Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 09:46 AM EDT

PDB ID	:	3DWJ
Title	:	Heme-proximal W188H mutant of inducible nitric oxide synthase
Authors	:	Tejero, J.; Biswas, A.; Wang, Z.-Q.; Haque, M.M.; Hemann, C.; Zweier, J.L.; Page, R.C.; Misra, S.; Stuehr, D.J.
Deposited on	:	2008-07-22
Resolution	:	2.75 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:

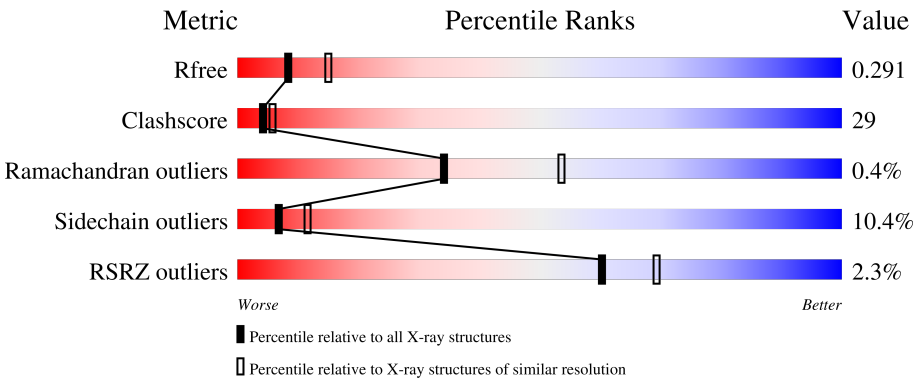
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	431	2% 52% 37% 6% 5%
1	B	431	2% 52% 37% 6% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7127 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.

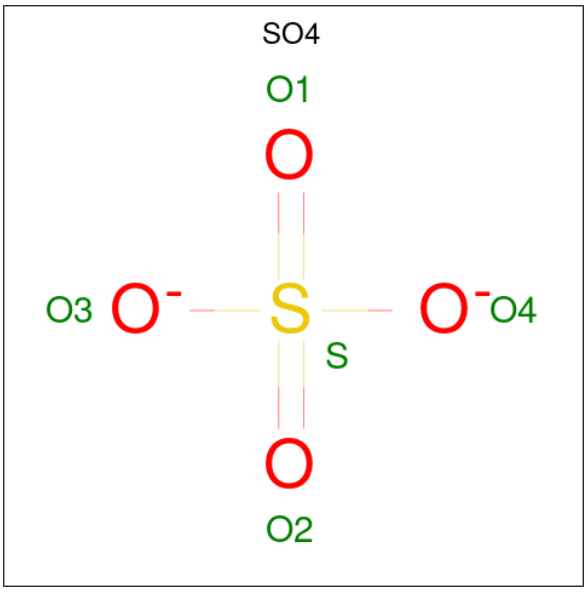
- Molecule 1 is a protein called Nitric oxide synthase, inducible.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	408	3331	2135	576	601	19	0	0	0
1	B	412	3346	2143	579	604	20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

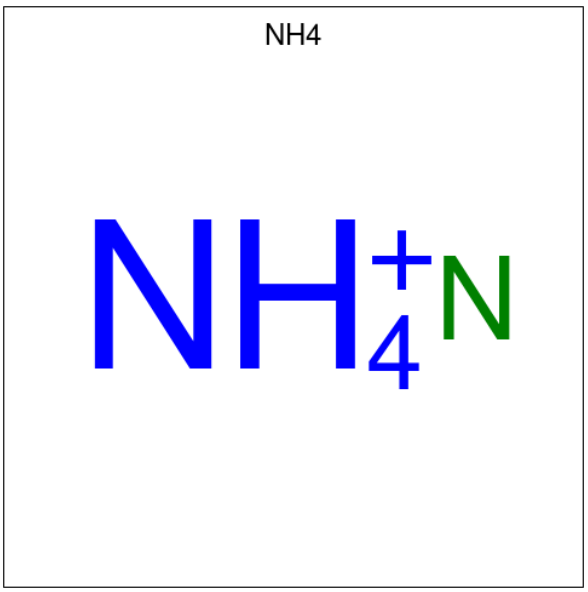
Chain	Residue	Modelled	Actual	Comment	Reference
A	188	HIS	TRP	engineered mutation	UNP P29477
B	188	HIS	TRP	engineered mutation	UNP P29477

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



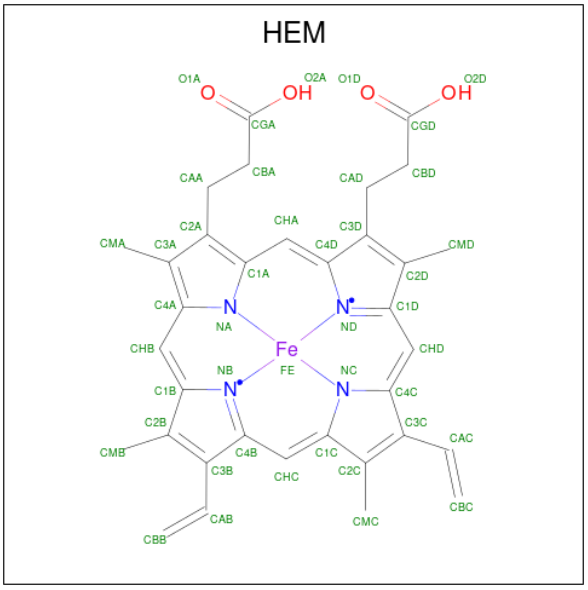
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



