Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 10:40 AM EDT

PDB ID	:	1N2N
Title	:	Crystal structure of cyanide complex of the oxygenase domain of inducible nitric oxide synthase.
Authors	:	Fedorov, R.; Ghosh, D.K.; Schlichting, I.
Deposited on	:	2002-10-23
Resolution	:	2.40 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:

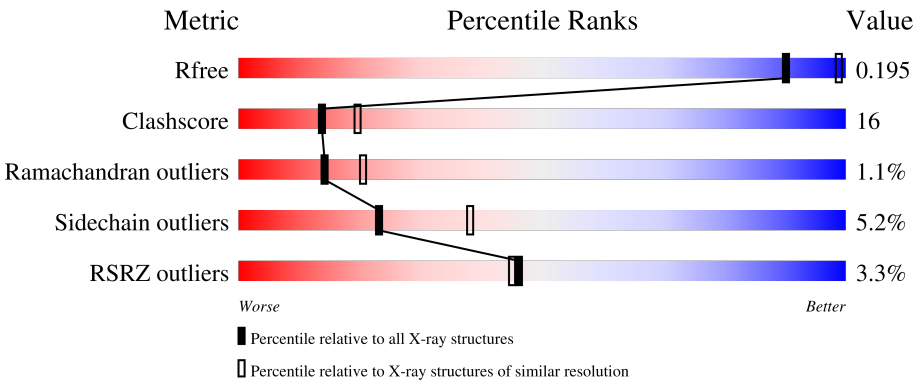
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	419	3% 70% 27% •
1	B	419	3% 67% 29% •

2 Entry composition (i)

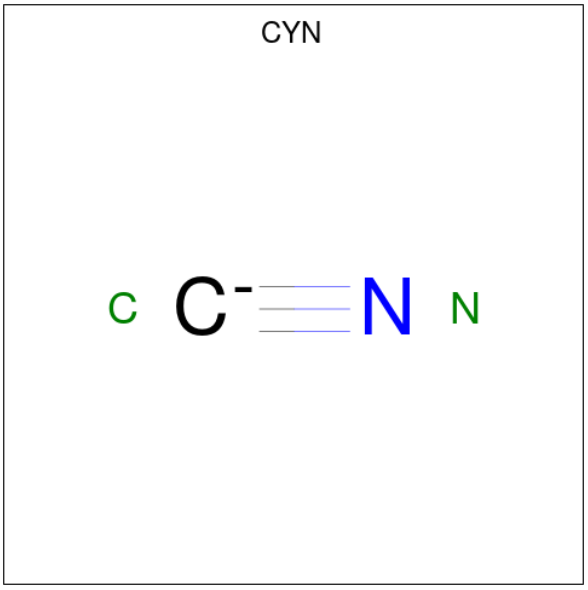
There are 7 unique types of molecules in this entry. The entry contains 7506 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Inducible Nitric Oxide Synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	419	3415	2189	588	617	21	0	0	0
1	B	419	3415	2189	588	617	21	0	0	0

- Molecule 2 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

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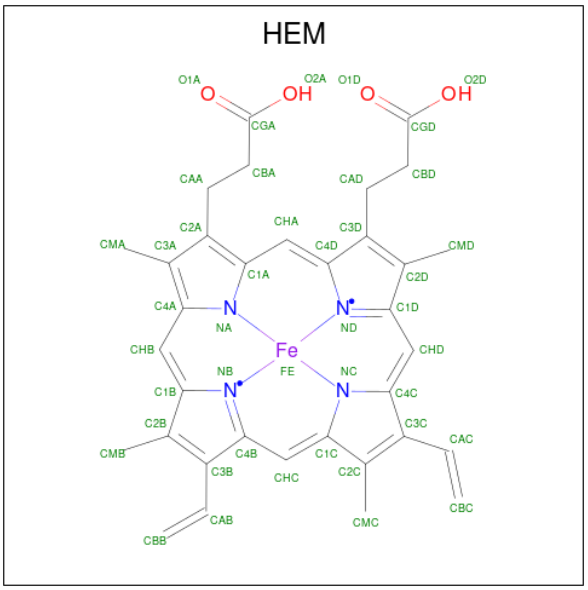
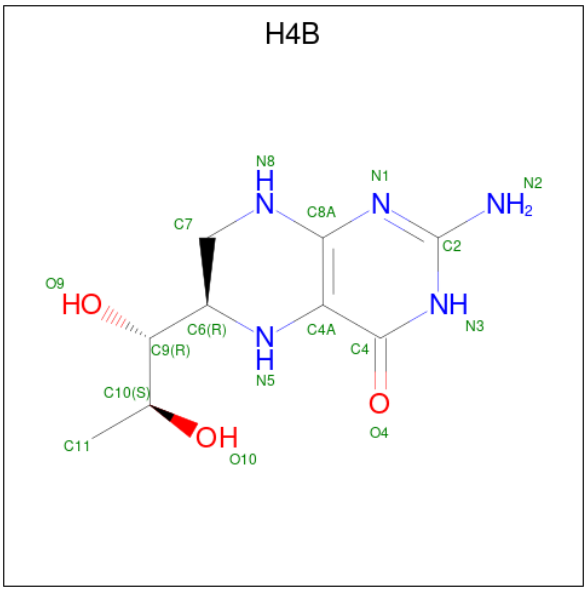
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	1	1	1	0	0

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



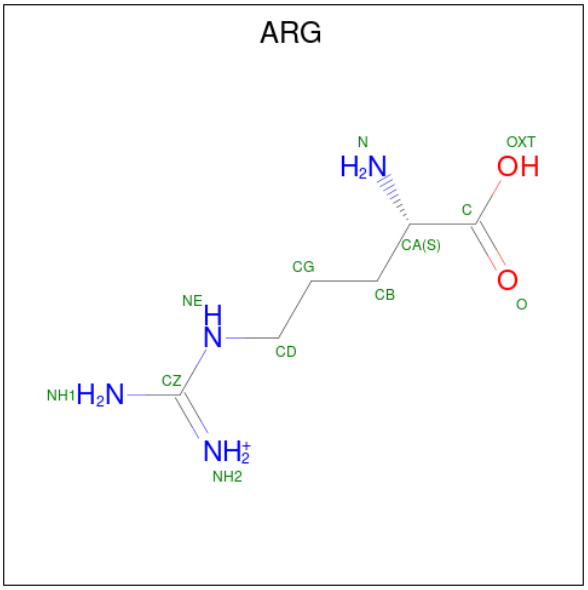
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
4	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
4	B	1	43	34	1	4	4	0	0

- Molecule 5 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		
5	A	1	17	9	5	3	0	0
5	B	1	17	9	5	3	0	0

- Molecule 6 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	11	6	4	1	0	0
6	B	1	11	6	4	1	0	0

- Molecule 7 is water.

