



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:11 PM UTC

PDB ID : 3E7G / pdb_00003e7g
Title : Structure of human INOSOX with inhibitor AR-C95791
Authors : Garcin, E.D.; Arvai, A.S.; Rosenfeld, R.J.; Kroeger, M.D.; Crane, B.R.; Andersson, G.; Andrews, G.; Hamley, P.J.; Mallinder, P.R.; Nicholls, D.J.; St-Gallay, S.A.; Tinker, A.C.; Gensmantel, N.P.; Mete, A.; Cheshire, D.R.; Connolly, S.; Stueh, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2008-08-18
Resolution : 2.20 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](#) ①) 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

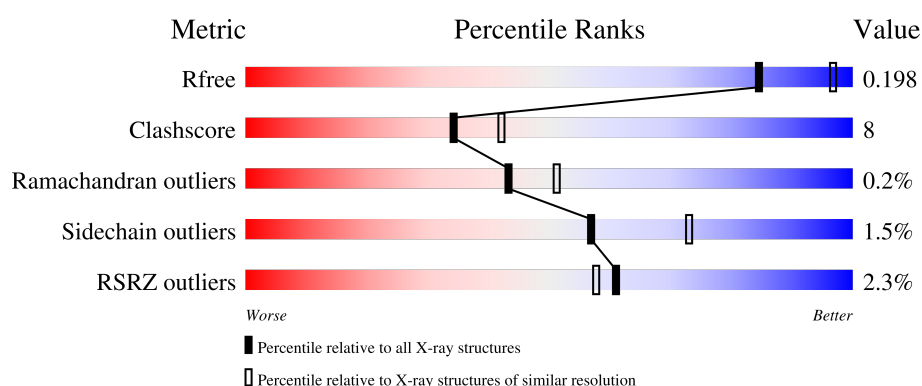
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	424	3% 78% 20% ..
1	B	424	3% 79% 19% ..
1	C	424	2% 82% 17% .
1	D	424	2% 76% 22% ..

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	H4B	A	902	X	-	-	-
4	H4B	D	3902	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14516 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.

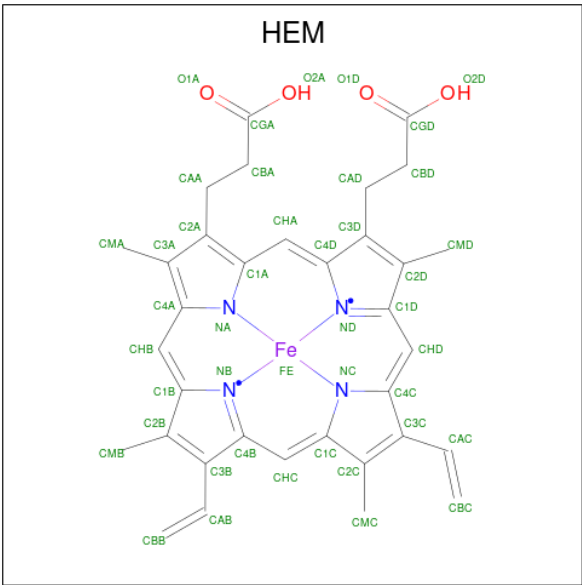
- Molecule 1 is a protein called Nitric oxide synthase, inducible.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3418	2186	597	613	22			
1	B	421	Total	C	N	O	S	0	0	0
			3418	2186	597	613	22			
1	C	423	Total	C	N	O	S	0	0	0
			3440	2198	600	620	22			
1	D	421	Total	C	N	O	S	0	0	0
			3418	2186	597	613	22			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

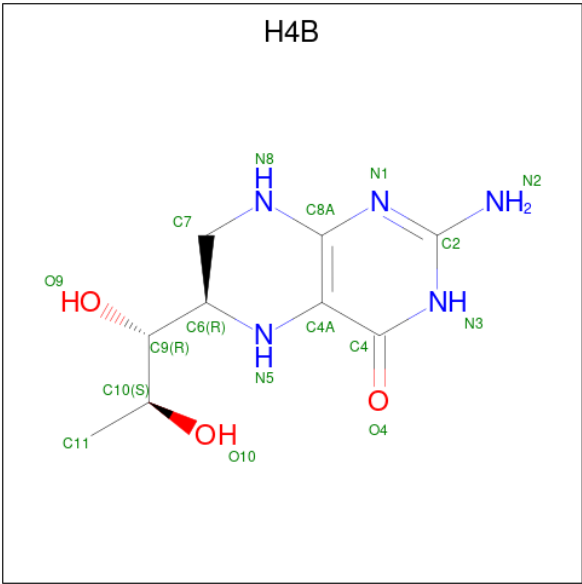
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



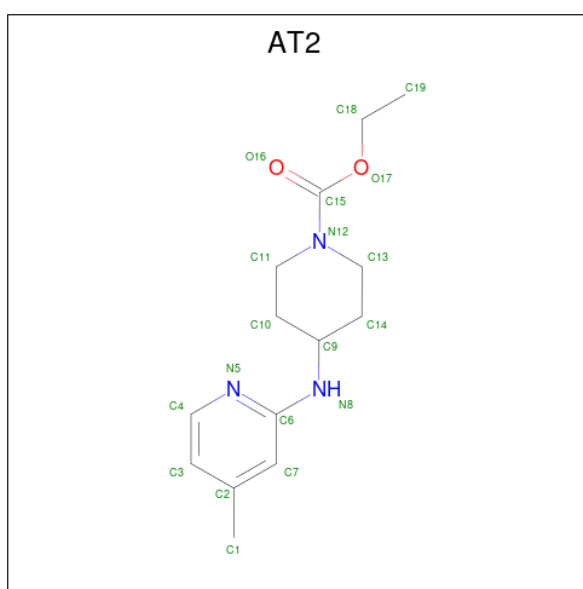
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: C₉H₁₅N₅O₃).



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

- Molecule 5 is ETHYL 4-[(4-METHYLPYRIDIN-2-YL)AMINO]PIPERIDINE-1-CARBOXYLATE (CCD ID: AT2) (formula: C₁₄H₂₁N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	14	3	2		
5	B	1	Total	C	N	O	0	0
			19	14	3	2		
5	C	1	Total	C	N	O	0	0
			19	14	3	2		
5	D	1	Total	C	N	O	0	0
			19	14	3	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	121	Total	O	0	0
			121	121		

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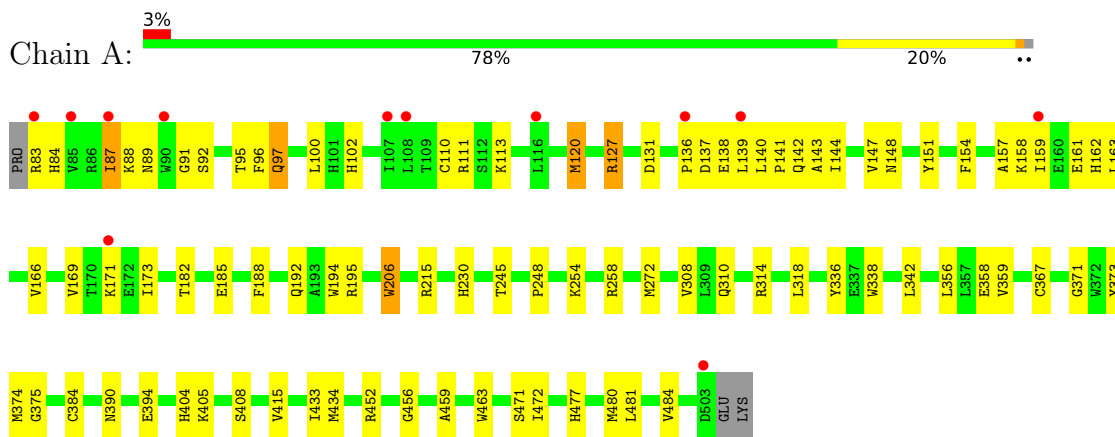
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	110	Total 110	O 110	0	0
6	C	137	Total 137	O 137	0	0
6	D	136	Total 136	O 136	0	0

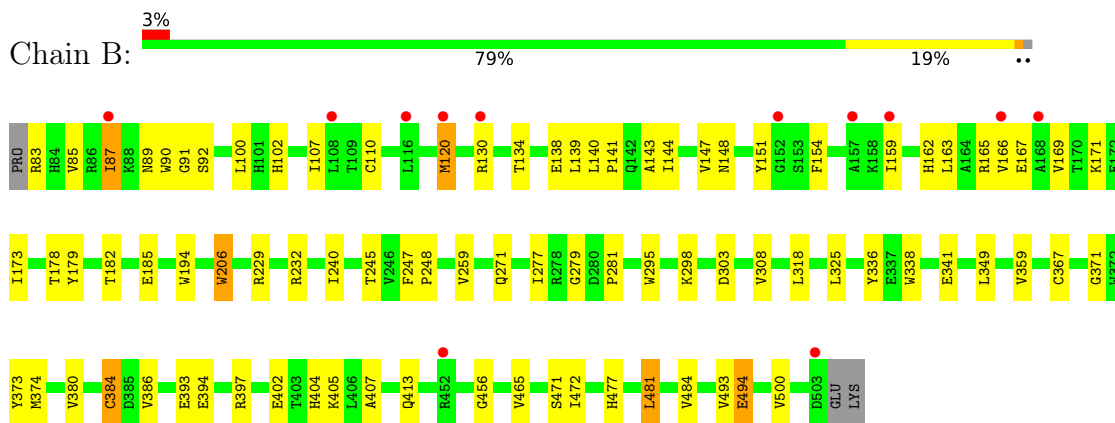
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

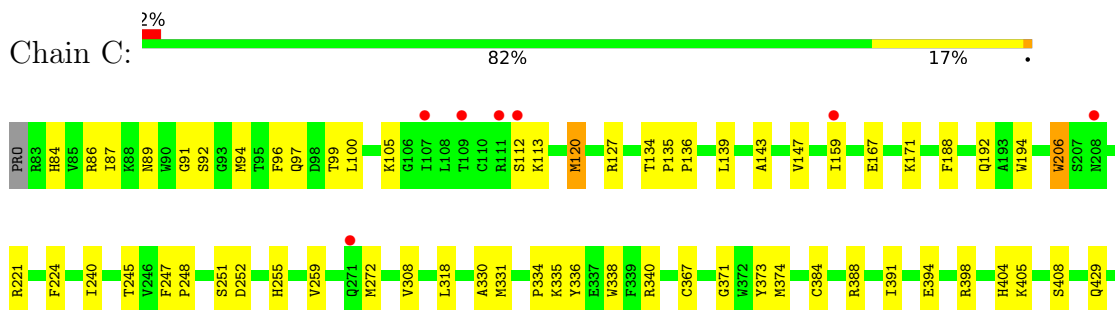
- Molecule 1: Nitric oxide synthase, inducible