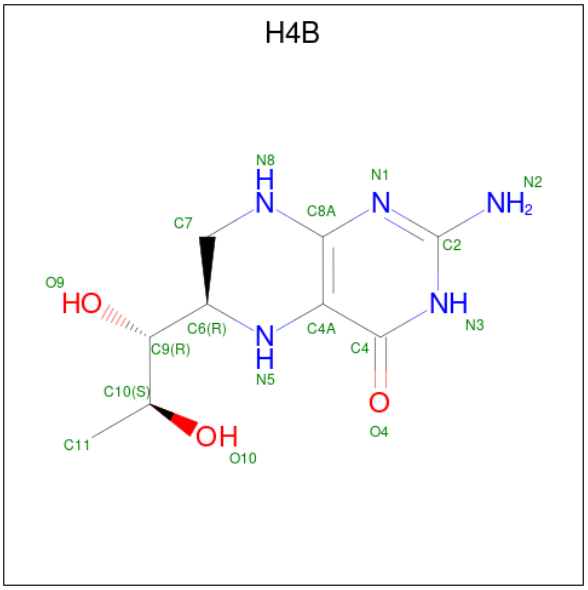
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 1 1	0	0
3	B	1	Total N 1 1	0	0

- 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
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 water.

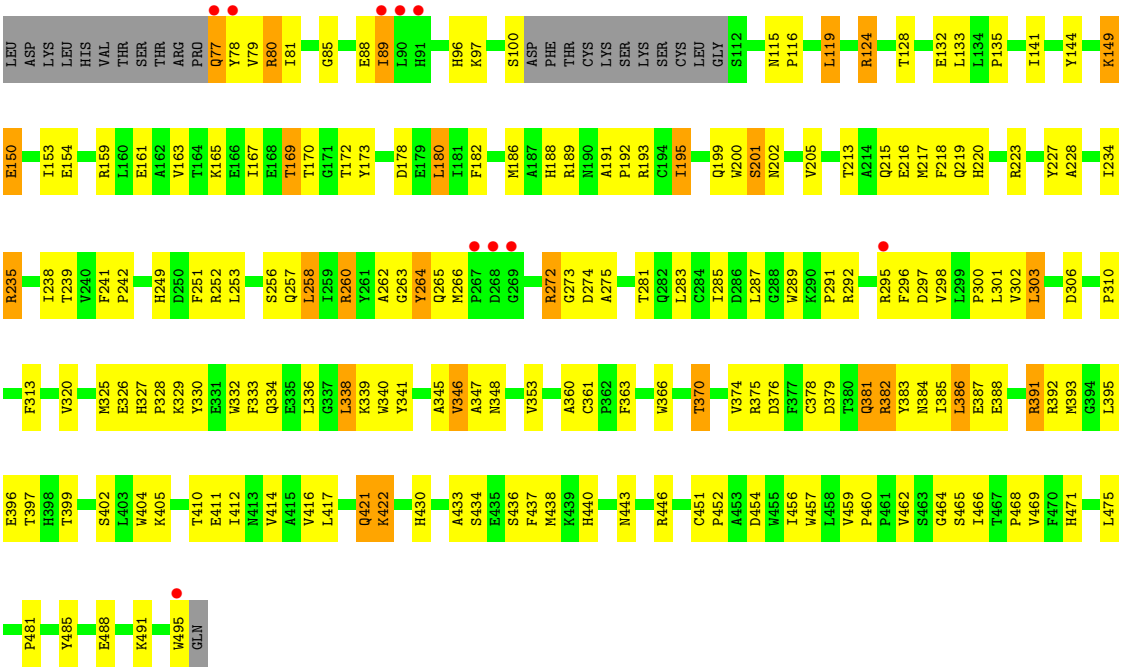
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	147	147	147	0	0
6	B	176	176	176	0	0

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.

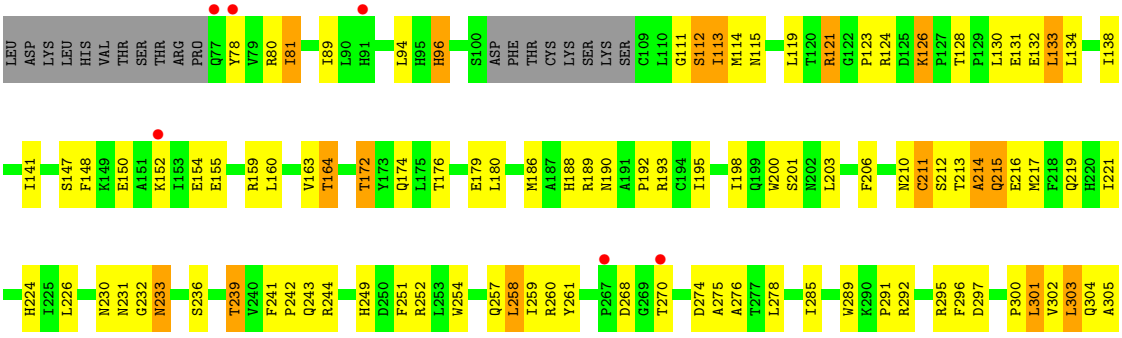
• Molecule 1: Nitric oxide synthase, inducible