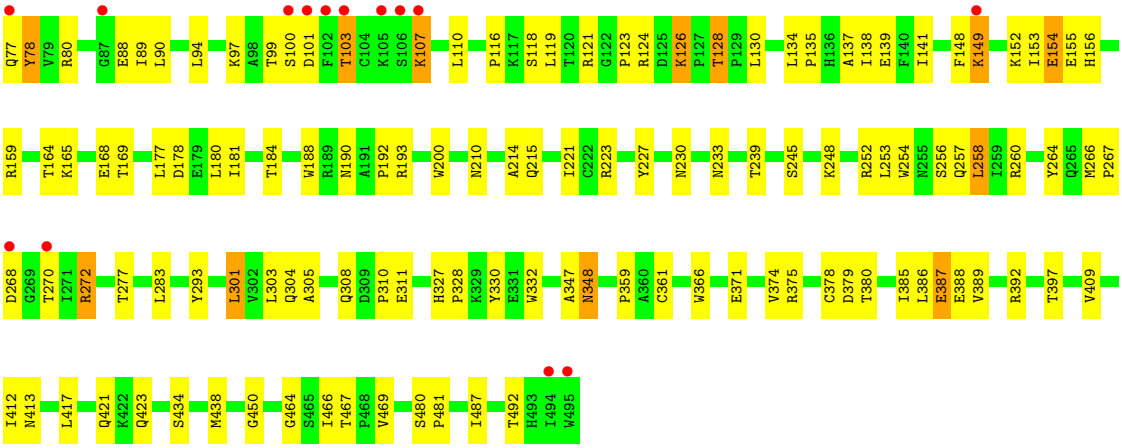
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	267	267	267	0	0
			Total	O		
7	B	263	263	263	0	0

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.

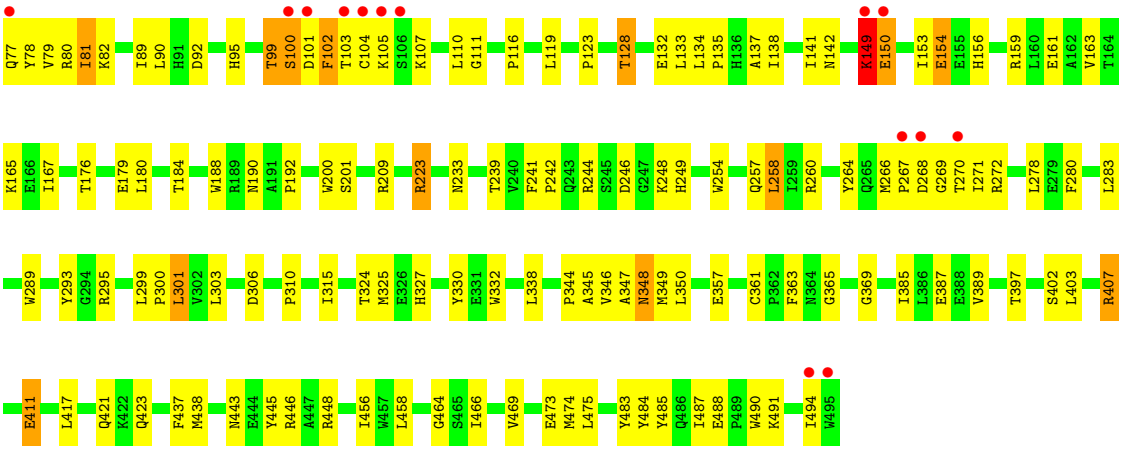
• Molecule 1: Inducible Nitric Oxide Synthase

Chain A:



• Molecule 1: Inducible Nitric Oxide Synthase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	214.80Å 214.80Å 117.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 96.0 (19.72-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.41Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.206 , 0.243 0.205 , 0.195	Depositor DCC
R_{free} test set	3038 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7506	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 2.09% 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: CYN, ZN, HEM, 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	0.41	0/3515	0.62	0/4778
1	B	0.41	0/3515	0.64	2/4778 (0.0%)
All	All	0.41	0/7030	0.63	2/9556 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	149	LYS	N-CA-C	-6.13	94.45	111.00
1	B	365	GLY	N-CA-C	-5.13	100.28	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	445	TYR	Sidechain

