



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:42 am BST

PDB ID : 3E6O  
Title : Structure of murine INOS oxygenase domain with inhibitor AR-C124355  
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 : 2008-08-15  
Resolution : 2.60 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](mailto: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.

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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

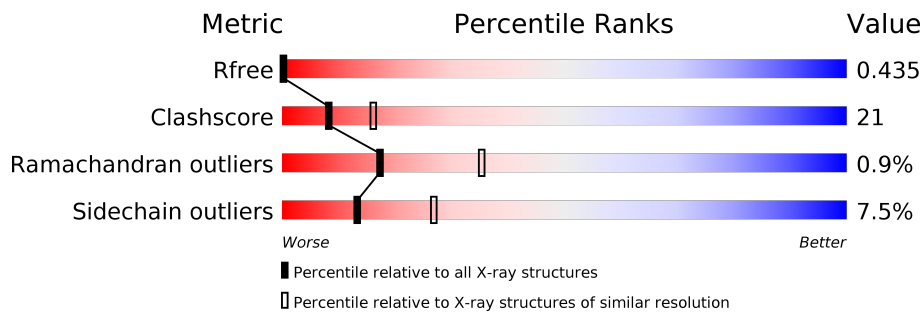
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	433	
1	B	433	

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	-	-	-

## 2 Entry composition i

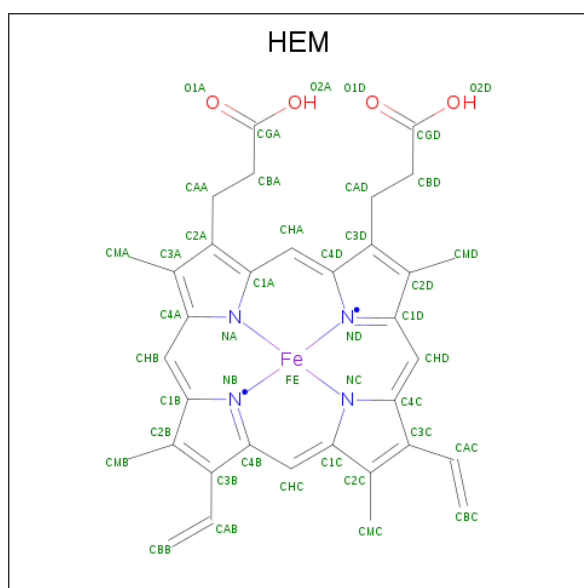
There are 5 unique types of molecules in this entry. The entry contains 7171 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	415	Total 3385	2171	582	612	20	0	0	0
1	B	410	Total 3347	2148	577	602	20	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



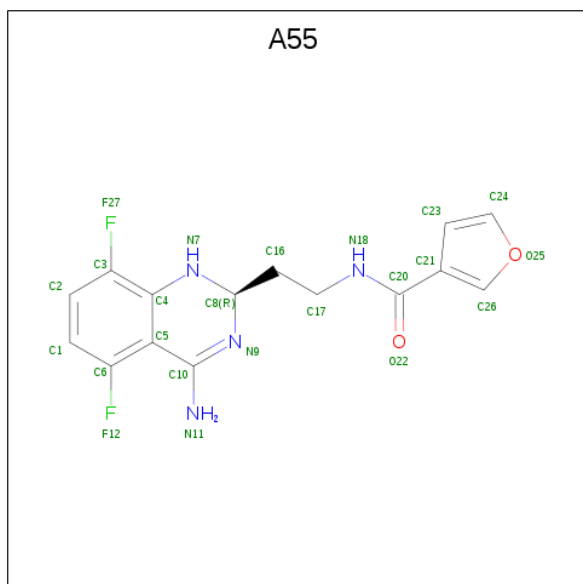
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	Total 43	34	1	4	4	0	0
2	B	1	Total 43	34	1	4	4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>).



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

- Molecule 4 is N-[2-(4-AMINO-5,8-DIFLUORO-1,2-DIHYDROQUINAZOLIN-2-YL)ETHYL]-3-FURAMIDE (three-letter code: A55) (formula: C<sub>15</sub>H<sub>14</sub>F<sub>2</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	A	1	23	15	2	4	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	B	1	23	15	2	4	2	0	0

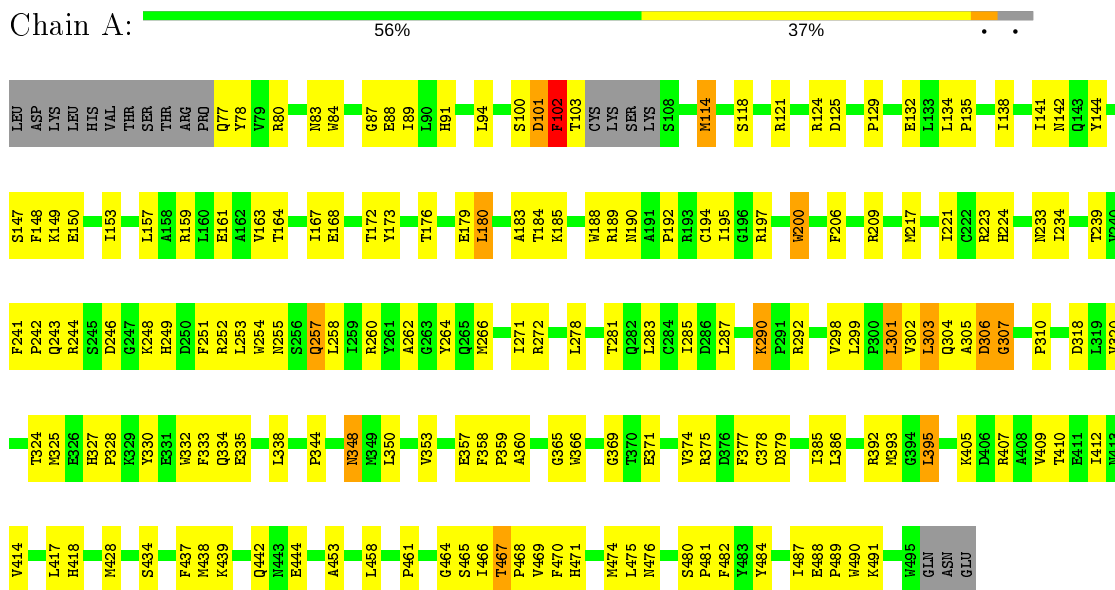
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total	O	0	0
			120	120		
5	B	153	Total	O	0	0
			153	153		

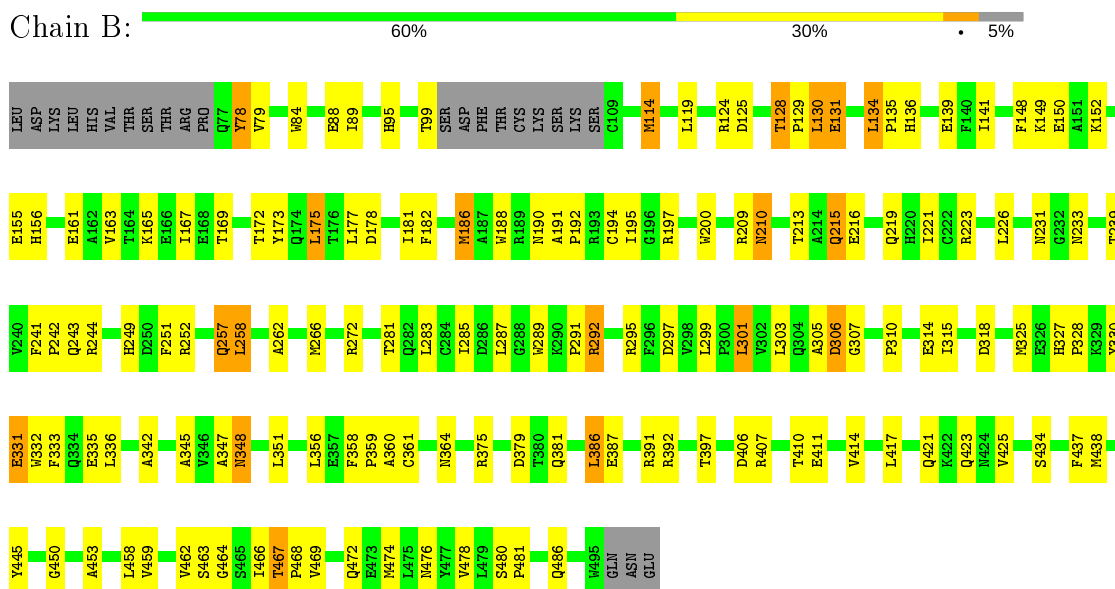
### 3 Residue-property plots [i](#)

