A	860	ACT	CH3-C	2.83	1.52	1.48
4	B	700	HEM	C1A-NA	2.63	1.41	1.36
6	B	800	JI7	C23-C22	2.61	1.43	1.38
5	B	760	H4B	C8A-N1	2.55	1.39	1.34
6	A	800	JI7	C5-C6	2.53	1.43	1.39
4	B	700	HEM	C4B-NB	2.45	1.41	1.36
6	A	800	JI7	C3-C4	2.31	1.42	1.39
3	B	860	ACT	CH3-C	2.24	1.51	1.48
5	B	760	H4B	C7-C6	2.22	1.54	1.52
5	A	760	H4B	C8A-N1	2.05	1.38	1.34
4	B	700	HEM	C4A-NA	2.02	1.40	1.36

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	760	H4B	C4-C4A-C8A	9.39	122.91	114.57
5	A	760	H4B	C4-C4A-C8A	9.39	122.91	114.57
4	A	700	HEM	CBA-CAA-C2A	-6.83	99.89	112.49
4	A	700	HEM	C4A-C3A-C2A	-5.95	102.86	107.00
5	B	760	H4B	C4-N3-C2	5.72	125.02	115.93
5	A	760	H4B	C4-N3-C2	5.70	124.98	115.93
5	A	760	H4B	N3-C2-N1	-5.07	117.47	125.42
5	B	760	H4B	N3-C2-N1	-4.83	117.84	125.42
6	B	800	JI7	C6-N1-C2	4.73	121.68	118.10
4	B	700	HEM	CBA-CAA-C2A	-3.94	105.21	112.49
5	B	760	H4B	N2-C2-N1	3.77	123.12	117.25
5	A	760	H4B	N2-C2-N1	3.71	123.03	117.25
5	A	760	H4B	C4A-C4-N3	-3.61	113.74	124.01
6	B	800	JI7	N6-C6-N1	3.56	122.12	116.49
5	B	760	H4B	C4A-C4-N3	-3.55	113.93	124.01
5	A	760	H4B	C2-N1-C8A	3.53	122.46	114.54