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	3415	0	3312	101	0
1	B	3415	0	3312	116	0
2	A	2	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	43	0	30	1	0
4	B	43	0	30	3	0
5	A	17	0	15	0	0
5	B	17	0	15	0	0
6	A	11	0	12	2	0
6	B	11	0	12	0	0
7	A	267	0	0	13	0
7	B	263	0	0	6	0
All	All	7506	0	6738	218	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (218) 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:124:ARG:HH12	1:A:128:THR:HB	1.02	1.08
1:A:103:THR:HG21	1:A:116:PRO:HB2	1.31	1.07
1:A:124:ARG:NH1	1:A:128:THR:HB	1.75	1.01
1:B:438:MET:HE2	1:B:469:VAL:HG22	1.51	0.90
1:B:77:GLN:HG2	1:B:78:TYR:H	1.38	0.87
1:B:190:ASN:ND2	1:B:448:ARG:HH22	1.73	0.87
1:A:272:ARG:HH11	1:A:272:ARG:HB2	1.40	0.85
1:B:134:LEU:O	1:B:138:ILE:HG12	1.78	0.83
1:A:77:GLN:HA	7:A:1094:HOH:O	1.83	0.77
1:A:128:THR:HG22	7:A:1187:HOH:O	1.85	0.76
1:A:438:MET:HE3	1:A:469:VAL:HG22	1.69	0.75
1:B:149:LYS:O	1:B:150:GLU:HG2	1.87	0.74
1:B:324:THR:H	1:B:423:GLN:HE22	1.34	0.73
1:A:153:ILE:HD12	1:A:153:ILE:H	1.54	0.72
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.26	0.71
1:B:80:ARG:HE	1:B:89:ILE:HG21	1.57	0.68
1:B:128:THR:HG21	7:B:2030:HOH:O	1.93	0.68
1:A:245:SER:HA	7:A:1179:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ARG:HG3	1:B:407:ARG:HH11	1.58	0.68
1:A:123:PRO:HG2	1:A:492:THR:HG21	1.76	0.67
1:B:417:LEU:O	1:B:421:GLN:HG3	1.94	0.67
1:B:246:ASP:OD2	1:B:248:LYS:HB2	1.94	0.67
1:B:132:GLU:O	1:B:135:PRO:HD2	1.95	0.66
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.78	0.66
1:A:107:LYS:NZ	1:A:107:LYS:HB3	2.11	0.66
1:B:260:ARG:HG2	7:B:2045:HOH:O	1.96	0.66
1:B:79:VAL:HG23	1:B:95:HIS:CE1	2.31	0.65
1:A:386:LEU:HB2	7:A:1099:HOH:O	1.96	0.65
1:A:103:THR:HG23	1:A:118:SER:CB	2.27	0.65
1:A:264:TYR:CE2	1:A:293:TYR:HA	2.31	0.65
1:A:88:GLU:C	1:A:89:ILE:HD12	2.18	0.65
1:B:81:ILE:HG22	1:B:90:LEU:HB2	1.79	0.65
1:B:270:THR:HG22	1:B:271:ILE:N	2.13	0.64
1:B:123:PRO:HD3	1:B:487:ILE:HD13	1.80	0.64
1:B:154:GLU:N	1:B:154:GLU:OE1	2.30	0.64
1:B:82:LYS:O	1:B:473:GLU:HG3	1.98	0.64
1:A:165:LYS:O	1:A:169:THR:HG23	1.97	0.64
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.33	0.63
1:A:366:TRP:H	4:A:900:HEM:HAB	1.63	0.63
1:A:305:ALA:O	1:A:308:GLN:HB2	2.00	0.62
1:A:100:SER:OG	1:A:101:ASP:N	2.32	0.61
1:B:190:ASN:HD21	1:B:448:ARG:HH22	1.48	0.61
1:B:77:GLN:HG2	1:B:78:TYR:N	2.14	0.61
1:A:103:THR:HG23	1:A:118:SER:OG	2.01	0.60
1:B:99:THR:HG22	1:B:100:SER:N	2.15	0.60
1:B:266:MET:HB3	1:B:267:PRO:HD2	1.83	0.60
1:A:248:LYS:NZ	1:A:248:LYS:HB3	2.16	0.60
1:A:304:GLN:HG3	1:A:308:GLN:O	2.02	0.59
1:B:438:MET:CE	1:B:469:VAL:HG22	2.30	0.59
1:A:387:GLU:HB2	7:A:1154:HOH:O	2.02	0.58
1:A:103:THR:HG23	1:A:118:SER:HB3	1.84	0.58
1:B:134:LEU:HB3	1:B:135:PRO:HD3	1.85	0.58
1:B:264:TYR:CE2	1:B:293:TYR:HA	2.39	0.58
1:B:295:ARG:NH2	1:B:338:LEU:HD23	2.19	0.58
1:A:80:ARG:HD3	7:A:1057:HOH:O	2.03	0.58
1:B:349:MET:HE2	4:B:900:HEM:HMD3	1.84	0.58
1:B:350:LEU:C	1:B:350:LEU:HD23	2.24	0.58
1:B:142:ASN:ND2	1:B:156:HIS:NE2	2.52	0.58
1:B:154:GLU:CD	1:B:154:GLU:H	2.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:HB2	1:B:107:LYS:NZ	2.19	0.57
1:B:494:ILE:H	1:B:494:ILE:HD12	1.70	0.57
1:B:295:ARG:HH21	1:B:338:LEU:HD23	1.70	0.57
1:B:385:ILE:O	1:B:389:VAL:HG23	2.05	0.56
1:A:487:ILE:HD12	1:A:487:ILE:N	2.19	0.56
1:B:102:PHE:CG	1:B:103:THR:N	2.73	0.56
1:A:375:ARG:O	1:A:379:ASP:HB2	2.05	0.56
1:A:110:LEU:HD12	1:A:110:LEU:N	2.21	0.56
1:A:389:VAL:HG21	1:A:412:ILE:HD11	1.88	0.56
1:A:374:VAL:O	1:A:378:CYS:HB2	2.06	0.56
1:A:330:TYR:HD2	1:A:332:TRP:HE1	1.53	0.55
1:A:124:ARG:NH1	1:A:128:THR:CB	2.61	0.55
1:A:94:LEU:HB3	1:A:450:GLY:HA3	1.89	0.55
1:A:258:LEU:HD13	1:A:347:ALA:HB2	1.88	0.55
1:A:388:GLU:OE1	1:A:392:ARG:HD2	2.07	0.55
1:B:485:TYR:OH	4:B:900:HEM:O2D	2.20	0.55
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.89	0.54
1:B:387:GLU:HG3	1:B:397:THR:HG21	1.90	0.54
1:A:423:GLN:HB3	7:A:1005:HOH:O	2.08	0.54
1:A:239:THR:O	1:A:361:CYS:HA	2.08	0.54
1:A:164:THR:O	1:A:168:GLU:HG3	2.07	0.54
1:B:266:MET:HE2	7:B:2061:HOH:O	2.08	0.54
1:A:327:HIS:ND1	1:A:328:PRO:HD2	2.23	0.54
1:B:190:ASN:HD22	1:B:448:ARG:HH22	1.51	0.54
1:B:223:ARG:HD2	7:B:1949:HOH:O	2.08	0.54
1:B:190:ASN:O	1:B:192:PRO:HD3	2.08	0.53
1:B:443:ASN:OD1	1:B:446:ARG:NH2	2.42	0.53
1:B:161:GLU:O	1:B:165:LYS:HG2	2.09	0.53
1:B:270:THR:HG22	1:B:271:ILE:H	1.72	0.53
1:A:215:GLN:NE2	7:A:1194:HOH:O	2.41	0.53
1:B:77:GLN:CG	1:B:78:TYR:H	2.18	0.53
1:B:349:MET:CE	4:B:900:HEM:HMD3	2.39	0.52
1:A:77:GLN:HG3	1:A:78:TYR:N	2.24	0.52
1:B:103:THR:HG23	1:B:116:PRO:HB2	1.92	0.52
1:B:349:MET:HG2	1:B:483:TYR:HB3	1.91	0.52
1:A:137:ALA:O	1:A:141:ILE:HG12	2.10	0.52
1:A:154:GLU:OE2	1:A:155:GLU:HG3	2.10	0.52
1:B:104:CYS:HA	1:B:110:LEU:HD12	1.91	0.51
1:B:149:LYS:HD2	1:B:150:GLU:N	2.25	0.51
1:B:407:ARG:HG3	1:B:407:ARG:NH1	2.22	0.51
1:B:103:THR:HG23	1:B:116:PRO:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.45	0.51
1:B:176:THR:OG1	1:B:179:GLU:HG3	2.11	0.51
1:B:487:ILE:N	1:B:487:ILE:HD12	2.25	0.51
1:A:303:LEU:O	1:A:310:PRO:HA	2.10	0.50
1:B:81:ILE:CD1	1:B:475:LEU:HD21	2.42	0.50
2:A:903:CYN:N	6:A:902:ARG:NH1	2.60	0.50
