



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:41 AM UTC

PDB ID : 3EAI / pdb_00003eai
Title : Structure of inhibited murine iNOS oxygenase domain
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.; Stuehr, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2008-08-25
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)
Xtrriage (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

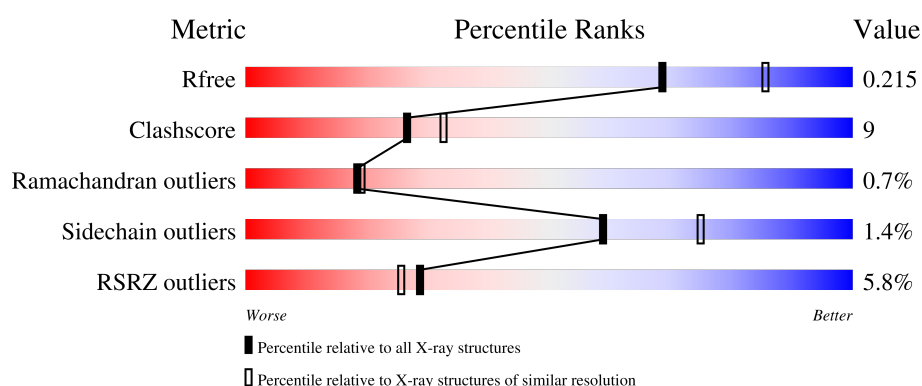
1 Overall quality at a glance

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	433	5% 72% 24% ..
1	B	433	6% 77% 19% ..

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
3	H4B	A	902	X	-	-	-
3	H4B	B	2902	X	-	-	-

2 Entry composition [i](#)

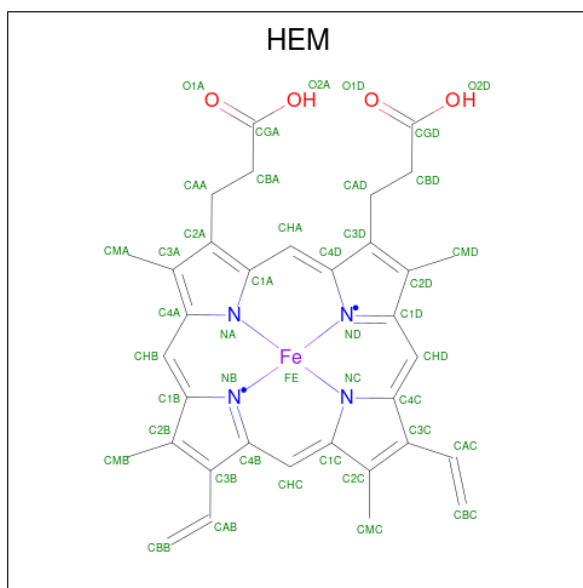
There are 6 unique types of molecules in this entry. The entry contains 7867 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

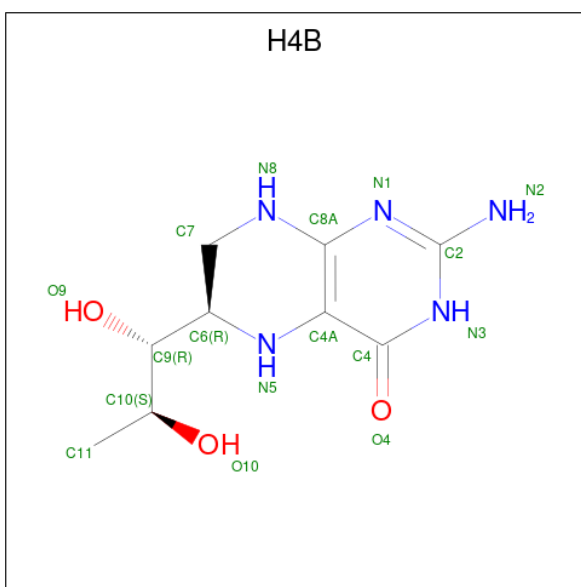
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3425	2195	590	619	21			
1	B	421	Total	C	N	O	S	0	0	0
			3421	2193	589	618	21			

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



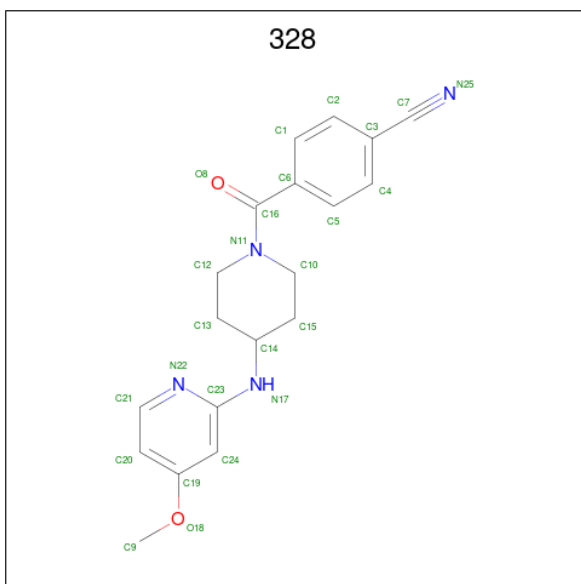
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 4 is 4-({4-[(4-methoxypyridin-2-yl)amino]piperidin-1-yl}carbonyl)benzonitrile (CCD ID: 328) (formula: C₁₉H₂₀N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			25	19	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			25	19	4	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

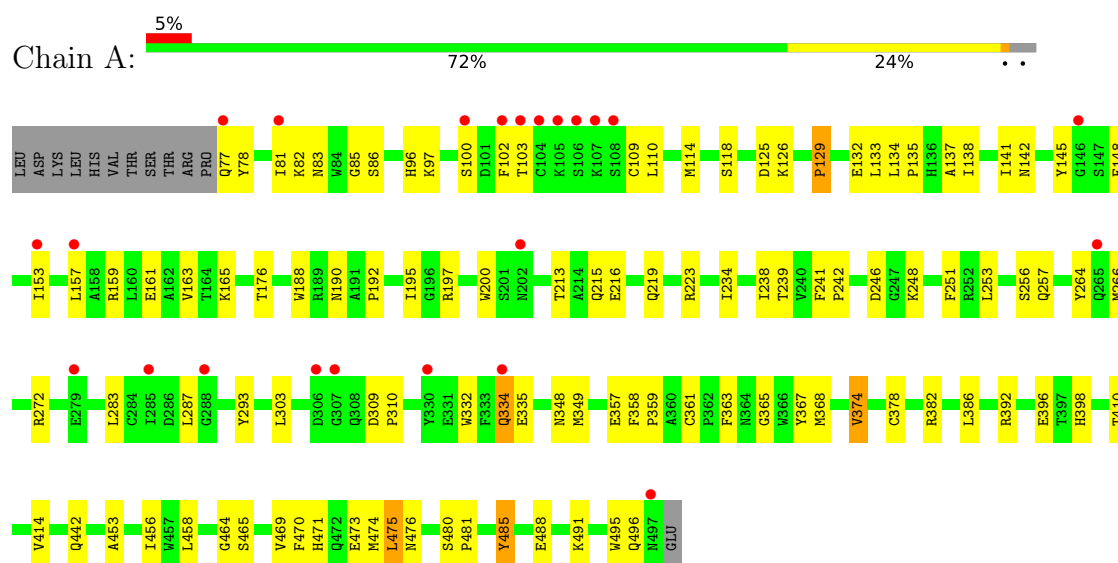
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	388	Total	O	0	0
			388	388		
6	B	443	Total	O	0	0
			443	443		