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. 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. 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, $\alpha$ , $\beta$ , $\gamma$	213.90Å 213.90Å 116.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.60 19.95 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.96-2.60) 92.4 (19.95-2.51)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.50Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.229 , 0.262 0.416 , 0.435	Depositor DCC
$R_{free}$ test set	2686 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtrriage
Anisotropy	0.786	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.74	EDS
Total number of atoms	7171	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, A55, H4B

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.40	0/3484	0.63	1/4737 (0.0%)
1	B	0.37	0/3445	0.62	0/4684
All	All	0.38	0/6929	0.63	1/9421 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	GLY	N-CA-C	-5.94	98.25	113.10

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	3385	0	3278	158	4
1	B	3347	0	3248	125	4
2	A	43	0	30	3	0
2	B	43	0	30	1	0
3	A	17	0	14	0	1
3	B	17	0	14	0	0
4	A	23	0	14	0	0
4	B	23	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	120	0	0	12	1
5	B	153	0	0	10	1
All	All	7171	0	6642	285	8

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 21.

All (285) 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:195:ILE:HB	5:B:1937:HOH:O	1.33	1.26
1:A:195:ILE:HB	5:A:1043:HOH:O	1.43	1.18
1:A:153:ILE:HD12	1:A:153:ILE:H	1.31	0.94
1:A:428:MET:HB3	5:A:1050:HOH:O	1.74	0.87
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.15	0.81
1:A:141:ILE:HD11	1:A:163:VAL:HG21	1.65	0.79
1:B:292:ARG:HH11	1:B:292:ARG:HB2	1.48	0.79
1:A:195:ILE:HG12	1:A:458:LEU:HD22	1.64	0.79
1:B:129:PRO:HB2	1:B:131:GLU:OE2	1.85	0.75
1:A:102:PHE:C	1:A:103:THR:HG23	2.06	0.74
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.67	0.74
1:A:217:MET:CE	1:A:303:LEU:HB3	2.18	0.73
1:A:290:LYS:CE	1:A:290:LYS:H	2.03	0.72
1:B:215:GLN:HG2	5:B:1949:HOH:O	1.89	0.71
1:A:189:ARG:HD2	1:A:200:TRP:CE3	2.26	0.71
1:A:281:THR:O	1:A:285:ILE:HG12	1.90	0.71
1:A:407:ARG:HG3	1:A:407:ARG:HH11	1.56	0.70
1:B:197:ARG:NE	5:B:2015:HOH:O	2.23	0.70
1:A:304:GLN:O	1:A:304:GLN:HG3	1.91	0.70
1:B:215:GLN:O	1:B:219:GLN:HG3	1.92	0.70
1:B:467:THR:CG2	1:B:469:VAL:HG22	2.22	0.68
1:A:102:PHE:O	1:A:102:PHE:CG	2.45	0.68
1:B:301:LEU:HD13	1:B:315:ILE:HD11	1.75	0.68
1:A:290:LYS:CD	1:A:290:LYS:H	2.08	0.67
1:A:102:PHE:O	1:A:103:THR:HG23	1.95	0.67
1:B:195:ILE:CG2	1:B:437:PHE:HB2	2.25	0.67
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.30	0.67
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.30	0.66
1:A:195:ILE:HD11	1:A:458:LEU:O	1.95	0.66
1:A:141:ILE:CD1	1:A:163:VAL:HG21	2.24	0.66
1:A:333:PHE:HB3	5:A:1099:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ASN:N	1:B:210:ASN:HD22	1.94	0.66
1:B:197:ARG:CZ	5:B:2015:HOH:O	2.43	0.65
1:A:252:ARG:HD3	1:A:359:PRO:HB2	1.77	0.65
1:B:190:ASN:O	1:B:192:PRO:HD3	1.97	0.65
1:A:465:SER:O	1:A:471:HIS:HE1	1.80	0.64
1:B:464:GLY:O	1:B:467:THR:HB	1.96	0.64
1:B:149:LYS:HG2	1:B:150:GLU:HG3	1.78	0.64
1:B:141:ILE:HD11	1:B:163:VAL:HG21	1.79	0.64
1:B:210:ASN:H	1:B:210:ASN:HD22	1.43	0.64
1:A:144:TYR:O	1:A:147:SER:HB3	1.97	0.64
1:B:244:ARG:HA	5:B:1958:HOH:O	1.96	0.64
1:A:217:MET:HE1	1:A:303:LEU:HB3	1.80	0.64
1:A:195:ILE:HG22	1:A:195:ILE:O	1.98	0.63
1:A:217:MET:HE2	1:A:305:ALA:HB2	1.81	0.62
1:B:195:ILE:HD11	1:B:458:LEU:O	2.00	0.62
1:A:217:MET:HE3	1:A:303:LEU:HB3	1.81	0.62
1:A:410:THR:O	1:A:414:VAL:HG23	2.00	0.62
1:A:124:ARG:HD3	5:A:1020:HOH:O	1.99	0.61
1:B:467:THR:HG21	1:B:469:VAL:HG22	1.81	0.61
1:A:290:LYS:HE3	1:A:290:LYS:H	1.65	0.61
1:B:292:ARG:NH1	1:B:297:ASP:HB3	2.16	0.61
1:A:334:GLN:HA	5:A:1098:HOH:O	2.00	0.61
1:B:209:ARG:O	1:B:242:PRO:HG3	2.00	0.61
1:A:206:PHE:HB2	1:A:239:THR:HG22	1.83	0.61
1:A:224:HIS:ND1	1:A:239:THR:HG23	2.16	0.61
1:B:249:HIS:C	1:B:306:ASP:O	2.39	0.60
1:A:84:TRP:NE1	1:A:114:MET:HG3	2.15	0.60
1:B:387:GLU:HG3	1:B:397:THR:HG21	1.84	0.60
1:B:195:ILE:HG22	1:B:195:ILE:O	2.02	0.60
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.84	0.60
1:A:332:TRP:CE3	1:A:392:ARG:HD2	2.37	0.59
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.84	0.59
1:A:246:ASP:OD2	1:A:248:LYS:HB3	2.02	0.59
1:B:177:LEU:O	1:B:181:ILE:HD13	2.03	0.59
1:B:210:ASN:H	1:B:210:ASN:ND2	1.99	0.59
1:B:301:LEU:HG	1:B:303:LEU:HD11	1.83	0.59
1:B:445:TYR:CE2	1:B:450:GLY:HA2	2.37	0.59
1:A:134:LEU:O	1:A:138:ILE:HG12	2.02	0.59
1:B:141:ILE:CD1	1:B:163:VAL:HG21	2.32	0.59
1:A:252:ARG:HB2	1:A:304:GLN:HG2	1.83	0.59
1:A:149:LYS:HG2	1:A:150:GLU:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.03	0.58
