Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 09:22 PM EST

PDB ID	:	3E68
Title	:	Structure of murine INOS oxygenase domain with inhibitor AR-C130232
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	:	2008-08-14
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 (i) 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 (i)) were used in the production of this report:

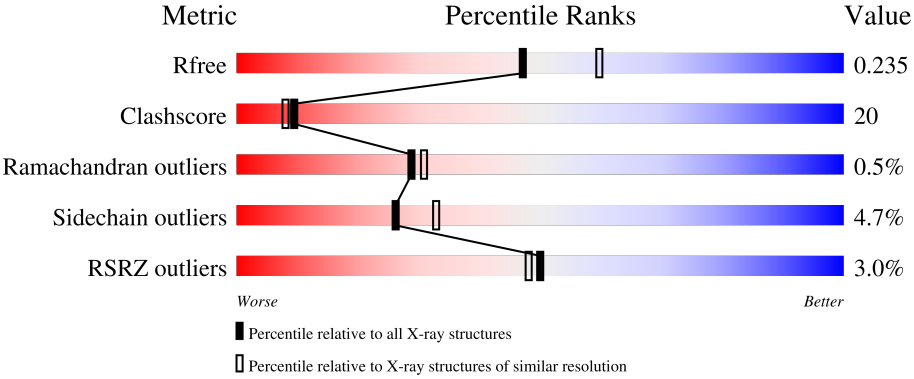
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	3% 63% 30% • •
1	B	433	2% 65% 26% • 5%

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
2	BOG	A	3100	-	-	-	X
6	H4B	A	902	X	-	-	-

2 Entry composition (i)

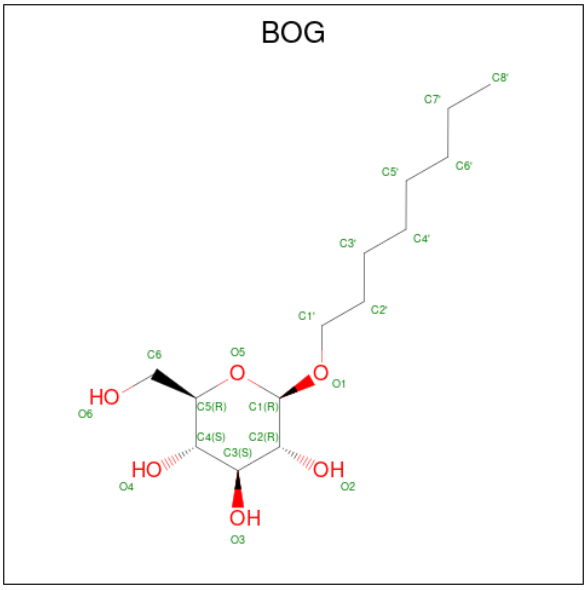
There are 8 unique types of molecules in this entry. The entry contains 7553 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

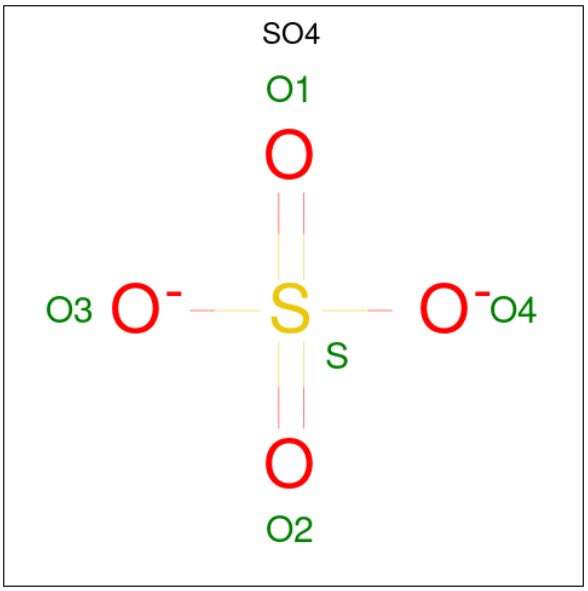
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	415	3385	2171	582	612	20	0	0	0
1	B	410	3347	2148	577	602	20	0	0	0

- Molecule 2 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



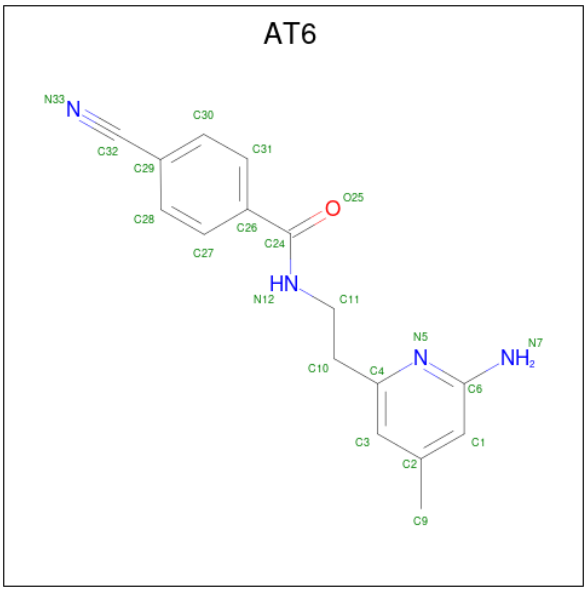
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	20	14	6	0	0
2	B	1	20	14	6	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



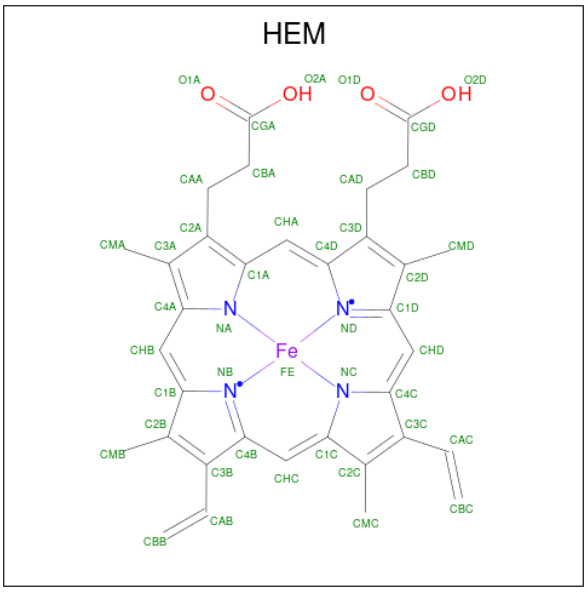
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is N-[2-(6-AMINO-4-METHYLPYRIDIN-2-YL)ETHYL]-4-CYANOBENZAMIDE (three-letter code: AT6) (formula: $C_{16}H_{16}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	21	16	4	1	0	0
			Total	C	N	O		
4	B	1	21	16	4	1	0	0

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



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

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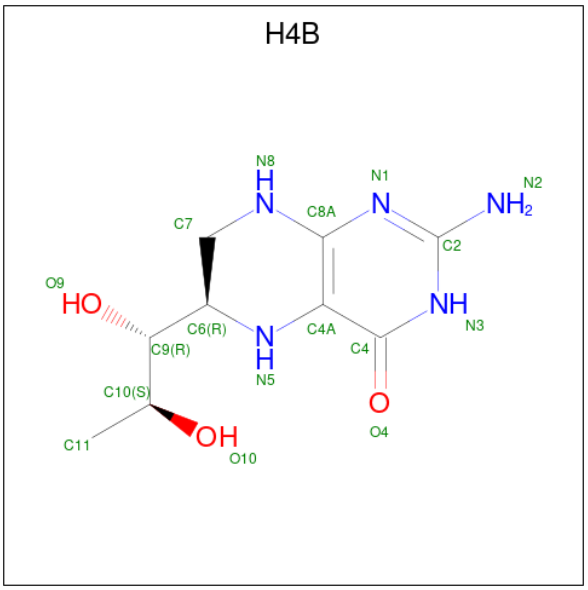
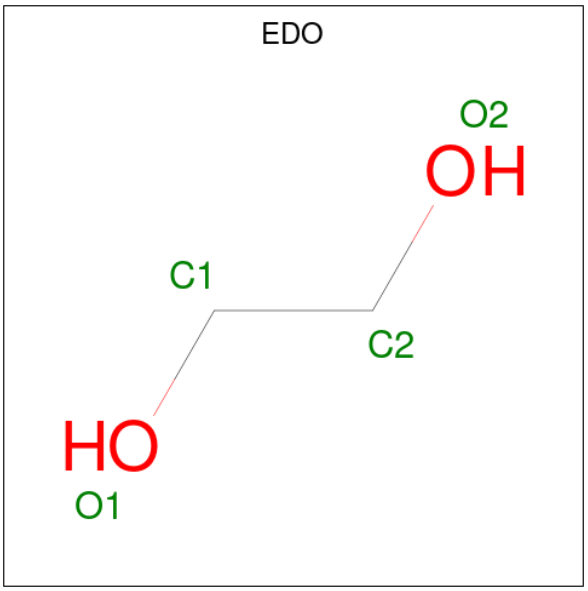
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0

- Molecule 6 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 8 is water.