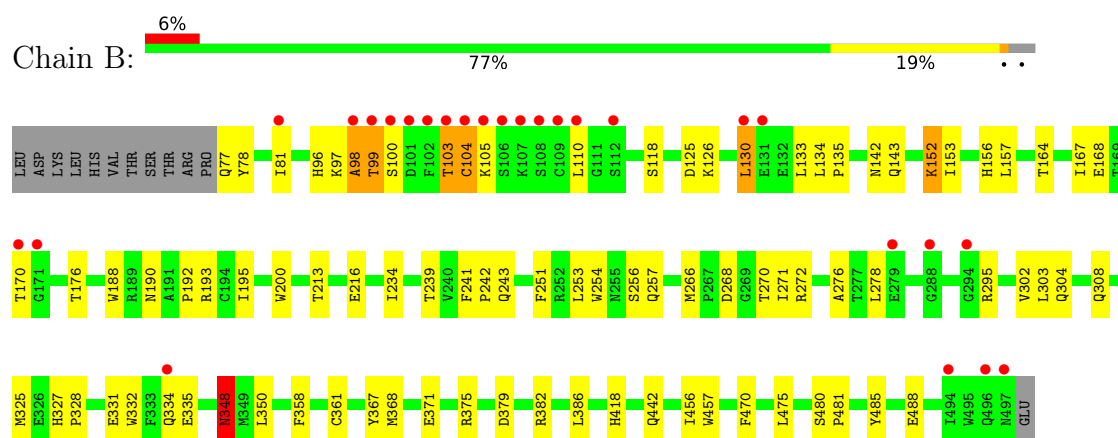
3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	213.11Å 213.11Å 116.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.20 19.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	85.3 (19.95-2.20) 85.2 (19.95-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , (Not available) 0.211 , 0.215	Depositor DCC
R_{free} test set	3389 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 69.3	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	0.95	EDS
Total number of atoms	7867	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: SO4, H4B, 328, 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	0.38	0/3525	0.91	14/4792 (0.3%)
1	B	0.40	0/3521	0.91	12/4787 (0.3%)
All	All	0.39	0/7046	0.91	26/9579 (0.3%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	368	MET	N-CA-C	-6.31	98.12	108.41
1	A	367	TYR	N-CA-C	6.20	118.78	110.35
1	A	368	MET	N-CA-C	-6.09	98.59	108.52
1	B	367	TYR	N-CA-C	5.97	118.25	110.43
1	B	251	PHE	N-CA-C	-5.95	99.97	109.96
1	A	485	TYR	N-CA-C	-5.93	102.00	110.59
1	A	348	ASN	N-CA-C	5.87	120.45	112.88
1	A	365	GLY	N-CA-C	-5.84	99.33	113.18
1	B	176	THR	N-CA-C	-5.79	103.06	110.53
1	A	358	PHE	CA-C-N	5.78	125.46	119.56
1	A	358	PHE	C-N-CA	5.78	125.46	119.56
1	B	485	TYR	N-CA-C	-5.67	102.36	110.59
1	B	303	LEU	N-CA-C	5.66	118.70	109.59
1	B	386	LEU	N-CA-C	5.63	117.86	111.11
1	B	253	LEU	N-CA-C	-5.61	99.38	108.52
1	B	133	LEU	N-CA-C	5.45	116.91	110.97
1	B	234	ILE	N-CA-C	5.44	116.43	109.30
1	A	386	LEU	N-CA-C	5.43	117.63	111.11
1	A	374	VAL	N-CA-C	5.38	116.19	111.56
1	A	251	PHE	N-CA-C	-5.35	100.58	109.46
1	B	325	MET	N-CA-C	5.31	117.37	109.25
1	A	176	THR	N-CA-C	-5.29	103.41	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	348	ASN	N-CA-C	5.26	119.01	112.59
1	A	253	LEU	N-CA-C	-5.22	100.22	108.73
1	A	197	ARG	N-CA-C	5.20	119.11	112.87
1	A	234	ILE	N-CA-C	5.01	116.67	109.51

There are no chirality outliers.

There are no planarity outliers.

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	3425	0	3318	67	0
1	B	3421	0	3312	59	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
3	A	17	0	14	1	0
3	B	17	0	13	2	0
4	A	25	0	20	2	0
4	B	25	0	20	2	0
5	A	10	0	0	0	0
5	B	10	0	0	0	0
6	A	388	0	0	3	2
6	B	443	0	0	8	1
All	All	7867	0	6757	128	2

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 9.