Chain A: 2% 52% 37% 6% 5%



• Molecule 1: Nitric oxide synthase, inducible

Chain B: 2% 52% 37% 6%



D306 G307 Q308 V312 F313 P316 P317 D318 L319 V320 L321 T324 M325 E326 H327 P328 K329 Y330 E331 W332 F333 Q334 E335 L336 G337 L338 K339 W340 Y341 A345 N348 L351 G355 F358 P359 A360 N364 Y367 M368 E371 V374 R375 C378 D379 T380 Q381 R382
Y383 L386 E387 E388 V389 G390 R391 R392 M393 G394 L395 E396 T397 H398 T399 S402 R407 A408 V409 T410 E411 I412 N413 V414 A415 V416 L417 K422 Q423 N424 V425 A433 S434 M438 K439 H440 M441 Q442 W457 L458 V459 P460 P461 G464 S465 P468 V469 F470 H471 Q472 E473
M474 L475 F482 Q486 I487 E488 P489 T492 H493 I494 W495 Q496

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	214.60Å 214.60Å 111.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.77 – 2.75 43.77 – 2.75	Depositor EDS
% Data completeness (in resolution range)	92.3 (43.77-2.75) 94.5 (43.77-2.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.77Å)	Xtriage
Refinement program	PHENIX phenix	Depositor
R, R_{free}	0.226 , 0.294 0.224 , 0.291	Depositor DCC
R_{free} test set	1898 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7127	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: NH4, H4B, SO4, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.43	0/3428	0.69	5/4660 (0.1%)
1	B	0.46	1/3443 (0.0%)	0.73	8/4683 (0.2%)
All	All	0.45	1/6871 (0.0%)	0.71	13/9343 (0.1%)

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	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382	ARG	C-N	-5.81	1.20	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	215	GLN	N-CA-CB	13.03	134.05	110.60
1	A	495	TRP	CB-CA-C	-11.46	87.47	110.40
1	B	113	ILE	N-CA-CB	-11.37	84.64	110.80
1	A	150	GLU	N-CA-CB	-10.55	91.61	110.60
1	B	215	GLN	N-CA-C	-9.37	85.70	111.00
1	B	112	SER	CB-CA-C	-7.56	95.74	110.10
1	B	383	TYR	N-CA-CB	7.12	123.41	110.60
1	B	214	ALA	N-CA-CB	6.55	119.28	110.10
1	B	112	SER	N-CA-C	6.34	128.12	111.00
1	A	150	GLU	CB-CA-C	-6.27	97.86	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	382	ARG	O-C-N	-6.03	113.05	122.70
1	A	329	LYS	CB-CA-C	5.39	121.18	110.40
1	A	149	LYS	N-CA-C	5.05	124.65	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	ARG	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	3331	0	3230	182	1
1	B	3346	0	3230	203	6
2	A	5	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
4	A	43	0	30	7	0
4	B	43	0	30	7	0
5	A	17	0	15	2	0
5	B	17	0	15	1	0
6	A	147	0	0	45	2
6	B	176	0	0	47	13
All	All	7127	0	6550	392	15

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 29.