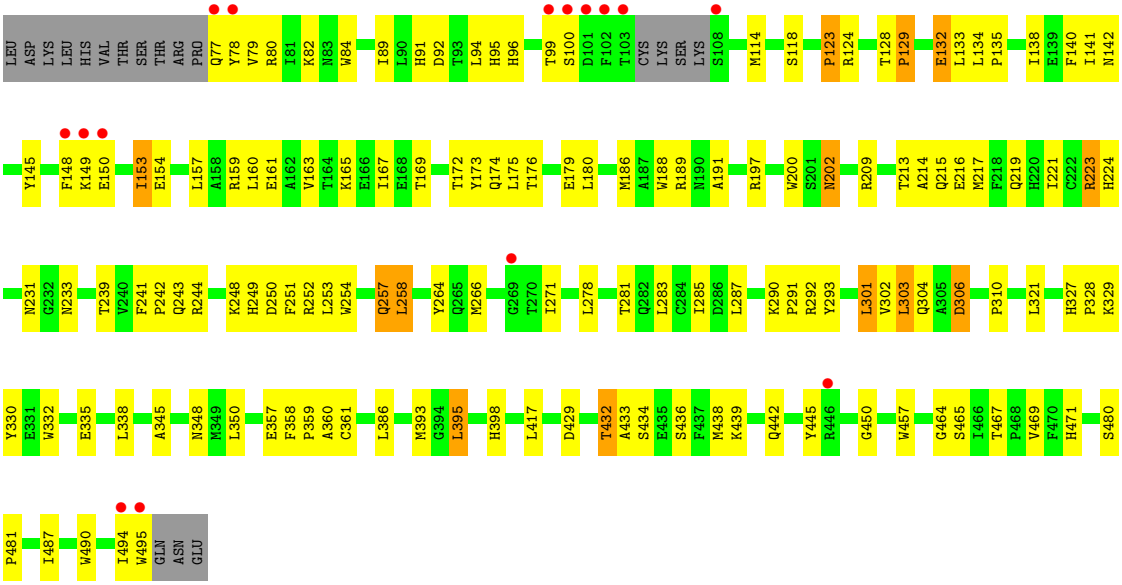
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	279	279	279	0	0
			Total	O		
8	B	291	291	291	0	0

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.

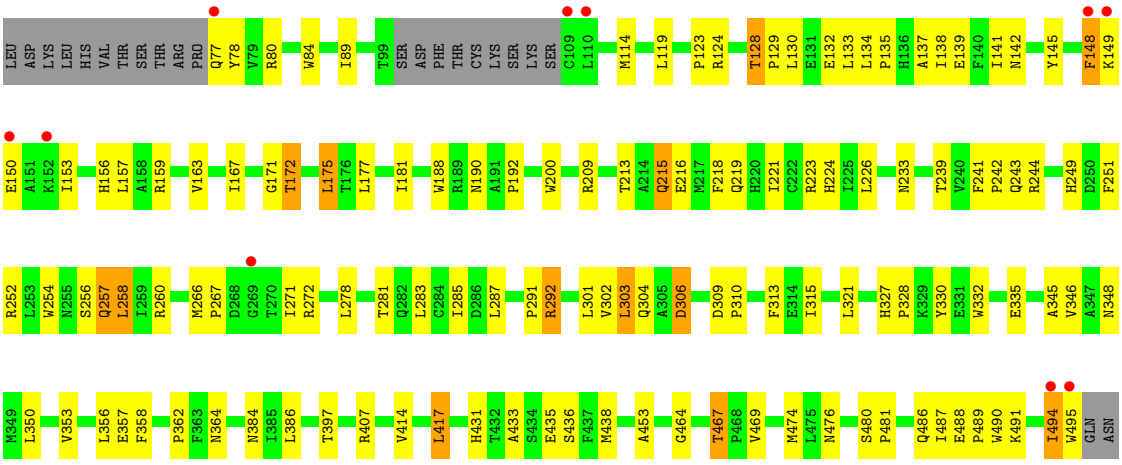
• Molecule 1: Nitric oxide synthase, inducible

Chain A:



• Molecule 1: Nitric oxide synthase, inducible

Chain B:



GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	213.78Å 213.78Å 115.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.63 – 2.20 19.63 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (19.63-2.20) 96.8 (19.63-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.275 0.233 , 0.235	Depositor DCC
R_{free} test set	3880 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.821	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 69.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7553	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, EDO, SO4, H4B, BOG, AT6

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	0/4737
1	B	0.39	0/3445	0.65	0/4684
All	All	0.40	0/6929	0.64	0/9421

There are no bond length outliers.

There are no bond angle outliers.

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	3277	147	0
1	B	3347	0	3247	118	0
2	A	20	0	28	1	0
2	B	20	0	28	0	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
4	A	21	0	16	1	0
4	B	21	0	16	0	0
5	A	43	0	30	1	0
5	B	43	0	30	2	0
6	A	17	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	17	0	14	0	0
7	A	12	0	18	1	0
7	B	12	0	18	3	0
8	A	279	0	0	11	1
8	B	291	0	0	6	1
All	All	7553	0	6736	269	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 20.