All (128) 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:81:ILE:HD11	1:B:475:LEU:HD13	1.49	0.93
1:A:153:ILE:H	1:A:153:ILE:HD12	1.50	0.76
1:A:83:ASN:ND2	1:A:85:GLY:H	1.85	0.74
1:B:77:GLN:O	1:B:96:HIS:HE1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:GLU:HB2	1:A:491:LYS:HE2	1.74	0.68
1:B:152:LYS:HZ2	1:B:152:LYS:HB3	1.58	0.68
1:B:81:ILE:HD11	1:B:475:LEU:CD1	2.23	0.67
2:A:901:HEM:HMC2	2:A:901:HEM:HBC2	1.75	0.67
1:A:129:PRO:HB2	1:A:132:GLU:HG3	1.78	0.66
1:A:469:VAL:HG13	1:A:474:MET:HE1	1.78	0.66
1:A:125:ASP:OD1	1:A:126:LYS:HG3	1.97	0.64
1:A:309:ASP:OD1	1:A:496:GLN:HG2	1.98	0.62
1:B:105:LYS:HD3	6:B:4610:HOH:O	2.00	0.61
1:A:83:ASN:HD22	1:A:86:SER:H	1.48	0.61
1:A:195:ILE:HD12	6:A:4332:HOH:O	2.00	0.60
1:B:190:ASN:O	1:B:192:PRO:HD3	2.01	0.60
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.83	0.60
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.37	0.60
1:B:304:GLN:HG3	1:B:308:GLN:O	2.02	0.59
1:A:103:THR:HG22	1:A:118:SER:OG	2.03	0.58
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.33	0.58
1:B:125:ASP:OD2	1:B:126:LYS:HG3	2.04	0.58
1:B:170:THR:HG21	6:B:4493:HOH:O	2.03	0.58
1:A:213:THR:OG1	1:A:216:GLU:HG3	2.04	0.58
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.39	0.57
1:A:239:THR:O	1:A:361:CYS:HA	2.04	0.57
1:B:152:LYS:HB3	1:B:152:LYS:NZ	2.19	0.57
1:A:145:TYR:HA	1:A:148:PHE:CE2	2.38	0.57
1:A:153:ILE:HD12	1:A:153:ILE:N	2.19	0.57
1:B:382:ARG:NH2	4:B:2905:328:H2	2.20	0.56
1:A:97:LYS:N	1:A:97:LYS:HD2	2.21	0.56
1:A:303:LEU:O	1:A:310:PRO:HA	2.06	0.56
1:A:266:MET:HE2	1:A:272:ARG:CZ	2.37	0.55
1:A:83:ASN:HD22	1:A:85:GLY:H	1.51	0.55
1:A:357:GLU:O	1:A:359:PRO:HD3	2.06	0.55
1:A:465:SER:O	1:A:471:HIS:HE1	1.89	0.55
1:B:256:SER:HB3	1:B:257:GLN:NE2	2.21	0.55
1:B:110:LEU:HD22	6:B:4611:HOH:O	2.06	0.55
1:A:332:TRP:CE3	1:A:392:ARG:HD2	2.42	0.54
1:B:334:GLN:NE2	1:B:335:GLU:HG3	2.22	0.54
1:A:349:MET:HE3	1:A:485:TYR:CD1	2.43	0.54
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.07	0.54
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.38	0.54
1:B:239:THR:O	1:B:361:CYS:HA	2.07	0.54
1:B:99:THR:HG22	6:B:4825:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASN:O	1:A:192:PRO:HD3	2.09	0.52
1:A:81:ILE:HD11	1:A:475:LEU:HD13	1.91	0.52
1:B:348:ASN:HB2	6:B:4535:HOH:O	2.09	0.52
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.46	0.51
1:A:153:ILE:H	1:A:153:ILE:CD1	2.19	0.51
1:A:246:ASP:OD1	1:A:248:LYS:HB2	2.10	0.51
1:B:331:GLU:O	1:B:334:GLN:HG3	2.10	0.51
1:A:83:ASN:ND2	1:A:86:SER:H	2.08	0.51
1:B:98:ALA:O	1:B:100:SER:N	2.44	0.51
1:A:382:ARG:NH2	4:A:905:328:H2	2.26	0.50
1:B:130:LEU:HD21	1:B:167:ILE:HG22	1.94	0.50
1:B:153:ILE:O	1:B:157:LEU:HG	2.12	0.50
1:A:134:LEU:O	1:A:138:ILE:HG12	2.12	0.50
1:A:215:GLN:O	1:A:219:GLN:HG3	2.11	0.50
1:A:137:ALA:O	1:A:141:ILE:HG12	2.12	0.49
1:B:103:THR:HG22	1:B:118:SER:OG	2.12	0.49
1:B:456:ILE:HG22	3:B:2902:H4B:H71	1.94	0.49
1:B:110:LEU:HD12	1:B:110:LEU:N	2.27	0.49
1:B:480:SER:HA	1:B:481:PRO:C	2.36	0.49
1:A:159:ARG:O	1:A:163:VAL:HG23	2.12	0.49
1:A:110:LEU:N	1:A:110:LEU:HD12	2.28	0.49
1:A:334:GLN:OE1	1:A:335:GLU:N	2.45	0.49
1:B:375:ARG:O	1:B:379:ASP:HB2	2.12	0.49
1:B:104:CYS:HA	1:B:110:LEU:CD1	2.43	0.49
1:B:142:ASN:OD1	1:B:156:HIS:NE2	2.45	0.48
1:B:98:ALA:O	1:B:99:THR:C	2.56	0.48
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.43	0.48
1:A:161:GLU:O	1:A:165:LYS:HD3	2.12	0.48
1:B:295:ARG:HD2	6:B:4545:HOH:O	2.13	0.48
1:B:78:TYR:C	1:B:78:TYR:CD1	2.92	0.47
1:A:470:PHE:C	1:A:470:PHE:CD1	2.93	0.47
1:B:143:GLN:HG3	6:B:4624:HOH:O	2.15	0.47
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.97	0.46
1:B:193:ARG:HB3	1:B:457:TRP:CE3	2.51	0.46
1:B:350:LEU:C	1:B:350:LEU:HD23	2.40	0.46
1:B:271:ILE:HD12	1:B:278:LEU:HD11	1.98	0.46
1:A:82:LYS:O	1:A:473:GLU:HG3	2.16	0.45
1:A:102:PHE:HA	6:A:4343:HOH:O	2.16	0.45
1:B:332:TRP:O	1:B:335:GLU:HB2	2.16	0.45
1:B:456:ILE:CG2	3:B:2902:H4B:H71	2.47	0.45
1:A:374:VAL:O	1:A:378:CYS:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.51	0.45
1:B:104:CYS:HA	1:B:110:LEU:HD13	1.98	0.45
1:B:97:LYS:C	1:B:99:THR:H	2.25	0.44
1:B:266:MET:HE2	1:B:272:ARG:CZ	2.48	0.44
1:A:81:ILE:HD11	1:A:475:LEU:CD1	2.48	0.44
1:A:78:TYR:CD1	1:A:78:TYR:C	2.96	0.44
1:A:382:ARG:CZ	4:A:905:328:H2	2.48	0.44
1:A:480:SER:HA	1:A:481:PRO:C	2.43	0.44
1:A:77:GLN:O	1:A:96:HIS:HE1	2.00	0.44
1:A:453:ALA:HB1	1:A:458:LEU:CD1	2.48	0.44
1:B:98:ALA:O	1:B:100:SER:O	2.36	0.43
1:B:164:THR:O	1:B:168:GLU:HG3	2.19	0.43
1:B:195:ILE:O	1:B:195:ILE:HG13	2.18	0.43
1:B:418:HIS:HD2	6:B:4721:HOH:O	2.01	0.43
1:A:256:SER:HB3	1:A:257:GLN:HE22	1.84	0.43
1:B:241:PHE:HB3	1:B:242:PRO:HD2	2.00	0.43
1:A:195:ILE:O	1:A:195:ILE:HG12	2.18	0.43
1:A:109:CYS:C	1:A:110:LEU:HD12	2.44	0.42
1:A:256:SER:HB3	1:A:257:GLN:NE2	2.33	0.42
1:A:334:GLN:OE1	1:A:335:GLU:HG3	2.19	0.42
1:B:488:GLU:H	1:B:488:GLU:CD	2.26	0.42
1:B:134:LEU:HB3	1:B:135:PRO:HD3	2.01	0.42
1:B:470:PHE:CD1	1:B:470:PHE:C	2.97	0.42
1:A:133:LEU:HD22	6:A:4180:HOH:O	2.18	0.42
1:A:309:ASP:OD2	1:A:495:TRP:HE3	2.03	0.42
1:B:81:ILE:HD13	1:B:81:ILE:HA	1.85	0.42
1:B:276:ALA:HB2	1:B:382:ARG:HD2	2.01	0.42
1:A:283:LEU:O	1:A:287:LEU:HG	2.19	0.42
1:A:396:GLU:C	1:A:398:HIS:H	2.27	0.42
1:A:410:THR:O	1:A:414:VAL:HG23	2.20	0.41
1:A:165:LYS:N	1:A:165:LYS:HD2	2.34	0.41
1:A:264:TYR:CE1	1:A:293:TYR:HA	2.55	0.41
1:A:153:ILE:HG22	1:A:157:LEU:HD23	2.03	0.41
1:B:371:GLU:OE2	4:B:2905:328:N22	2.53	0.41
1:A:97:LYS:N	1:A:97:LYS:CD	2.84	0.41
1:A:102:PHE:HZ	1:A:476:ASN:ND2	2.18	0.41
1:B:268:ASP:OD1	1:B:270:THR:HG23	2.21	0.41
1:A:238:ILE:HG13	1:A:363:PHE:HB3	2.02	0.40
1:B:254:TRP:HB2	1:B:302:VAL:HB	2.02	0.40
2:B:2901:HEM:HBC2	2:B:2901:HEM:HMC1	2.03	0.40
1:A:138:ILE:O	1:A:142:ASN:ND2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ILE:CG2	3:A:902:H4B:H71	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:4789:HOH:O	6:B:4330:HOH:O[12_556]	1.94	0.26
6:A:4196:HOH:O	6:A:4210:HOH:O[11_655]	2.06	0.14