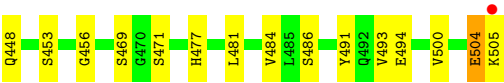


- Molecule 1: Nitric oxide synthase, inducible

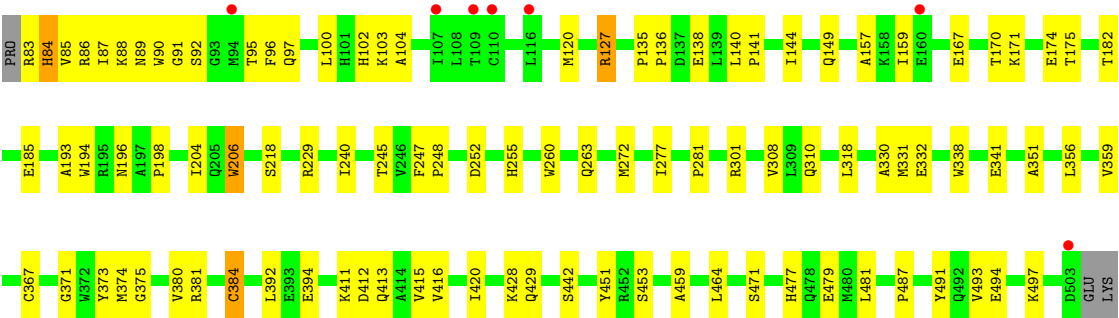
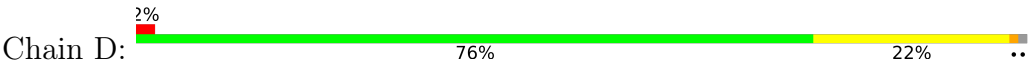


- Molecule 1: Nitric oxide synthase, inducible





● Molecule 1: Nitric oxide synthase, inducible



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.21Å 158.67Å 191.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.51 – 2.20 39.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.2 (39.51-2.20) 90.2 (39.51-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.10Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.182 , 0.213 0.173 , 0.198	Depositor DCC
R_{free} test set	7159 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.8	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	0.97	EDS
Total number of atoms	14516	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 3.39% 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: ZN, H4B, HEM, AT2

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	0.54	0/3517	0.96	13/4774 (0.3%)
1	B	0.53	0/3517	0.95	10/4774 (0.2%)
1	C	0.54	0/3539	0.97	19/4801 (0.4%)
1	D	0.52	0/3517	0.94	12/4774 (0.3%)
All	All	0.53	0/14090	0.95	54/19123 (0.3%)

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

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

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	MET	N-CA-C	-8.29	95.72	109.07
1	C	159	ILE	N-CA-C	7.72	119.43	110.62
1	C	373	TYR	N-CA-C	7.30	120.80	110.50
1	D	374	MET	N-CA-C	-7.08	97.70	109.24
1	D	206	TRP	N-CA-C	7.01	120.73	111.75
1	C	374	MET	N-CA-C	-6.96	97.86	109.07
1	B	374	MET	N-CA-C	-6.82	98.08	109.07
1	B	373	TYR	N-CA-C	6.75	120.02	110.50
1	C	206	TRP	N-CA-C	6.66	120.28	111.75
1	A	206	TRP	N-CA-C	6.62	120.22	111.75
1	D	373	TYR	N-CA-C	6.47	119.63	110.50
1	B	240	ILE	N-CA-C	6.44	117.74	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	VAL	N-CA-C	6.43	117.37	107.99
1	D	453	SER	N-CA-C	6.33	118.26	111.36
1	B	206	TRP	N-CA-C	6.31	119.82	111.75
1	D	240	ILE	N-CA-C	6.26	118.47	109.51
1	A	375	GLY	N-CA-C	6.26	120.47	112.83
1	A	371	GLY	N-CA-C	-6.17	100.95	110.77
1	C	484	VAL	N-CA-C	5.90	116.61	107.99
1	D	375	GLY	N-CA-C	5.85	119.97	112.83
1	C	240	ILE	N-CA-C	5.74	116.82	109.30
1	A	373	TYR	N-CA-C	5.70	118.54	110.50
1	C	259	VAL	N-CA-C	-5.68	99.57	107.80
1	B	139	LEU	N-CA-C	5.65	117.52	111.36
1	C	504	GLU	N-CA-C	-5.59	101.17	109.11
1	A	390	ASN	N-CA-C	5.54	118.98	111.17
1	D	491	TYR	N-CA-C	-5.54	103.38	110.53
1	C	491	TYR	N-CA-C	-5.50	103.43	110.53
1	C	384	CYS	N-CA-C	5.49	120.85	113.72
1	A	408	SER	N-CA-C	-5.48	106.55	113.18
1	D	371	GLY	N-CA-C	-5.45	100.25	113.18
1	D	381	ARG	N-CA-C	5.45	117.08	111.03
1	B	465	VAL	CA-C-N	5.44	123.63	119.66
1	B	465	VAL	C-N-CA	5.44	123.63	119.66
1	D	420	ILE	N-CA-C	-5.44	105.23	110.72
1	C	408	SER	N-CA-C	-5.43	106.66	113.28
1	C	272	MET	CA-C-N	5.41	124.87	119.24
1	C	272	MET	C-N-CA	5.41	124.87	119.24
1	A	88	LYS	N-CA-C	5.39	118.25	109.24
1	B	371	GLY	N-CA-C	-5.37	100.45	113.18
1	A	159	ILE	N-CA-C	5.36	116.09	110.62
1	A	258	ARG	N-CA-C	5.36	117.22	109.07
1	C	139	LEU	N-CA-C	5.35	116.92	111.14
1	C	453	SER	N-CA-C	5.28	116.72	111.07
1	B	384	CYS	N-CA-C	5.25	120.55	113.72
1	D	331	MET	N-CA-C	5.21	118.10	109.46
1	C	371	GLY	N-CA-C	-5.15	100.97	113.18
1	A	384	CYS	N-CA-C	5.11	119.66	113.38
1	B	349	LEU	N-CA-C	5.09	117.86	108.69
1	C	331	MET	N-CA-C	5.09	117.91	109.46
1	C	391	ILE	CB-CA-C	-5.08	104.92	111.88
1	C	112	SER	N-CA-C	-5.08	106.35	112.54
1	A	342	LEU	N-CA-C	-5.05	106.38	112.54
1	D	384	CYS	N-CA-C	5.01	119.54	113.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	451	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	3418	0	3318	57	0
1	B	3418	0	3317	52	0
1	C	3440	0	3339	48	0
1	D	3418	0	3317	65	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	43	0	30	0	0
3	B	43	0	30	0	0
3	C	43	0	30	1	0
3	D	43	0	30	0	0
4	A	17	0	14	1	0
4	B	17	0	14	2	0
4	C	17	0	15	1	0
4	D	17	0	14	0	0
5	A	19	0	21	0	0
5	B	19	0	21	0	0
5	C	19	0	21	0	0
5	D	19	0	21	0	0
6	A	121	0	0	0	0
6	B	110	0	0	1	0
6	C	137	0	0	1	0
6	D	136	0	0	5	0
All	All	14516	0	13552	210	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 8.