1:B:438:MET:HG3	1:B:468:PRO:HB2	1.86	0.58
1:A:290:LYS:H	1:A:290:LYS:HD2	1.68	0.58
1:B:149:LYS:HG2	1:B:150:GLU:N	2.19	0.58
1:B:281:THR:O	1:B:285:ILE:HG12	2.04	0.58
1:A:249:HIS:C	1:A:306:ASP:O	2.42	0.57
1:A:149:LYS:HG2	1:A:150:GLU:N	2.19	0.57
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.34	0.57
1:A:407:ARG:HG3	1:A:407:ARG:NH1	2.20	0.56
1:A:223:ARG:HD3	5:A:1061:HOH:O	2.04	0.56
1:B:195:ILE:HG23	1:B:437:PHE:HB2	1.87	0.56
1:A:132:GLU:O	1:A:135:PRO:HD2	2.06	0.56
1:B:84:TRP:CD1	1:B:114:MET:HE2	2.41	0.56
1:B:156:HIS:ND1	5:B:1922:HOH:O	2.33	0.56
1:B:410:THR:O	1:B:414:VAL:HG13	2.06	0.56
1:B:195:ILE:HG22	1:B:437:PHE:HB2	1.87	0.56
1:B:130:LEU:HD21	1:B:167:ILE:HG22	1.87	0.55
1:B:221:ILE:HD12	1:B:303:LEU:HD21	1.88	0.55
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.88	0.55
1:B:292:ARG:HH11	1:B:292:ARG:CB	2.18	0.55
1:A:439:LYS:O	1:A:442:GLN:HG2	2.07	0.54
1:B:152:LYS:HD2	1:B:155:GLU:OE2	2.07	0.54
1:B:239:THR:O	1:B:361:CYS:HA	2.07	0.54
1:B:445:TYR:HA	1:B:450:GLY:H	1.73	0.54
1:A:209:ARG:O	1:A:242:PRO:HG3	2.07	0.54
1:A:283:LEU:O	1:A:287:LEU:HG	2.07	0.54
1:A:176:THR:OG1	1:A:179:GLU:HG3	2.08	0.54
1:A:405:LYS:O	1:A:409:VAL:HG23	2.08	0.54
1:A:129:PRO:HB2	1:A:132:GLU:HG3	1.90	0.53
1:B:175:LEU:HD13	1:B:356:LEU:CD1	2.37	0.53
1:A:189:ARG:HD2	1:A:200:TRP:CZ3	2.42	0.53
1:A:290:LYS:HD3	1:A:292:ARG:HH22	1.74	0.53
1:A:438:MET:HG3	1:A:468:PRO:HB2	1.90	0.53
1:A:332:TRP:O	1:A:335:GLU:HB2	2.08	0.53
1:B:195:ILE:HG12	1:B:458:LEU:HD22	1.91	0.53
1:B:191:ALA:O	1:B:197:ARG:NH1	2.42	0.53
1:A:195:ILE:CG2	1:A:437:PHE:HB2	2.38	0.52
1:B:330:TYR:HB3	1:B:332:TRP:CE2	2.44	0.52
1:B:131:GLU:CD	1:B:131:GLU:H	2.13	0.52
1:A:303:LEU:O	1:A:310:PRO:HA	2.09	0.52
1:B:331:GLU:HA	1:B:331:GLU:OE1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PHE:HD2	1:A:239:THR:HG22	1.74	0.52
1:A:257:GLN:OE1	1:A:260:ARG:NH1	2.36	0.52
1:B:387:GLU:O	1:B:391:ARG:HG3	2.09	0.52
1:A:264:TYR:HB2	1:A:266:MET:CE	2.40	0.52
1:B:194:CYS:O	1:B:197:ARG:HG3	2.10	0.52
1:B:332:TRP:O	1:B:335:GLU:HB2	2.09	0.52
1:A:262:ALA:HB2	1:A:299:LEU:CD2	2.40	0.52
1:A:480:SER:HA	1:A:481:PRO:C	2.29	0.52
1:A:172:THR:OG1	1:A:173:TYR:N	2.42	0.51
1:A:185:LYS:O	1:A:189:ARG:HG3	2.09	0.51
1:B:177:LEU:HD13	1:B:181:ILE:HD13	1.91	0.51
1:B:438:MET:CE	1:B:469:VAL:HG12	2.41	0.51
1:B:78:TYR:CD1	1:B:78:TYR:C	2.84	0.51
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.45	0.51
1:B:333:PHE:HA	1:B:336:LEU:CD2	2.40	0.51
1:A:159:ARG:O	1:A:163:VAL:HG23	2.10	0.51
1:A:434:SER:HB3	1:A:468:PRO:HD2	1.91	0.51
1:A:453:ALA:HB3	1:A:474:MET:HB3	1.91	0.51
1:A:301:LEU:HB3	1:A:303:LEU:HD13	1.91	0.51
1:A:290:LYS:N	1:A:290:LYS:HE3	2.25	0.51
1:A:438:MET:HE2	1:A:469:VAL:HG12	1.94	0.50
1:A:164:THR:O	1:A:168:GLU:HG2	2.12	0.50
1:A:464:GLY:O	1:A:467:THR:HB	2.12	0.50
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.40	0.50
1:A:190:ASN:O	1:A:192:PRO:HD3	2.12	0.50
1:B:124:ARG:HH21	1:B:128:THR:HB	1.76	0.50
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.26	0.50
1:A:153:ILE:HD12	1:A:153:ILE:N	2.14	0.50
1:B:165:LYS:O	1:B:169:THR:HG23	2.12	0.50
1:B:434:SER:HB3	1:B:468:PRO:HD2	1.94	0.50
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.76	0.50
1:B:251:PHE:O	1:B:360:ALA:HB2	2.11	0.50
1:A:327:HIS:ND1	1:A:328:PRO:HD2	2.27	0.50
1:A:195:ILE:HG23	1:A:437:PHE:HB2	1.94	0.50
1:B:188:TRP:CZ3	1:B:200:TRP:HA	2.47	0.50
1:A:233:ASN:ND2	5:A:1066:HOH:O	2.44	0.49
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.94	0.49
1:A:438:MET:CE	1:A:469:VAL:HG12	2.42	0.49
1:A:298:VAL:HG21	1:A:320:VAL:HG11	1.93	0.49
1:B:379:ASP:HB3	1:B:381:GLN:OE1	2.12	0.49
1:B:411:GLU:O	1:B:414:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.28	0.49
1:A:467:THR:HG21	1:A:469:VAL:HG22	1.95	0.49
1:B:195:ILE:HG23	1:B:437:PHE:CB	2.43	0.49
1:A:129:PRO:HG3	5:A:1021:HOH:O	2.13	0.48
1:A:88:GLU:HG2	1:A:89:ILE:N	2.28	0.48
1:B:445:TYR:CZ	1:B:450:GLY:HA2	2.48	0.48
1:A:290:LYS:HG2	1:A:292:ARG:HH12	1.77	0.48
1:B:131:GLU:CD	1:B:131:GLU:N	2.67	0.48
1:B:330:TYR:HB3	1:B:332:TRP:NE1	2.29	0.48
1:A:467:THR:CG2	1:A:469:VAL:HG22	2.44	0.48
1:A:244:ARG:HD2	1:A:357:GLU:OE2	2.13	0.48
1:A:78:TYR:CD1	1:A:78:TYR:C	2.87	0.48
1:B:295:ARG:HD2	5:B:2027:HOH:O	2.14	0.48
1:B:252:ARG:HD3	1:B:359:PRO:HB2	1.96	0.47
1:B:285:ILE:CD1	1:B:291:PRO:HB3	2.44	0.47
1:A:132:GLU:C	1:A:135:PRO:HD2	2.35	0.47
1:A:330:TYR:HD2	1:A:332:TRP:HE1	1.62	0.47
1:B:303:LEU:O	1:B:310:PRO:HA	2.15	0.47
1:A:180:LEU:O	1:A:184:THR:HG23	2.14	0.47
1:A:252:ARG:CD	1:A:359:PRO:HB2	2.44	0.47
1:A:301:LEU:HB3	1:A:303:LEU:CD1	2.45	0.47
1:A:348:ASN:ND2	1:A:348:ASN:H	2.13	0.47
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.44	0.47