5	B	760	H4B	C2-N1-C8A	3.46	122.29	114.54
5	B	760	H4B	C4-C4A-N5	-3.20	116.44	119.12
5	A	760	H4B	C4A-N5-C6	-3.17	112.54	121.16
6	A	800	JI7	C6-N1-C2	3.13	120.47	118.10
5	B	760	H4B	C4A-N5-C6	-2.74	113.71	121.16
6	A	800	JI7	N6-C6-N1	2.70	120.76	116.49
4	A	700	HEM	CMA-C3A-C2A	2.47	129.61	124.94
6	B	800	JI7	C4-C3-C2	-2.47	118.70	120.32
5	A	760	H4B	C4-C4A-N5	-2.46	117.05	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	HEM	CMB-C2B-C3B	2.14	128.69	124.68
4	B	700	HEM	CBD-CAD-C3D	2.08	116.31	112.48
4	B	700	HEM	CMB-C2B-C3B	2.04	128.50	124.68

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	800	JI7	C4'-C3'-N8-C9
6	B	800	JI7	C2'-C3'-N8-C9
7	B	880	GOL	O1-C1-C2-C3
6	A	800	JI7	C4'-C3'-N8-C9
6	A	800	JI7	C2'-C3'-N8-C9
6	A	800	JI7	C10-C9-N8-C3'
6	B	800	JI7	N11-C10-C9-N8
6	A	800	JI7	N11-C10-C9-N8
6	B	800	JI7	C9-C10-N11-C12
6	A	800	JI7	C9-C10-N11-C12
7	B	880	GOL	O1-C1-C2-O2
5	B	760	H4B	O10-C10-C9-C6
5	B	760	H4B	O10-C10-C9-O9
5	B	760	H4B	C11-C10-C9-C6
6	B	800	JI7	C10-C9-N8-C3'

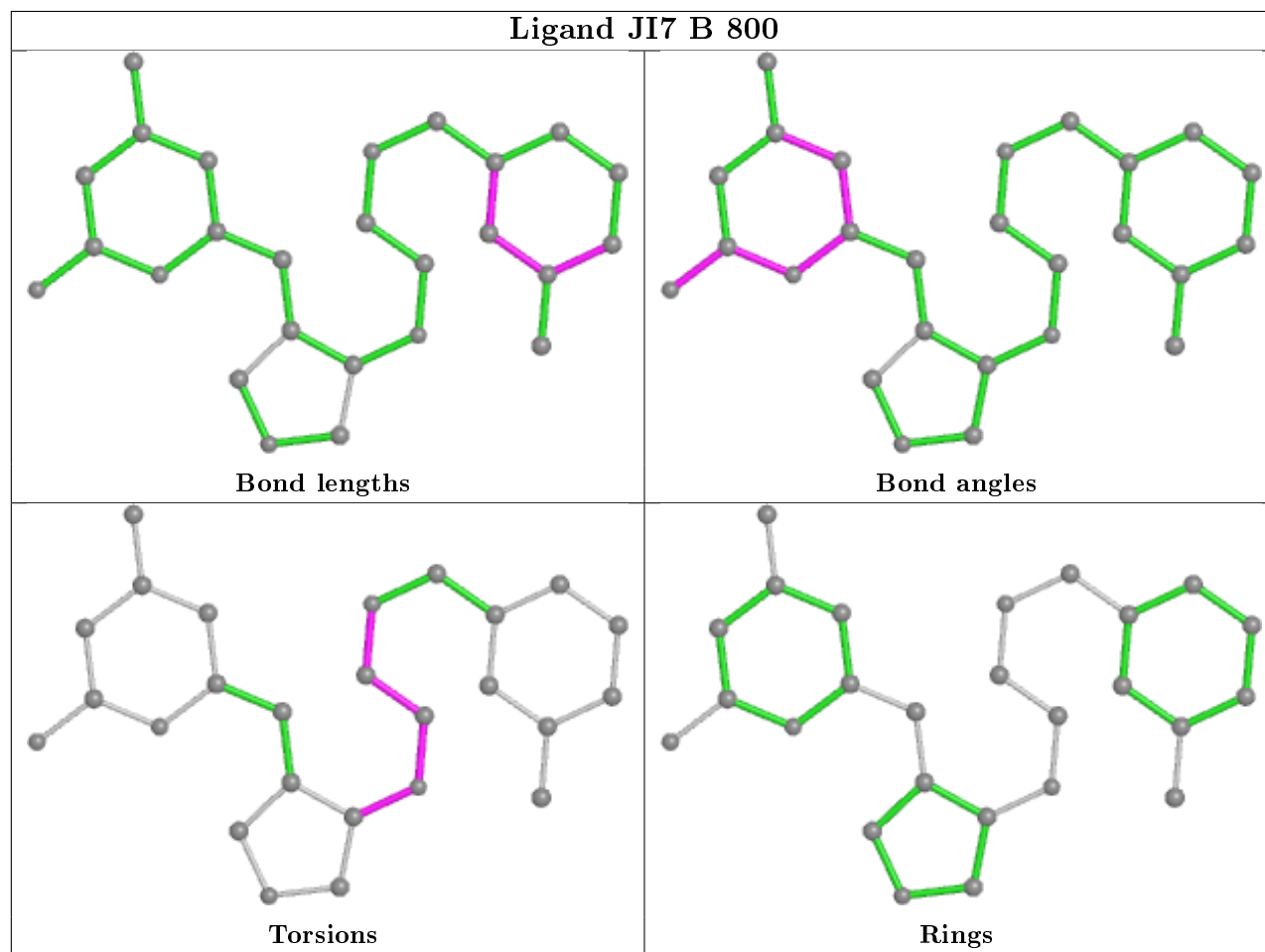
There are no ring outliers.