All (269) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:THR:HG22	1:A:216:GLU:OE1	1.76	0.86
1:A:134:LEU:O	1:A:138:ILE:HG12	1.79	0.83
1:B:464:GLY:O	1:B:467:THR:HG22	1.78	0.81
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.65	0.79
1:A:304:GLN:O	1:A:304:GLN:HG3	1.83	0.78
1:B:215:GLN:HG2	8:B:2152:HOH:O	1.84	0.77
1:B:252:ARG:HB2	1:B:304:GLN:HG2	1.67	0.77
1:B:285:ILE:HD12	1:B:291:PRO:HD3	1.68	0.75
1:B:292:ARG:NH1	1:B:292:ARG:HB3	2.02	0.74
1:A:176:THR:OG1	1:A:179:GLU:HG3	1.88	0.74
1:B:321:LEU:HD11	7:B:4101:EDO:H11	1.69	0.74
1:B:292:ARG:HB3	1:B:292:ARG:HH11	1.53	0.73
1:B:304:GLN:O	1:B:304:GLN:HG3	1.90	0.72
1:B:494:ILE:H	1:B:494:ILE:HD12	1.54	0.72
1:A:223:ARG:HD2	8:A:2045:HOH:O	1.89	0.71
1:A:153:ILE:HD12	1:A:154:GLU:H	1.55	0.71
1:B:303:LEU:HD23	1:B:313:PHE:CD2	2.26	0.71
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.20	0.70
1:B:130:LEU:HD21	1:B:167:ILE:HG22	1.73	0.70
1:A:467:THR:CG2	1:A:469:VAL:HG22	2.20	0.70
1:A:153:ILE:O	1:A:157:LEU:HD13	1.92	0.70
1:A:141:ILE:CD1	1:A:163:VAL:HG21	2.23	0.69
1:A:217:MET:CE	1:A:303:LEU:HB3	2.20	0.69
1:B:244:ARG:HA	8:B:2161:HOH:O	1.91	0.69
1:A:159:ARG:O	1:A:163:VAL:HG23	1.93	0.69
1:B:129:PRO:HG2	1:B:132:GLU:HG2	1.73	0.69
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.29	0.68
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.31	0.66
1:A:467:THR:HG22	1:A:469:VAL:HG22	1.78	0.65
1:A:271:ILE:HD13	1:A:278:LEU:HD11	1.78	0.65
1:B:386:LEU:HB2	8:B:2193:HOH:O	1.96	0.65
1:A:132:GLU:O	1:A:135:PRO:HD2	1.97	0.65
1:A:209:ARG:O	1:A:242:PRO:HG3	1.98	0.64
1:A:163:VAL:O	1:A:167:ILE:HG13	1.97	0.64
1:A:213:THR:HG23	1:A:216:GLU:H	1.61	0.64
1:A:283:LEU:O	1:A:287:LEU:HG	1.96	0.64
1:B:159:ARG:O	1:B:163:VAL:HG23	1.99	0.63
1:B:163:VAL:O	1:B:167:ILE:HG13	1.98	0.63
1:A:77:GLN:O	1:A:96:HIS:HE1	1.82	0.63
1:A:429:ASP:OD2	1:A:432:THR:HG23	1.99	0.63
1:B:467:THR:HG23	1:B:469:VAL:HG22	1.80	0.63
1:A:99:THR:CG2	1:A:100:SER:N	2.61	0.62
1:B:80:ARG:NH2	1:B:89:ILE:HD13	2.14	0.62
1:B:223:ARG:HG3	1:B:223:ARG:HH11	1.63	0.62
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.35	0.62
1:A:264:TYR:HB2	1:A:266:MET:HE2	1.82	0.61
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.36	0.60
1:A:439:LYS:O	1:A:442:GLN:HG2	2.01	0.60
1:A:217:MET:HE1	1:A:303:LEU:HB3	1.82	0.60
1:A:123:PRO:HD3	1:A:487:ILE:HD12	1.83	0.60
1:A:78:TYR:CE1	1:A:91:HIS:ND1	2.69	0.60
1:A:141:ILE:HD11	1:A:163:VAL:HG21	1.84	0.60
1:A:254:TRP:CZ3	1:A:490:TRP:HB3	2.37	0.60
1:A:221:ILE:HD12	1:A:303:LEU:HD21	1.84	0.60
1:A:132:GLU:C	1:A:135:PRO:HD2	2.22	0.59
1:A:217:MET:HE3	1:A:303:LEU:HB3	1.83	0.59
1:A:138:ILE:HG23	1:A:160:LEU:HD22	1.85	0.59
1:B:130:LEU:HD13	1:B:130:LEU:O	2.02	0.59
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.33	0.59
1:A:285:ILE:HD12	1:A:291:PRO:HD3	1.84	0.59
1:B:249:HIS:C	1:B:306:ASP:O	2.40	0.59
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.17	0.58
1:A:141:ILE:HD13	1:A:163:VAL:HG21	1.85	0.58
1:B:494:ILE:HD12	1:B:494:ILE:N	2.18	0.58
1:A:281:THR:O	1:A:285:ILE:HG12	2.04	0.58
1:B:215:GLN:O	1:B:219:GLN:HG3	2.04	0.58
1:A:252:ARG:HD3	1:A:359:PRO:HB2	1.86	0.58
1:A:433:ALA:O	1:A:436:SER:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ARG:HH21	1:B:489:PRO:HD3	1.68	0.57
1:A:465:SER:O	1:A:471:HIS:HE1	1.88	0.57
1:B:134:LEU:O	1:B:138:ILE:HG13	2.04	0.57
1:A:264:TYR:HB2	1:A:266:MET:CE	2.34	0.57
5:B:1901:HEM:HMC1	5:B:1901:HEM:HBC2	1.87	0.57
1:A:285:ILE:HD11	1:A:291:PRO:HB3	1.87	0.57
1:A:99:THR:HG22	1:A:100:SER:N	2.20	0.57
1:B:271:ILE:HD13	1:B:278:LEU:HD11	1.87	0.57
1:B:303:LEU:O	1:B:310:PRO:HA	2.04	0.57
1:A:303:LEU:O	1:A:310:PRO:HA	2.04	0.56
1:B:303:LEU:HD23	1:B:313:PHE:HD2	1.70	0.56
1:A:215:GLN:HG3	1:A:219:GLN:NE2	2.21	0.55
1:A:249:HIS:C	1:A:306:ASP:O	2.44	0.55
1:A:215:GLN:NE2	8:A:2044:HOH:O	2.39	0.55
1:A:434:SER:CB	1:A:467:THR:HG23	2.37	0.55
1:B:266:MET:HB3	1:B:267:PRO:HD2	1.87	0.55
1:A:145:TYR:HA	1:A:148:PHE:CE2	2.42	0.54
1:A:149:LYS:HD3	1:A:150:GLU:HG3	1.89	0.54
1:A:161:GLU:HB3	8:A:2470:HOH:O	2.06	0.54
1:B:301:LEU:HB3	1:B:303:LEU:HD21	1.89	0.54
1:A:243:GLN:HB3	1:A:358:PHE:CE2	2.43	0.54
1:A:124:ARG:NH1	1:A:128:THR:OG1	2.42	0.53
1:B:332:TRP:O	1:B:335:GLU:HB2	2.08	0.53
1:B:303:LEU:N	1:B:303:LEU:HD22	2.22	0.53
5:A:901:HEM:HBC2	5:A:901:HEM:HMC2	1.91	0.53
1:A:153:ILE:CD1	1:A:154:GLU:H	2.21	0.53
1:B:453:ALA:HB3	1:B:474:MET:HB3	1.90	0.53
1:B:77:GLN:HE21	1:B:78:TYR:HD2	1.57	0.53
1:B:224:HIS:HD2	1:B:239:THR:OG1	1.93	0.52
1:B:190:ASN:O	1:B:192:PRO:HD3	2.09	0.52
1:A:467:THR:HG21	1:A:469:VAL:HG22	1.88	0.52
1:B:145:TYR:HE2	1:B:159:ARG:HG2	1.73	0.52
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.92	0.52
1:A:84:TRP:CE2	1:A:114:MET:HG3	2.45	0.52
1:A:251:PHE:O	1:A:360:ALA:HB2	2.10	0.52
1:A:145:TYR:HA	1:A:148:PHE:HE2	1.72	0.52
1:B:78:TYR:CD1	1:B:78:TYR:C	2.84	0.52
1:B:244:ARG:NH1	1:B:357:GLU:OE2	2.43	0.52
1:A:244:ARG:HD2	1:A:357:GLU:OE2	2.10	0.51
1:B:252:ARG:HB2	1:B:304:GLN:CG	2.38	0.51
4:A:905:AT6:H27	8:A:2320:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:TRP:O	1:A:335:GLU:HB2	2.09	0.51
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.93	0.51
1:B:251:PHE:O	1:B:252:ARG:HG2	2.11	0.51
1:A:129:PRO:HG3	8:A:2016:HOH:O	2.11	0.51
1:A:213:THR:CG2	1:A:216:GLU:HG3	2.40	0.51
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.41	0.51
1:B:153:ILE:O	1:B:156:HIS:HB3	2.10	0.51
1:A:145:TYR:HE2	1:A:159:ARG:HG2	1.76	0.51
1:A:252:ARG:HB2	1:A:304:GLN:HG2	1.91	0.51
1:A:253:LEU:HD12	1:A:253:LEU:N	2.25	0.51
1:A:480:SER:HA	1:A:481:PRO:C	2.30	0.51
1:B:433:ALA:O	1:B:436:SER:HB3	2.10	0.51
1:A:327:HIS:CG	1:A:328:PRO:HD2	2.46	0.50
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.93	0.50
1:B:353:VAL:HG23	1:B:481:PRO:HG3	1.93	0.50
1:A:231:ASN:ND2	8:A:2405:HOH:O	2.44	0.50
1:B:283:LEU:O	1:B:287:LEU:HG	2.12	0.50
1:A:328:PRO:O	1:A:329:LYS:HD2	2.12	0.50
1:A:386:LEU:HB2	8:A:2084:HOH:O	2.12	0.49
1:B:132:GLU:C	1:B:135:PRO:HD2	2.32	0.49
1:B:301:LEU:HD13	1:B:315:ILE:HD11	1.94	0.49
1:B:281:THR:O	1:B:285:ILE:HG12	2.12	0.49
1:A:134:LEU:HD11	1:A:138:ILE:HD11	1.93	0.49
1:B:171:GLY:O	1:B:172:THR:HB	2.12	0.49
1:B:149:LYS:O	1:B:150:GLU:HB2	2.13	0.49