All (392) 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:396:GLU:CB	6:B:1193:HOH:O	1.70	1.29
1:A:195:ILE:HD11	6:A:1006:HOH:O	1.11	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASP:HB2	6:A:1048:HOH:O	1.09	1.21
1:B:216:GLU:OE1	6:B:1189:HOH:O	1.52	1.21
1:A:124:ARG:NH2	6:A:1015:HOH:O	1.71	1.21
1:A:462:VAL:HB	6:A:1028:HOH:O	1.37	1.19
1:B:213:THR:OG1	1:B:216:GLU:HB2	1.41	1.17
1:B:216:GLU:HB2	6:B:1189:HOH:O	1.44	1.14
1:A:382:ARG:NH1	6:A:977:HOH:O	1.78	1.11
1:A:326:GLU:OE2	1:A:422:LYS:HE3	1.52	1.08
1:A:334:GLN:OE1	6:A:1039:HOH:O	1.71	1.06
1:B:213:THR:O	6:B:1040:HOH:O	1.71	1.06
1:A:77:GLN:O	6:A:992:HOH:O	1.77	1.02
1:A:235:ARG:HG3	1:A:235:ARG:HH11	1.26	1.00
1:B:132:GLU:OE1	6:B:1142:HOH:O	1.79	1.00
1:A:169:THR:HG22	1:A:170:THR:HG23	1.44	0.99
1:B:386:LEU:HB2	6:B:1165:HOH:O	1.62	0.98
1:B:396:GLU:OE2	6:B:1110:HOH:O	1.80	0.97
1:A:297:ASP:CB	6:A:1048:HOH:O	1.79	0.97
1:B:471:HIS:NE2	6:B:1135:HOH:O	1.98	0.97
1:B:371:GLU:OE1	6:B:1155:HOH:O	1.84	0.94
1:A:213:THR:OG1	1:A:216:GLU:HG3	1.68	0.94
1:B:132:GLU:CB	6:B:1152:HOH:O	2.14	0.94
1:A:381:GLN:HB3	6:A:1046:HOH:O	1.67	0.93
1:B:132:GLU:HB2	6:B:1152:HOH:O	1.69	0.93
1:A:266:MET:O	6:A:1013:HOH:O	1.85	0.93
1:B:396:GLU:HB2	6:B:1193:HOH:O	1.41	0.91
1:B:195:ILE:HG21	1:B:368:MET:HE3	1.51	0.91
1:A:376:ASP:OD1	1:A:382:ARG:NH2	2.04	0.90
1:B:214:ALA:O	1:B:313:PHE:CZ	2.24	0.90
1:B:213:THR:OG1	1:B:216:GLU:CB	2.19	0.90
1:A:201:SER:HA	6:A:922:HOH:O	1.72	0.89
1:B:96:HIS:ND1	6:B:1153:HOH:O	2.05	0.89
1:B:321:LEU:HD12	6:B:1180:HOH:O	1.73	0.87
1:A:80:ARG:NH2	6:A:954:HOH:O	1.69	0.86
1:B:224:HIS:HD1	1:B:239:THR:HG22	1.39	0.86
1:B:285:ILE:HD12	1:B:291:PRO:HD3	1.55	0.86
1:B:150:GLU:HG2	6:B:1179:HOH:O	1.72	0.86
1:A:274:ASP:OD1	6:A:1003:HOH:O	1.94	0.85
1:A:124:ARG:NE	6:A:1047:HOH:O	2.09	0.85
1:A:165:LYS:O	1:A:169:THR:HB	1.77	0.84
1:B:141:ILE:HD11	1:B:163:VAL:HG21	1.60	0.83
1:B:224:HIS:HD1	1:B:239:THR:CG2	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:THR:HG21	1:B:133:LEU:CD1	2.09	0.83
1:A:274:ASP:OD2	6:A:1003:HOH:O	1.96	0.83
1:A:100:SER:O	6:A:1020:HOH:O	1.96	0.82
1:A:85:GLY:HA2	6:A:1046:HOH:O	1.79	0.81
1:A:274:ASP:CG	6:A:1003:HOH:O	2.19	0.81
1:A:116:PRO:HG2	1:A:119:LEU:HB2	1.61	0.80
1:B:132:GLU:OE2	6:B:1152:HOH:O	1.98	0.80
1:A:385:ILE:HD11	1:A:412:ILE:HD13	1.64	0.79
1:B:396:GLU:N	6:B:1193:HOH:O	2.16	0.78
1:A:159:ARG:O	1:A:163:VAL:HG23	1.84	0.78
1:A:393:MET:HB3	1:A:395:LEU:HD13	1.65	0.78
1:A:150:GLU:HB2	6:A:1012:HOH:O	1.83	0.78
1:A:161:GLU:O	1:A:165:LYS:HG2	1.84	0.77
1:B:128:THR:CB	1:B:133:LEU:HD13	2.14	0.77
1:A:436:SER:HB3	6:A:913:HOH:O	1.85	0.77
1:B:396:GLU:HB3	6:B:1193:HOH:O	1.52	0.76
1:A:382:ARG:NH2	6:A:1032:HOH:O	2.17	0.76
1:B:128:THR:CG2	1:B:133:LEU:HD13	2.16	0.76
1:A:169:THR:CG2	1:A:170:THR:HG23	2.15	0.76
1:A:438:MET:HE2	1:A:469:VAL:HG12	1.68	0.76
1:A:260:ARG:HB3	6:A:1000:HOH:O	1.85	0.76
1:B:214:ALA:O	1:B:313:PHE:HZ	1.68	0.76
1:B:128:THR:HG21	1:B:133:LEU:HD13	1.68	0.75
1:B:124:ARG:NH1	6:B:1146:HOH:O	2.18	0.74
1:B:471:HIS:CD2	6:B:1135:HOH:O	2.40	0.73
1:A:77:GLN:HE21	1:A:78:TYR:N	1.85	0.73
1:B:332:TRP:HE3	1:B:392:ARG:NH1	1.87	0.73
1:A:376:ASP:OD1	1:A:382:ARG:CZ	2.37	0.72
1:A:85:GLY:HA2	1:A:381:GLN:HE21	1.53	0.72