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	419/433 (97%)	389 (93%)	28 (7%)	2 (0%)	24	27
1	B	419/433 (97%)	388 (93%)	27 (6%)	4 (1%)	12	11
All	All	838/866 (97%)	777 (93%)	55 (7%)	6 (1%)	18	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	SER
1	B	99	THR
1	B	104	CYS
1	A	464	GLY
1	B	103	THR
1	B	98	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	367/381 (96%)	361 (98%)	6 (2%)	55	71
1	B	366/381 (96%)	362 (99%)	4 (1%)	65	79
All	All	733/762 (96%)	723 (99%)	10 (1%)	59	75

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	MET
1	A	129	PRO
1	A	223	ARG
1	A	334	GLN
1	A	442	GLN
1	A	475	LEU
1	B	130	LEU
1	B	152	LYS
1	B	348	ASN
1	B	442	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	96	HIS
1	A	115	ASN
1	A	142	ASN
1	A	202	ASN
1	A	215	GLN
1	A	219	GLN
1	A	384	ASN
1	A	421	GLN
1	A	431	HIS
1	A	442	GLN
1	A	471	HIS
1	A	486	GLN
1	A	493	HIS
1	B	96	HIS
1	B	115	ASN

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Mol	Chain	Res	Type
1	B	199	GLN
1	B	202	ASN
1	B	215	GLN
1	B	220	HIS
1	B	348	ASN
1	B	384	ASN
1	B	421	GLN
1	B	486	GLN
1	B	493	HIS

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](#)

10 ligands are modelled in this entry.

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	SO4	A	3002	-	4,4,4	0.36	0	6,6,6	0.06	0
3	H4B	B	2902	-	17,18,18	2.69	3 (17%)	14,26,26	6.72	13 (92%)
4	328	A	905	-	27,27,27	1.90	8 (29%)	35,36,36	1.77	11 (31%)
5	SO4	B	3003	-	4,4,4	0.38	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	901	1	50,50,50	1.33	7 (14%)	67,82,82	1.08	3 (4%)
2	HEM	B	2901	1	50,50,50	1.37	6 (12%)	67,82,82	1.08	4 (5%)
5	SO4	B	3004	-	4,4,4	0.36	0	6,6,6	0.10	0
5	SO4	A	3001	-	4,4,4	0.39	0	6,6,6	0.14	0
3	H4B	A	902	-	17,18,18	2.69	3 (17%)	14,26,26	6.51	11 (78%)
4	328	B	2905	-	27,27,27	1.95	7 (25%)	35,36,36	1.68	10 (28%)

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	H4B	B	2902	-	1/1/3/5	2/8/17/17	0/2/2/2
4	328	A	905	-	-	4/16/26/26	0/3/3/3
2	HEM	A	901	1	-	2/14/54/54	-
2	HEM	B	2901	1	-	1/14/54/54	-
3	H4B	A	902	-	1/1/3/5	5/8/17/17	0/2/2/2
4	328	B	2905	-	-	3/16/26/26	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2902	H4B	C7-N8	-8.35	1.38	1.46
3	A	902	H4B	C7-N8	-8.23	1.38	1.46
3	A	902	H4B	C7-C6	-5.71	1.46	1.52
3	B	2902	H4B	C7-C6	-5.62	1.46	1.52
4	A	905	328	C15-C14	3.97	1.61	1.52
4	B	2905	328	C5-C6	3.91	1.45	1.39
4	B	2905	328	C15-C14	3.70	1.60	1.52
4	A	905	328	C5-C6	3.63	1.44	1.39
4	B	2905	328	C2-C1	3.56	1.44	1.38
4	A	905	328	C2-C1	3.54	1.44	1.38
2	B	2901	HEM	FE-ND	3.28	2.05	1.94
2	A	901	HEM	FE-ND	3.16	2.04	1.94
4	A	905	328	C1-C6	2.93	1.43	1.39
4	B	2905	328	C2-C3	2.92	1.45	1.39
4	B	2905	328	C1-C6	2.91	1.43	1.39
2	A	901	HEM	FE-NC	2.88	2.04	1.95
3	A	902	H4B	C4-N3	-2.87	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2905	328	C16-N11	2.86	1.40	1.34
2	A	901	HEM	CAC-C3C	-2.83	1.39	1.47
2	B	2901	HEM	FE-NC	2.81	2.04	1.95
4	A	905	328	C2-C3	2.74	1.45	1.39
2	B	2901	HEM	CAC-C3C	-2.70	1.40	1.47
2	A	901	HEM	FE-NB	2.70	2.03	1.94
3	B	2902	H4B	C4-N3	-2.70	1.33	1.38
2	A	901	HEM	CAB-C3B	-2.69	1.40	1.47
4	A	905	328	C16-N11	2.69	1.40	1.34
2	B	2901	HEM	FE-NB	2.45	2.02	1.94
2	B	2901	HEM	CAB-C3B	-2.42	1.40	1.47
2	B	2901	HEM	CBC-CAC	2.11	1.40	1.30
4	A	905	328	C24-C19	2.05	1.42	1.39
4	B	2905	328	C24-C19	2.04	1.42	1.39
4	A	905	328	C23-N22	2.03	1.37	1.34
2	A	901	HEM	FE-NA	2.01	2.01	1.95
2	A	901	HEM	C4D-ND	-2.00	1.36	1.40