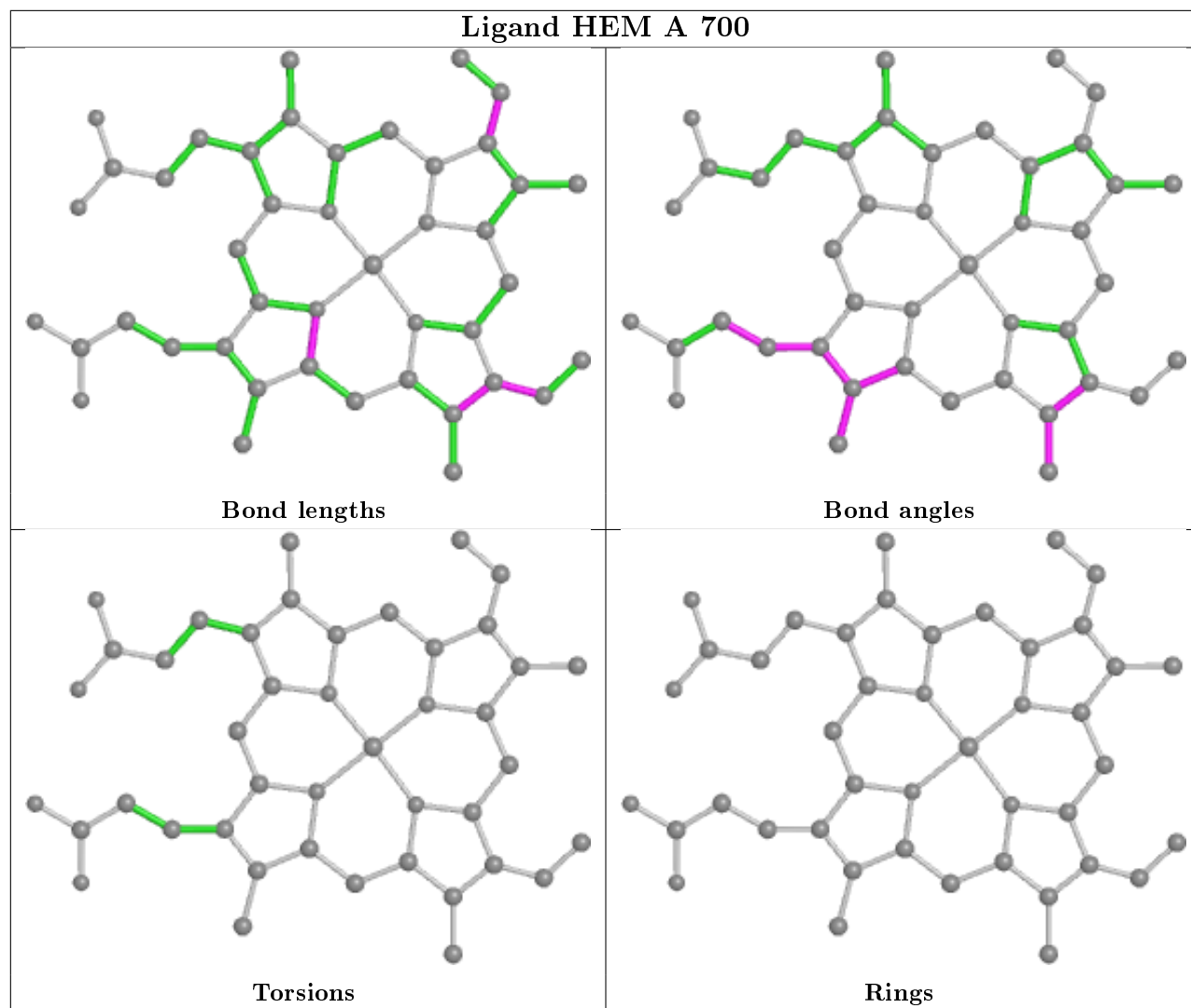
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	760	H4B	1	0
6	B	800	JI7	4	0
4	A	700	HEM	4	0
5	B	760	H4B	2	0
6	A	800	JI7	3	0
4	B	700	HEM	5	0

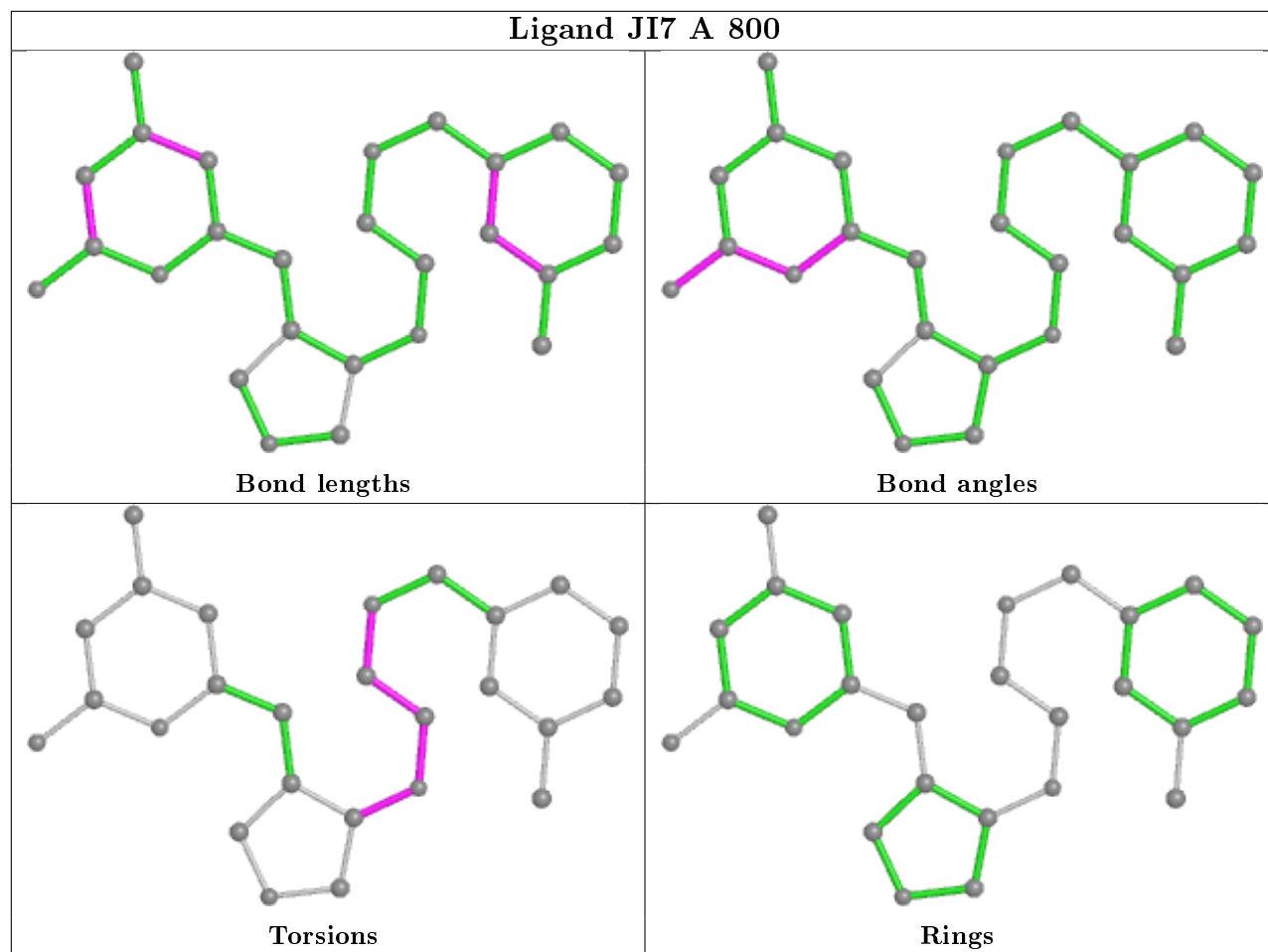
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

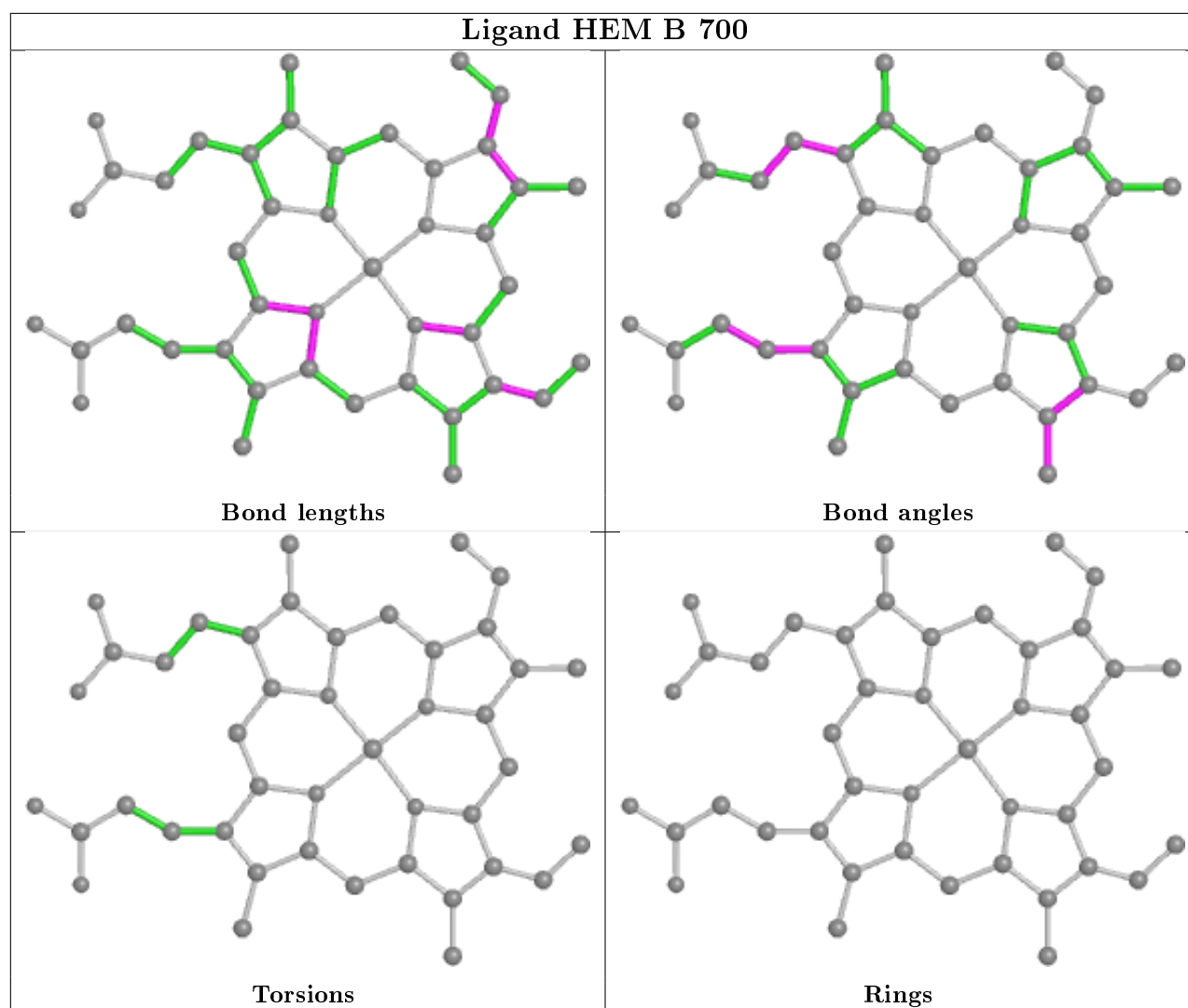
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand JI7 A 800