1:A:260:ARG:HD2	6:A:975:HOH:O	1.88	0.72
1:A:200:TRP:CE3	6:A:922:HOH:O	2.43	0.72
4:B:901:HEM:O1A	6:B:1151:HOH:O	2.08	0.71
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.19	0.71
1:B:126:LYS:HE2	6:B:1146:HOH:O	1.89	0.71
1:B:128:THR:HB	1:B:133:LEU:HD13	1.70	0.71
1:B:80:ARG:HE	1:B:89:ILE:HD13	1.55	0.70
1:A:275:ALA:HB3	1:A:381:GLN:O	1.91	0.70
1:A:262:ALA:HB3	6:A:1048:HOH:O	1.91	0.69
1:A:417:LEU:O	1:A:421:GLN:HG2	1.91	0.69
1:A:89:ILE:HD13	1:A:89:ILE:H	1.57	0.69
1:A:438:MET:CE	1:A:469:VAL:HA	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:THR:OG1	1:A:216:GLU:CG	2.41	0.68
1:B:96:HIS:CE1	6:B:1153:HOH:O	2.42	0.68
1:B:252:ARG:NH2	1:B:489:PRO:HD3	2.09	0.68
1:A:438:MET:HE2	1:A:469:VAL:CG1	2.23	0.68
1:B:114:MET:O	6:B:1080:HOH:O	2.12	0.68
1:A:438:MET:CE	1:A:469:VAL:HG12	2.24	0.67
1:A:375:ARG:HH21	5:A:902:H4B:C4	2.08	0.67
1:B:128:THR:HG21	1:B:133:LEU:HD12	1.75	0.67
1:B:410:THR:O	1:B:414:VAL:HG13	1.95	0.67
1:A:410:THR:O	1:A:414:VAL:HG23	1.95	0.66
1:B:494:ILE:HD11	6:B:1094:HOH:O	1.94	0.66
1:B:390:GLY:HA2	6:B:1037:HOH:O	1.96	0.66
4:A:901:HEM:HBB2	6:A:1025:HOH:O	1.96	0.66
1:A:213:THR:HG1	1:A:216:GLU:HG3	1.60	0.66
1:A:235:ARG:HG3	1:A:235:ARG:NH1	1.97	0.66
1:A:433:ALA:O	6:A:913:HOH:O	2.14	0.66
1:A:153:ILE:HD12	1:A:153:ILE:H	1.59	0.66
1:A:235:ARG:HH11	1:A:235:ARG:CG	2.07	0.65
1:A:289:TRP:CE2	1:A:300:PRO:HD3	2.31	0.65
1:B:325:MET:HE3	1:B:325:MET:HA	1.79	0.65
1:B:334:GLN:CG	6:B:1104:HOH:O	2.44	0.65
1:B:210:ASN:O	1:B:210:ASN:CG	2.30	0.65
3:A:497:NH4:N	6:A:1043:HOH:O	2.30	0.64
1:A:326:GLU:OE2	1:A:422:LYS:CE	2.39	0.64
1:A:201:SER:CA	6:A:922:HOH:O	2.39	0.62
1:B:334:GLN:HG2	6:B:1104:HOH:O	1.98	0.62
1:B:211:CYS:SG	6:B:1040:HOH:O	2.56	0.62
1:B:396:GLU:HG3	1:B:399:THR:HB	1.81	0.62
1:B:244:ARG:HA	6:B:1072:HOH:O	1.99	0.62
1:B:148:PHE:HE1	1:B:152:LYS:HD2	1.65	0.62
1:A:303:LEU:O	1:A:310:PRO:HA	2.00	0.62
1:A:85:GLY:HA2	1:A:381:GLN:NE2	2.15	0.61
1:A:375:ARG:NH2	5:A:902:H4B:O4	2.33	0.61
1:B:292:ARG:HB2	1:B:297:ASP:OD2	2.00	0.61
1:B:188:HIS:CD2	4:B:901:HEM:C4C	2.88	0.61
1:A:217:MET:HE3	1:A:303:LEU:HB3	1.83	0.61
1:A:223:ARG:HD3	6:A:956:HOH:O	1.99	0.61
1:A:285:ILE:HD12	1:A:291:PRO:HG3	1.83	0.61
1:A:465:SER:O	1:A:471:HIS:HE1	1.84	0.61
1:B:132:GLU:HB3	6:B:1152:HOH:O	1.90	0.61
1:A:265:GLN:HG3	1:A:265:GLN:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:LEU:HD11	1:B:164:THR:HG23	1.82	0.61
4:B:901:HEM:HMC1	4:B:901:HEM:HBC2	1.83	0.61
1:A:149:LYS:HG2	1:A:150:GLU:HG3	1.83	0.60
1:B:226:LEU:HD23	1:B:226:LEU:O	2.02	0.60
1:B:408:ALA:O	1:B:412:ILE:HG13	2.00	0.60
1:B:422:LYS:CG	1:B:423:GLN:HG3	2.32	0.60
1:A:375:ARG:NH1	1:A:379:ASP:OD1	2.34	0.60
1:A:393:MET:CE	1:A:411:GLU:HG3	2.32	0.60
1:A:199:GLN:HE22	1:A:202:ASN:HD22	1.50	0.60
1:B:148:PHE:CE1	1:B:152:LYS:HD2	2.37	0.60
1:B:188:HIS:CD2	4:B:901:HEM:C3C	2.89	0.59
1:B:388:GLU:HA	1:B:388:GLU:OE2	2.02	0.59
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.31	0.59
1:B:334:GLN:C	1:B:336:LEU:H	2.06	0.58
1:B:141:ILE:CD1	1:B:163:VAL:HG21	2.32	0.58
1:B:465:SER:O	1:B:471:HIS:HE1	1.86	0.58
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.85	0.58
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.85	0.58
1:B:381:GLN:H	1:B:381:GLN:NE2	2.02	0.58