All (210) 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:D:260:TRP:HE1	1:D:310:GLN:HE21	1.07	1.00
1:D:260:TRP:HE1	1:D:310:GLN:NE2	1.65	0.93
1:A:192:GLN:HE22	1:A:195:ARG:HH11	1.22	0.86
1:A:272:MET:HE1	1:D:272:MET:HE1	1.58	0.86
1:C:505:LYS:HG2	1:C:505:LYS:O	1.79	0.82
1:C:505:LYS:O	1:C:505:LYS:CG	2.33	0.77
1:B:144:ILE:HD12	1:B:166:VAL:HG13	1.69	0.75
1:A:89:ASN:HD22	1:A:92:SER:H	1.33	0.75
1:D:89:ASN:ND2	1:D:92:SER:H	1.86	0.73
1:A:140:LEU:O	1:A:144:ILE:HG12	1.89	0.72
1:D:167:GLU:O	1:D:171:LYS:HD3	1.89	0.71
1:D:170:THR:O	1:D:174:GLU:HG3	1.90	0.70
1:A:89:ASN:ND2	1:A:92:SER:H	1.89	0.70
1:D:89:ASN:HD22	1:D:92:SER:H	1.40	0.69
1:C:167:GLU:O	1:C:171:LYS:HD3	1.93	0.69
1:C:94:MET:HE2	1:C:96:PHE:CE2	2.28	0.67
1:D:135:PRO:HB2	1:D:138:GLU:HG3	1.77	0.67
1:B:405:LYS:HE2	1:B:407:ALA:HB3	1.75	0.67
1:D:140:LEU:O	1:D:144:ILE:HG12	1.95	0.67
1:D:140:LEU:HB3	1:D:141:PRO:HD3	1.78	0.65
1:D:83:ARG:O	1:D:84:HIS:HB3	1.95	0.65
1:A:83:ARG:O	1:A:102:HIS:HE1	1.80	0.64
1:C:120:MET:HE2	1:D:90:TRP:CE2	2.35	0.62
1:C:221:ARG:NH2	1:C:221:ARG:HG3	2.14	0.62
1:C:221:ARG:HG3	1:C:221:ARG:HH21	1.65	0.62
1:A:89:ASN:ND2	1:A:91:GLY:H	1.99	0.61
1:D:87:ILE:HG21	1:D:481:LEU:HD13	1.83	0.61
3:C:2901:HEM:HBC2	3:C:2901:HEM:HMC2	1.83	0.61
1:A:404:HIS:CD2	1:A:405:LYS:HG3	2.35	0.60
1:D:196:ASN:O	1:D:198:PRO:HD3	2.01	0.60
1:B:89:ASN:HD22	1:B:92:SER:H	1.49	0.60
1:B:182:THR:OG1	1:B:185:GLU:HG3	2.02	0.60
1:A:215:ARG:O	1:A:248:PRO:HG3	2.02	0.60
1:D:260:TRP:NE1	1:D:310:GLN:HE21	1.90	0.59
1:D:89:ASN:ND2	1:D:91:GLY:H	2.00	0.59
1:C:94:MET:HE1	1:C:448:GLN:HG2	1.85	0.59
1:B:159:ILE:O	1:B:163:LEU:HD23	2.01	0.59
1:B:87:ILE:HD11	1:B:481:LEU:HD13	1.84	0.59
1:C:471:SER:O	1:C:477:HIS:HE1	1.87	0.58
1:C:221:ARG:HD2	6:C:6120:HOH:O	2.02	0.58
1:D:330:ALA:H	1:D:429:GLN:HE22	1.49	0.58
1:A:87:ILE:HD11	1:A:481:LEU:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:MET:HE2	1:C:96:PHE:CZ	2.38	0.57
1:D:301:ARG:HD3	6:D:7132:HOH:O	2.03	0.57
1:C:504:GLU:CD	1:C:504:GLU:O	2.47	0.57
1:A:308:VAL:HG22	1:A:318:LEU:CD2	2.35	0.57
1:B:232:ARG:NH1	1:B:325:LEU:HD21	2.20	0.57
1:A:158:LYS:HD2	1:A:161:GLU:OE2	2.04	0.57
1:B:308:VAL:HG22	1:B:318:LEU:CD2	2.35	0.57
1:B:338:TRP:O	1:B:341:GLU:HB2	2.04	0.56
1:C:340:ARG:HG3	1:C:340:ARG:HH21	1.70	0.56
1:B:143:ALA:O	1:B:147:VAL:HG23	2.06	0.56
1:C:143:ALA:O	1:C:147:VAL:HG23	2.06	0.56
1:C:308:VAL:HG22	1:C:318:LEU:CD2	2.35	0.55
1:A:182:THR:OG1	1:A:185:GLU:HG3	2.07	0.55
1:D:471:SER:O	1:D:477:HIS:HE1	1.90	0.55
1:B:295:TRP:CZ2	1:B:298:LYS:HE2	2.41	0.55
1:B:295:TRP:HZ2	1:B:298:LYS:HE2	1.71	0.55
1:A:169:VAL:O	1:A:173:ILE:HG13	2.07	0.54
1:D:356:LEU:C	1:D:356:LEU:HD23	2.32	0.54
1:C:86:ARG:HH21	1:C:97:GLN:NE2	2.05	0.54
1:B:471:SER:O	1:B:477:HIS:HE1	1.90	0.54
1:A:194:TRP:CE3	1:A:206:TRP:HA	2.42	0.54
1:C:87:ILE:HG21	1:C:481:LEU:HD13	1.91	0.53
1:A:188:PHE:CZ	1:A:192:GLN:HG3	2.44	0.53
1:B:130:ARG:NH2	1:B:134:THR:OG1	2.42	0.53
1:C:84:HIS:CE1	1:C:97:GLN:HE21	2.26	0.53
1:D:413:GLN:NE2	6:D:7134:HOH:O	2.42	0.53
1:A:131:ASP:O	1:A:254:LYS:HE3	2.10	0.52
1:A:100:LEU:HB3	1:A:456:GLY:HA3	1.92	0.52
1:B:83:ARG:O	1:B:102:HIS:HE1	1.91	0.52
1:C:334:PRO:O	1:C:335:LYS:HD3	2.09	0.52
1:A:162:HIS:O	1:A:166:VAL:HG23	2.10	0.52
1:B:89:ASN:ND2	1:B:91:GLY:H	2.06	0.52
1:D:182:THR:OG1	1:D:185:GLU:HG3	2.09	0.52
1:B:162:HIS:O	1:B:166:VAL:HG23	2.10	0.52
1:B:165:ARG:O	1:B:169:VAL:HG23	2.09	0.52
1:B:500:VAL:HG23	1:B:500:VAL:O	2.09	0.51
1:D:204:ILE:HG21	1:D:442:SER:OG	2.10	0.51
1:B:336:TYR:HB3	1:B:338:TRP:CE2	2.45	0.51
1:C:100:LEU:HB3	1:C:456:GLY:HA3	1.92	0.51
1:D:252:ASP:OD1	1:D:255:HIS:HD2	1.93	0.51
1:D:277:ILE:HG21	1:D:281:PRO:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:HIS:CD2	1:A:97:GLN:NE2	2.80	0.50
1:B:386:VAL:HG22	6:B:5090:HOH:O	2.10	0.50
1:B:138:GLU:O	1:B:141:PRO:HD2	2.12	0.50
1:C:188:PHE:CZ	1:C:192:GLN:HG3	2.47	0.50
1:B:402:GLU:HB3	1:B:404:HIS:CE1	2.47	0.50
1:A:136:PRO:HA	1:A:139:LEU:HB3	1.94	0.49
1:C:84:HIS:HB3	1:C:99:THR:HG22	1.94	0.49
1:B:140:LEU:O	1:B:144:ILE:HG12	2.13	0.49
1:A:111:ARG:NH2	1:A:113:LYS:HE2	2.28	0.49
1:C:89:ASN:HD22	1:C:92:SER:H	1.60	0.49
1:C:120:MET:CG	4:C:2902:H4B:H9	2.43	0.49
1:C:388:ARG:HH11	1:C:388:ARG:HG3	1.78	0.49
1:D:84:HIS:CE1	1:D:97:GLN:HE21	2.31	0.49
1:A:84:HIS:CD2	1:A:97:GLN:HE22	2.31	0.48
1:A:452:ARG:HG2	1:A:452:ARG:HH21	1.78	0.48
1:B:169:VAL:O	1:B:173:ILE:HG13	2.14	0.48
1:A:95:THR:HG22	1:A:96:PHE:N	2.29	0.48
1:A:245:THR:O	1:A:367:CYS:HA	2.14	0.48
1:D:171:LYS:O	1:D:175:THR:HG23	2.14	0.47
1:D:194:TRP:CZ3	1:D:206:TRP:HA	2.49	0.47
1:D:85:VAL:HB	1:D:481:LEU:HD21	1.96	0.47
1:A:415:VAL:HG11	1:B:472:ILE:HG13	1.97	0.47
1:B:151:TYR:HA	1:B:154:PHE:CD2	2.50	0.47
1:B:247:PHE:HB3	1:B:248:PRO:CD	2.44	0.47
1:B:298:LYS:HE3	1:B:303:ASP:HB3	1.97	0.47
1:D:412:ASP:O	1:D:416:VAL:HG23	2.14	0.47
1:A:113:LYS:NZ	1:B:102:HIS:O	2.47	0.47
1:A:194:TRP:CZ3	1:A:206:TRP:HA	2.49	0.46
1:D:392:LEU:HB2	6:D:7131:HOH:O	2.16	0.46
1:B:120:MET:HG2	4:B:1902:H4B:H9	1.98	0.46
1:D:308:VAL:HG22	1:D:318:LEU:CD2	2.45	0.46
1:C:247:PHE:HB3	1:C:248:PRO:CD	2.46	0.46
1:B:100:LEU:HB3	1:B:456:GLY:HA3	1.98	0.46
1:C:194:TRP:CE3	1:C:206:TRP:HA	2.51	0.46
1:A:143:ALA:O	1:A:147:VAL:HG23	2.16	0.46
1:B:194:TRP:CE3	1:B:206:TRP:HA	2.51	0.46
1:C:245:THR:O	1:C:367:CYS:HA	2.15	0.46
1:B:245:THR:O	1:B:367:CYS:HA	2.16	0.46
1:C:120:MET:HE2	1:D:90:TRP:CD2	2.50	0.46
1:B:159:ILE:HG22	1:B:163:LEU:HD23	1.98	0.45
1:D:86:ARG:CZ	1:D:95:THR:HG21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:LYS:O	1:D:479:GLU:HG3	2.16	0.45
1:D:194:TRP:CE3	1:D:206:TRP:HA	2.51	0.45
1:D:229:ARG:HD3	6:D:7064:HOH:O	2.16	0.45
1:A:83:ARG:C	1:A:102:HIS:HE1	2.23	0.45
1:A:272:MET:HE1	1:D:272:MET:CE	2.38	0.45
1:A:138:GLU:O	1:A:142:GLN:HG3	2.16	0.45
1:B:271:GLN:HA	1:B:277:ILE:HD13	1.99	0.45
1:D:135:PRO:HA	1:D:136:PRO:HD3	1.90	0.45
1:B:229:ARG:HH21	1:B:229:ARG:HG2	1.82	0.45
1:B:144:ILE:HG22	1:B:148:ASN:HD21	1.82	0.45
1:C:221:ARG:HH22	1:C:224:PHE:HD2	1.65	0.45
1:D:247:PHE:HB3	1:D:248:PRO:CD	2.47	0.45
1:B:85:VAL:HB	1:B:481:LEU:HD21	1.99	0.44
1:D:411:LYS:O	1:D:415:VAL:HG23	2.17	0.44
1:A:144:ILE:HG22	1:A:148:ASN:ND2	2.32	0.44
1:D:332:GLU:OE1	1:D:428:LYS:NZ	2.37	0.44
1:A:144:ILE:HG22	1:A:148:ASN:HD21	1.83	0.44
1:B:107:ILE:HD11	1:B:484:VAL:HG11	1.97	0.44
1:B:167:GLU:O	1:B:171:LYS:HD3	2.18	0.44
1:C:87:ILE:HG21	1:C:481:LEU:CD1	2.46	0.44
1:C:394:GLU:O	1:C:398:ARG:HG3	2.16	0.44
1:B:178:THR:OG1	1:B:179:TYR:N	2.51	0.44
1:A:120:MET:HG3	1:B:90:TRP:NE1	2.33	0.44
1:A:356:LEU:C	1:A:356:LEU:HD23	2.42	0.44
1:C:89:ASN:ND2	1:C:91:GLY:H	2.16	0.44
1:D:247:PHE:HB3	1:D:248:PRO:HD2	2.00	0.43
1:D:86:ARG:HG3	1:D:95:THR:HG23	1.99	0.43
1:A:471:SER:O	1:A:477:HIS:HE1	2.01	0.43
1:D:88:LYS:HE3	1:D:90:TRP:CE2	2.53	0.43
1:A:140:LEU:CD1	1:A:173:ILE:HD12	2.48	0.43
1:B:279:GLY:O	1:B:281:PRO:HD3	2.19	0.43
1:C:87:ILE:HG13	1:C:96:PHE:HB2	2.01	0.43
1:C:330:ALA:H	1:C:429:GLN:HE22	1.66	0.43
1:A:336:TYR:HB3	1:A:338:TRP:CE2	2.54	0.43
1:B:394:GLU:HA	1:B:397:ARG:NH1	2.33	0.43
1:A:127:ARG:NH1	1:A:358:GLU:HG3	2.34	0.43
1:A:310:GLN:HG3	1:A:314:ARG:O	2.19	0.43
1:C:252:ASP:OD1	1:C:255:HIS:HD2	2.01	0.43
1:D:245:THR:O	1:D:367:CYS:HA	2.18	0.43
1:B:380:VAL:O	1:B:384:CYS:HB2	2.19	0.43
1:C:336:TYR:HB3	1:C:338:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:HIS:CE1	1:C:405:LYS:HE3	2.54	0.43
1:D:127:ARG:HA	1:D:127:ARG:HD3	1.76	0.43
1:C:251:SER:OG	1:C:252:ASP:N	2.53	0.42
1:D:494:GLU:HG3	1:D:497:LYS:HE3	2.00	0.42
1:A:138:GLU:C	1:A:141:PRO:HD2	2.43	0.42
1:A:137:ASP:OD2	1:A:137:ASP:N	2.51	0.42
1:D:89:ASN:HD22	1:D:92:SER:N	2.13	0.42
1:A:138:GLU:O	1:A:141:PRO:HD2	2.18	0.42
1:A:472:ILE:O	1:A:472:ILE:HG22	2.20	0.42
1:B:393:GLU:OE2	1:B:397:ARG:NH2	2.52	0.42
1:D:149:GLN:NE2	6:D:7068:HOH:O	2.51	0.42
1:B:120:MET:CG	4:B:1902:H4B:H9	2.50	0.41
1:C:120:MET:HE2	1:D:90:TRP:CZ2	2.55	0.41
1:A:87:ILE:HD13	1:A:87:ILE:HA	1.71	0.41
1:C:340:ARG:HG3	1:C:340:ARG:NH2	2.35	0.41
1:D:95:THR:CG2	1:D:96:PHE:N	2.83	0.41
1:B:87:ILE:HD11	1:B:481:LEU:CD1	2.50	0.41
1:D:159:ILE:H	1:D:159:ILE:HG13	1.67	0.41
1:A:84:HIS:ND1	1:A:84:HIS:C	2.78	0.41
1:C:469:SER:OG	1:D:412:ASP:OD2	2.30	0.41
1:D:193:ALA:HB2	1:D:487:PRO:HB2	2.03	0.41
1:D:263:GLN:HA	1:D:351:ALA:O	2.21	0.41
1:A:171:LYS:HD2	1:A:171:LYS:N	2.35	0.41
1:C:134:THR:HA	1:C:135:PRO:HD3	1.86	0.41
1:D:86:ARG:NE	1:D:95:THR:HG21	2.36	0.41
1:D:100:LEU:CD1	1:D:103:LYS:HD2	2.51	0.41
1:D:338:TRP:O	1:D:341:GLU:HB2	2.20	0.41
1:A:110:CYS:HB3	1:B:110:CYS:HB3	2.02	0.41
1:A:230:HIS:CD2	1:A:230:HIS:C	2.99	0.41
1:A:463:TRP:HA	4:A:902:H4B:N1	2.36	0.41
1:C:113:LYS:NZ	1:D:102:HIS:O	2.54	0.41
1:C:127:ARG:HA	1:C:127:ARG:HD3	1.92	0.41
1:D:380:VAL:O	1:D:384:CYS:HB2	2.21	0.41
1:A:272:MET:CE	1:D:272:MET:HE1	2.39	0.41
1:C:113:LYS:NZ	1:D:102:HIS:HA	2.36	0.41
1:D:493:VAL:O	1:D:494:GLU:C	2.64	0.41
1:A:89:ASN:ND2	1:A:91:GLY:N	2.67	0.40
1:C:105:LYS:HE2	1:C:486:SER:HB2	2.04	0.40
1:A:151:TYR:HA	1:A:154:PHE:CD2	2.56	0.40
1:A:433:ILE:HG13	1:A:434:MET:N	2.36	0.40
1:A:459:ALA:HB3	1:A:480:MET:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ILE:HD13	1:B:87:ILE:HA	1.76	0.40
1:C:493:VAL:O	1:C:494:GLU:C	2.63	0.40
1:B:493:VAL:O	1:B:494:GLU:C	2.64	0.40
1:D:459:ALA:HB1	1:D:464:LEU:CD1	2.52	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	419/424 (99%)	402 (96%)	16 (4%)	1 (0%)	43	51
1	B	419/424 (99%)	398 (95%)	21 (5%)	0	100	100
1	C	421/424 (99%)	400 (95%)	21 (5%)	0	100	100
1	D	419/424 (99%)	401 (96%)	15 (4%)	3 (1%)	18	19
All	All	1678/1696 (99%)	1601 (95%)	73 (4%)	4 (0%)	43	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	84	HIS
1	D	104	ALA
1	D	157	ALA
1	A	157	ALA