1:A:253:LEU:HD22	1:A:347:ALA:HB1	1.93	0.50
1:A:257:GLN:HG3	1:A:260:ARG:HD2	1.93	0.50
1:A:413:ASN:ND2	7:A:1097:HOH:O	2.44	0.50
1:B:327:HIS:NE2	1:B:411:GLU:HG3	2.27	0.49
1:A:153:ILE:O	1:A:156:HIS:HB3	2.12	0.49
1:B:349:MET:HG3	1:B:484:TYR:O	2.12	0.49
1:B:348:ASN:H	1:B:348:ASN:ND2	2.11	0.49
1:A:330:TYR:HD2	1:A:332:TRP:NE1	2.11	0.48
1:B:488:GLU:HG3	1:B:491:LYS:HD2	1.95	0.48
1:A:190:ASN:O	1:A:192:PRO:HD3	2.14	0.48
1:B:327:HIS:HE2	1:B:411:GLU:HG3	1.78	0.48
1:B:271:ILE:HD13	1:B:278:LEU:HD11	1.96	0.48
1:A:272:ARG:HH11	1:A:272:ARG:CB	2.19	0.47
1:B:137:ALA:O	1:B:141:ILE:HG12	2.14	0.47
1:B:301:LEU:HD22	1:B:315:ILE:HG12	1.95	0.47
1:A:107:LYS:HB3	1:A:107:LYS:HZ3	1.78	0.47
1:B:104:CYS:HA	1:B:110:LEU:CD1	2.44	0.47
1:A:266:MET:SD	1:A:272:ARG:NH1	2.87	0.47
1:B:402:SER:O	1:B:403:LEU:HB2	2.14	0.47
1:B:103:THR:O	1:B:110:LEU:HD13	2.14	0.47
1:B:110:LEU:HD12	1:B:110:LEU:H	1.80	0.47
1:A:260:ARG:HE	1:A:277:THR:HG21	1.80	0.47
1:A:148:PHE:CD2	1:A:152:LYS:HD3	2.50	0.47
1:A:88:GLU:O	1:A:89:ILE:HD12	2.15	0.46
1:B:133:LEU:HD22	1:B:167:ILE:HD13	1.95	0.46
1:B:153:ILE:O	1:B:156:HIS:HB3	2.15	0.46
1:A:126:LYS:NZ	1:A:126:LYS:HB3	2.30	0.46
1:B:133:LEU:HD23	1:B:133:LEU:C	2.36	0.46
1:A:103:THR:HG21	1:A:116:PRO:CB	2.23	0.46
1:A:266:MET:CE	1:A:272:ARG:HH12	2.28	0.46
1:B:81:ILE:HD11	1:B:475:LEU:CD2	2.45	0.46
1:A:385:ILE:O	1:A:389:VAL:HG23	2.15	0.46
1:B:270:THR:CG2	1:B:271:ILE:N	2.79	0.46
1:B:301:LEU:HG	1:B:303:LEU:HD21	1.98	0.46
1:B:132:GLU:C	1:B:135:PRO:HD2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:ILE:HD12	1:B:494:ILE:N	2.31	0.46
1:A:267:PRO:HD2	7:A:1116:HOH:O	2.16	0.45
1:A:327:HIS:CG	1:A:328:PRO:HD2	2.51	0.45
1:A:434:SER:OG	1:A:467:THR:HB	2.17	0.45
1:B:346:VAL:HB	1:B:363:PHE:CE1	2.52	0.45
1:A:177:LEU:O	1:A:181:ILE:HG13	2.17	0.45
1:B:107:LYS:HB2	1:B:107:LYS:HZ2	1.80	0.45
1:A:154:GLU:CD	1:A:154:GLU:N	2.71	0.44
1:A:252:ARG:HD3	1:A:359:PRO:HB2	1.99	0.44
1:B:159:ARG:O	1:B:163:VAL:HG23	2.17	0.44
1:A:89:ILE:CG2	1:A:90:LEU:N	2.79	0.44
1:B:303:LEU:O	1:B:310:PRO:HA	2.17	0.44
1:A:434:SER:OG	1:A:469:VAL:HG23	2.17	0.44
1:A:260:ARG:HH21	1:A:277:THR:HG23	1.82	0.44
1:B:258:LEU:HB2	1:B:345:ALA:HB3	1.98	0.44
1:B:244:ARG:HD2	1:B:357:GLU:OE2	2.17	0.44
1:B:100:SER:HB3	1:B:101:ASP:H	1.58	0.44
1:B:254:TRP:CE3	1:B:283:LEU:HD21	2.52	0.44
1:A:254:TRP:HE3	1:A:283:LEU:HD21	1.82	0.44
1:B:272:ARG:HD2	7:B:2061:HOH:O	2.18	0.44
1:A:78:TYR:C	1:A:78:TYR:CD1	2.90	0.44
1:B:254:TRP:HE3	1:B:283:LEU:HD21	1.82	0.44
1:A:152:LYS:HE2	1:A:155:GLU:OE2	2.17	0.43
1:B:92:ASP:CG	1:B:475:LEU:HD12	2.38	0.43
1:A:348:ASN:HD22	1:A:348:ASN:H	1.66	0.43
1:A:267:PRO:HB2	7:A:1116:HOH:O	2.19	0.43
1:A:152:LYS:HE2	1:A:155:GLU:CD	2.39	0.43
1:B:78:TYR:CD1	1:B:78:TYR:C	2.92	0.43
1:B:289:TRP:CE2	1:B:300:PRO:HD3	2.53	0.43
1:A:121:ARG:HA	1:A:121:ARG:HD3	1.72	0.43
1:B:466:ILE:O	1:B:466:ILE:HG22	2.18	0.43
1:B:348:ASN:N	1:B:348:ASN:HD22	2.17	0.43
1:A:260:ARG:HE	1:A:277:THR:CG2	2.32	0.42
1:B:437:PHE:CE2	1:B:458:LEU:HD13	2.54	0.42
1:A:248:LYS:HB3	1:A:248:LYS:HZ2	1.82	0.42
1:A:487:ILE:N	1:A:487:ILE:CD1	2.82	0.42
1:A:466:ILE:HG22	1:A:466:ILE:O	2.18	0.42
1:A:417:LEU:O	1:A:421:GLN:HG3	2.19	0.42
1:B:81:ILE:HD11	1:B:475:LEU:HD21	2.01	0.42
1:A:159:ARG:HA	7:A:1188:HOH:O	2.19	0.42
1:A:230:ASN:ND2	1:A:233:ASN:HB3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ASN:HD22	1:A:348:ASN:N	2.18	0.42
1:B:487:ILE:HD12	1:B:487:ILE:H	1.85	0.42
1:A:130:LEU:C	1:A:130:LEU:HD23	2.39	0.42
1:A:180:LEU:O	1:A:184:THR:HG23	2.20	0.42
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.54	0.42
1:A:371:GLU:OE1	6:A:902:ARG:N	2.53	0.42
1:A:438:MET:CE	1:A:469:VAL:HA	2.50	0.42
1:A:268:ASP:OD1	1:A:270:THR:N	2.49	0.42
1:B:111:GLY:O	1:B:456:ILE:HD12	2.20	0.42
1:B:258:LEU:HD13	1:B:347:ALA:HB2	2.00	0.42
1:B:330:TYR:HB3	1:B:332:TRP:CE2	2.55	0.41
1:A:480:SER:HA	1:A:481:PRO:C	2.41	0.41
1:B:133:LEU:HD23	1:B:133:LEU:O	2.19	0.41
1:B:239:THR:O	1:B:361:CYS:HA	2.19	0.41
1:B:209:ARG:O	1:B:242:PRO:HG3	2.21	0.41
1:B:344:PRO:O	1:B:344:PRO:HG2	2.20	0.41
1:B:153:ILE:N	1:B:154:GLU:OE1	2.54	0.41
1:A:397:THR:O	1:A:397:THR:CG2	2.69	0.41
1:B:249:HIS:HB3	1:B:306:ASP:OD1	2.21	0.41
1:A:227:TYR:CD1	1:A:227:TYR:C	2.94	0.41
1:B:161:GLU:OE2	1:B:165:LYS:NZ	2.54	0.41
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.51	0.41
1:B:438:MET:HE3	1:B:469:VAL:HA	2.02	0.41
1:B:474:MET:HB3	1:B:474:MET:HE2	1.87	0.41
1:B:180:LEU:O	1:B:184:THR:HG23	2.21	0.41
1:B:241:PHE:HB3	1:B:242:PRO:HD2	2.02	0.41
1:B:348:ASN:H	1:B:348:ASN:HD22	1.68	0.41
1:A:193:ARG:HD2	7:A:962:HOH:O	2.20	0.40
1:B:280:PHE:HD2	1:B:299:LEU:HD13	1.85	0.40
1:A:214:ALA:HB3	1:A:311:GLU:OE1	2.21	0.40
1:B:81:ILE:HG22	1:B:81:ILE:O	2.22	0.40
1:B:260:ARG:NH2	7:B:2099:HOH:O	2.54	0.40
1:A:134:LEU:O	1:A:138:ILE:HG13	2.20	0.40
1:B:258:LEU:HD12	1:B:258:LEU:HA	1.85	0.40
1:A:149:LYS:O	1:A:149:LYS:HD2	2.22	0.40
1:B:254:TRP:CZ3	1:B:490:TRP:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	417/419 (100%)	388 (93%)	27 (6%)	2 (0%)	29 41
1	B	417/419 (100%)	384 (92%)	26 (6%)	7 (2%)	9 11
All	All	834/838 (100%)	772 (93%)	53 (6%)	9 (1%)	14 20