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2902	H4B	C11-C10-C9	15.90	131.59	112.11
3	B	2902	H4B	O9-C9-C10	-11.93	86.44	109.14
3	A	902	H4B	O9-C9-C10	-11.02	88.16	109.14
3	A	902	H4B	O4-C4-C4A	-9.34	104.73	127.26
3	A	902	H4B	C4A-C4-N3	8.67	135.95	112.13
3	A	902	H4B	C11-C10-C9	8.21	122.17	112.11
3	A	902	H4B	C2-N3-C4	-7.84	110.88	125.11
3	B	2902	H4B	O4-C4-C4A	-7.77	108.53	127.26
3	A	902	H4B	C4-C4A-N5	7.56	136.88	116.27
3	A	902	H4B	O10-C10-C11	-7.22	88.09	109.68
3	B	2902	H4B	N2-C2-N1	-6.54	106.90	119.67
3	A	902	H4B	N2-C2-N1	-5.98	107.99	119.67
3	B	2902	H4B	C2-N1-C8A	-4.90	104.71	113.36
3	B	2902	H4B	C4-C4A-N5	4.67	128.99	116.27
3	B	2902	H4B	C4A-C4-N3	4.21	123.70	112.13
3	B	2902	H4B	O4-C4-N3	4.07	127.77	120.11
3	B	2902	H4B	C2-N3-C4	-3.98	117.89	125.11
3	A	902	H4B	O9-C9-C6	-3.81	100.14	109.28
4	A	905	328	C20-C21-N22	-3.75	119.38	123.97
4	B	2905	328	C21-N22-C23	3.72	122.53	117.21
4	A	905	328	C21-N22-C23	3.72	122.52	117.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2905	328	C20-C21-N22	-3.61	119.55	123.97
2	A	901	HEM	CMD-C2D-C1D	3.59	130.64	125.03
3	B	2902	H4B	O10-C10-C11	-3.51	99.19	109.68
3	A	902	H4B	N2-C2-N3	3.49	124.13	116.76
4	A	905	328	C15-C10-N11	-3.45	103.91	110.66
3	B	2902	H4B	N3-C2-N1	3.40	129.54	123.32
3	B	2902	H4B	N2-C2-N3	3.22	123.56	116.76
4	A	905	328	C15-C14-N17	3.04	115.67	110.77
4	B	2905	328	C15-C10-N11	-3.01	104.76	110.66
4	A	905	328	C6-C16-N11	2.95	122.34	118.66
4	B	2905	328	C15-C14-N17	2.82	115.32	110.77
2	B	2901	HEM	CMD-C2D-C1D	2.79	129.40	125.03
4	B	2905	328	C24-C23-N22	-2.69	119.39	122.92
4	A	905	328	C21-C20-C19	2.60	120.42	118.01
2	B	2901	HEM	CHC-C4B-NB	-2.58	121.65	124.42
3	A	902	H4B	N3-C2-N1	2.49	127.88	123.32
4	B	2905	328	C6-C16-N11	2.48	121.76	118.66
4	A	905	328	C24-C23-N22	-2.46	119.70	122.92
4	A	905	328	C13-C14-N17	-2.43	106.85	110.77
4	B	2905	328	C9-O18-C19	2.39	122.63	117.50
4	A	905	328	C13-C12-N11	-2.39	105.98	110.66
4	A	905	328	O8-C16-C6	-2.38	115.56	120.29
4	B	2905	328	C21-C20-C19	2.31	120.15	118.01
4	A	905	328	C9-O18-C19	2.24	122.31	117.50
4	B	2905	328	C13-C14-N17	-2.20	107.23	110.77
2	B	2901	HEM	CAB-C3B-C2B	-2.17	121.37	128.43
4	B	2905	328	O8-C16-C6	-2.16	116.01	120.29
3	B	2902	H4B	O9-C9-C6	2.12	114.36	109.28
2	B	2901	HEM	CAD-C3D-C4D	2.06	128.28	124.70
2	A	901	HEM	CMA-C3A-C4A	2.02	128.50	125.42
2	A	901	HEM	CAD-C3D-C2D	-2.01	124.10	127.87