4:B:901:HEM:HBC2	4:B:901:HEM:CMC	2.34	0.58
1:B:193:ARG:HD3	1:B:457:TRP:CD2	2.38	0.58
1:A:382:ARG:NE	6:A:1003:HOH:O	2.36	0.58
1:B:190:ASN:O	1:B:192:PRO:HD3	2.04	0.58
1:B:215:GLN:HE21	1:B:219:GLN:HE21	1.50	0.58
1:B:340:TRP:HZ3	1:B:383:TYR:CE1	2.22	0.57
1:A:217:MET:CE	1:A:303:LEU:HB3	2.35	0.57
1:B:381:GLN:HE21	1:B:381:GLN:N	2.03	0.57
1:B:232:GLY:O	1:B:425:VAL:HA	2.04	0.57
1:B:396:GLU:CG	1:B:399:THR:HB	2.34	0.57
1:A:216:GLU:HG2	6:A:1010:HOH:O	2.04	0.57
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.40	0.57
1:B:334:GLN:C	1:B:336:LEU:N	2.59	0.56
1:B:375:ARG:NH1	1:B:379:ASP:OD2	2.38	0.56
1:B:368:MET:CE	1:B:433:ALA:HB1	2.36	0.56
1:A:391:ARG:NH1	6:A:1021:HOH:O	1.88	0.56
1:B:141:ILE:HD13	1:B:159:ARG:HG3	1.88	0.56
1:B:368:MET:CE	1:B:433:ALA:CB	2.83	0.56
1:B:261:TYR:CE1	1:B:296:PHE:HB3	2.42	0.55
1:A:200:TRP:CD2	6:A:922:HOH:O	2.59	0.55
1:B:434:SER:HB3	1:B:468:PRO:HD2	1.87	0.55
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:PHE:HE1	6:B:1160:HOH:O	1.89	0.55
1:A:438:MET:HE3	1:A:469:VAL:HA	1.89	0.54
1:B:126:LYS:HD3	1:B:126:LYS:N	2.22	0.54
1:A:393:MET:HE3	1:A:411:GLU:HG3	1.87	0.54
1:B:348:ASN:HD22	1:B:348:ASN:H	1.56	0.54
1:A:485:TYR:OH	4:A:901:HEM:O2D	2.15	0.54
1:B:333:PHE:O	1:B:336:LEU:HB2	2.08	0.54
1:A:327:HIS:CE1	1:A:328:PRO:HD2	2.41	0.53
1:A:327:HIS:ND1	1:A:328:PRO:HD2	2.23	0.53
1:B:217:MET:HG2	1:B:241:PHE:CE2	2.43	0.53
1:A:163:VAL:HG13	1:A:173:TYR:CD2	2.43	0.53
1:A:218:PHE:HB2	1:A:303:LEU:CD2	2.38	0.53
1:A:333:PHE:O	1:A:336:LEU:HB2	2.09	0.53
1:A:370:THR:HG21	1:A:430:HIS:HB3	1.91	0.53
1:B:334:GLN:O	1:B:336:LEU:N	2.41	0.53
1:A:292:ARG:HB2	1:A:297:ASP:OD2	2.09	0.53
1:B:318:ASP:HB2	6:B:1190:HOH:O	2.08	0.53
1:B:80:ARG:NE	1:B:89:ILE:HD13	2.21	0.52
1:A:133:LEU:HD22	1:A:167:ILE:CD1	2.40	0.52
1:A:260:ARG:HA	1:A:341:TYR:CE1	2.44	0.52
1:B:340:TRP:CZ3	1:B:383:TYR:CE1	2.98	0.52
1:B:367:TYR:HD2	6:B:1169:HOH:O	1.92	0.52
1:A:77:GLN:NE2	1:A:78:TYR:N	2.56	0.52
1:A:217:MET:HG2	1:A:241:PHE:CE1	2.44	0.52
1:A:266:MET:SD	1:A:272:ARG:HD2	2.50	0.52
1:A:434:SER:HB3	1:A:468:PRO:HD2	1.92	0.52
1:A:283:LEU:O	1:A:287:LEU:HG	2.10	0.52
1:B:422:LYS:HG2	1:B:423:GLN:HG3	1.92	0.51
1:A:188:HIS:CD2	4:A:901:HEM:C3C	2.97	0.51
1:A:370:THR:CG2	1:A:430:HIS:HB3	2.40	0.51
4:A:901:HEM:HBC2	4:A:901:HEM:CMC	2.39	0.51
1:B:368:MET:HE2	1:B:433:ALA:CB	2.40	0.51
1:B:318:ASP:CG	6:B:1166:HOH:O	2.50	0.51
1:B:121:ARG:HG3	6:B:1167:HOH:O	2.11	0.51
1:B:276:ALA:HB2	6:B:1062:HOH:O	2.10	0.51
1:B:330:TYR:HB3	1:B:332:TRP:NE1	2.26	0.51
1:A:77:GLN:HG3	1:A:78:TYR:H	1.77	0.50
1:A:193:ARG:HG2	1:A:457:TRP:CG	2.46	0.50
1:A:263:GLY:HA2	1:A:272:ARG:O	2.11	0.50
1:B:217:MET:CE	1:B:305:ALA:HB2	2.42	0.50
1:A:346:VAL:HG13	1:A:363:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:HIS:O	1:A:443:ASN:HB2	2.12	0.50
1:B:304:GLN:HG3	1:B:308:GLN:O	2.12	0.50
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.92	0.50
1:A:281:THR:O	1:A:285:ILE:HG12	2.10	0.50
1:B:493:HIS:CG	1:B:494:ILE:N	2.80	0.50
1:A:264:TYR:CD1	1:A:264:TYR:N	2.79	0.50
1:B:214:ALA:O	1:B:313:PHE:CE2	2.64	0.50
1:B:210:ASN:O	1:B:210:ASN:OD1	2.30	0.50
1:B:285:ILE:HD12	1:B:291:PRO:CD	2.36	0.50
1:B:465:SER:O	1:B:471:HIS:CE1	2.64	0.50