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	THR
1	B	99	THR
1	B	150	GLU
1	B	102	PHE
1	B	105	LYS
1	B	269	GLY
1	B	464	GLY
1	A	464	GLY
1	B	369	GLY

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	367/367 (100%)	346 (94%)	21 (6%)	20 33
1	B	367/367 (100%)	350 (95%)	17 (5%)	27 43
All	All	734/734 (100%)	696 (95%)	38 (5%)	23 38

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
1	A	97	LYS
1	A	103	THR
1	A	107	LYS
1	A	119	LEU
1	A	126	LYS
1	A	128	THR
1	A	139	GLU
1	A	149	LYS
1	A	154	GLU
1	A	178	ASP
1	A	210	ASN
1	A	223	ARG
1	A	256	SER
1	A	258	LEU
1	A	272	ARG
1	A	301	LEU
1	A	348	ASN
1	A	380	THR
1	A	387	GLU
1	A	409	VAL
1	B	81	ILE
1	B	100	SER
1	B	119	LEU
1	B	128	THR
1	B	149	LYS
1	B	154	GLU
1	B	201	SER
1	B	223	ARG
1	B	233	ASN
1	B	257	GLN
1	B	258	LEU
1	B	268	ASP
1	B	301	LEU
1	B	325	MET
1	B	348	ASN
1	B	407	ARG
1	B	411	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) 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	143	GLN
1	A	174	GLN
1	A	215	GLN
1	A	219	GLN
1	A	257	GLN
1	A	334	GLN
1	A	348	ASN
1	A	418	HIS
1	A	486	GLN
1	B	142	ASN
1	B	143	GLN
1	B	174	GLN
1	B	190	ASN
1	B	202	ASN
1	B	215	GLN
1	B	219	GLN
1	B	231	ASN
1	B	233	ASN
1	B	257	GLN
1	B	348	ASN
1	B	421	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CYN	A	903	4	0,1,1	-	-	-		
5	H4B	B	1901	-	16,18,18	2.24	5 (31%)	11,26,26	4.13	7 (63%)
5	H4B	A	901	-	16,18,18	2.11	4 (25%)	11,26,26	4.12	7 (63%)
6	ARG	B	1902	-	9,10,11	0.53	0	5,11,13	0.37	0
4	HEM	B	900	7,1	41,50,50	1.38	5 (12%)	45,82,82	1.50	5 (11%)
4	HEM	A	900	2,1	41,50,50	1.37	5 (12%)	45,82,82	1.16	2 (4%)
6	ARG	A	902	-	9,10,11	0.57	0	5,11,13	0.49	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
5	H4B	B	1901	-	-	0/8/17/17	0/2/2/2
5	H4B	A	901	-	-	0/8/17/17	0/2/2/2
6	ARG	B	1902	-	-	0/8/9/11	-
4	HEM	B	900	7,1	-	4/12/54/54	-
4	HEM	A	900	2,1	-	4/12/54/54	-
6	ARG	A	902	-	-	0/8/9/11	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1901	H4B	C4-N3	5.47	1.42	1.33
5	A	901	H4B	C4-N3	5.08	1.41	1.33
5	B	1901	H4B	C4A-N5	4.47	1.47	1.38
5	A	901	H4B	C4A-N5	4.39	1.47	1.38
4	A	900	HEM	C3C-CAC	-4.07	1.39	1.47
5	B	1901	H4B	C6-N5	3.88	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	900	HEM	C3C-CAC	-3.74	1.40	1.47
5	A	901	H4B	C6-N5	3.36	1.52	1.45
4	A	900	HEM	CAB-C3B	-3.17	1.38	1.47
4	B	900	HEM	CAB-C3B	-3.03	1.39	1.47
4	B	900	HEM	C3C-C2C	-2.98	1.36	1.40
4	A	900	HEM	CBB-CAB	2.80	1.44	1.30
4	B	900	HEM	CBB-CAB	2.72	1.43	1.30
4	A	900	HEM	C3C-C2C	-2.48	1.36	1.40
5	A	901	H4B	C8A-N1	2.45	1.39	1.34
4	B	900	HEM	CBC-CAC	2.40	1.45	1.29
5	B	1901	H4B	C8A-N1	2.36	1.39	1.34
5	B	1901	H4B	C7-N8	2.33	1.48	1.44
4	A	900	HEM	CBC-CAC	2.32	1.44	1.29