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	902	H4B	C6
3	B	2902	H4B	C6

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	H4B	N5-C6-C9-O9

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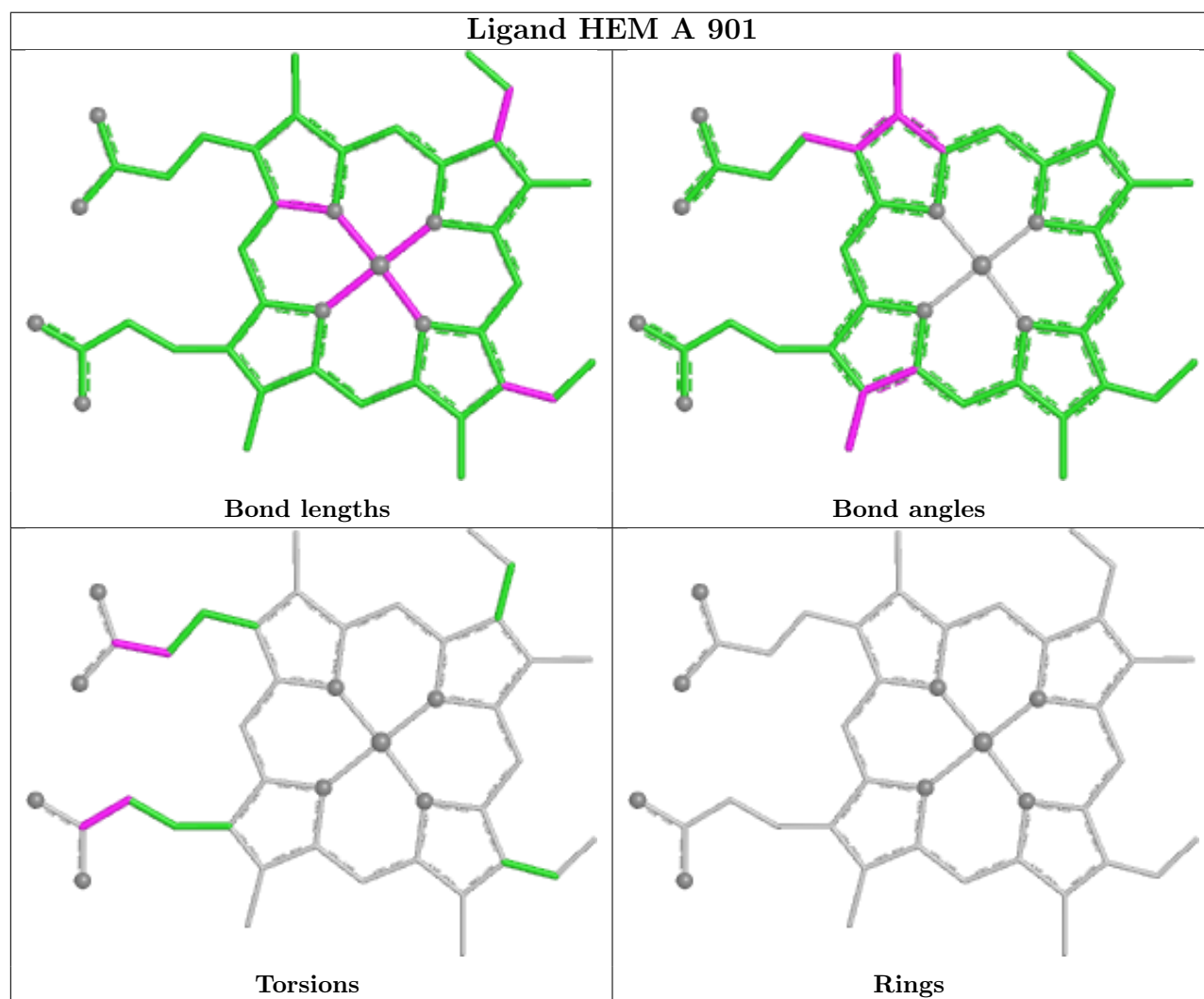
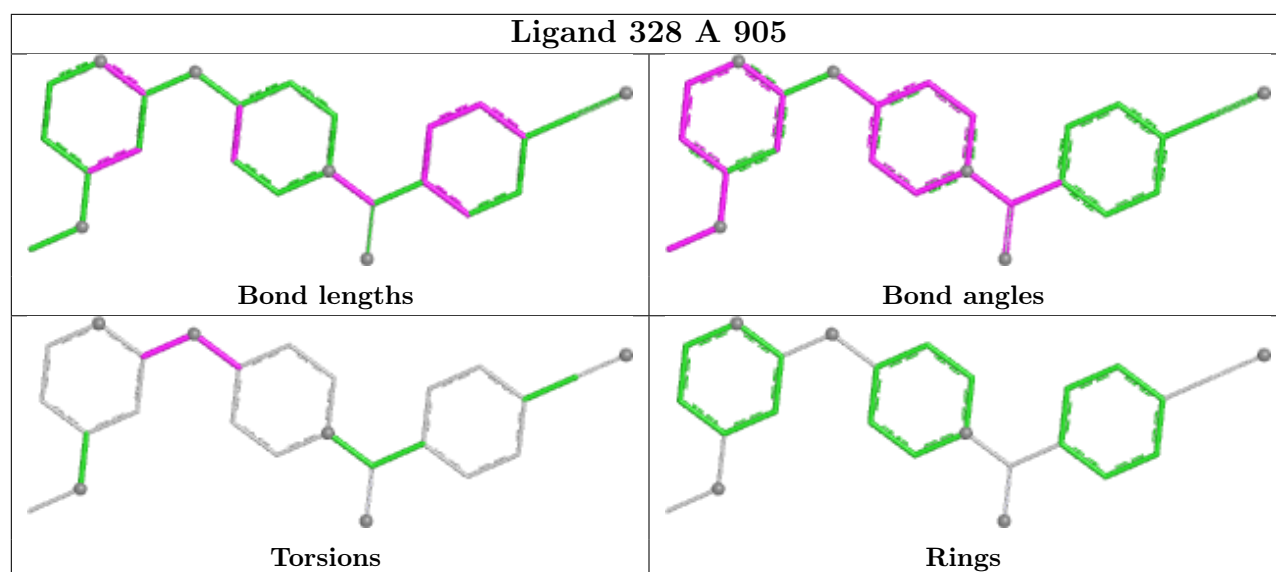
Mol	Chain	Res	Type	Atoms
3	A	902	H4B	C7-C6-C9-O9
3	A	902	H4B	C7-C6-C9-C10
3	A	902	H4B	O10-C10-C9-C6
3	B	2902	H4B	N5-C6-C9-O9
3	B	2902	H4B	C7-C6-C9-C10
4	A	905	328	N22-C23-N17-C14
4	A	905	328	C13-C14-N17-C23
4	A	905	328	C15-C14-N17-C23
4	B	2905	328	C13-C14-N17-C23
4	B	2905	328	C15-C14-N17-C23
3	A	902	H4B	O10-C10-C9-O9
2	B	2901	HEM	C4B-C3B-CAB-CBB
4	A	905	328	C24-C23-N17-C14
4	B	2905	328	N22-C23-N17-C14
2	A	901	HEM	CAA-CBA-CGA-O2A
2	A	901	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

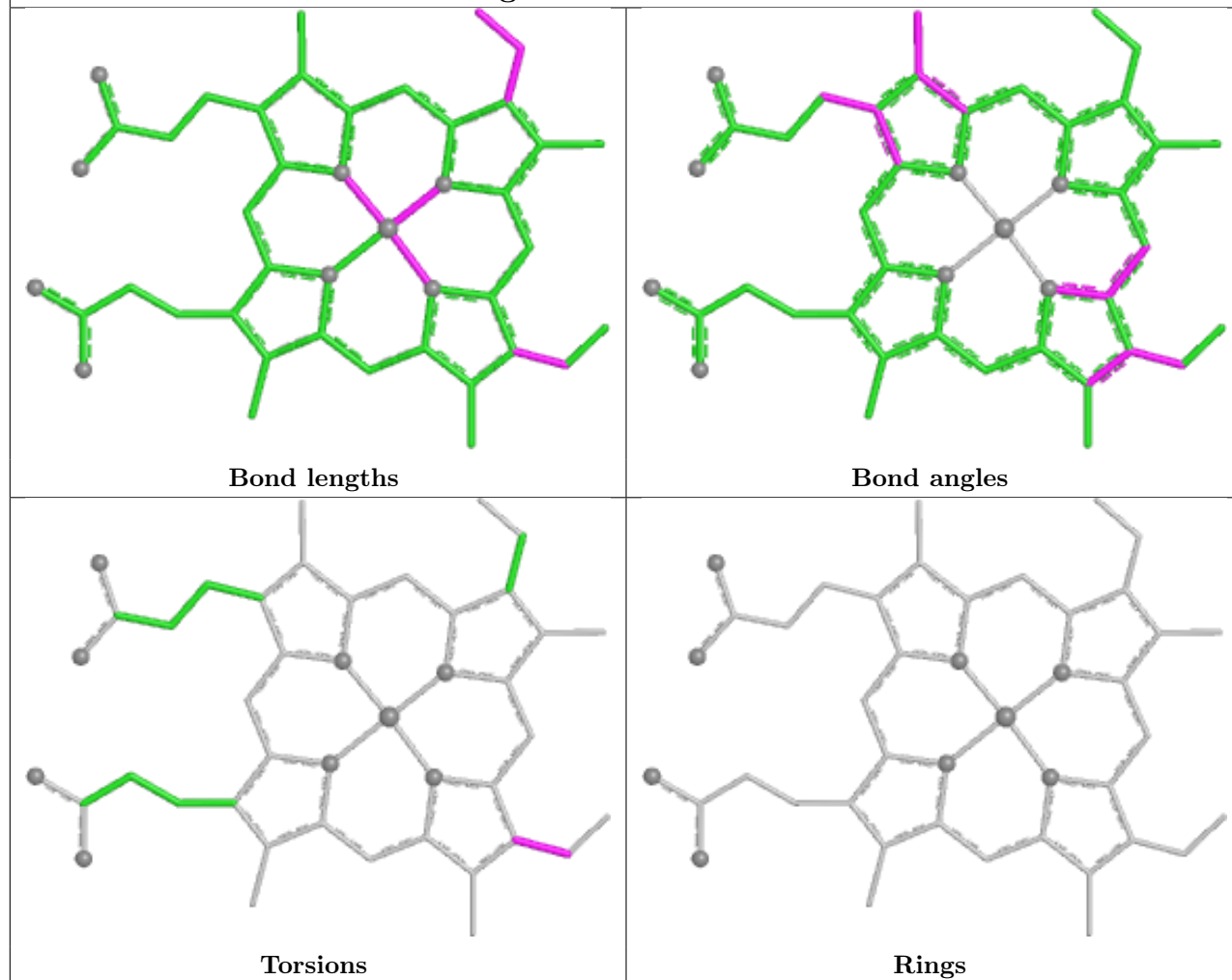
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2902	H4B	2	0
4	A	905	328	2	0
2	A	901	HEM	1	0
2	B	2901	HEM	1	0
3	A	902	H4B	1	0
4	B	2905	328	2	0