1:B:397:THR:HG22	1:B:397:THR:O	2.11	0.49
1:A:328:PRO:C	1:A:329:LYS:HD2	2.32	0.49
1:B:467:THR:CG2	1:B:469:VAL:HG22	2.41	0.49
1:B:153:ILE:O	1:B:157:LEU:HG	2.13	0.49
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.94	0.49
1:B:138:ILE:O	1:B:142:ASN:ND2	2.45	0.49
1:A:78:TYR:C	1:A:78:TYR:CD1	2.86	0.48
1:A:80:ARG:NH1	1:A:89:ILE:HG21	2.28	0.48
1:B:137:ALA:O	1:B:141:ILE:HD13	2.12	0.48
1:A:429:ASP:CG	1:A:432:THR:HG23	2.34	0.48
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.95	0.48
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.49	0.48
1:B:258:LEU:HD22	1:B:345:ALA:HB1	1.96	0.48
1:A:140:PHE:HE2	1:A:175:LEU:HD22	1.78	0.48
1:A:434:SER:HB3	1:A:467:THR:HG23	1.95	0.48
1:B:132:GLU:O	1:B:135:PRO:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ARG:NH1	1:B:486:GLN:CD	2.68	0.47
1:A:350:LEU:C	1:A:350:LEU:HD23	2.35	0.47
1:B:252:ARG:NH1	1:B:486:GLN:OE1	2.47	0.47
1:B:266:MET:HE1	1:B:272:ARG:NH2	2.29	0.47
1:A:99:THR:CG2	1:A:100:SER:H	2.27	0.47
1:A:138:ILE:O	1:A:142:ASN:ND2	2.48	0.47
1:B:488:GLU:OE2	1:B:491:LYS:HE2	2.15	0.47
1:A:202:ASN:C	1:A:202:ASN:HD22	2.19	0.47
1:A:186:MET:HE1	1:A:189:ARG:HH11	1.81	0.46
1:A:285:ILE:CD1	1:A:291:PRO:HD3	2.45	0.46
1:A:302:VAL:C	1:A:303:LEU:HD12	2.36	0.46
1:B:177:LEU:C	1:B:177:LEU:HD13	2.35	0.46
1:A:128:THR:O	1:A:129:PRO:C	2.54	0.46
1:A:321:LEU:HD11	7:A:3101:EDO:H22	1.96	0.46
1:B:209:ARG:O	1:B:242:PRO:HG3	2.16	0.46
1:B:407:ARG:HG3	8:B:2202:HOH:O	2.14	0.46
1:B:487:ILE:N	1:B:487:ILE:HD12	2.30	0.46
1:A:79:VAL:HG23	1:A:95:HIS:CE1	2.50	0.46
1:A:304:GLN:O	1:A:304:GLN:CG	2.61	0.46
1:A:133:LEU:CD2	1:A:167:ILE:HD13	2.45	0.46
1:A:133:LEU:HD22	1:A:167:ILE:HD13	1.98	0.46
1:A:303:LEU:N	1:A:303:LEU:CD1	2.79	0.46
1:B:346:VAL:O	1:B:362:PRO:HA	2.16	0.46
1:B:488:GLU:O	1:B:491:LYS:HB2	2.15	0.46
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.51	0.46
1:B:215:GLN:CG	8:B:2152:HOH:O	2.55	0.46
1:A:123:PRO:CD	1:A:487:ILE:HD12	2.44	0.46
1:B:258:LEU:HB2	1:B:345:ALA:HB3	1.97	0.46
1:B:224:HIS:HE1	1:B:364:ASN:OD1	1.98	0.45
1:B:256:SER:HB2	1:B:257:GLN:OE1	2.16	0.45
1:A:264:TYR:CE1	1:A:293:TYR:HA	2.51	0.45
1:A:124:ARG:HD2	1:A:244:ARG:HD3	1.98	0.45
1:A:264:TYR:CD1	1:A:293:TYR:HA	2.52	0.45
1:B:124:ARG:HG3	1:B:124:ARG:HH11	1.82	0.45
1:A:134:LEU:CD1	1:A:138:ILE:HD11	2.47	0.45
1:B:145:TYR:CD1	1:B:148:PHE:HZ	2.35	0.45
1:B:285:ILE:CD1	1:B:291:PRO:HB3	2.47	0.45
1:B:414:VAL:HG13	7:B:4104:EDO:O2	2.16	0.45
1:A:92:ASP:O	1:A:95:HIS:CE1	2.70	0.45
1:A:239:THR:O	1:A:361:CYS:HA	2.17	0.45
1:A:248:LYS:O	1:A:248:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:HIS:HB2	8:A:2088:HOH:O	2.17	0.45
1:A:129:PRO:O	1:A:132:GLU:HG3	2.17	0.44
1:A:214:ALA:O	1:A:217:MET:HB2	2.17	0.44
1:B:123:PRO:HD3	1:B:487:ILE:HD13	1.99	0.44
1:A:99:THR:HG23	1:A:100:SER:H	1.83	0.44
1:A:133:LEU:C	1:A:133:LEU:HD23	2.38	0.44
1:A:494:ILE:HD12	1:A:495:TRP:H	1.83	0.44
1:B:149:LYS:HG2	1:B:150:GLU:HG3	1.99	0.44
1:A:290:LYS:HA	1:A:291:PRO:HD2	1.85	0.44
1:A:350:LEU:HD21	1:A:357:GLU:HB2	2.00	0.44
1:B:494:ILE:H	1:B:494:ILE:CD1	2.10	0.44
1:A:258:LEU:HB2	1:A:345:ALA:HB3	2.00	0.44
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.17	0.44
1:A:445:TYR:HA	1:A:450:GLY:H	1.82	0.43
1:A:84:TRP:NE1	1:A:114:MET:HG3	2.33	0.43
1:A:464:GLY:O	1:A:467:THR:HB	2.19	0.43
1:B:330:TYR:HB3	1:B:332:TRP:CE2	2.53	0.43
1:A:250:ASP:HB2	8:A:2344:HOH:O	2.19	0.43
1:A:358:PHE:CD1	1:A:358:PHE:N	2.86	0.43
1:B:84:TRP:NE1	1:B:114:MET:HG3	2.33	0.43
1:B:175:LEU:HD13	1:B:356:LEU:CD1	2.49	0.43
1:B:188:TRP:CZ3	1:B:200:TRP:HA	2.53	0.43
1:A:213:THR:HG22	1:A:216:GLU:CG	2.48	0.43
1:B:141:ILE:N	1:B:141:ILE:HD12	2.33	0.43
1:B:223:ARG:HG3	1:B:223:ARG:NH1	2.30	0.43
1:A:429:ASP:OD1	1:A:432:THR:HG23	2.19	0.43
1:A:457:TRP:HA	6:A:902:H4B:N1	2.34	0.43
1:B:438:MET:HE2	1:B:469:VAL:HG12	2.00	0.43
1:A:301:LEU:HG	1:A:303:LEU:HD11	2.01	0.42
1:B:350:LEU:HB2	1:B:486:GLN:CD	2.38	0.42
1:A:358:PHE:HB3	8:A:2080:HOH:O	2.19	0.42
1:B:384:ASN:CG	1:B:384:ASN:O	2.58	0.42
1:A:165:LYS:O	1:A:169:THR:HG23	2.19	0.42
1:A:213:THR:HG22	1:A:216:GLU:CD	2.36	0.42
1:B:133:LEU:HD13	1:B:133:LEU:O	2.20	0.42
1:A:186:MET:CE	1:A:189:ARG:HH11	2.32	0.42
1:B:139:GLU:HG3	8:B:2382:HOH:O	2.20	0.42
1:B:330:TYR:HB3	1:B:332:TRP:NE1	2.34	0.42
1:B:309:ASP:HB3	1:B:495:TRP:CZ3	2.55	0.42
1:B:438:MET:CE	1:B:469:VAL:HG12	2.50	0.42
1:B:251:PHE:C	1:B:252:ARG:HG2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:HD11	1:B:181:ILE:HD11	2.02	0.42
1:B:302:VAL:CG1	1:B:310:PRO:HB2	2.50	0.42
1:A:82:LYS:HD3	1:A:84:TRP:CE2	2.55	0.42
1:A:221:ILE:O	1:A:224:HIS:HB3	2.20	0.42
1:A:438:MET:HA	1:A:438:MET:CE	2.50	0.42
1:A:191:ALA:O	1:A:197:ARG:CZ	2.67	0.42
1:B:218:PHE:CE1	1:B:313:PHE:HB3	2.55	0.42
1:A:202:ASN:C	1:A:202:ASN:ND2	2.73	0.41
1:A:153:ILE:HD12	1:A:153:ILE:N	2.35	0.41
1:A:242:PRO:HG2	1:A:251:PHE:CZ	2.55	0.41
1:B:252:ARG:NH2	1:B:489:PRO:HD3	2.33	0.41
1:B:257:GLN:OE1	1:B:260:ARG:NH1	2.54	0.41
1:A:129:PRO:HB2	1:A:132:GLU:HG3	2.02	0.41
1:A:244:ARG:NH1	1:A:357:GLU:OE2	2.48	0.41
1:A:257:GLN:CB	1:A:345:ALA:O	2.68	0.41
1:A:393:MET:HB2	1:A:395:LEU:HD22	2.03	0.41
1:A:165:LYS:HB2	1:A:165:LYS:HE3	1.87	0.41
1:A:494:ILE:HD12	1:A:495:TRP:N	2.36	0.41
1:A:172:THR:HG23	1:A:173:TYR:N	2.36	0.41
1:A:163:VAL:HG13	1:A:173:TYR:CD2	2.56	0.41
1:A:174:GLN:HA	8:A:2020:HOH:O	2.21	0.41
1:B:254:TRP:CZ3	1:B:490:TRP:HB3	2.55	0.41
1:B:453:ALA:O	1:B:476:ASN:HB2	2.21	0.41
1:B:304:GLN:O	1:B:304:GLN:CG	2.65	0.41
1:B:417:LEU:HB3	7:B:4104:EDO:H12	2.02	0.41
1:B:431:HIS:O	1:B:435:GLU:HG3	2.21	0.41
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.93	0.40
1:B:84:TRP:CE2	1:B:114:MET:HG3	2.56	0.40
1:B:224:HIS:CD2	1:B:239:THR:OG1	2.74	0.40
1:B:283:LEU:HD23	1:B:283:LEU:C	2.41	0.40
5:B:1901:HEM:HBC2	5:B:1901:HEM:CMC	2.52	0.40
1:A:134:LEU:N	1:A:135:PRO:CD	2.84	0.40
1:B:480:SER:HA	1:B:481:PRO:C	2.42	0.40
1:B:124:ARG:HH21	1:B:128:THR:HB	1.87	0.40
1:B:397:THR:O	1:B:397:THR:CG2	2.70	0.40
1:A:138:ILE:HG21	2:A:3100:BOG:H7'1	2.02	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)
8:B:2368:HOH:O	8:B:2499:HOH:O[9_766]	1.99	0.21
8:A:2473:HOH:O	8:A:2473:HOH:O[9_765]	2.00	0.20