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1901	H4B	C8A-C4A-C4	8.45	122.08	114.57
5	A	901	H4B	C8A-C4A-C4	8.35	121.99	114.57
5	A	901	H4B	C2-N3-C4	5.96	125.40	115.93
5	B	1901	H4B	C2-N3-C4	5.90	125.31	115.93
5	B	1901	H4B	N1-C2-N3	-5.28	117.13	125.42
5	A	901	H4B	N1-C2-N3	-5.21	117.25	125.42
4	B	900	HEM	C2C-C3C-C4C	-4.28	103.91	106.90
4	B	900	HEM	C4B-CHC-C1C	4.26	128.18	122.56
5	A	901	H4B	C2-N1-C8A	3.64	122.69	114.54
5	A	901	H4B	N2-C2-N1	3.59	122.83	117.25
5	B	1901	H4B	C2-N1-C8A	3.59	122.58	114.54
5	A	901	H4B	C4A-C4-N3	-3.49	114.08	124.01
5	B	1901	H4B	C4A-C4-N3	-3.49	114.10	124.01
5	B	1901	H4B	N2-C2-N1	3.47	122.64	117.25
5	A	901	H4B	C4A-N5-C6	-3.21	112.44	121.16
5	B	1901	H4B	C4A-N5-C6	-3.08	112.77	121.16
4	B	900	HEM	CHC-C4B-NB	-3.05	121.12	124.43
4	A	900	HEM	C4C-CHD-C1D	2.86	126.33	122.56
4	A	900	HEM	C4B-CHC-C1C	2.84	126.31	122.56
4	B	900	HEM	C4C-CHD-C1D	2.61	126.01	122.56
4	B	900	HEM	CAB-C3B-C2B	-2.14	121.56	128.60

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	900	HEM	C2B-C3B-CAB-CBB
4	A	900	HEM	C4B-C3B-CAB-CBB
4	B	900	HEM	CAD-CBD-CGD-O2D
4	A	900	HEM	CAA-CBA-CGA-O2A
4	B	900	HEM	CAA-CBA-CGA-O2A
4	B	900	HEM	CAD-CBD-CGD-O1D
4	A	900	HEM	CAA-CBA-CGA-O1A
4	B	900	HEM	CAA-CBA-CGA-O1A

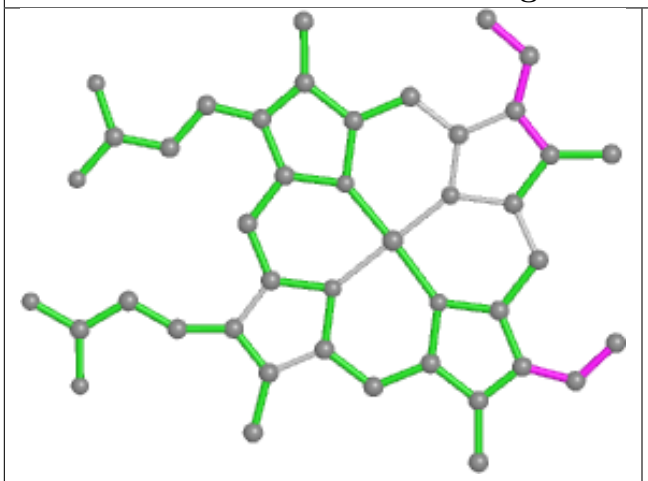
There are no ring outliers.

4 monomers are involved in 6 short contacts:

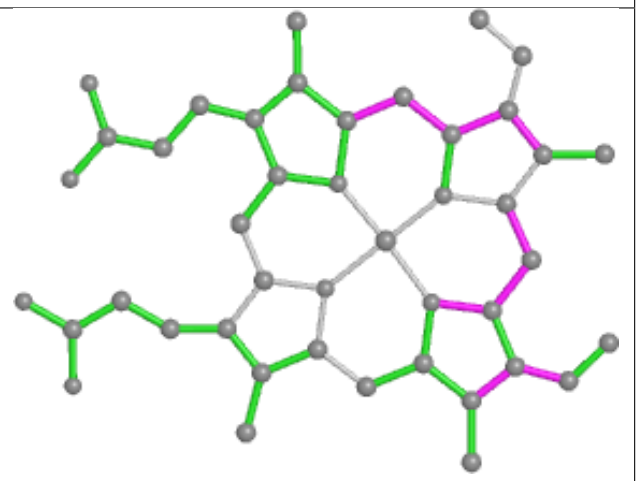
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	903	CYN	1	0
4	B	900	HEM	3	0
4	A	900	HEM	1	0
6	A	902	ARG	2	0

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 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.