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	405/416 (97%)	0.02	19 (4%) 31 38	31, 47, 73, 101	0
1	B	405/416 (97%)	0.10	12 (2%) 50 57	31, 51, 77, 117	0
All	All	810/832 (97%)	0.06	31 (3%) 40 47	31, 49, 75, 117	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	PRO	12.6
1	B	120	PRO	5.8
1	B	259	GLN	3.7
1	A	259	GLN	3.5
1	A	160	ALA	3.5
1	A	120	PRO	3.5
1	A	123	GLU	3.4
1	A	121	PRO	3.3
1	B	121	PRO	3.1
1	A	161	SER	2.9
1	B	142	ARG	2.8
1	A	91	GLN	2.7
1	B	277	ILE	2.7
1	A	156	GLU	2.6
1	A	67	GLY	2.6
1	A	239	GLY	2.6
1	A	126	LEU	2.5
1	A	69	LYS	2.5
1	A	122	ALA	2.4
1	A	99	ARG	2.4
1	B	123	GLU	2.4
1	B	223	ARG	2.4
1	A	311	LEU	2.3
1	B	122	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	278	GLN	2.2
1	A	261	GLY	2.2
1	B	260	ASP	2.1
1	A	168	ARG	2.1
1	B	143	SER	2.0
1	A	90	SER	2.0
1	B	144	GLY	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.

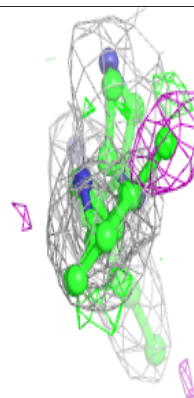
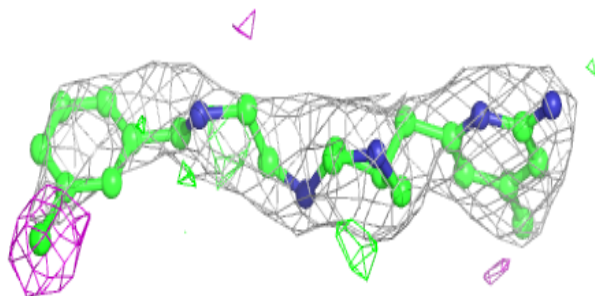
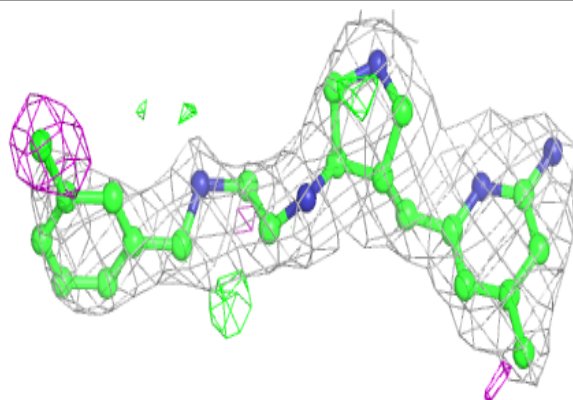
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	JI7	A	800	26/26	0.86	0.29	29,51,88,88	0