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%)	368 (90%)	41 (10%)	2 (0%)	29	31
1	B	406/433 (94%)	373 (92%)	31 (8%)	2 (0%)	29	31
All	All	817/866 (94%)	741 (91%)	72 (9%)	4 (0%)	29	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	THR
1	B	306	ASP
1	A	306	ASP
1	A	123	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%)	344 (95%)	19 (5%)	23	28
1	B	358/381 (94%)	343 (96%)	15 (4%)	30	38
All	All	721/762 (95%)	687 (95%)	34 (5%)	26	33

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LEU
1	A	118	SER
1	A	129	PRO
1	A	132	GLU
1	A	153	ILE
1	A	180	LEU
1	A	202	ASN
1	A	223	ARG
1	A	233	ASN
1	A	257	GLN
1	A	258	LEU
1	A	292	ARG
1	A	301	LEU
1	A	303	LEU
1	A	338	LEU
1	A	348	ASN
1	A	395	LEU
1	A	417	LEU
1	A	432	THR
1	B	119	LEU
1	B	128	THR
1	B	148	PHE
1	B	175	LEU
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	303	LEU
1	B	348	ASN
1	B	417	LEU
1	B	467	THR
1	B	494	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	202	ASN
1	A	204	GLN

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Mol	Chain	Res	Type
1	A	215	GLN
1	A	219	GLN
1	A	231	ASN
1	A	233	ASN
1	A	334	GLN
1	A	348	ASN
1	A	442	GLN
1	A	471	HIS
1	B	77	GLN
1	B	91	HIS
1	B	220	HIS
1	B	224	HIS
1	B	231	ASN
1	B	233	ASN
1	B	334	GLN
1	B	348	ASN
1	B	421	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

19 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	HEM	B	1901	1	41,50,50	1.29	6 (14%)	45,82,82	1.67	9 (20%)
4	AT6	A	905	-	22,22,22	1.27	3 (13%)	29,29,29	1.54	4 (13%)
4	AT6	B	1905	-	22,22,22	1.45	3 (13%)	29,29,29	1.67	6 (20%)
3	SO4	A	3003	-	4,4,4	0.33	0	6,6,6	0.07	0
7	EDO	B	4102	-	3,3,3	0.45	0	2,2,2	0.68	0
7	EDO	B	4104	-	3,3,3	0.51	0	2,2,2	0.64	0
6	H4B	A	902	-	16,18,18	1.91	3 (18%)	11,26,26	1.97	5 (45%)
5	HEM	A	901	-	41,50,50	1.22	3 (7%)	45,82,82	1.33	5 (11%)
3	SO4	B	4004	-	4,4,4	0.32	0	6,6,6	0.12	0
7	EDO	B	4101	-	3,3,3	0.68	0	2,2,2	0.45	0
2	BOG	A	3100	-	20,20,20	0.95	2 (10%)	25,25,25	0.61	0
7	EDO	A	3101	-	3,3,3	0.64	0	2,2,2	0.50	0
3	SO4	B	4003	-	4,4,4	0.33	0	6,6,6	0.08	0
7	EDO	A	3104	-	3,3,3	0.51	0	2,2,2	0.63	0
3	SO4	A	3005	-	4,4,4	0.32	0	6,6,6	0.09	0
7	EDO	A	3102	-	3,3,3	0.46	0	2,2,2	0.65	0
2	BOG	B	4100	-	20,20,20	0.92	1 (5%)	25,25,25	0.65	0
6	H4B	B	1902	-	16,18,18	1.96	3 (18%)	11,26,26	2.01	5 (45%)
3	SO4	A	3004	-	4,4,4	0.27	0	6,6,6	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	4104	-	-	0/1/1/1	-
6	H4B	A	902	-	1/1/3/5	4/8/17/17	0/2/2/2
4	AT6	B	1905	-	-	2/12/12/12	0/2/2/2
7	EDO	A	3104	-	-	0/1/1/1	-
5	HEM	B	1901	1	-	2/12/54/54	-
5	HEM	A	901	-	-	0/12/54/54	-
7	EDO	B	4102	-	-	0/1/1/1	-
7	EDO	A	3102	-	-	0/1/1/1	-
2	BOG	B	4100	-	-	1/11/31/31	0/1/1/1
7	EDO	B	4101	-	-	0/1/1/1	-
4	AT6	A	905	-	-	2/12/12/12	0/2/2/2
2	BOG	A	3100	-	-	1/11/31/31	0/1/1/1
7	EDO	A	3101	-	-	0/1/1/1	-
6	H4B	B	1902	-	-	0/8/17/17	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1902	H4B	C7-C6	-6.45	1.46	1.52
6	A	902	H4B	C7-C6	-6.01	1.46	1.52
6	B	1902	H4B	C7-N8	-3.56	1.38	1.44
6	A	902	H4B	C7-N8	-3.35	1.39	1.44
5	B	1901	HEM	CAB-C3B	-2.84	1.39	1.47
2	B	4100	BOG	O1-C1	2.70	1.44	1.40
6	A	902	H4B	C4A-N5	-2.68	1.32	1.38
5	A	901	HEM	CAB-C3B	-2.56	1.40	1.47
5	B	1901	HEM	CHA-C4D	2.55	1.41	1.35
2	A	3100	BOG	O1-C1	2.55	1.44	1.40
4	B	1905	AT6	C1-C2	2.50	1.43	1.39
5	B	1901	HEM	C2C-C1C	2.39	1.48	1.42
4	B	1905	AT6	C31-C26	2.34	1.43	1.39
6	B	1902	H4B	C4A-N5	-2.32	1.33	1.38
5	B	1901	HEM	C3C-CAC	-2.28	1.43	1.47
2	A	3100	BOG	O5-C1	2.28	1.47	1.41
5	B	1901	HEM	FE-NB	2.19	2.07	1.96
4	A	905	AT6	C4-N5	2.18	1.38	1.34
5	B	1901	HEM	C3B-C4B	2.17	1.49	1.44
4	A	905	AT6	C1-C2	2.13	1.42	1.39
4	B	1905	AT6	C27-C26	2.10	1.42	1.39
5	A	901	HEM	C2C-C1C	2.09	1.47	1.42
4	A	905	AT6	C31-C30	2.09	1.42	1.38
5	A	901	HEM	CHA-C4D	2.08	1.40	1.35