1:A:487:ILE:N	1:A:487:ILE:HD12	2.30	0.47
1:A:102:PHE:C	1:A:103:THR:O	2.53	0.47
1:A:360:ALA:HA	5:A:1075:HOH:O	2.14	0.47
1:B:438:MET:HE2	1:B:469:VAL:HG12	1.97	0.47
2:A:901:HEM:HMC1	2:A:901:HEM:HBC2	1.97	0.47
1:A:103:THR:O	1:A:103:THR:OG1	2.31	0.46
1:A:80:ARG:NH1	5:A:1136:HOH:O	2.48	0.46
1:A:78:TYR:CE1	1:A:91:HIS:ND1	2.82	0.46
1:A:189:ARG:HH21	1:A:444:GLU:CD	2.19	0.46
1:A:243:GLN:HB3	1:A:358:PHE:CE2	2.50	0.46
1:A:393:MET:HB2	1:A:395:LEU:HD22	1.96	0.46
1:B:292:ARG:HD3	1:B:292:ARG:N	2.30	0.46
1:A:305:ALA:O	1:A:307:GLY:N	2.49	0.46
1:B:194:CYS:O	1:B:197:ARG:NH1	2.49	0.46
1:A:290:LYS:CD	1:A:290:LYS:N	2.77	0.46
1:A:253:LEU:HD12	1:A:253:LEU:N	2.30	0.46
1:A:290:LYS:N	1:A:290:LYS:HD2	2.30	0.46
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ILE:HD13	1:A:278:LEU:HD11	1.99	0.45
1:A:375:ARG:O	1:A:379:ASP:HB2	2.16	0.45
1:B:213:THR:N	1:B:216:GLU:OE1	2.50	0.45
1:A:100:SER:C	1:A:101:ASP:O	2.53	0.45
1:A:328:PRO:HB3	1:A:418:HIS:CD2	2.51	0.45
1:A:102:PHE:O	1:A:102:PHE:CD1	2.70	0.45
1:B:375:ARG:O	1:B:379:ASP:HB2	2.16	0.45
1:A:385:ILE:HD11	1:A:412:ILE:HD13	1.98	0.45
1:A:488:GLU:HB3	1:A:490:TRP:CE2	2.52	0.44
1:A:194:CYS:HB2	2:A:901:HEM:ND	2.32	0.44
1:B:190:ASN:O	1:B:192:PRO:CD	2.65	0.44
1:A:290:LYS:HG2	1:A:292:ARG:NH1	2.32	0.44
1:A:77:GLN:O	1:A:78:TYR:HB3	2.18	0.44
1:B:258:LEU:HD13	1:B:347:ALA:HB2	1.99	0.44
1:A:371:GLU:O	1:A:375:ARG:HB2	2.17	0.44
1:B:480:SER:HA	1:B:481:PRO:C	2.38	0.44
1:A:195:ILE:HG12	1:A:458:LEU:CD2	2.42	0.44
1:A:102:PHE:O	1:A:103:THR:CG2	2.65	0.44
1:A:290:LYS:CD	1:A:292:ARG:HH22	2.29	0.44
1:B:141:ILE:HD11	1:B:163:VAL:HG11	2.00	0.44
1:B:88:GLU:C	1:B:89:ILE:HD12	2.38	0.44
1:A:83:ASN:O	1:A:87:GLY:N	2.50	0.44
1:B:453:ALA:O	1:B:476:ASN:HB2	2.17	0.44
1:A:206:PHE:CD2	1:A:239:THR:HG22	2.53	0.43
1:A:167:ILE:HA	1:A:172:THR:O	2.18	0.43
1:A:377:PHE:O	1:A:385:ILE:HG12	2.17	0.43
1:B:188:TRP:HB2	2:B:1901:HEM:CBC	2.48	0.43
1:B:351:LEU:HB3	1:B:358:PHE:HB2	1.99	0.43
1:B:466:ILE:O	1:B:466:ILE:HG22	2.18	0.43
1:A:290:LYS:CG	1:A:292:ARG:HH12	2.30	0.43
1:B:342:ALA:HB1	1:B:425:VAL:HG11	2.00	0.43
1:B:292:ARG:HH12	1:B:297:ASP:HB3	1.82	0.43
1:A:194:CYS:SG	1:A:197:ARG:HG3	2.58	0.43
1:B:177:LEU:HD13	1:B:177:LEU:C	2.39	0.43
1:B:195:ILE:CG1	1:B:458:LEU:HD22	2.49	0.43
1:B:348:ASN:H	1:B:348:ASN:HD22	1.67	0.43
1:A:188:TRP:CD2	1:A:200:TRP:HA	2.53	0.43
1:A:221:ILE:HD12	1:A:303:LEU:HD21	2.01	0.43
1:A:266:MET:SD	1:A:272:ARG:HD3	2.58	0.43
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.79	0.43
1:A:350:LEU:HD23	1:A:350:LEU:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:NH2	1:A:89:ILE:HD13	2.34	0.43
1:B:262:ALA:HB2	1:B:299:LEU:CD2	2.49	0.43
1:A:234:ILE:HG21	1:A:366:TRP:HB3	2.01	0.42
1:B:134:LEU:HB3	1:B:135:PRO:HD3	2.00	0.42
1:B:136:HIS:O	1:B:139:GLU:HB3	2.19	0.42
1:A:242:PRO:HG2	1:A:251:PHE:CZ	2.54	0.42
1:A:134:LEU:HB3	1:A:135:PRO:HD3	2.02	0.42
2:A:901:HEM:CMC	2:A:901:HEM:HBC2	2.49	0.42
1:A:466:ILE:HG22	1:A:466:ILE:O	2.20	0.42
1:A:482:PHE:HB3	1:A:484:TYR:CE1	2.54	0.42
1:A:80:ARG:HH22	1:A:89:ILE:HD13	1.84	0.42
1:A:124:ARG:CD	5:A:1020:HOH:O	2.63	0.42
1:B:223:ARG:HD3	5:B:1950:HOH:O	2.19	0.42
1:B:289:TRP:NE1	1:B:314:GLU:OE1	2.51	0.42
1:A:374:VAL:O	1:A:378:CYS:HB2	2.20	0.42
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.55	0.42
1:A:195:ILE:HG21	1:A:195:ILE:HD13	1.81	0.42
1:A:327:HIS:CG	1:A:328:PRO:HD2	2.55	0.42
1:A:153:ILE:H	1:A:153:ILE:CD1	2.06	0.41
1:A:453:ALA:O	1:A:476:ASN:HB2	2.20	0.41
1:B:182:PHE:CZ	1:B:186:MET:HE2	2.53	0.41
1:B:188:TRP:CD2	1:B:200:TRP:HA	2.55	0.41
1:B:257:GLN:CB	1:B:345:ALA:O	2.68	0.41
1:B:175:LEU:HD13	1:B:356:LEU:HD11	2.02	0.41
1:B:79:VAL:HG23	1:B:95:HIS:NE2	2.34	0.41
1:A:121:ARG:HD3	1:A:121:ARG:HA	1.87	0.41
1:B:472:GLN:O	1:B:474:MET:HG2	2.20	0.41
1:B:175:LEU:HD13	1:B:356:LEU:HD12	2.03	0.41
1:B:345:ALA:HB2	1:B:364:ASN:HB3	2.03	0.41
1:B:486:GLN:HB2	5:B:1917:HOH:O	2.20	0.41
1:A:303:LEU:N	1:A:303:LEU:CD1	2.83	0.41
1:A:444:GLU:OE1	1:A:444:GLU:HA	2.20	0.41
1:B:283:LEU:O	1:B:287:LEU:HG	2.20	0.41
1:B:305:ALA:O	1:B:307:GLY:N	2.53	0.41
1:A:183:ALA:HB2	1:A:353:VAL:HG21	2.03	0.41
1:A:262:ALA:HB2	1:A:299:LEU:HG	2.03	0.41
1:A:407:ARG:HD2	5:A:1117:HOH:O	2.21	0.41
1:B:163:VAL:O	1:B:167:ILE:HG13	2.21	0.41
1:B:333:PHE:O	1:B:336:LEU:HD23	2.21	0.41
1:A:489:PRO:C	1:A:491:LYS:H	2.25	0.41
1:B:386:LEU:HB2	5:B:1990:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:TRP:CE3	1:B:392:ARG:HD2	2.56	0.40
1:B:266:MET:CE	1:B:272:ARG:HE	2.34	0.40
1:B:257:GLN:HB3	1:B:257:GLN:HE21	1.68	0.40
1:A:254:TRP:HB2	1:A:302:VAL:HB	2.04	0.40
1:A:438:MET:HE3	1:A:469:VAL:HA	2.03	0.40
1:A:488:GLU:O	1:A:491:LYS:HB2	2.22	0.40
1:B:161:GLU:CG	1:B:165:LYS:HE2	2.51	0.40
1:B:172:THR:OG1	1:B:173:TYR:N	2.54	0.40