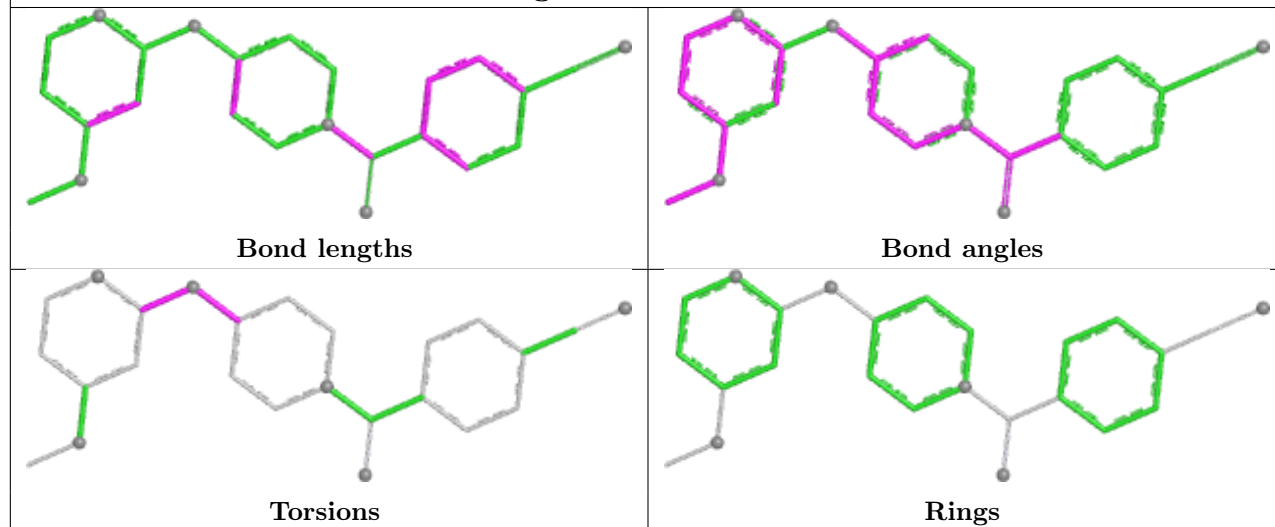
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand HEM B 2901



Ligand 328 B 2905



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	421/433 (97%)	0.37	23 (5%) 30 27	27, 45, 70, 95	0
1	B	421/433 (97%)	0.20	26 (6%) 26 23	25, 42, 67, 96	0
All	All	842/866 (97%)	0.29	49 (5%) 29 25	25, 44, 70, 96	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	99	THR	6.7
1	A	103	THR	5.0
1	A	104	CYS	4.7
1	B	103	THR	4.6
1	B	104	CYS	4.4
1	B	98	ALA	3.6
1	A	102	PHE	3.5
1	B	100	SER	3.5
1	B	497	ASN	3.4
1	A	108	SER	3.2
1	B	494	ILE	3.1
1	B	105	LYS	3.0
1	A	202	ASN	2.9
1	A	334	GLN	2.9
1	B	101	ASP	2.9
1	B	102	PHE	2.8
1	A	107	LYS	2.8
1	B	334	GLN	2.8
1	A	77	GLN	2.7
1	A	306	ASP	2.7
1	A	105	LYS	2.7
1	B	107	LYS	2.6
1	B	496	GLN	2.6
1	B	108	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	106	SER	2.5
1	A	153	ILE	2.4
1	B	171	GLY	2.4
1	B	294	GLY	2.4
1	A	265	GLN	2.4
1	B	279	GLU	2.4
1	A	307	GLY	2.3
1	B	288	GLY	2.3
1	A	288	GLY	2.3
1	B	106	SER	2.3
1	A	497	ASN	2.2
1	B	131	GLU	2.2
1	A	100	SER	2.2
1	B	112	SER	2.2
1	A	81	ILE	2.2
1	A	330	TYR	2.1
1	B	81	ILE	2.1
1	A	279	GLU	2.1
1	B	109	CYS	2.1
1	A	285	ILE	2.1
1	B	110	LEU	2.1
1	B	130	LEU	2.1
1	B	170	THR	2.0
1	A	157	LEU	2.0
1	A	146	GLY	2.0