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1905	AT6	C6-N5-C4	5.57	122.32	118.10
5	B	1901	HEM	C4B-CHC-C1C	5.55	129.89	122.56
4	A	905	AT6	C6-N5-C4	5.07	121.94	118.10
5	A	901	HEM	C4B-CHC-C1C	3.92	127.72	122.56
5	B	1901	HEM	C4C-CHD-C1D	3.80	127.58	122.56
5	B	1901	HEM	C2C-C3C-C4C	-3.76	104.27	106.90
6	A	902	H4B	C8A-C4A-C4	3.45	117.63	114.57
5	A	901	HEM	C4C-CHD-C1D	3.33	126.96	122.56
5	B	1901	HEM	CMD-C2D-C1D	3.15	129.84	125.04
6	B	1902	H4B	C8A-C4A-C4	3.02	117.26	114.57
5	A	901	HEM	C2C-C3C-C4C	-2.93	104.85	106.90
6	B	1902	H4B	C2-N3-C4	2.92	120.56	115.93
6	A	902	H4B	C2-N3-C4	2.86	120.47	115.93
6	B	1902	H4B	C2-N1-C8A	2.83	120.88	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1902	H4B	C4-C4A-N5	2.80	121.47	119.12
4	A	905	AT6	N7-C6-N5	2.74	120.82	116.49
4	A	905	AT6	C10-C4-N5	2.74	120.03	115.95
6	A	902	H4B	C2-N1-C8A	2.70	120.59	114.54
5	B	1901	HEM	CAD-C3D-C2D	-2.69	122.87	127.88
4	B	1905	AT6	C10-C4-N5	2.69	119.95	115.95
4	B	1905	AT6	O25-C24-C26	-2.64	116.23	120.94
4	B	1905	AT6	N7-C6-N5	2.63	120.64	116.49
4	B	1905	AT6	C3-C4-N5	-2.53	120.22	122.90
6	A	902	H4B	C4-C4A-N5	2.33	121.08	119.12
4	A	905	AT6	C3-C4-N5	-2.33	120.43	122.90
5	B	1901	HEM	CHC-C4B-NB	-2.31	121.92	124.43
6	B	1902	H4B	N1-C2-N3	-2.30	121.81	125.42
5	B	1901	HEM	CHC-C4B-C3B	2.29	128.08	124.57
4	B	1905	AT6	C26-C24-N12	2.26	121.94	117.09
6	A	902	H4B	N1-C2-N3	-2.25	121.89	125.42
5	A	901	HEM	C4B-C3B-C2B	-2.24	105.34	107.11
5	A	901	HEM	CMC-C2C-C3C	2.21	128.81	124.68
5	B	1901	HEM	CAD-C3D-C4D	2.06	128.26	124.66
5	B	1901	HEM	C1D-C2D-C3D	-2.02	104.83	106.96

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	902	H4B	C6

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	902	H4B	C7-C6-C9-O9
6	A	902	H4B	C7-C6-C9-C10
2	B	4100	BOG	O1-C1'-C2'-C3'
4	B	1905	AT6	C11-C10-C4-N5
2	A	3100	BOG	O1-C1'-C2'-C3'
4	B	1905	AT6	C11-C10-C4-C3
6	A	902	H4B	N5-C6-C9-O9
4	A	905	AT6	C11-C10-C4-N5
4	A	905	AT6	C11-C10-C4-C3
6	A	902	H4B	N5-C6-C9-C10
5	B	1901	HEM	CAA-CBA-CGA-O2A
5	B	1901	HEM	CAA-CBA-CGA-O1A

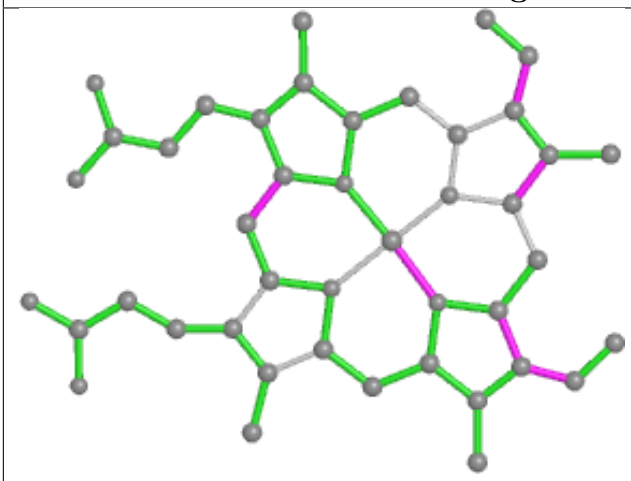
There are no ring outliers.

8 monomers are involved in 10 short contacts:

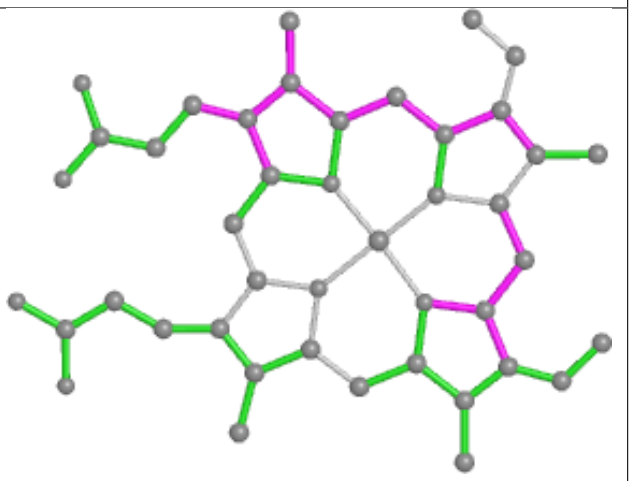
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1901	HEM	2	0
4	A	905	AT6	1	0
7	B	4104	EDO	2	0
6	A	902	H4B	1	0
5	A	901	HEM	1	0
7	B	4101	EDO	1	0
2	A	3100	BOG	1	0
7	A	3101	EDO	1	0

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 then 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.