1:A:388:GLU:O	1:A:392:ARG:HG2	2.12	0.50
1:B:133:LEU:HD11	1:B:355:GLY:O	2.11	0.50
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.46	0.49
1:B:80:ARG:HE	1:B:89:ILE:CD1	2.25	0.49
1:B:188:HIS:NE2	4:B:901:HEM:C1C	2.80	0.49
1:B:285:ILE:HD13	1:B:289:TRP:HE3	1.76	0.49
1:B:332:TRP:CE3	1:B:392:ARG:NH1	2.74	0.49
1:A:227:TYR:O	1:A:235:ARG:NH1	2.45	0.49
1:A:437:PHE:O	1:A:440:HIS:HB3	2.12	0.49
1:B:152:LYS:HE2	1:B:155:GLU:CD	2.32	0.49
1:B:316:PRO:O	1:B:319:LEU:N	2.43	0.49
1:B:303:LEU:HD13	1:B:303:LEU:N	2.27	0.49
1:B:398:HIS:HB2	6:B:1110:HOH:O	2.12	0.49
1:A:154:GLU:CD	1:A:154:GLU:H	2.15	0.49
1:A:327:HIS:CG	1:A:328:PRO:CD	2.96	0.49
1:A:336:LEU:HB3	1:A:338:LEU:HD22	1.94	0.49
1:A:188:HIS:CD2	4:A:901:HEM:C4C	3.01	0.48
1:B:134:LEU:HD11	1:B:138:ILE:HD11	1.94	0.48
1:B:224:HIS:ND1	1:B:239:THR:HG22	2.20	0.48
1:B:249:HIS:HA	1:B:307:GLY:HA3	1.95	0.48
1:A:215:GLN:O	1:A:219:GLN:HG3	2.13	0.48
4:A:901:HEM:HBC2	4:A:901:HEM:HMC1	1.95	0.48
1:B:147:SER:C	1:B:148:PHE:HD2	2.16	0.48
1:B:217:MET:HG2	1:B:241:PHE:CZ	2.48	0.48
1:B:320:VAL:HG12	1:B:320:VAL:O	2.13	0.48
1:B:438:MET:CE	1:B:469:VAL:HG12	2.43	0.48
1:A:223:ARG:NH1	6:A:974:HOH:O	2.34	0.48
1:B:148:PHE:N	1:B:148:PHE:CD2	2.82	0.48
1:B:332:TRP:HE3	1:B:392:ARG:HH11	1.58	0.48
1:B:134:LEU:CD1	1:B:138:ILE:HD11	2.43	0.48
1:B:198:ILE:HB	6:B:1162:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:MET:HE1	1:B:433:ALA:CB	2.44	0.48
1:B:422:LYS:HG3	1:B:423:GLN:HG3	1.94	0.48
1:A:178:ASP:C	6:A:916:HOH:O	2.51	0.48
1:A:251:PHE:O	1:A:252:ARG:HB3	2.14	0.48
1:B:217:MET:HB2	6:B:1040:HOH:O	2.14	0.47
1:B:289:TRP:CG	1:B:300:PRO:HG3	2.49	0.47
1:B:131:GLU:OE1	1:B:131:GLU:N	2.30	0.47
1:B:289:TRP:CD1	1:B:300:PRO:HG3	2.50	0.47
1:B:295:ARG:HB3	1:B:296:PHE:CE2	2.49	0.47
1:B:399:THR:HG22	1:B:399:THR:O	2.13	0.47
1:B:289:TRP:CE2	1:B:300:PRO:HD3	2.49	0.47
1:A:78:TYR:HD1	1:A:79:VAL:N	2.12	0.47
1:B:148:PHE:HD2	1:B:148:PHE:N	2.12	0.47
1:B:254:TRP:CE2	1:B:489:PRO:HB2	2.50	0.47
1:A:218:PHE:CE2	1:A:313:PHE:HB3	2.50	0.47
1:A:77:GLN:CG	1:A:78:TYR:H	2.26	0.47
1:A:132:GLU:O	1:A:135:PRO:HD2	2.15	0.47
1:B:221:ILE:CG2	1:B:301:LEU:HD21	2.45	0.47
1:A:393:MET:CE	1:A:411:GLU:CG	2.93	0.47
1:B:213:THR:C	1:B:215:GLN:H	2.15	0.47
1:B:368:MET:O	1:B:371:GLU:HB2	2.14	0.47
1:A:326:GLU:HB3	1:A:334:GLN:HG2	1.97	0.47
1:B:216:GLU:CB	6:B:1189:HOH:O	2.20	0.47
1:A:189:ARG:HD2	1:A:200:TRP:CZ3	2.50	0.47
1:A:216:GLU:O	1:A:220:HIS:HD2	1.97	0.47
1:A:252:ARG:HA	1:A:360:ALA:HB2	1.97	0.46
1:B:130:LEU:N	1:B:130:LEU:HD23	2.30	0.46
1:A:327:HIS:CE1	1:A:330:TYR:CD1	3.03	0.46
1:B:303:LEU:HD22	1:B:313:PHE:CD2	2.50	0.46
1:B:348:ASN:HD22	1:B:348:ASN:N	2.10	0.46
1:A:332:TRP:CH2	1:A:392:ARG:HB2	2.50	0.46
1:A:385:ILE:CD1	1:A:412:ILE:HD13	2.40	0.46
1:B:138:ILE:HG23	1:B:160:LEU:HD22	1.96	0.46
1:A:258:LEU:HD22	1:A:345:ALA:HB1	1.97	0.46
1:A:396:GLU:HA	6:A:965:HOH:O	2.14	0.46
1:B:198:ILE:HD12	1:B:440:HIS:HB2	1.98	0.46
1:B:258:LEU:HD22	1:B:345:ALA:HB1	1.98	0.46
1:A:438:MET:HE2	1:A:469:VAL:HA	1.95	0.46
1:B:275:ALA:O	1:B:278:LEU:HB2	2.16	0.46
1:A:399:THR:O	1:A:402:SER:HB3	2.16	0.45
1:A:172:THR:HG23	1:A:173:TYR:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLN:HG2	1:A:421:GLN:H	1.42	0.45