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	365/370 (99%)	358 (98%)	7 (2%)	50	66
1	B	365/370 (99%)	358 (98%)	7 (2%)	50	66
1	C	368/370 (100%)	365 (99%)	3 (1%)	73	85
1	D	365/370 (99%)	360 (99%)	5 (1%)	59	75
All	All	1463/1480 (99%)	1441 (98%)	22 (2%)	57	73

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

Mol	Chain	Res	Type
1	A	87	ILE
1	A	97	GLN
1	A	120	MET
1	A	127	ARG
1	A	163	LEU
1	A	359	VAL
1	A	394	GLU
1	B	87	ILE
1	B	120	MET
1	B	259	VAL
1	B	359	VAL
1	B	413	GLN
1	B	481	LEU
1	B	494	GLU
1	C	120	MET
1	C	136	PRO
1	C	500	VAL
1	D	120	MET
1	D	127	ARG
1	D	218	SER
1	D	359	VAL
1	D	394	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	A	89	ASN
1	A	97	GLN

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Mol	Chain	Res	Type
1	A	102	HIS
1	A	148	ASN
1	A	192	GLN
1	A	210	GLN
1	A	239	ASN
1	A	255	HIS
1	A	283	ASN
1	A	312	ASN
1	A	404	HIS
1	A	413	GLN
1	A	429	GLN
1	A	477	HIS
1	A	492	GLN
1	A	502	GLN
1	B	89	ASN
1	B	97	GLN
1	B	102	HIS
1	B	148	ASN
1	B	149	GLN
1	B	271	GLN
1	B	288	GLN
1	B	413	GLN
1	B	424	HIS
1	B	427	GLN
1	B	477	HIS
1	B	482	ASN
1	C	89	ASN
1	C	97	GLN
1	C	102	HIS
1	C	142	GLN
1	C	149	GLN
1	C	208	ASN
1	C	255	HIS
1	C	288	GLN
1	C	390	ASN
1	C	404	HIS
1	C	424	HIS
1	C	427	GLN
1	C	429	GLN
1	C	449	ASN
1	C	477	HIS
1	C	502	GLN

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Mol	Chain	Res	Type
1	D	89	ASN
1	D	97	GLN
1	D	208	ASN
1	D	239	ASN
1	D	255	HIS
1	D	283	ASN
1	D	310	GLN
1	D	413	GLN
1	D	424	HIS
1	D	429	GLN
1	D	448	GLN
1	D	477	HIS
1	D	502	GLN

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 14 ligands modelled in this entry, 2 are 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	$\# Z > 2$
3	HEM	D	3901	1	50,50,50	1.51	9 (18%)	67,82,82	1.02	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	H4B	B	1902	-	17,18,18	2.72	4 (23%)	14,26,26	1.98	5 (35%)
4	H4B	D	3902	-	17,18,18	2.95	3 (17%)	14,26,26	1.93	5 (35%)
4	H4B	A	902	-	17,18,18	2.79	4 (23%)	14,26,26	1.93	4 (28%)
5	AT2	C	2906	-	20,20,20	1.93	6 (30%)	25,26,26	1.30	3 (12%)
5	AT2	D	3906	-	20,20,20	1.89	5 (25%)	25,26,26	1.42	3 (12%)
3	HEM	C	2901	1	50,50,50	1.64	11 (22%)	67,82,82	1.04	3 (4%)
3	HEM	B	1901	1	50,50,50	1.52	7 (14%)	67,82,82	0.82	2 (2%)
5	AT2	B	1906	-	20,20,20	1.82	5 (25%)	25,26,26	1.45	4 (16%)
3	HEM	A	901	1	50,50,50	1.61	9 (18%)	67,82,82	1.01	2 (2%)
5	AT2	A	906	-	20,20,20	1.80	5 (25%)	25,26,26	1.42	3 (12%)
4	H4B	C	2902	-	17,18,18	2.56	3 (17%)	14,26,26	1.91	5 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	D	3901	1	-	1/14/54/54	-
4	H4B	B	1902	-	-	2/8/17/17	0/2/2/2
4	H4B	D	3902	-	1/1/3/5	4/8/17/17	0/2/2/2
4	H4B	A	902	-	1/1/3/5	6/8/17/17	0/2/2/2
5	AT2	C	2906	-	-	0/11/21/21	0/2/2/2
5	AT2	D	3906	-	-	0/11/21/21	0/2/2/2
3	HEM	C	2901	1	-	1/14/54/54	-
3	HEM	B	1901	1	-	2/14/54/54	-
5	AT2	B	1906	-	-	0/11/21/21	0/2/2/2
3	HEM	A	901	1	-	1/14/54/54	-
5	AT2	A	906	-	-	0/11/21/21	0/2/2/2
4	H4B	C	2902	-	-	0/8/17/17	0/2/2/2