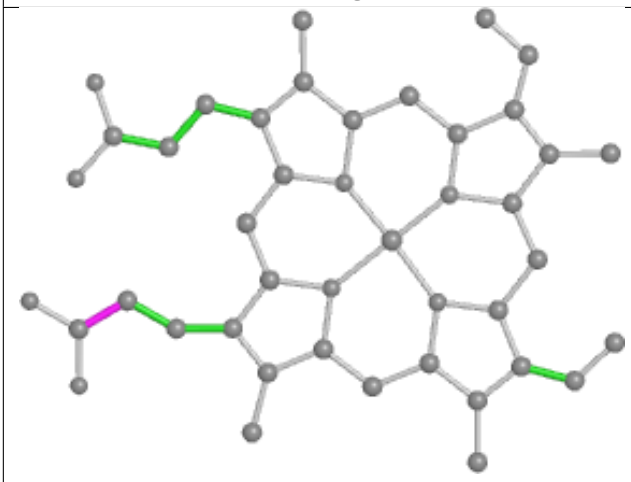
Ligand HEM B 1901



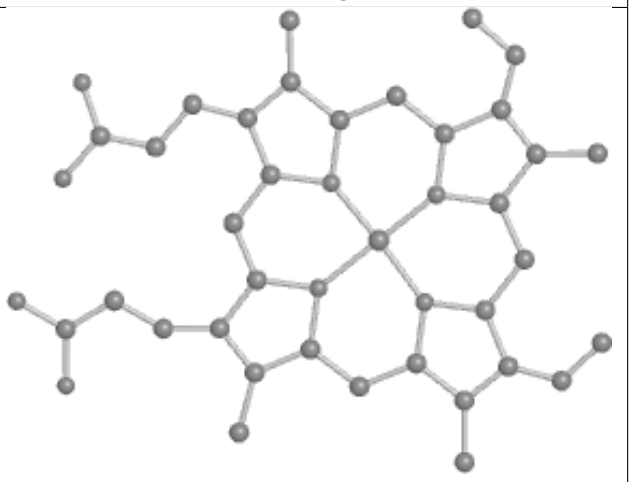
Bond lengths



Bond angles

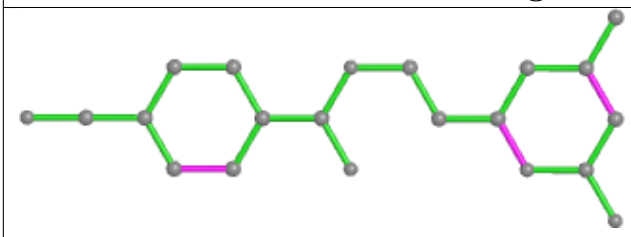


Torsions

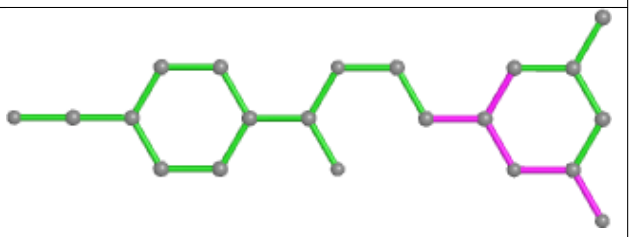


Rings

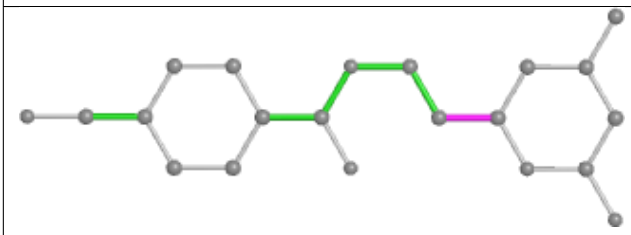
Ligand AT6 A 905



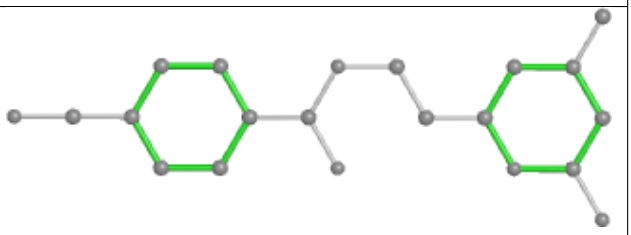
Bond lengths



Bond angles

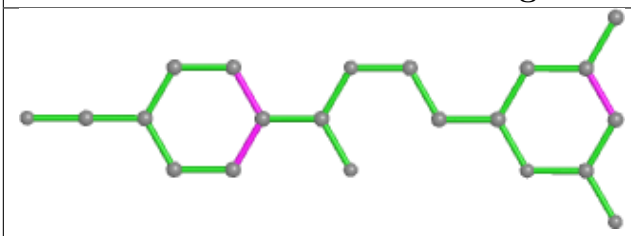


Torsions

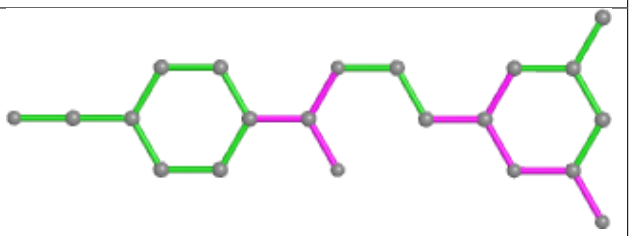


Rings

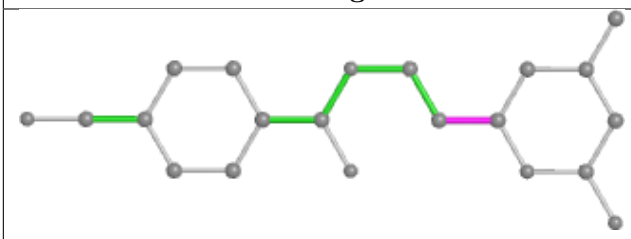
Ligand AT6 B 1905



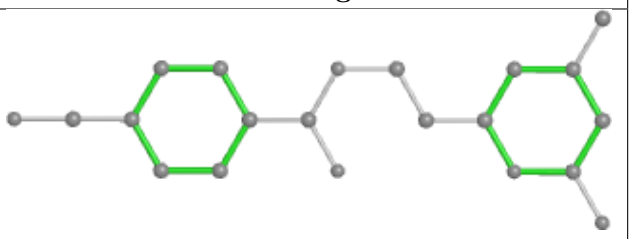
Bond lengths



Bond angles

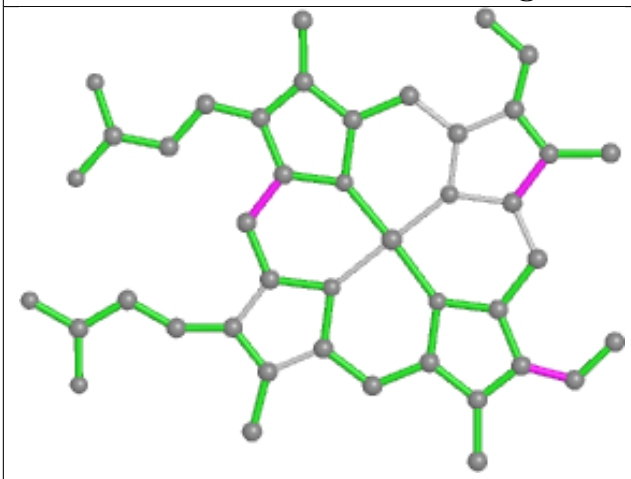


Torsions

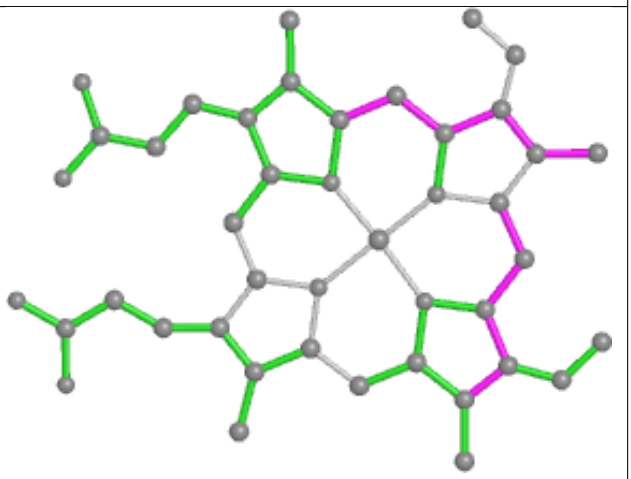


Rings

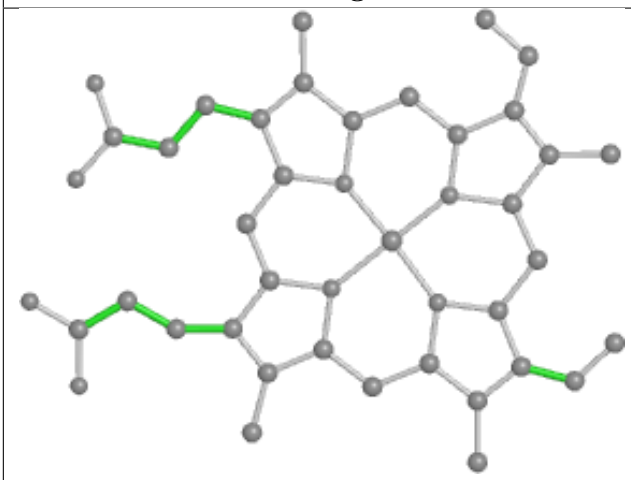
Ligand HEM A 901



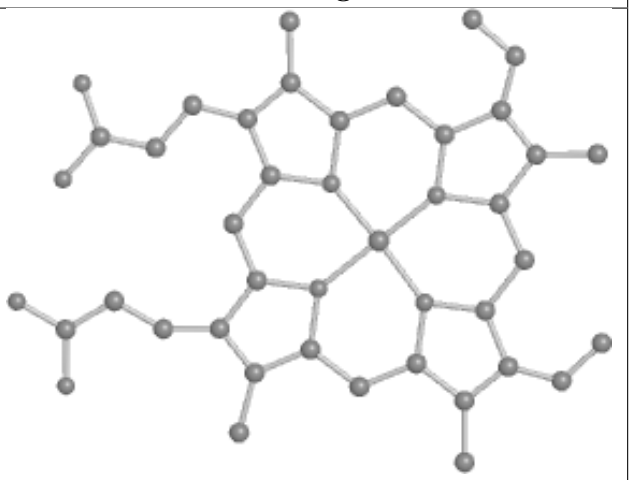
Bond lengths



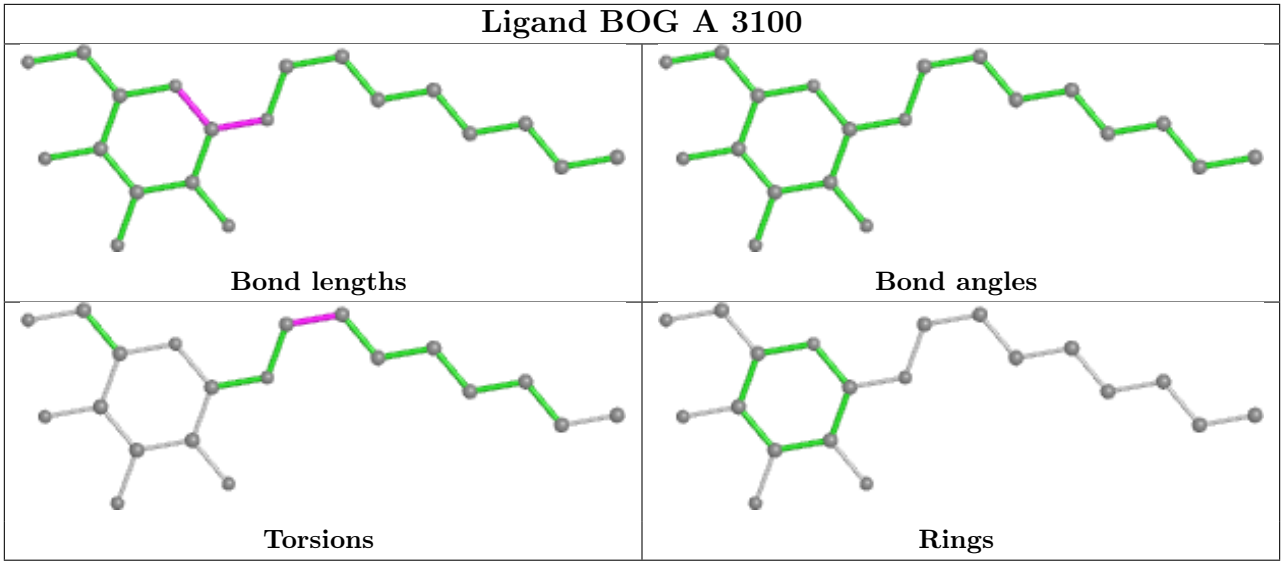
Bond angles

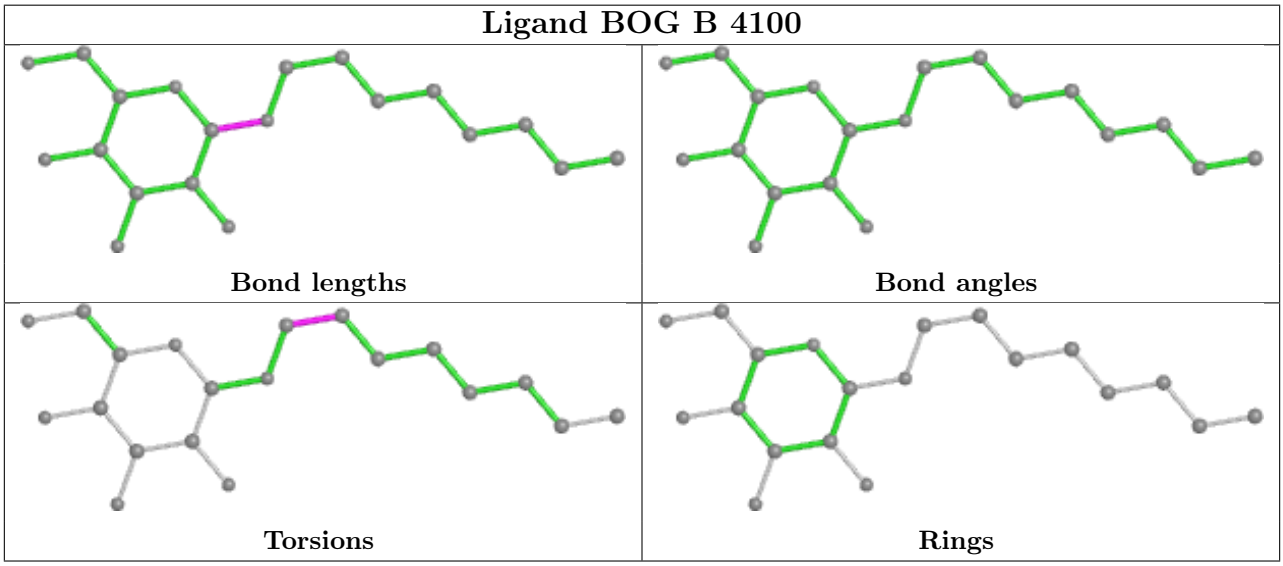


Torsions



Rings





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	415/433 (95%)	0.01	15 (3%)	42	41	25, 46, 78, 106	0
1	B	410/433 (94%)	-0.08	10 (2%)	59	56	21, 45, 74, 91	0
All	All	825/866 (95%)	-0.03	25 (3%)	50	48	21, 46, 75, 106	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	THR	7.2
1	A	495	TRP	5.4
1	A	102	PHE	4.6
1	A	101	ASP	4.6
1	A	494	ILE	4.5
1	A	149	LYS	4.4
1	A	108	SER	4.1
1	A	100	SER	3.9
1	B	110	LEU	3.5
1	B	494	ILE	3.5
1	A	150	GLU	3.4
1	B	495	TRP	3.2
1	B	150	GLU	3.1
1	B	149	LYS	3.0
1	B	109	CYS	2.9
1	A	78	TYR	2.9
1	A	77	GLN	2.8
1	A	269	GLY	2.7
1	A	99	THR	2.7
1	A	148	PHE	2.4
1	A	446	ARG	2.3
1	B	77	GLN	2.3
1	B	148	PHE	2.2
1	B	269	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	152	LYS	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

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

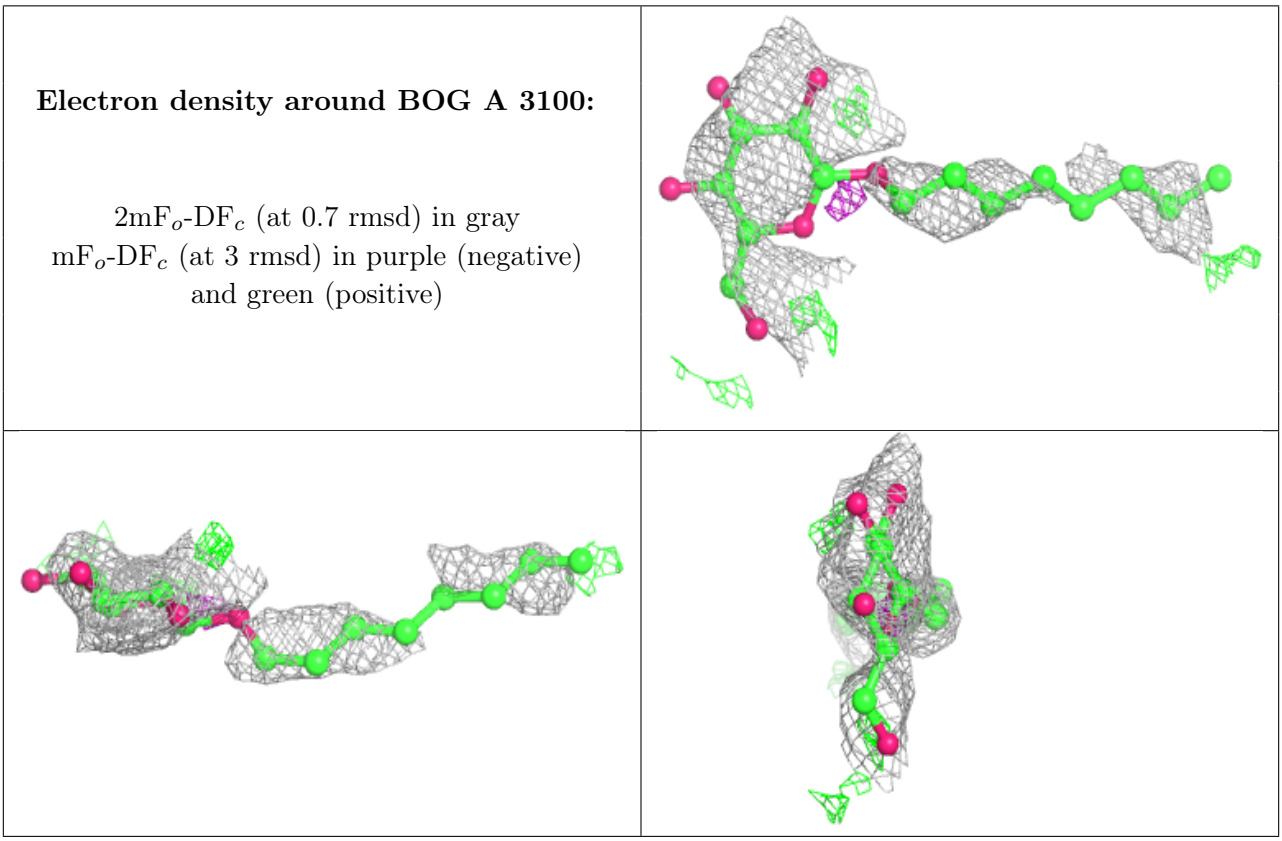
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BOG	A	3100	20/20	0.72	0.49	89,101,103,104	0
7	EDO	A	3101	4/4	0.75	0.37	63,65,66,68	0
3	SO4	A	3004	5/5	0.78	0.18	111,112,112,113	0
2	BOG	B	4100	20/20	0.82	0.25	80,83,84,86	0
3	SO4	A	3003	5/5	0.85	0.20	111,111,111,111	0
7	EDO	B	4101	4/4	0.86	0.22	64,65,66,66	0
7	EDO	B	4104	4/4	0.86	0.19	67,68,68,70	0
3	SO4	B	4003	5/5	0.91	0.13	107,108,109,109	0
3	SO4	A	3005	5/5	0.92	0.18	99,99,100,100	0
7	EDO	A	3102	4/4	0.92	0.13	42,42,44,45	0
7	EDO	B	4102	4/4	0.93	0.12	42,42,43,43	0
3	SO4	B	4004	5/5	0.93	0.17	98,99,100,101	0
7	EDO	A	3104	4/4	0.95	0.14	59,60,60,60	0
4	AT6	A	905	21/21	0.95	0.11	25,36,38,43	0
4	AT6	B	1905	21/21	0.95	0.11	26,36,42,45	0
6	H4B	A	902	17/17	0.97	0.08	28,30,37,37	0
6	H4B	B	1902	17/17	0.97	0.08	29,31,36,38	0
5	HEM	A	901	43/43	0.98	0.10	24,28,31,35	0
5	HEM	B	1901	43/43	0.98	0.09	20,28,31,34	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.