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

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 ⓘ

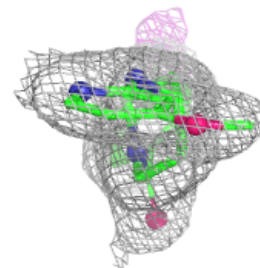
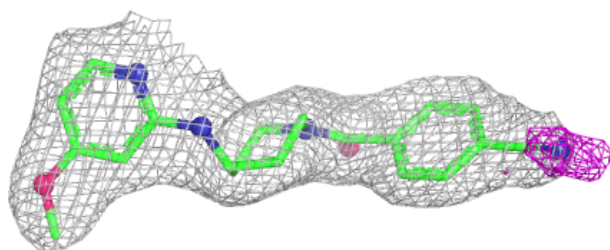
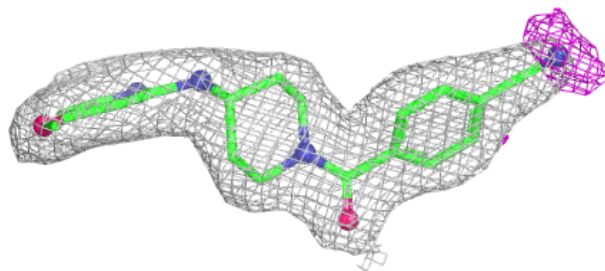
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	SO4	B	3003	5/5	0.73	0.13	104,104,105,106	0
5	SO4	B	3004	5/5	0.76	0.14	97,98,99,100	0
5	SO4	A	3001	5/5	0.78	0.10	106,106,106,106	0
5	SO4	A	3002	5/5	0.85	0.11	93,94,94,94	0
4	328	A	905	25/25	0.95	0.08	24,28,31,37	0
4	328	B	2905	25/25	0.95	0.08	21,26,28,32	0
3	H4B	A	902	17/17	0.97	0.05	23,30,35,35	0
2	HEM	A	901	43/43	0.98	0.06	25,28,30,33	0
3	H4B	B	2902	17/17	0.98	0.04	23,28,33,34	0
2	HEM	B	2901	43/43	0.99	0.05	19,25,29,30	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.

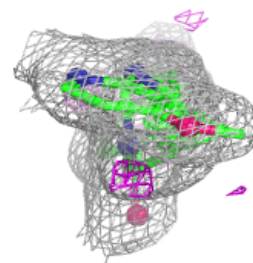
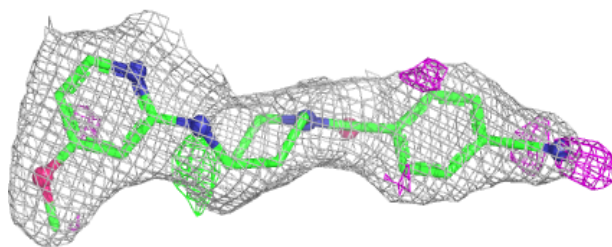
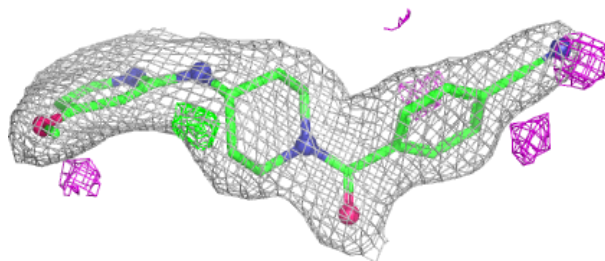
Electron density around 328 A 905:

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



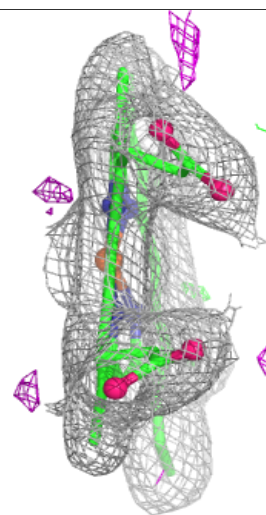
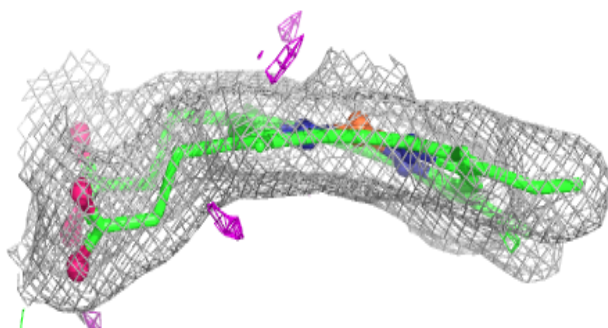
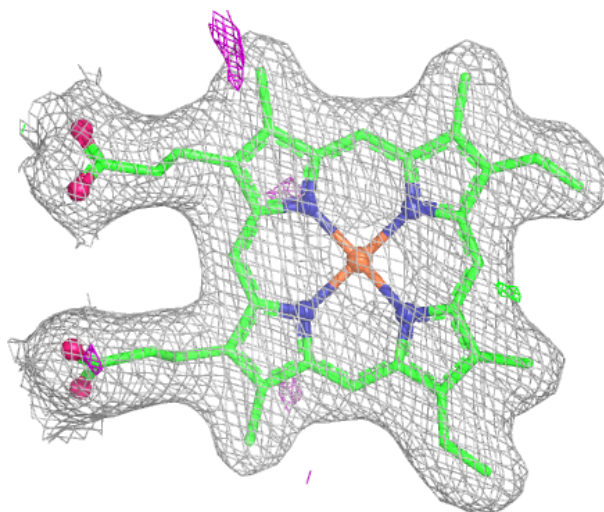
Electron density around 328 B 2905:

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



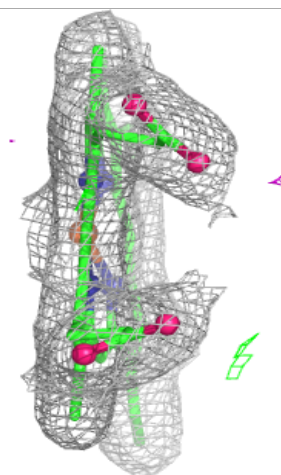
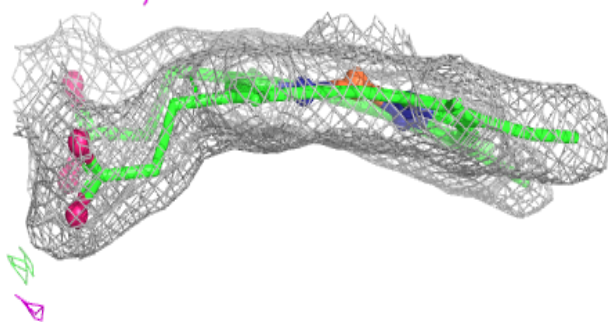
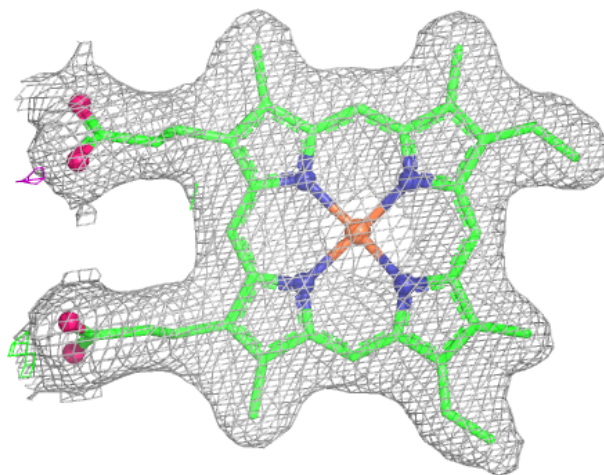
Electron density around HEM A 901:

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



Electron density around HEM B 2901:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.