All (8) 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)
1:B:406:ASP:OD2	1:B:463:SER:OG[9_766]	1.72	0.48
1:A:103:THR:CG2	1:A:118:SER:OG[11_655]	1.87	0.33
1:B:231:ASN:N	1:B:318:ASP:OD2[11_656]	1.99	0.21
1:B:318:ASP:N	5:B:1954:HOH:O[11_656]	1.99	0.21
1:A:470:PHE:O	3:A:902:H4B:O9[11_655]	2.00	0.20
1:A:461:PRO:O	1:A:464:GLY:N[11_655]	2.12	0.08
1:B:99:THR:OG1	1:B:478:VAL:O[9_766]	2.12	0.08
1:A:318:ASP:OD2	5:A:1065:HOH:O[9_765]	2.19	0.01

## 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	411/433 (95%)	370 (90%)	35 (8%)	6 (2%)	10 21
1	B	406/433 (94%)	367 (90%)	38 (9%)	1 (0%)	47 71
All	All	817/866 (94%)	737 (90%)	73 (9%)	7 (1%)	17 35

All (7) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	102	PHE
1	A	200	TRP
1	A	306	ASP
1	B	306	ASP
1	A	307	GLY
1	A	369	GLY
1	A	344	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	363/381 (95%)	339 (93%)	24 (7%)	16	33
1	B	358/381 (94%)	328 (92%)	30 (8%)	11	21
All	All	721/762 (95%)	667 (92%)	54 (8%)	13	27

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	101	ASP
1	A	102	PHE
1	A	114	MET
1	A	125	ASP
1	A	148	PHE
1	A	157	LEU
1	A	161	GLU
1	A	180	LEU
1	A	255	ASN
1	A	257	GLN
1	A	258	LEU
1	A	290	LYS
1	A	301	LEU
1	A	303	LEU
1	A	324	THR
1	A	325	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	338	LEU
1	A	348	ASN
1	A	386	LEU
1	A	395	LEU
1	A	417	LEU
1	A	467	THR
1	A	475	LEU
1	B	78	TYR
1	B	114	MET
1	B	119	LEU
1	B	125	ASP
1	B	128	THR
1	B	130	LEU
1	B	131	GLU
1	B	134	LEU
1	B	148	PHE
1	B	175	LEU
1	B	178	ASP
1	B	186	MET
1	B	210	ASN
1	B	215	GLN
1	B	226	LEU
1	B	233	ASN
1	B	257	GLN
1	B	258	LEU
1	B	292	ARG
1	B	301	LEU
1	B	325	MET
1	B	331	GLU
1	B	348	ASN
1	B	386	LEU
1	B	407	ARG
1	B	417	LEU
1	B	421	GLN
1	B	423	GLN
1	B	462	VAL
1	B	467	THR

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	77	GLN

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Mol	Chain	Res	Type
1	A	96	HIS
1	A	142	ASN
1	A	202	ASN
1	A	204	GLN
1	A	215	GLN
1	A	219	GLN
1	A	231	ASN
1	A	233	ASN
1	A	249	HIS
1	A	348	ASN
1	A	471	HIS
1	B	96	HIS
1	B	210	ASN
1	B	231	ASN
1	B	233	ASN
1	B	348	ASN
1	B	423	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

6 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
2	HEM	A	901	-	27,50,50	1.40	4 (14%)	17,82,82	1.52	4 (23%)
3	H4B	A	902	-	16,18,18	1.83	3 (18%)	11,26,26	1.90	5 (45%)
2	HEM	B	1901	-	27,50,50	1.80	7 (25%)	17,82,82	1.23	2 (11%)
3	H4B	B	1902	-	16,18,18	2.04	3 (18%)	11,26,26	1.97	5 (45%)
4	A55	A	903	-	18,25,25	1.73	5 (27%)	20,35,35	1.84	3 (15%)
4	A55	B	904	-	18,25,25	1.72	2 (11%)	20,35,35	1.74	4 (20%)

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
2	HEM	A	901	-	-	0/6/54/54	-
3	H4B	A	902	-	1/1/3/5	4/8/17/17	0/2/2/2
2	HEM	B	1901	-	-	0/6/54/54	-
3	H4B	B	1902	-	-	0/8/17/17	0/2/2/2
4	A55	A	903	-	-	2/9/22/22	0/2/3/3
4	A55	B	904	-	-	1/9/22/22	0/2/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1902	H4B	C7-C6	-6.78	1.45	1.52
3	A	902	H4B	C7-C6	-5.74	1.46	1.52
4	B	904	A55	C23-C21	4.98	1.49	1.42
4	A	903	A55	C23-C21	4.42	1.48	1.42
2	B	1901	HEM	C3B-C2B	-4.27	1.34	1.40
2	B	1901	HEM	C3B-CAB	-4.11	1.39	1.47
2	B	1901	HEM	C3C-CAC	-3.81	1.40	1.47
3	B	1902	H4B	C7-N8	-3.68	1.38	1.44
2	A	901	HEM	C3C-CAC	-3.52	1.40	1.47
3	A	902	H4B	C7-N8	-3.38	1.39	1.44
2	A	901	HEM	C3B-CAB	-2.62	1.42	1.47
4	A	903	A55	C1-C2	2.49	1.43	1.38
2	B	1901	HEM	C4D-C3D	2.44	1.48	1.42
3	A	902	H4B	C4A-N5	-2.38	1.33	1.38
4	A	903	A55	C1-C6	2.35	1.42	1.37
4	A	903	A55	O22-C20	2.29	1.28	1.23
3	B	1902	H4B	C4A-N5	-2.26	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	C3B-C2B	-2.18	1.37	1.40
2	B	1901	HEM	C1C-C2C	2.18	1.47	1.42
2	B	1901	HEM	C4A-NA	2.08	1.40	1.36
4	A	903	A55	C2-C3	2.05	1.42	1.37
2	A	901	HEM	C1D-ND	2.03	1.40	1.36
4	B	904	A55	O22-C20	2.03	1.27	1.23
2	B	1901	HEM	C1A-NA	2.03	1.40	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	A55	C5-C4-C3	5.09	121.82	117.55
4	B	904	A55	C5-C4-C3	4.80	121.57	117.55
3	B	1902	H4B	C4-C4A-N5	3.17	121.78	119.12
2	A	901	HEM	CBA-CAA-C2A	-3.10	106.77	112.49
3	A	902	H4B	C4-C4A-N5	2.98	121.63	119.12
3	A	902	H4B	C4-C4A-C8A	2.97	117.20	114.57
3	B	1902	H4B	C4-C4A-C8A	2.87	117.12	114.57
4	A	903	A55	C2-C3-C4	-2.82	119.70	122.88
3	B	1902	H4B	C4-N3-C2	2.72	120.25	115.93
3	A	902	H4B	C4-N3-C2	2.62	120.09	115.93
2	A	901	HEM	C1D-C2D-C3D	-2.53	105.24	107.00
3	B	1902	H4B	C2-N1-C8A	2.49	120.12	114.54
4	B	904	A55	C2-C3-C4	-2.46	120.10	122.88
4	B	904	A55	C16-C8-N7	-2.42	105.80	111.33
2	B	1901	HEM	C1D-C2D-C3D	-2.37	105.35	107.00
3	A	902	H4B	N3-C2-N1	-2.26	121.87	125.42
2	A	901	HEM	CMC-C2C-C3C	2.26	128.90	124.68
4	B	904	A55	N11-C10-N9	2.24	121.87	118.70
3	B	1902	H4B	N3-C2-N1	-2.21	121.96	125.42
3	A	902	H4B	C2-N1-C8A	2.20	119.47	114.54
4	A	903	A55	C1-C6-C5	-2.19	119.66	123.58
2	A	901	HEM	CMD-C2D-C1D	2.08	131.65	128.46
2	B	1901	HEM	CMA-C3A-C4A	-2.03	125.34	128.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	902	H4B	C6