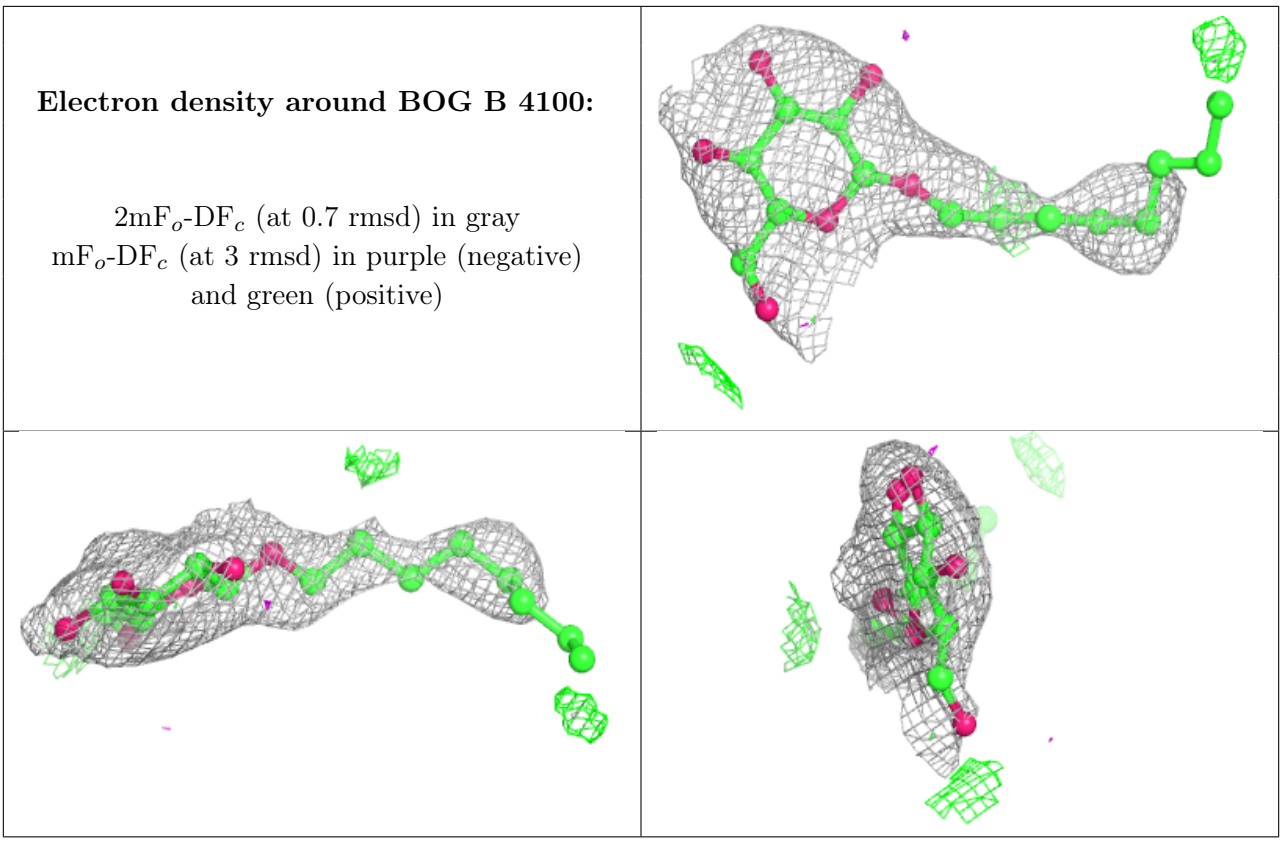
Electron density around BOG A 3100:

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



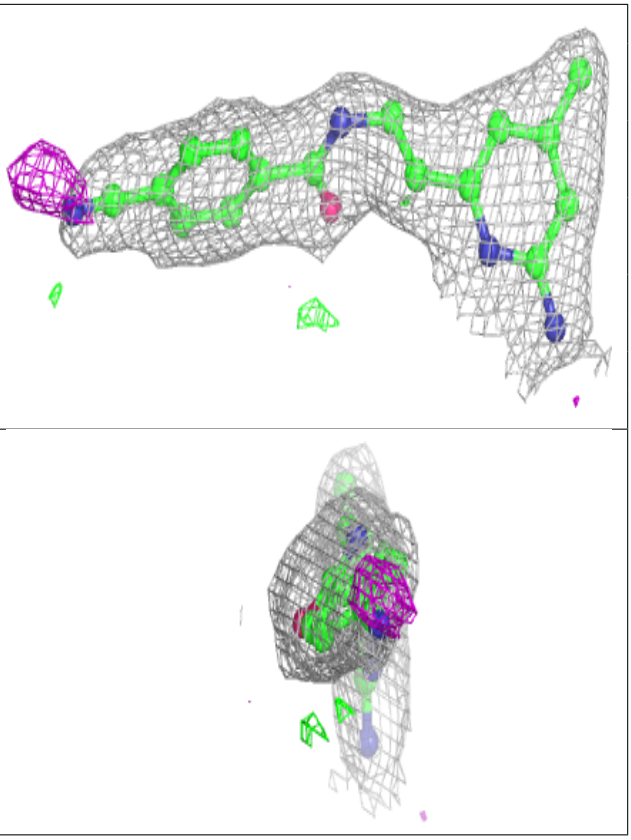
Electron density around BOG B 4100:

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



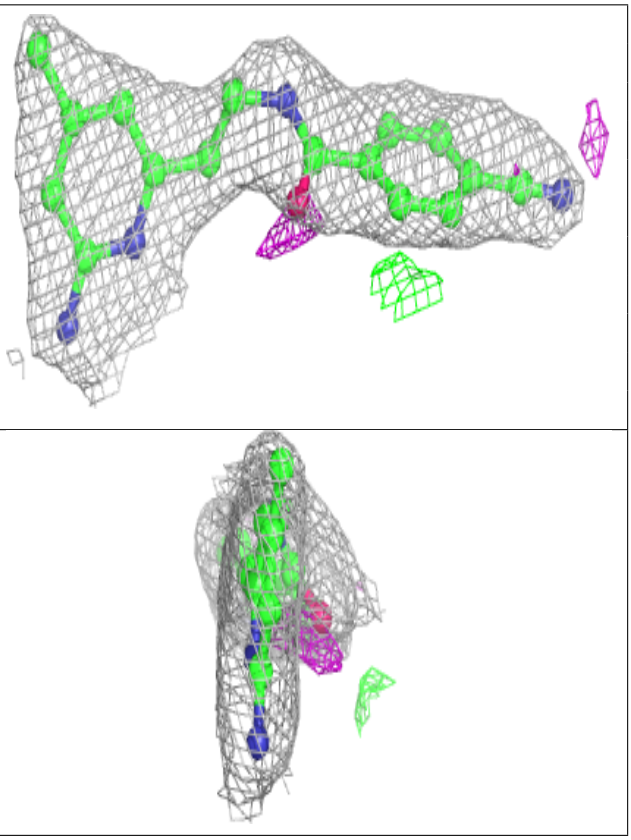
Electron density around AT6 A 905:

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



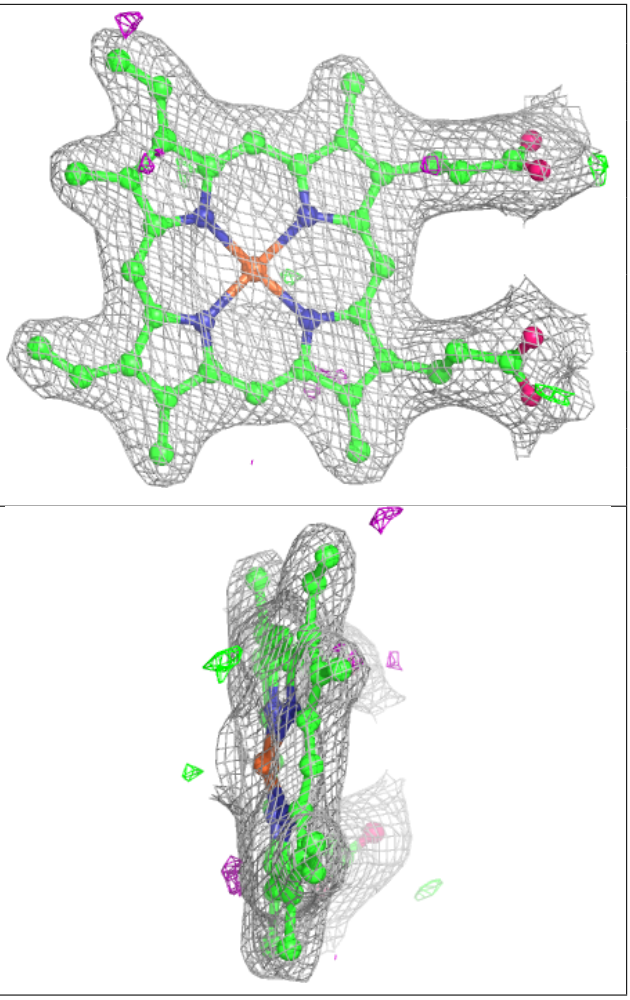
Electron density around AT6 B 1905:

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



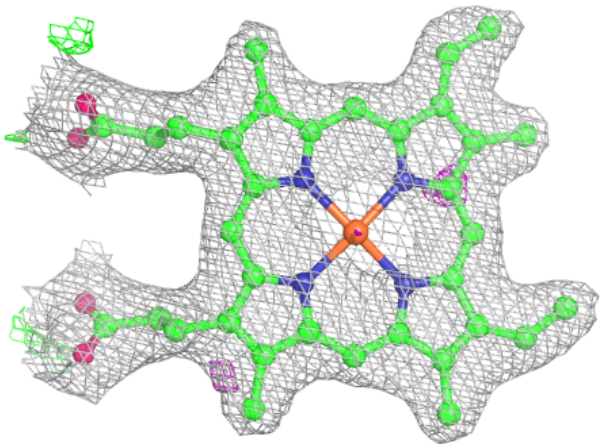
Electron density around HEM A 901:

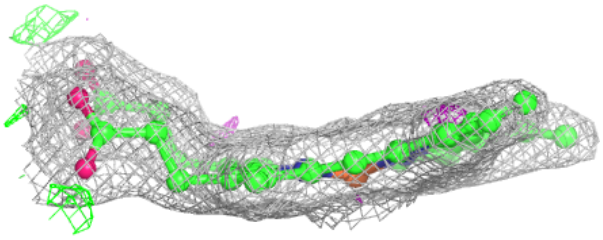
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

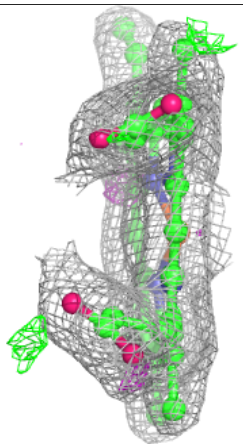


Electron density around HEM B 1901:

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







6.5 Other polymers (i)

There are no such residues in this entry.