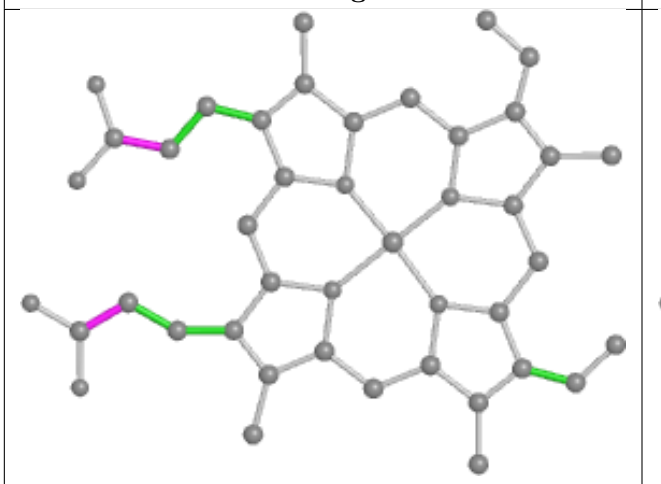
Ligand HEM B 900



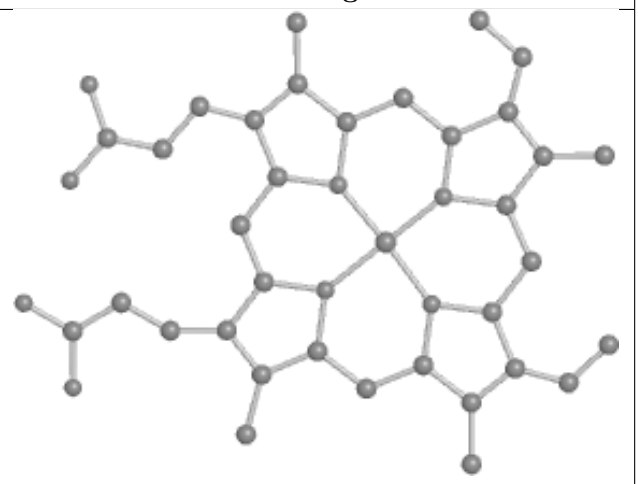
Bond lengths



Bond angles

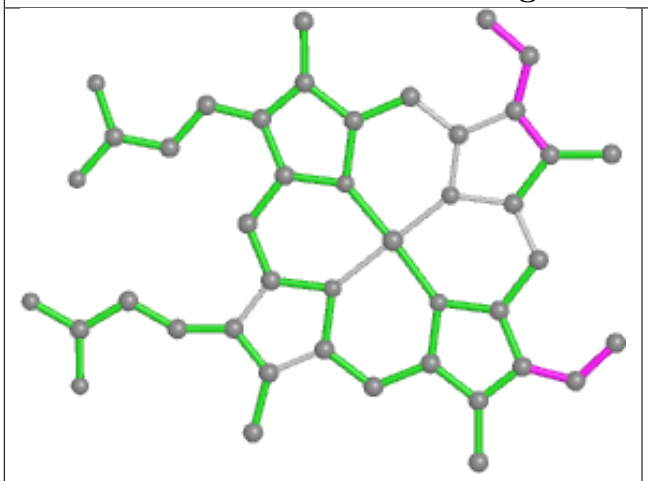


Torsions

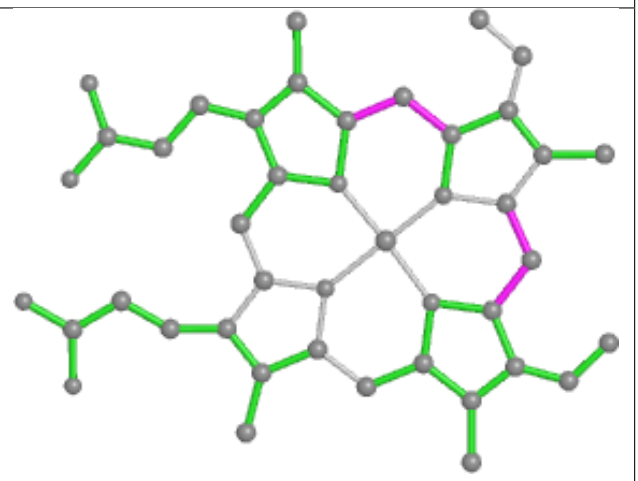


Rings

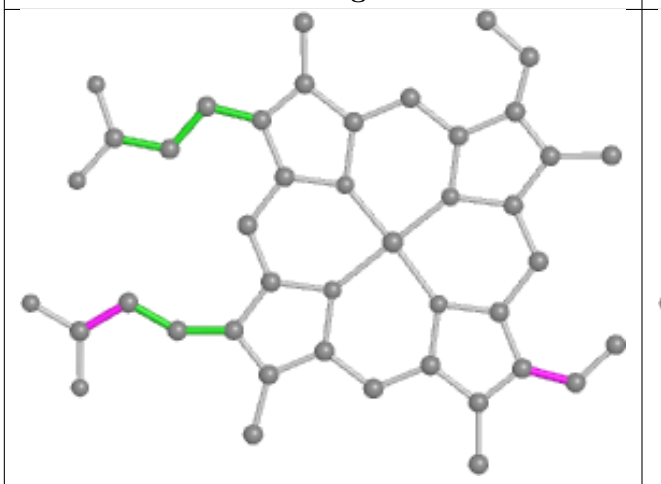
Ligand HEM A 900



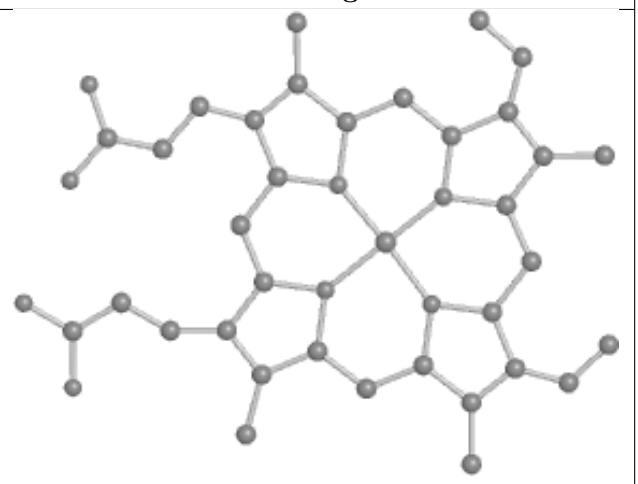
Bond lengths



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	419/419 (100%)	-0.18	14 (3%)	46	45	32, 46, 66, 85	0
1	B	419/419 (100%)	-0.22	14 (3%)	46	45	31, 46, 67, 84	0
All	All	838/838 (100%)	-0.20	28 (3%)	46	45	31, 46, 67, 85	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	SER	5.8
1	B	106	SER	5.5
1	A	77	GLN	3.7
1	A	101	ASP	3.5
1	A	100	SER	3.4
1	A	103	THR	3.3
1	B	150	GLU	3.2
1	B	103	THR	3.1
1	A	494	ILE	3.0
1	B	270	THR	3.0
1	A	102	PHE	2.9
1	B	268	ASP	2.8
1	B	495	TRP	2.7
1	A	270	THR	2.7
1	B	100	SER	2.6
1	A	107	LYS	2.6
1	A	149	LYS	2.4
1	A	495	TRP	2.4
1	B	77	GLN	2.2
1	A	268	ASP	2.2
1	B	101	ASP	2.2
1	B	494	ILE	2.1