All (7) torsion outliers are listed below:

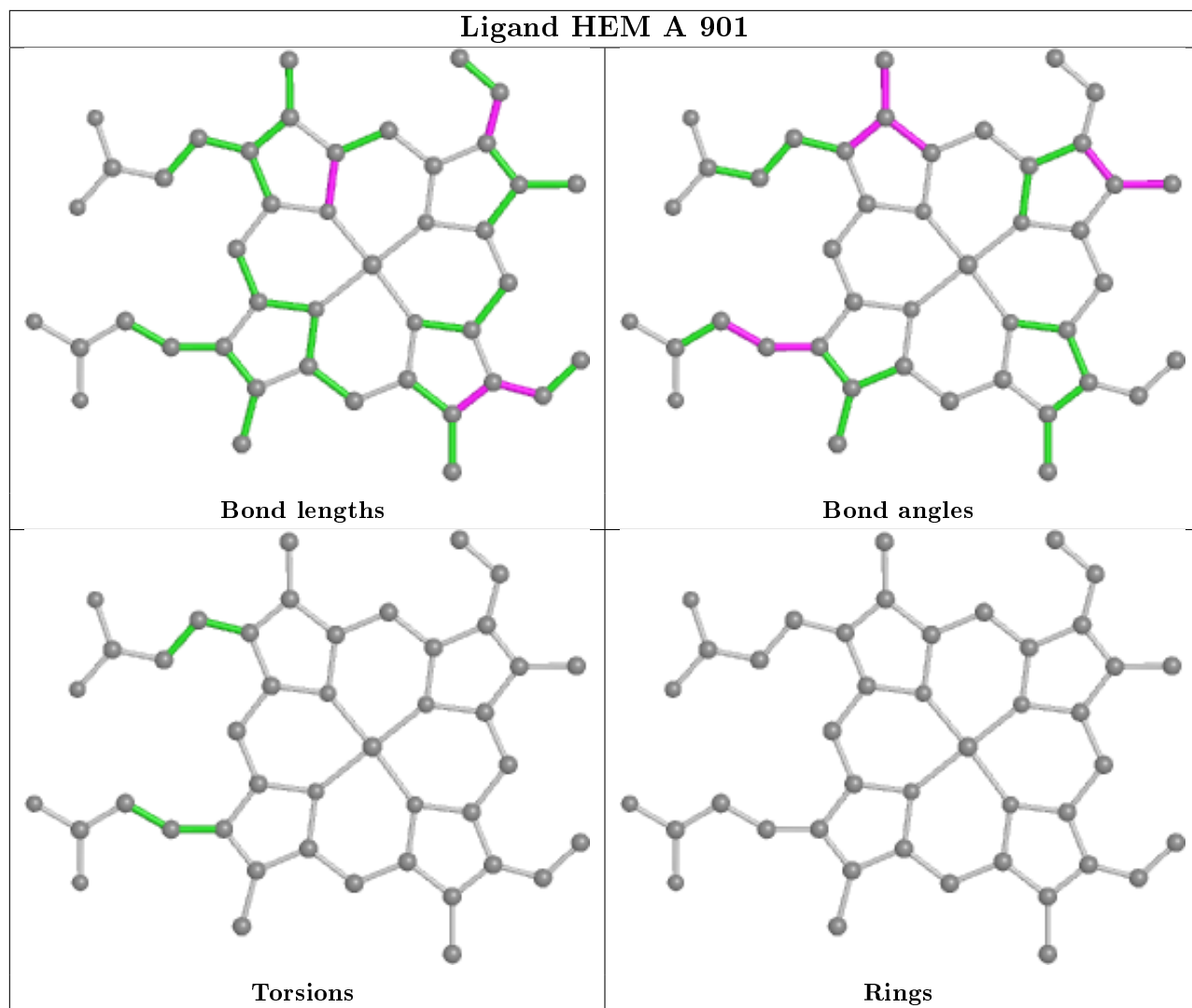
Mol	Chain	Res	Type	Atoms
3	A	902	H4B	N5-C6-C9-O9
3	A	902	H4B	C7-C6-C9-O9
3	A	902	H4B	C7-C6-C9-C10
4	A	903	A55	N18-C20-C21-C26
4	B	904	A55	C17-C16-C8-N7
3	A	902	H4B	N5-C6-C9-C10
4	A	903	A55	O22-C20-C21-C26

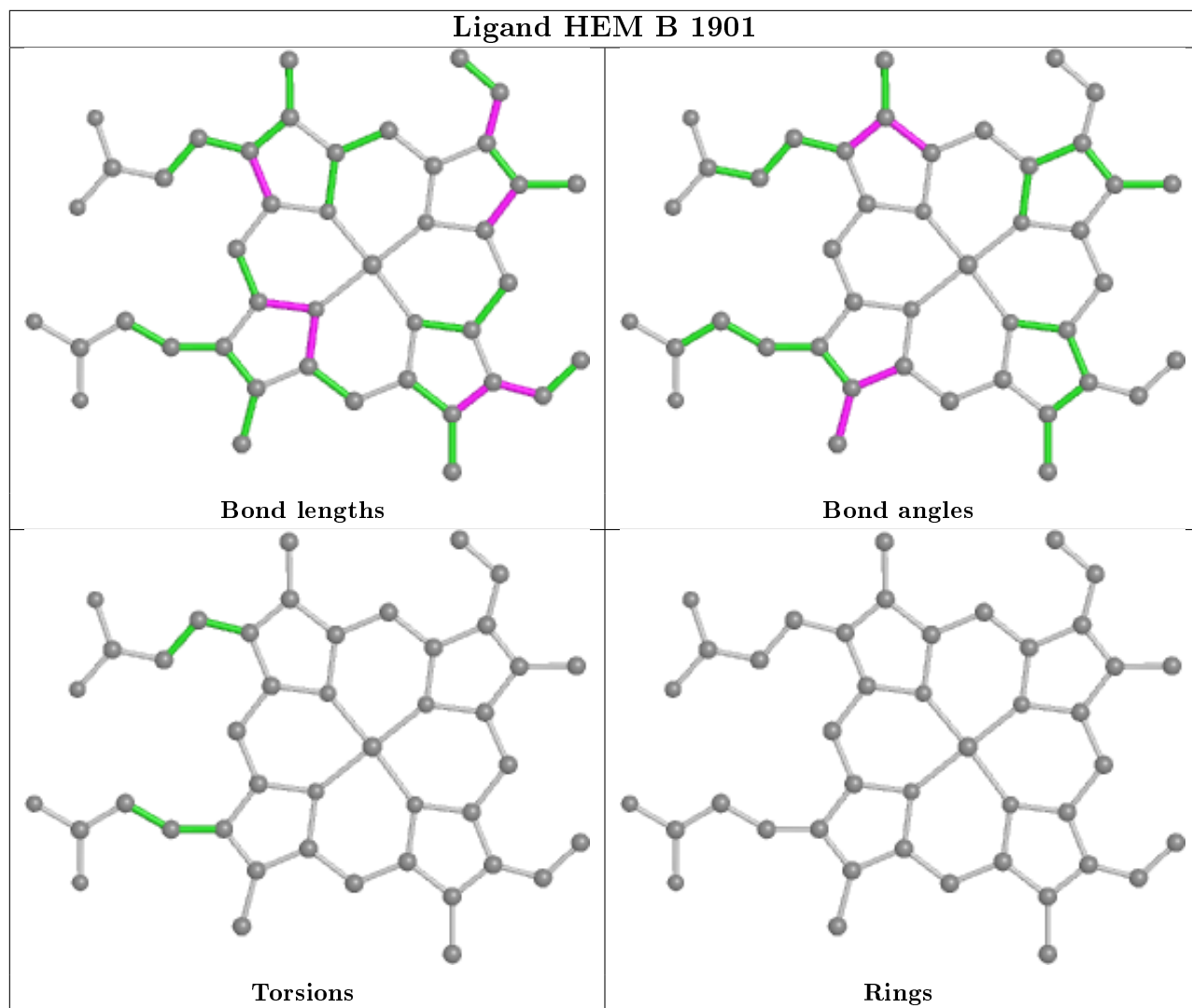
There are no ring outliers.