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3902	H4B	C7-N8	-8.16	1.38	1.46
4	A	902	H4B	C7-C6	-7.43	1.45	1.52
4	D	3902	H4B	C7-C6	-7.41	1.45	1.52
4	B	1902	H4B	C7-N8	-7.35	1.39	1.46
4	A	902	H4B	C7-N8	-7.33	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2902	H4B	C7-N8	-7.14	1.39	1.46
4	B	1902	H4B	C7-C6	-6.75	1.45	1.52
4	C	2902	H4B	C7-C6	-5.79	1.46	1.52
3	C	2901	HEM	FE-NB	5.42	2.11	1.94
3	B	1901	HEM	FE-NB	4.82	2.09	1.94
5	C	2906	AT2	O16-C15	4.76	1.28	1.21
5	C	2906	AT2	C6-N5	4.53	1.42	1.34
5	A	906	AT2	O16-C15	4.48	1.27	1.21
5	D	3906	AT2	O16-C15	4.42	1.27	1.21
5	D	3906	AT2	C6-N5	4.18	1.41	1.34
5	A	906	AT2	C6-N5	4.07	1.41	1.34
3	A	901	HEM	FE-NA	4.03	2.08	1.95
5	B	1906	AT2	O16-C15	4.00	1.27	1.21
3	A	901	HEM	FE-NB	3.66	2.06	1.94
3	D	3901	HEM	FE-NB	3.60	2.06	1.94
3	D	3901	HEM	FE-NC	3.50	2.06	1.95
3	B	1901	HEM	FE-ND	3.49	2.05	1.94
3	A	901	HEM	FE-NC	3.46	2.06	1.95
5	B	1906	AT2	C6-N5	3.45	1.40	1.34
3	B	1901	HEM	FE-NC	3.45	2.06	1.95
5	B	1906	AT2	C10-C9	3.29	1.59	1.52
3	B	1901	HEM	FE-NA	3.23	2.05	1.95
3	D	3901	HEM	FE-NA	3.17	2.05	1.95
3	A	901	HEM	CAB-C3B	-3.08	1.39	1.47
4	D	3902	H4B	C4-N3	-3.01	1.33	1.38
3	C	2901	HEM	FE-ND	2.98	2.04	1.94
3	D	3901	HEM	C1B-NB	-2.96	1.35	1.40
3	C	2901	HEM	C4D-C3D	2.93	1.50	1.45
4	B	1902	H4B	C4-N3	-2.91	1.33	1.38
5	D	3906	AT2	C4-N5	2.90	1.40	1.34
4	C	2902	H4B	C4-N3	-2.90	1.33	1.38
5	C	2906	AT2	C4-N5	2.87	1.40	1.34
3	C	2901	HEM	FE-NA	2.86	2.04	1.95
4	A	902	H4B	C4-N3	-2.85	1.33	1.38
3	D	3901	HEM	FE-ND	2.85	2.03	1.94
5	B	1906	AT2	C4-N5	2.85	1.40	1.34
3	A	901	HEM	C1D-ND	-2.81	1.33	1.38
3	D	3901	HEM	CAC-C3C	-2.77	1.40	1.47
3	A	901	HEM	FE-ND	2.71	2.03	1.94
5	D	3906	AT2	C10-C9	2.55	1.57	1.52
3	C	2901	HEM	CAB-C3B	-2.54	1.40	1.47
3	B	1901	HEM	CAB-C3B	-2.54	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	906	AT2	C4-N5	2.52	1.39	1.34
3	C	2901	HEM	CMC-C2C	2.52	1.55	1.50
5	A	906	AT2	C3-C4	2.43	1.43	1.38
3	D	3901	HEM	CHC-C1C	2.39	1.43	1.38
3	C	2901	HEM	C3B-C4B	2.37	1.49	1.44
5	C	2906	AT2	C10-C9	2.34	1.57	1.52
5	D	3906	AT2	C3-C4	2.34	1.43	1.38
3	C	2901	HEM	C3C-C2C	2.28	1.41	1.37
3	C	2901	HEM	CAC-C3C	-2.28	1.41	1.47
5	B	1906	AT2	C3-C4	2.26	1.42	1.38
3	B	1901	HEM	CAC-C3C	-2.24	1.41	1.47
3	A	901	HEM	C3B-C4B	2.19	1.49	1.44
3	D	3901	HEM	CAB-C3B	-2.17	1.41	1.47
3	A	901	HEM	C1A-NA	-2.16	1.35	1.39
5	C	2906	AT2	C3-C4	2.15	1.42	1.38
4	A	902	H4B	C4A-N5	-2.14	1.32	1.37
3	C	2901	HEM	C3C-C4C	-2.13	1.42	1.46
5	A	906	AT2	C10-C9	2.10	1.56	1.52
3	C	2901	HEM	FE-NC	2.07	2.02	1.95
4	B	1902	H4B	C8A-N1	-2.03	1.33	1.36
3	B	1901	HEM	C1B-NB	-2.02	1.36	1.40
3	D	3901	HEM	CBC-CAC	2.02	1.40	1.30
5	C	2906	AT2	C7-C6	2.02	1.44	1.39
3	A	901	HEM	CMA-C3A	2.00	1.54	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1902	H4B	C2-N1-C8A	4.30	120.95	113.36
4	D	3902	H4B	C2-N1-C8A	4.28	120.92	113.36
4	C	2902	H4B	C2-N1-C8A	4.16	120.71	113.36
4	A	902	H4B	O4-C4-C4A	-3.84	117.99	127.26
4	B	1902	H4B	O4-C4-C4A	-3.65	118.45	127.26
4	A	902	H4B	C2-N1-C8A	3.62	119.75	113.36
4	C	2902	H4B	O4-C4-C4A	-3.62	118.53	127.26
4	D	3902	H4B	O4-C4-C4A	-3.55	118.71	127.26
5	A	906	AT2	C3-C4-N5	-2.94	120.37	123.97
3	A	901	HEM	CAB-C3B-C2B	-2.93	118.90	128.43
5	B	1906	AT2	C3-C4-N5	-2.90	120.42	123.97
5	B	1906	AT2	C7-C6-N5	-2.90	119.12	122.92
5	D	3906	AT2	C3-C4-N5	-2.84	120.50	123.97
3	C	2901	HEM	CAB-C3B-C2B	-2.80	119.31	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	H4B	C4A-C4-N3	2.72	119.60	112.13
4	B	1902	H4B	C4A-C4-N3	2.72	119.59	112.13
4	D	3902	H4B	C4A-C4-N3	2.69	119.51	112.13
5	A	906	AT2	C7-C6-N5	-2.69	119.40	122.92
5	C	2906	AT2	C3-C4-N5	-2.65	120.72	123.97
5	D	3906	AT2	C7-C6-N5	-2.65	119.44	122.92
4	C	2902	H4B	C4A-C4-N3	2.65	119.40	112.13
4	A	902	H4B	C2-N3-C4	-2.63	120.35	125.11
3	C	2901	HEM	CBD-CAD-C3D	-2.52	105.57	112.53
5	C	2906	AT2	C7-C6-N5	-2.52	119.61	122.92
4	B	1902	H4B	C2-N3-C4	-2.49	120.60	125.11
3	A	901	HEM	CBD-CAD-C3D	-2.49	105.66	112.53
5	D	3906	AT2	O16-C15-N12	-2.42	119.82	124.30
5	A	906	AT2	O16-C15-N12	-2.38	119.89	124.30
5	C	2906	AT2	O16-C15-N12	-2.27	120.10	124.30
5	B	1906	AT2	O16-C15-N12	-2.27	120.10	124.30
4	C	2902	H4B	C2-N3-C4	-2.25	121.03	125.11
3	B	1901	HEM	C3B-C2B-C1B	2.17	108.04	106.41
4	D	3902	H4B	C2-N3-C4	-2.17	121.18	125.11
3	D	3901	HEM	C3B-C2B-C1B	2.12	108.00	106.41
3	D	3901	HEM	CAB-C3B-C2B	-2.12	121.55	128.43
3	C	2901	HEM	CAB-C3B-C4B	2.11	133.71	124.39
5	B	1906	AT2	C4-N5-C6	2.09	120.20	117.21
4	B	1902	H4B	C4-C4A-N5	2.07	121.92	116.27
3	D	3901	HEM	C4B-C3B-C2B	-2.06	105.38	107.28
3	B	1901	HEM	C4B-C3B-C2B	-2.06	105.39	107.28
4	D	3902	H4B	C4-C4A-N5	2.05	121.86	116.27
4	C	2902	H4B	C4-C4A-N5	2.03	121.81	116.27

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	902	H4B	C6
4	D	3902	H4B	C6

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	H4B	N5-C6-C9-O9
4	A	902	H4B	N5-C6-C9-C10
4	A	902	H4B	C7-C6-C9-O9
4	A	902	H4B	C7-C6-C9-C10

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Mol	Chain	Res	Type	Atoms
4	B	1902	H4B	C7-C6-C9-O9
4	B	1902	H4B	C7-C6-C9-C10
4	D	3902	H4B	N5-C6-C9-O9
4	D	3902	H4B	C7-C6-C9-O9
4	D	3902	H4B	C7-C6-C9-C10
3	A	901	HEM	C4B-C3B-CAB-CBB
4	D	3902	H4B	N5-C6-C9-C10
3	C	2901	HEM	C4B-C3B-CAB-CBB
4	A	902	H4B	O10-C10-C9-O9
4	A	902	H4B	C11-C10-C9-O9
3	B	1901	HEM	CAA-CBA-CGA-O2A
3	D	3901	HEM	CAA-CBA-CGA-O2A
3	B	1901	HEM	CAA-CBA-CGA-O1A

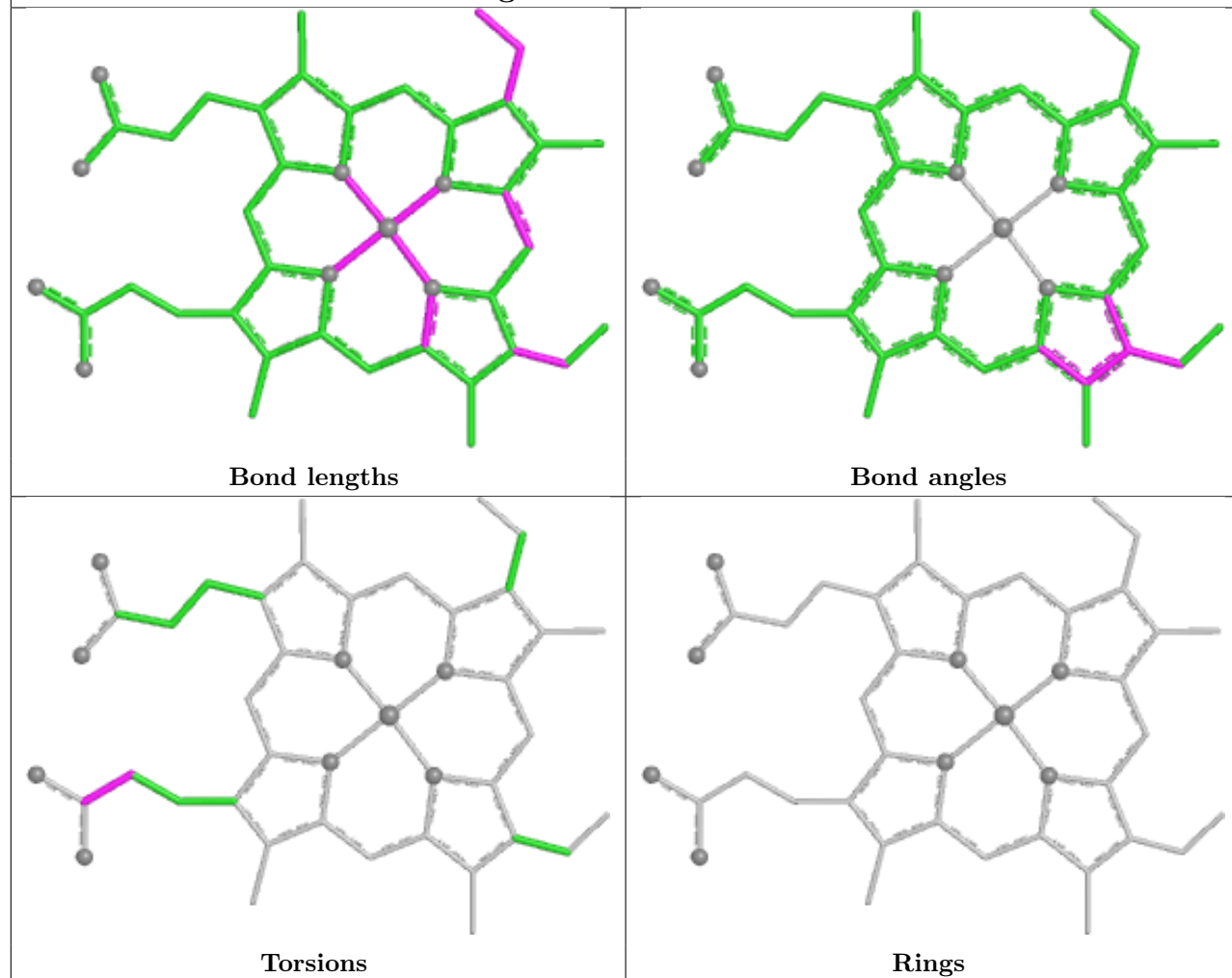
There are no ring outliers.

4 monomers are involved in 5 short contacts:

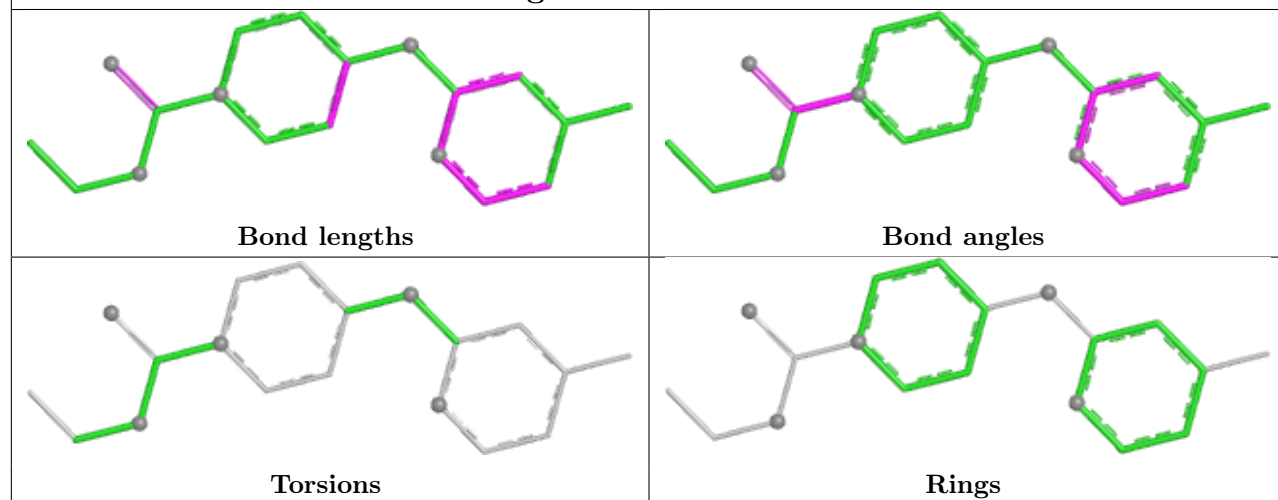
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1902	H4B	2	0
4	A	902	H4B	1	0
3	C	2901	HEM	1	0
4	C	2902	H4B	1	0

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.