6	JI7	B	800	26/26	0.89	0.26	38,50,86,87	0
7	GOL	A	880	6/6	0.92	0.21	66,66,69,69	0
7	GOL	B	880	6/6	0.92	0.29	69,71,74,75	0
5	H4B	B	760	17/17	0.93	0.21	54,61,71,72	0
5	H4B	A	760	17/17	0.95	0.17	58,61,64,64	0
3	ACT	A	860	4/4	0.97	0.14	44,45,46,47	0
3	ACT	B	860	4/4	0.97	0.21	45,50,50,57	0
2	CAC	B	850	3/5	0.97	0.14	87,87,88,89	0
4	HEM	B	700	43/43	0.98	0.17	29,34,62,69	0
4	HEM	A	700	43/43	0.98	0.16	26,35,60,63	0
2	CAC	A	850	3/5	0.99	0.09	61,61,63,71	0
8	ZN	B	900	1/1	0.99	0.06	43,43,43,43	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.

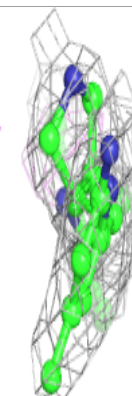
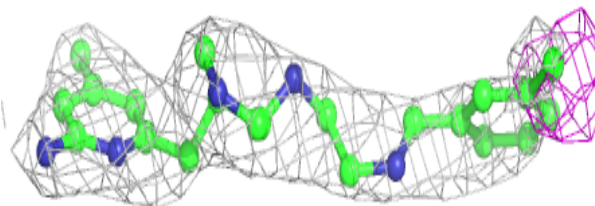
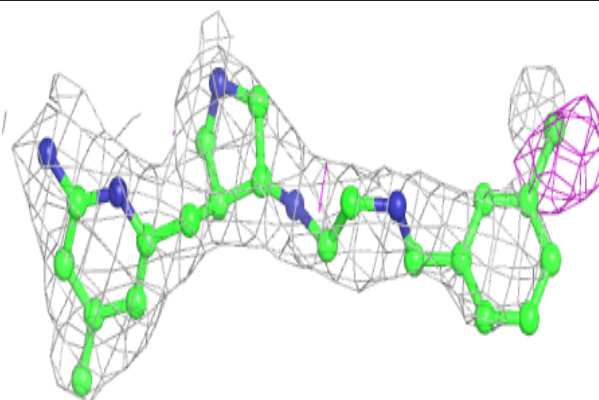
Electron density around JI7 A 800:

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



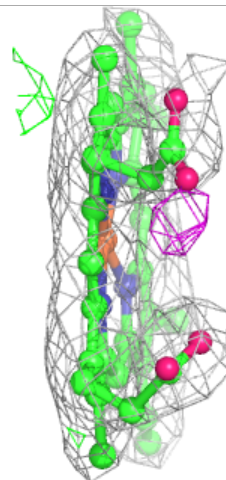
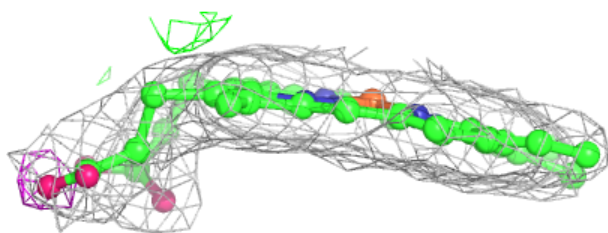
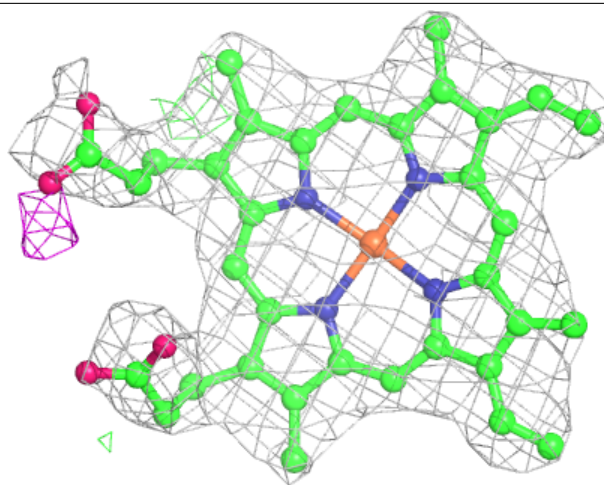
Electron density around JI7 B 800:

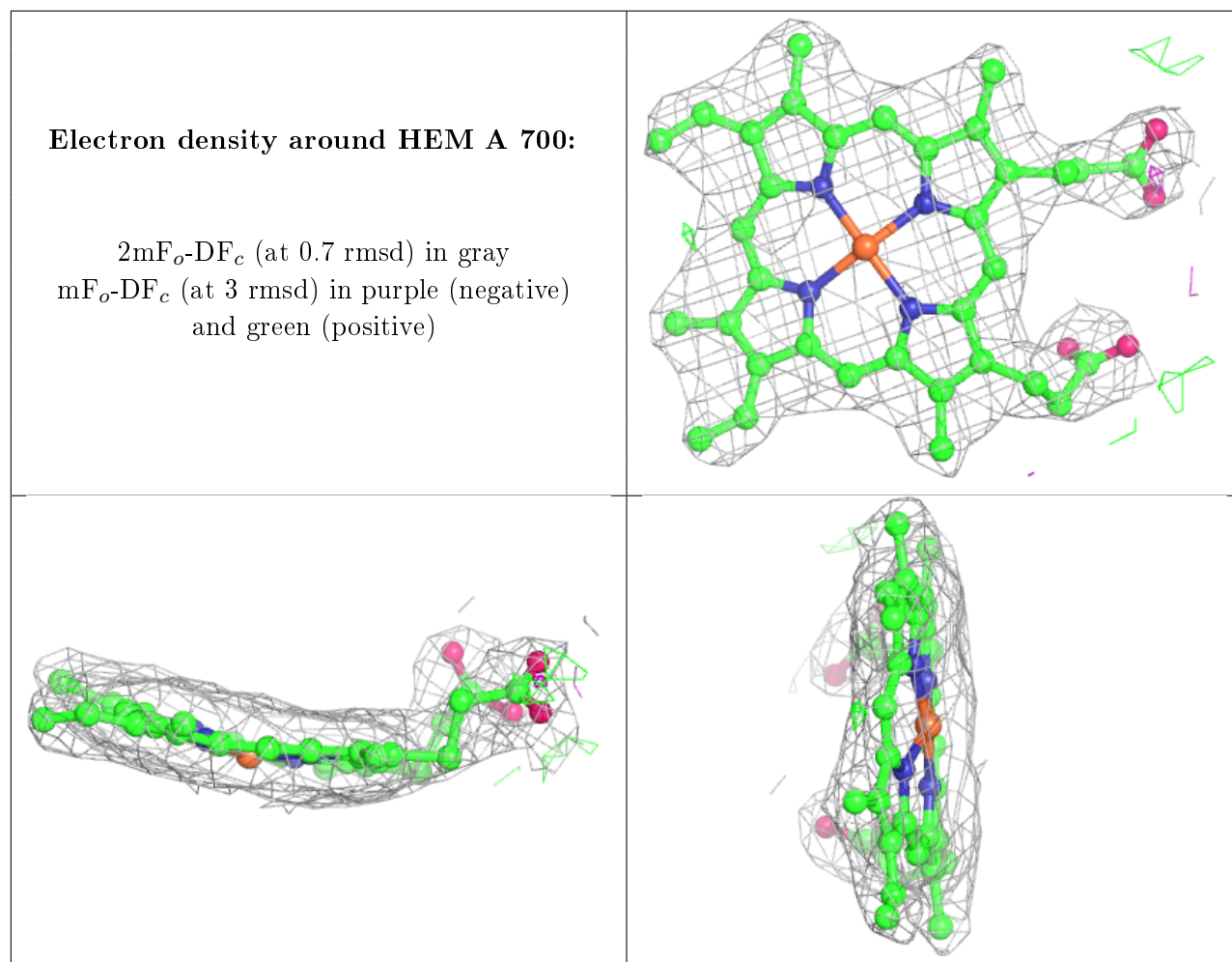
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 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.