3 monomers are involved in 5 short contacts:

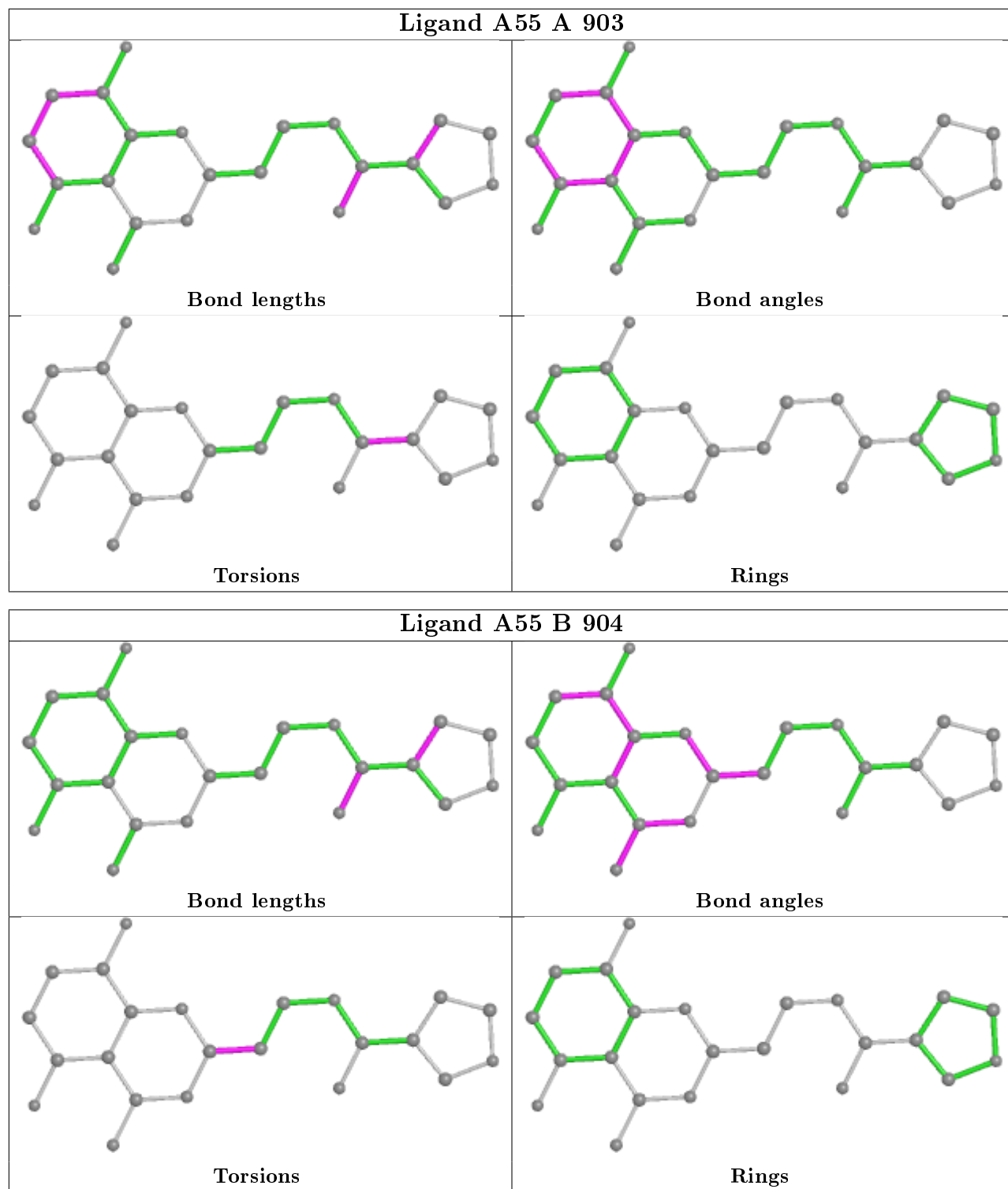
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	HEM	3	0
3	A	902	H4B	0	1
2	B	1901	HEM	1	0

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.









## 5.7 Other polymers [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

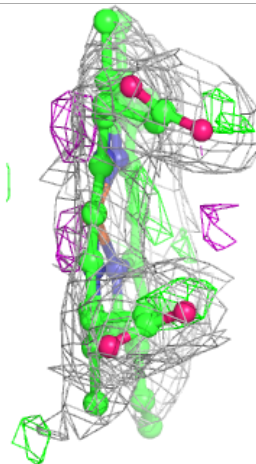
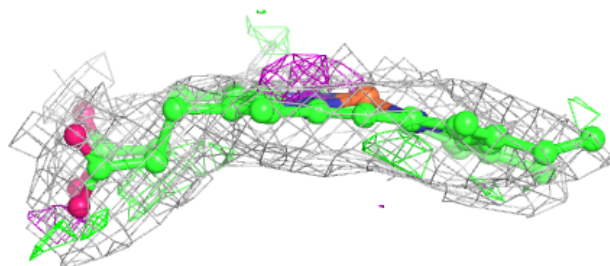
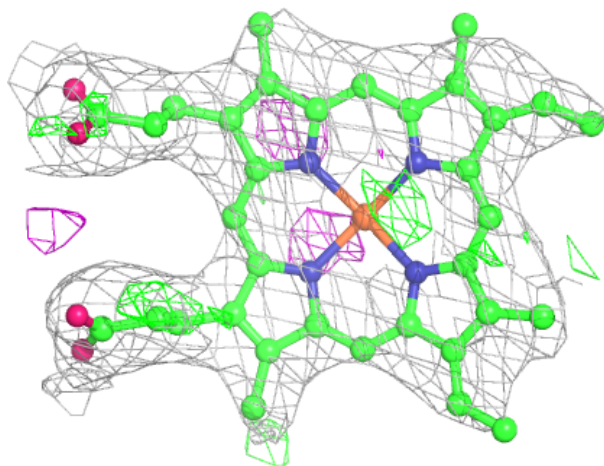
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