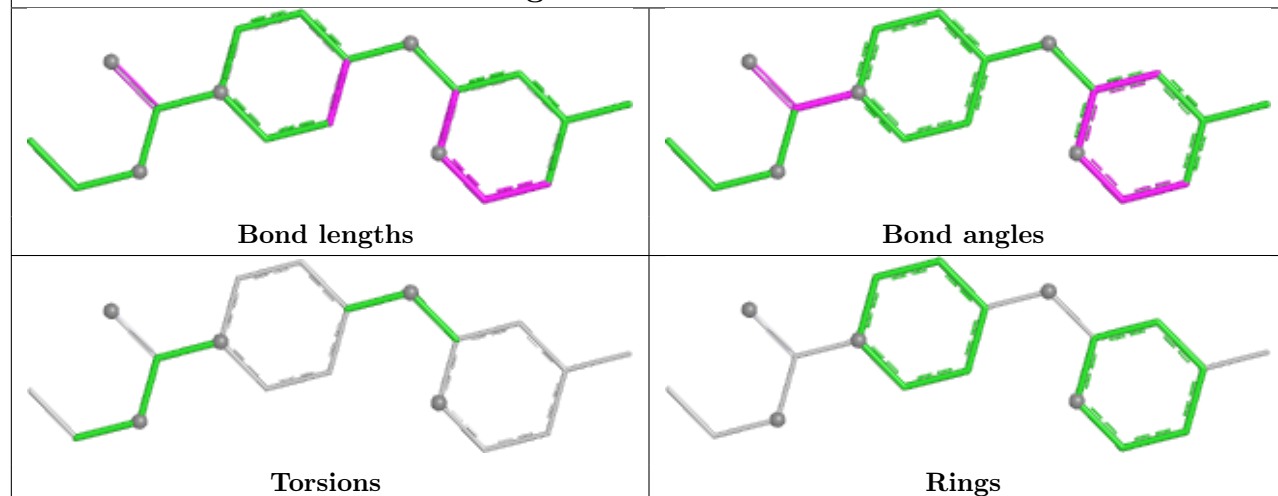
Ligand HEM D 3901



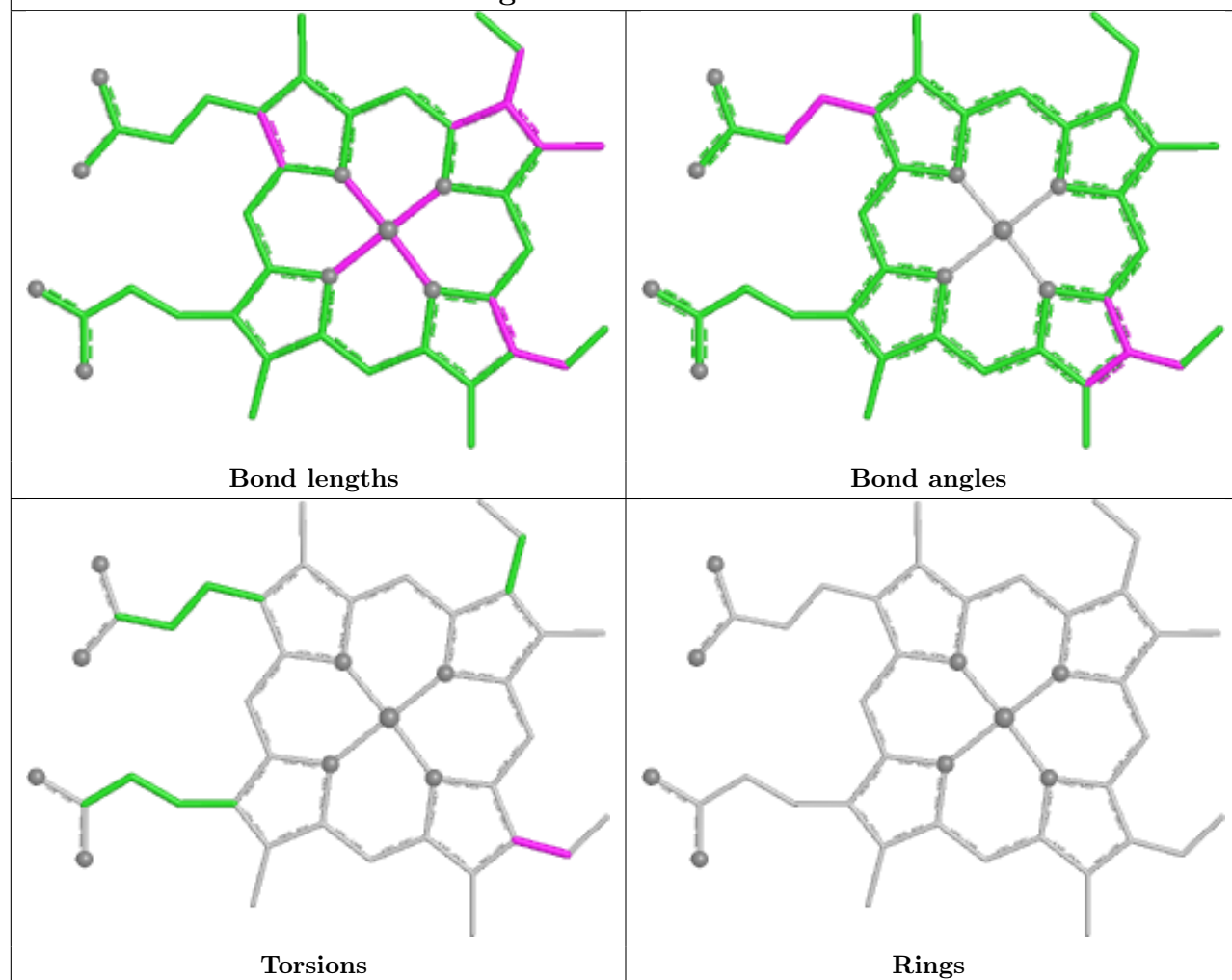
Ligand AT2 C 2906



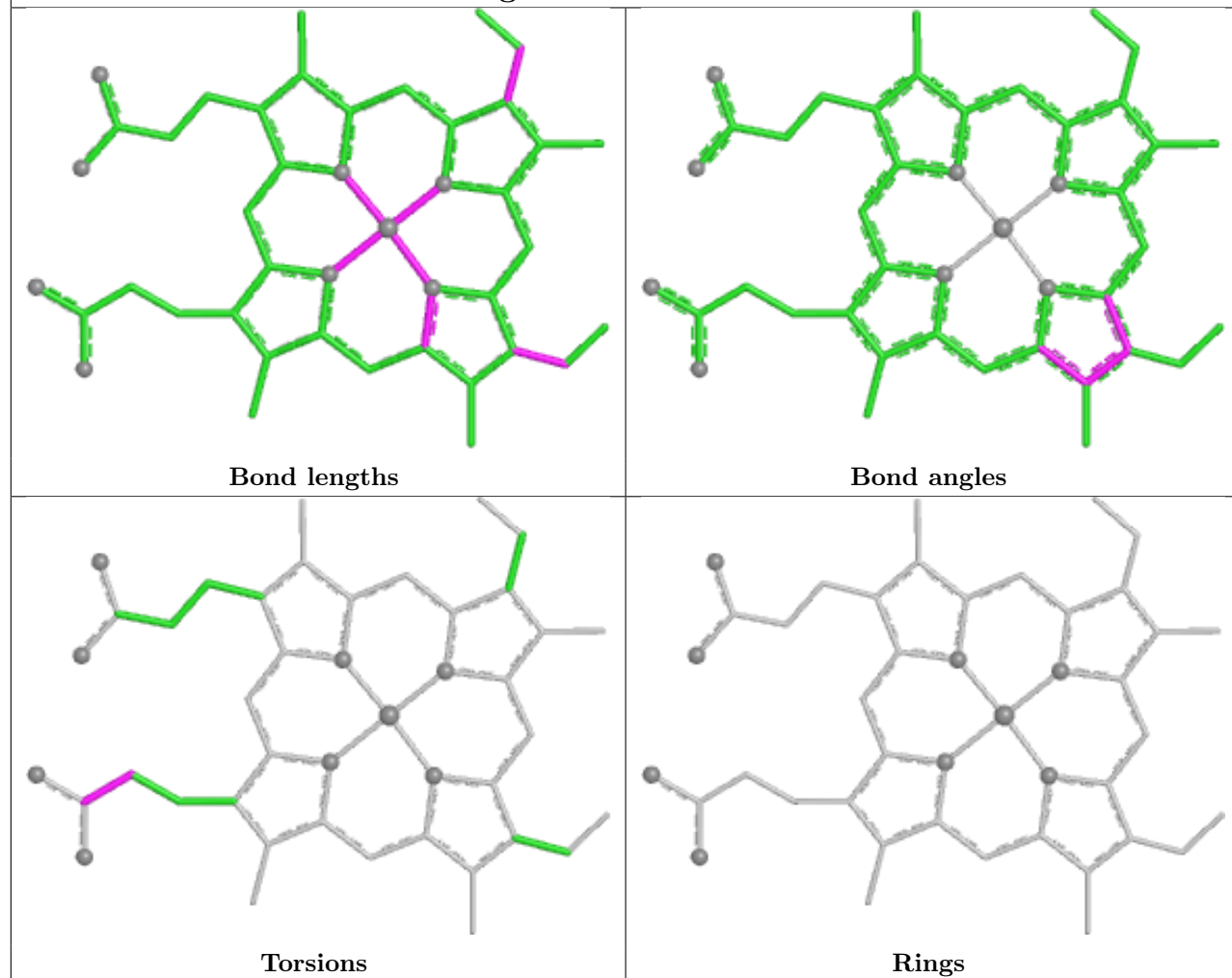
Ligand AT2 D 3906



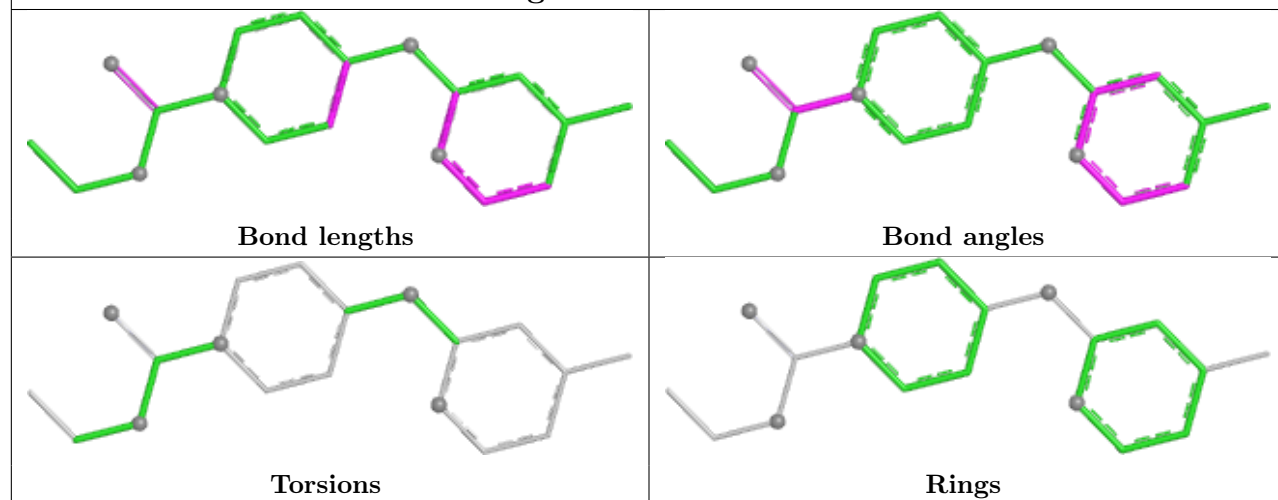
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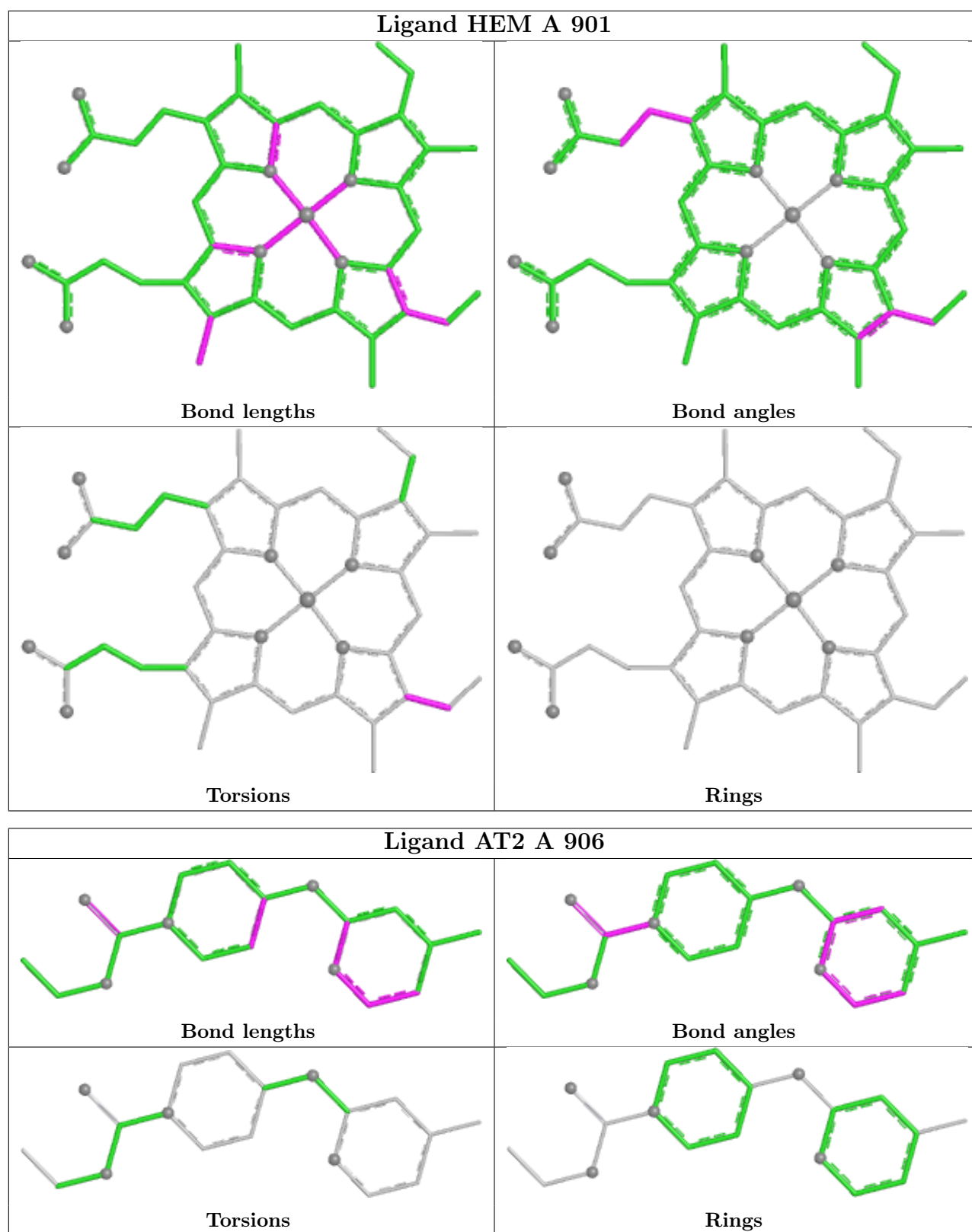


Ligand HEM B 1901



Ligand AT2 B 1906





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	421/424 (99%)	0.10	12 (2%) 53 50	29, 46, 79, 95	0
1	B	421/424 (99%)	0.14	12 (2%) 53 50	30, 48, 80, 101	0
1	C	423/424 (99%)	-0.10	8 (1%) 66 63	25, 43, 73, 92	0
1	D	421/424 (99%)	-0.06	7 (1%) 69 66	29, 45, 75, 93	0
All	All	1686/1696 (99%)	0.02	39 (2%) 61 58	25, 45, 77, 101	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	503	ASP	5.0
1	A	503	ASP	4.4
1	B	503	ASP	4.2
1	B	159	ILE	3.1
1	A	90	TRP	3.0
1	A	107	ILE	2.9
1	D	107	ILE	2.9
1	C	111	ARG	2.8
1	A	116	LEU	2.7
1	D	110	CYS	2.7
1	D	94	MET	2.7
1	D	160	GLU	2.6
1	C	505	LYS	2.6
1	A	83	ARG	2.6
1	B	152	GLY	2.6
1	C	107	ILE	2.6
1	B	130	ARG	2.5
1	C	112	SER	2.5
1	C	159	ILE	2.5
1	B	108	LEU	2.3
1	A	171	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	87	ILE	2.3
1	B	116	LEU	2.3
1	A	85	VAL	2.3
1	D	116	LEU	2.3
1	A	136	PRO	2.3
1	C	109	THR	2.3
1	C	271	GLN	2.2
1	D	109	THR	2.2