1	A	87	GLY	2.1
1	A	105	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	105	LYS	2.1
1	B	149	LYS	2.0
1	B	104	CYS	2.0
1	B	267	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

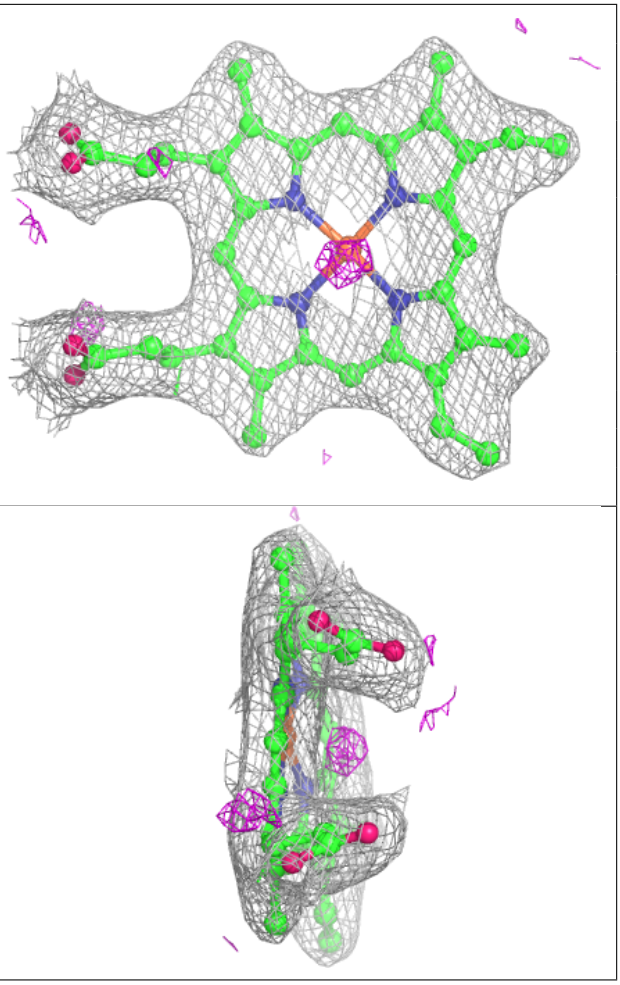
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

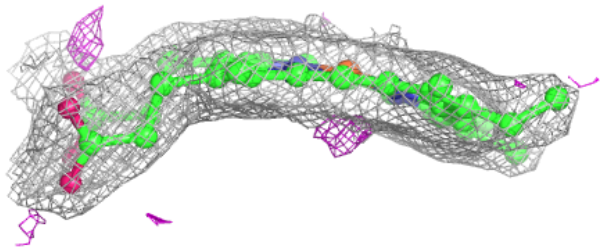
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ARG	A	902	11/12	0.87	0.17	46,50,53,54	0
6	ARG	B	1902	11/12	0.88	0.19	50,54,59,59	0
3	ZN	B	950	1/1	0.95	0.23	46,46,46,46	1
3	ZN	A	950	1/1	0.96	0.25	46,46,46,46	1
2	CYN	A	903	2/2	0.97	0.15	38,38,38,40	0
5	H4B	A	901	17/17	0.98	0.09	29,32,35,36	0
5	H4B	B	1901	17/17	0.98	0.09	33,35,38,42	0
4	HEM	A	900	43/43	0.98	0.11	30,35,38,40	0
4	HEM	B	900	43/43	0.98	0.10	32,35,37,41	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 HEM A 900:

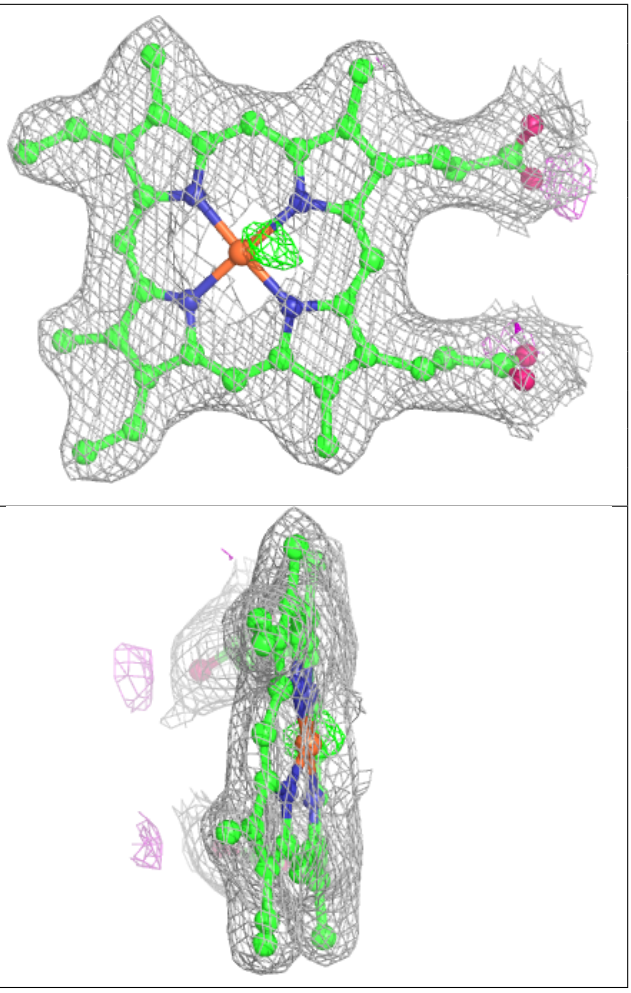
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEM B 900:

$2mF_o$-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.