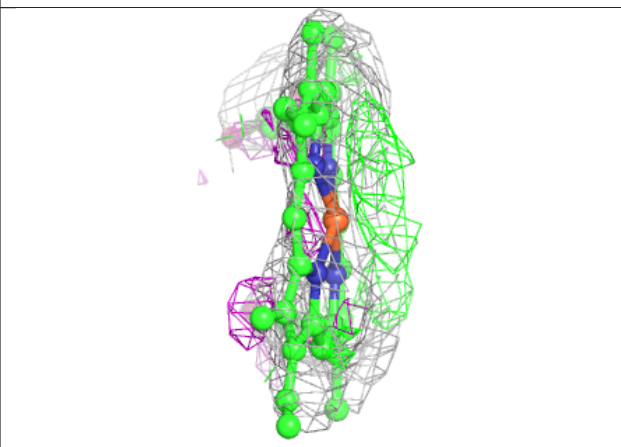
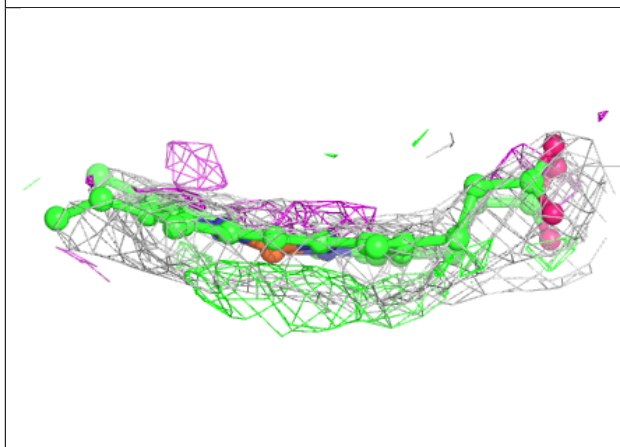
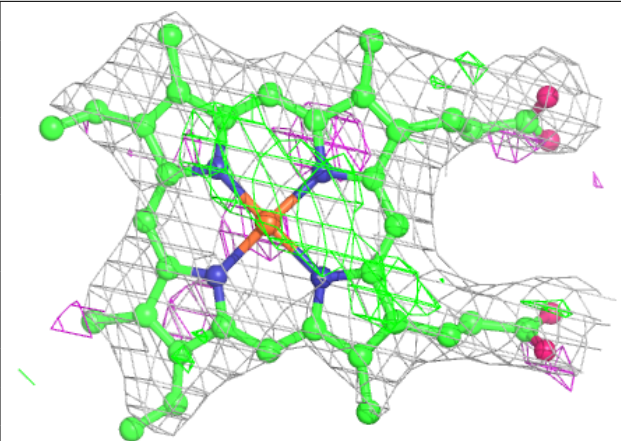
**Electron density around HEM A 901:**

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

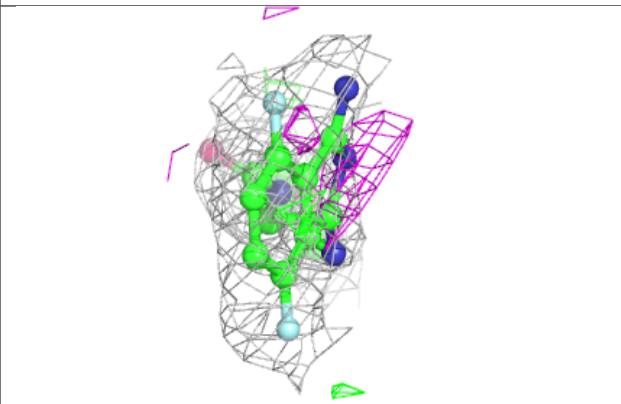
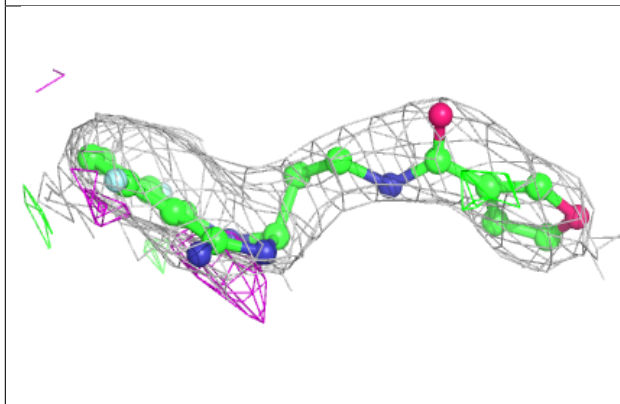
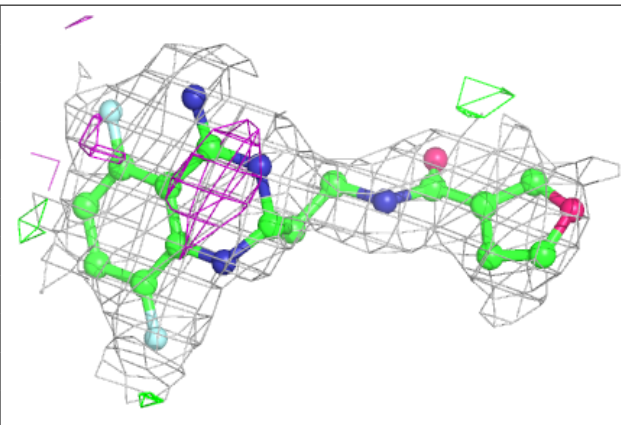


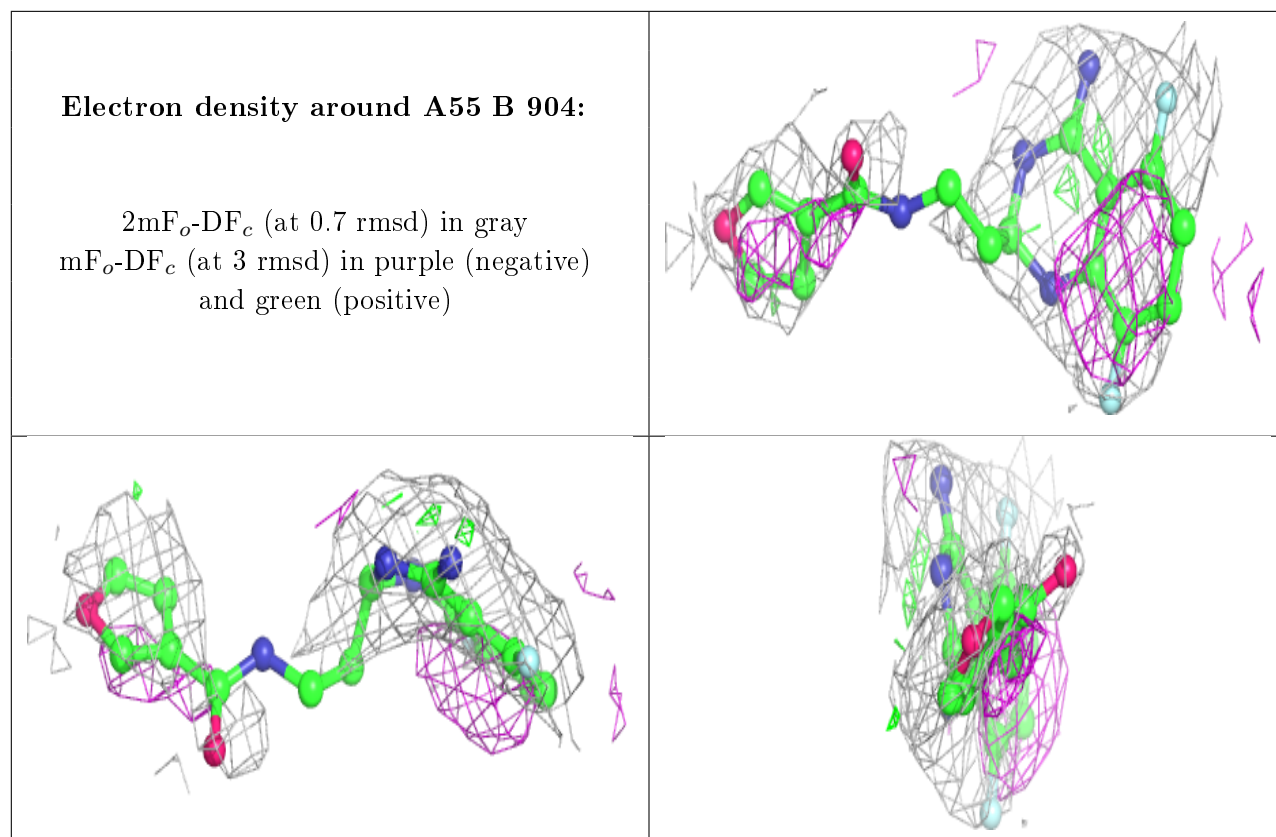
**Electron density around HEM B 1901:**

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

**Electron density around A55 A 903:**

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





## 6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.