1	B	168	ALA	2.2
1	B	87	ILE	2.2
1	B	120	MET	2.2
1	B	452	ARG	2.1
1	A	159	ILE	2.1
1	A	139	LEU	2.1
1	A	108	LEU	2.1
1	B	166	VAL	2.1
1	B	157	ALA	2.0
1	C	208	ASN	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	H4B	B	1902	17/17	0.92	0.11	58,59,65,65	0
4	H4B	A	902	17/17	0.93	0.11	53,55,62,63	0
4	H4B	C	2902	17/17	0.93	0.11	61,63,67,67	0
4	H4B	D	3902	17/17	0.94	0.12	57,59,65,66	0
5	AT2	B	1906	19/19	0.96	0.07	27,30,37,37	0

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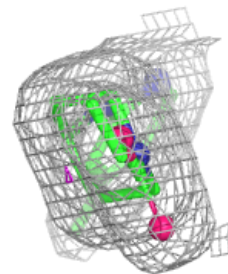
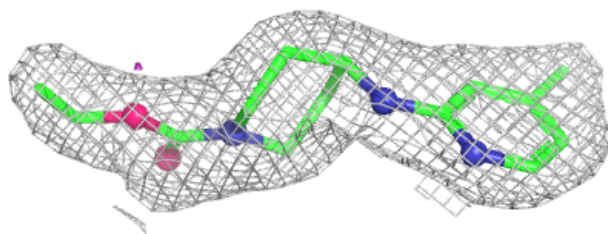
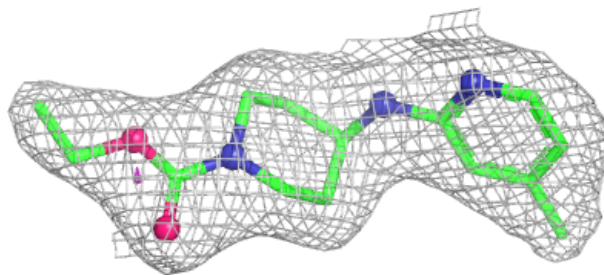
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	AT2	C	2906	19/19	0.97	0.05	24,27,34,34	0
5	AT2	D	3906	19/19	0.97	0.06	27,31,37,38	0
2	ZN	A	3001	1/1	0.98	0.04	72,72,72,72	0
2	ZN	C	3002	1/1	0.98	0.07	73,73,73,73	0
5	AT2	A	906	19/19	0.98	0.06	27,29,31,31	0
3	HEM	A	901	43/43	0.99	0.05	29,31,34,39	0
3	HEM	B	1901	43/43	0.99	0.05	32,34,37,39	0
3	HEM	C	2901	43/43	0.99	0.05	25,29,34,38	0
3	HEM	D	3901	43/43	0.99	0.06	30,32,39,43	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.

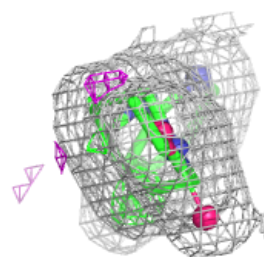
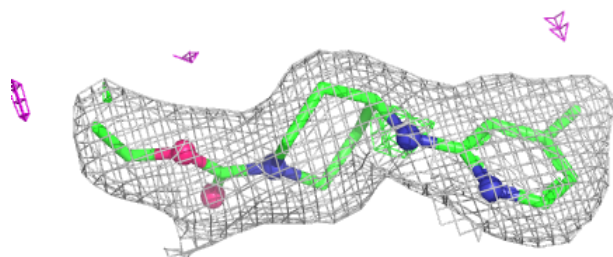
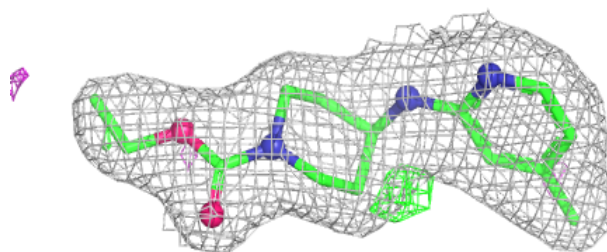
Electron density around AT2 B 1906:

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

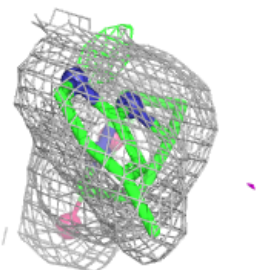
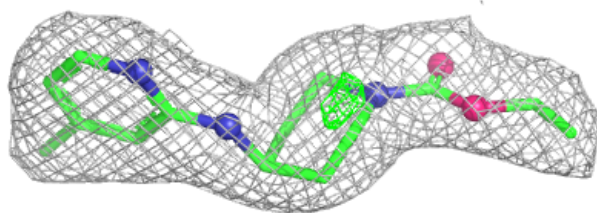
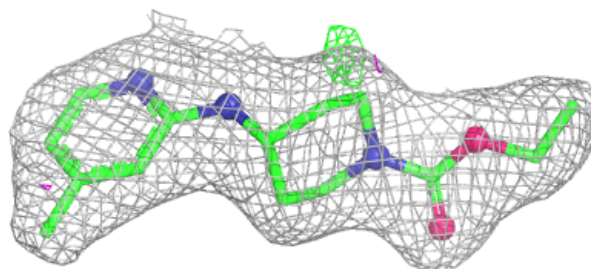


Electron density around AT2 C 2906:

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

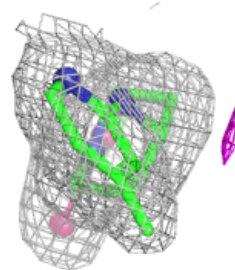
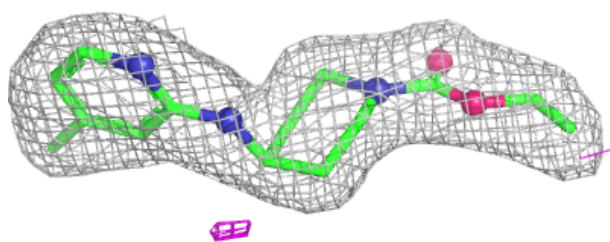
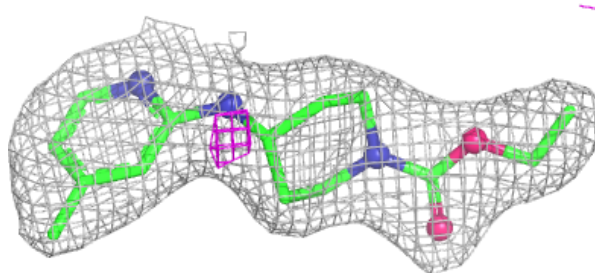
**Electron density around AT2 D 3906:**

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



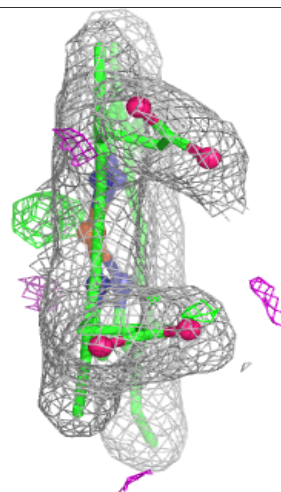
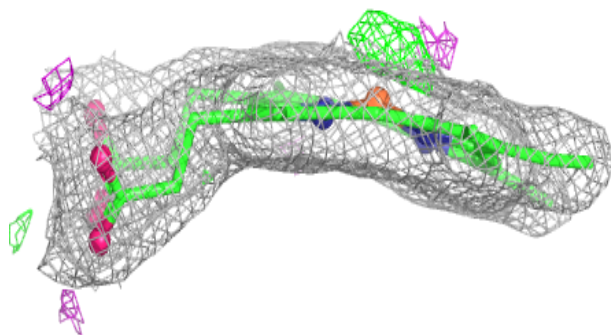
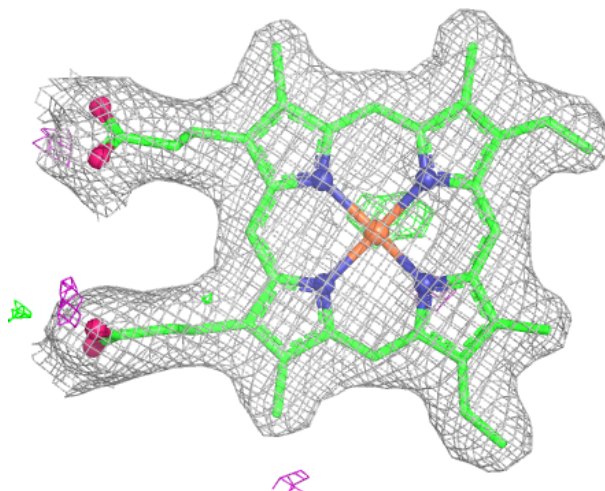
Electron density around AT2 A 906:

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



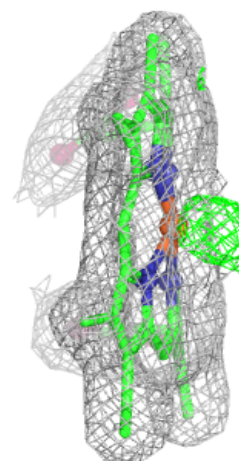
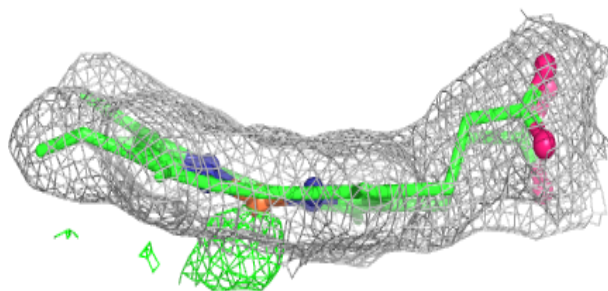
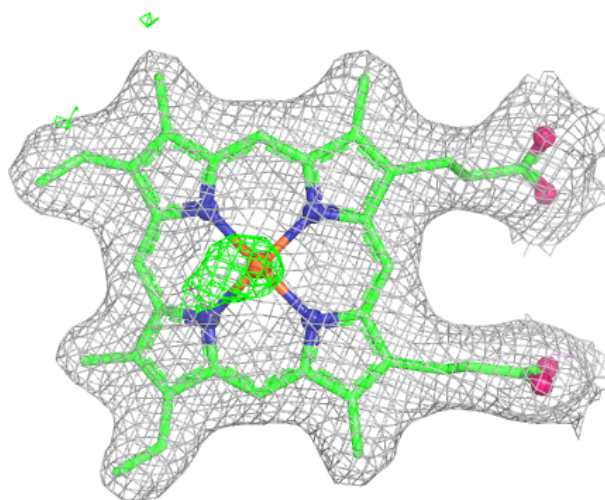
Electron density around HEM A 901:

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



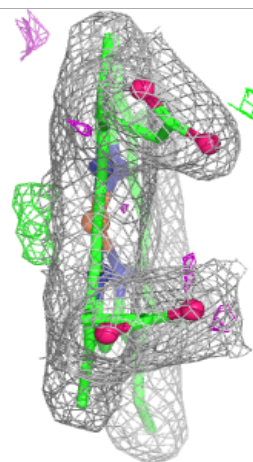
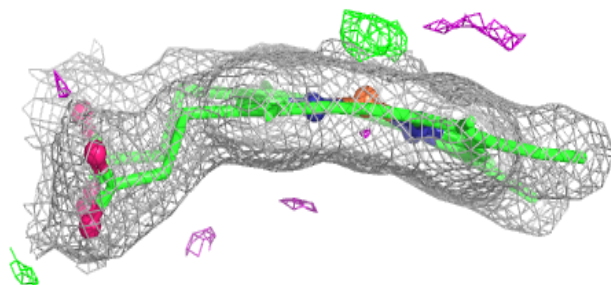
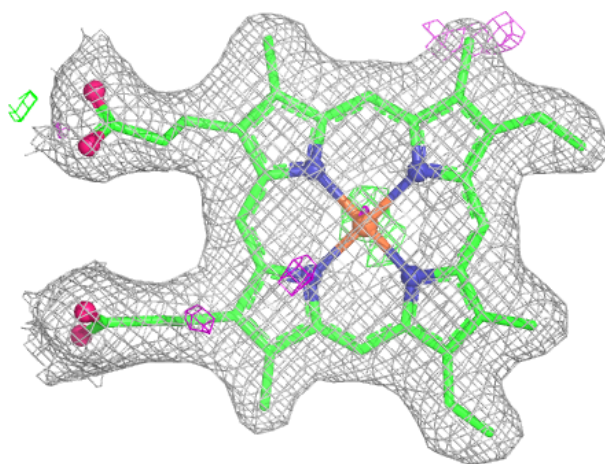
Electron density around HEM B 1901:

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



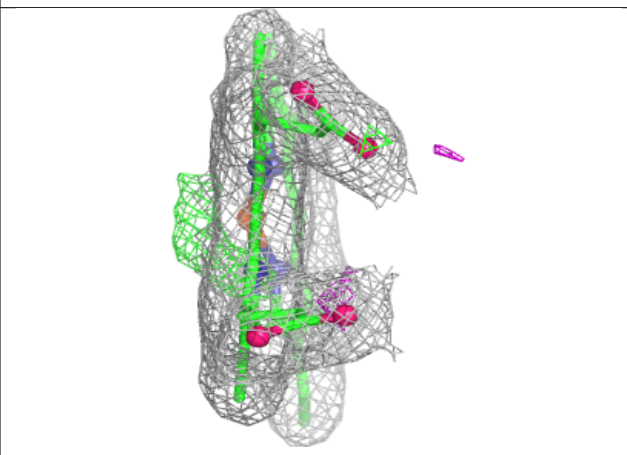
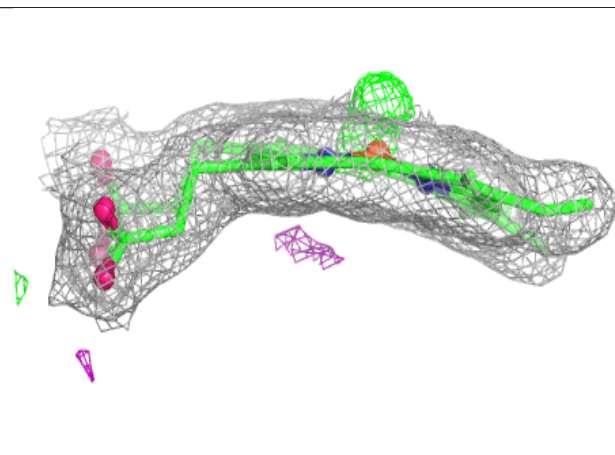
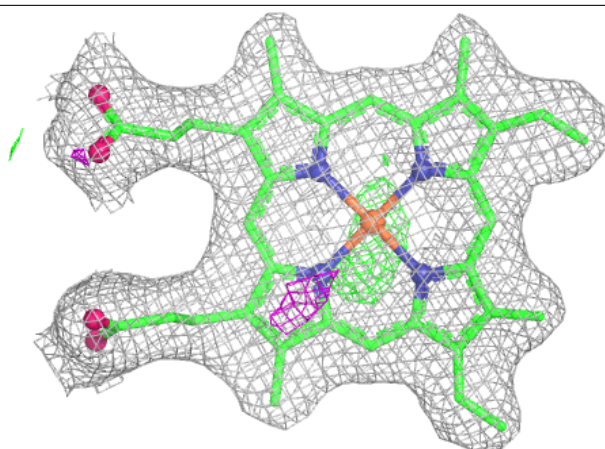
Electron density around HEM C 2901:

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



Electron density around HEM D 3901:

$2mF_o-DF_c$ (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.