1:A:451:CYS:O	1:A:452:PRO:C	2.52	0.45
1:A:325:MET:CE	1:A:416:VAL:HG22	2.46	0.45
1:B:206:PHE:HB2	1:B:239:THR:HB	1.99	0.45
1:A:386:LEU:HD13	1:A:405:LYS:HG2	1.99	0.45
1:B:351:LEU:HB3	1:B:358:PHE:HB2	1.98	0.45
1:A:144:TYR:CE2	1:A:178:ASP:O	2.70	0.45
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.72	0.45
1:A:340:TRP:HZ3	1:A:383:TYR:CE1	2.35	0.45
1:A:438:MET:HG3	1:A:468:PRO:HB2	1.98	0.45
1:B:126:LYS:CE	6:B:1146:HOH:O	2.57	0.45
1:B:230:ASN:HB3	1:B:233:ASN:O	2.16	0.45
1:B:374:VAL:HG11	1:B:461:PRO:HB2	1.99	0.45
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.67	0.45
1:A:382:ARG:CD	6:A:1003:HOH:O	2.64	0.45
1:B:211:CYS:SG	1:B:212:SER:N	2.89	0.45
1:A:296:PHE:CE1	1:A:339:LYS:O	2.69	0.44
1:A:133:LEU:HD22	1:A:167:ILE:HD13	1.99	0.44
1:B:251:PHE:O	1:B:360:ALA:HB2	2.17	0.44
1:A:257:GLN:HG2	1:A:260:ARG:HE	1.83	0.44
1:B:80:ARG:HH21	1:B:89:ILE:HD12	1.82	0.44
1:B:81:ILE:HD13	1:B:81:ILE:HA	1.74	0.44
1:A:298:VAL:HG21	1:A:320:VAL:HG11	1.98	0.44
1:A:466:ILE:HG22	1:A:466:ILE:O	2.18	0.44
1:B:174:GLN:HA	6:B:1108:HOH:O	2.17	0.44
1:A:302:VAL:HG12	1:A:310:PRO:HB2	1.99	0.44
1:A:459:VAL:HA	1:A:460:PRO:HD3	1.85	0.44
1:B:186:MET:O	1:B:189:ARG:HB3	2.18	0.44
1:A:258:LEU:HD13	1:A:347:ALA:HB2	2.00	0.44
1:B:114:MET:O	1:B:115:ASN:OD1	2.36	0.44
1:B:134:LEU:O	1:B:138:ILE:HG12	2.18	0.44
1:B:172:THR:OG1	6:B:1161:HOH:O	2.21	0.44
1:B:495:TRP:O	1:B:496:GLN:C	2.57	0.44
1:B:154:GLU:H	1:B:154:GLU:HG2	1.51	0.43
1:A:253:LEU:HD12	1:A:253:LEU:N	2.33	0.43
1:A:395:LEU:HD23	1:A:404:TRP:HB2	2.00	0.43
1:A:257:GLN:HE21	1:A:260:ARG:NE	2.15	0.43
1:A:301:LEU:HB3	1:A:303:LEU:CD1	2.48	0.43
1:A:301:LEU:HB3	1:A:303:LEU:HD13	2.01	0.43
1:A:374:VAL:O	1:A:378:CYS:HB2	2.19	0.43
1:B:442:GLN:H	1:B:442:GLN:HG2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:MET:CB	1:A:395:LEU:HD13	2.43	0.43
1:A:96:HIS:CE1	6:A:992:HOH:O	2.70	0.43
1:B:78:TYR:CD1	1:B:78:TYR:C	2.92	0.43
1:A:182:PHE:N	6:A:916:HOH:O	2.28	0.43
1:B:215:GLN:HG3	1:B:219:GLN:HE21	1.84	0.43
1:A:273:GLY:HA2	1:A:295:ARG:HA	2.00	0.43
1:A:381:GLN:HB3	1:A:381:GLN:HE21	1.58	0.43
1:A:205:VAL:HG22	1:A:238:ILE:CG2	2.48	0.43
1:B:336:LEU:HA	1:B:336:LEU:HD12	1.81	0.43
1:B:411:GLU:OE1	1:B:411:GLU:HA	2.19	0.43
1:B:457:TRP:HA	5:B:902:H4B:N1	2.34	0.43
1:A:85:GLY:CA	6:A:1046:HOH:O	2.51	0.42
1:A:465:SER:O	1:A:471:HIS:CE1	2.67	0.42
1:B:274:ASP:OD1	1:B:274:ASP:C	2.58	0.42
1:B:89:ILE:HD11	6:B:1088:HOH:O	2.19	0.42
1:A:296:PHE:HB3	1:A:339:LYS:HE3	2.02	0.42
1:B:213:THR:C	1:B:215:GLN:N	2.72	0.42
1:B:302:VAL:C	1:B:303:LEU:HD13	2.40	0.42
1:B:224:HIS:ND1	1:B:239:THR:CG2	2.72	0.42
1:B:386:LEU:HD23	1:B:386:LEU:HA	1.89	0.42
1:B:325:MET:HA	1:B:325:MET:CE	2.46	0.42
1:B:438:MET:HG3	1:B:468:PRO:HB2	2.00	0.42
1:B:176:THR:O	1:B:179:GLU:HB2	2.20	0.42
1:B:224:HIS:NE2	1:B:364:ASN:ND2	2.68	0.42
1:B:407:ARG:NE	6:B:1185:HOH:O	1.82	0.42
1:A:124:ARG:NH1	1:A:128:THR:OG1	2.53	0.41
1:A:330:TYR:HB3	1:A:332:TRP:NE1	2.35	0.41
1:B:257:GLN:NE2	1:B:260:ARG:CD	2.82	0.41
1:B:332:TRP:CZ3	1:B:392:ARG:HB2	2.55	0.41
1:B:259:ILE:HG22	1:B:341:TYR:CG	2.55	0.41
1:B:374:VAL:O	1:B:378:CYS:HB2	2.21	0.41
1:A:186:MET:O	1:A:189:ARG:HB3	2.20	0.41
1:A:191:ALA:HA	1:A:192:PRO:HD2	1.91	0.41
1:A:417:LEU:HD11	6:A:980:HOH:O	2.20	0.41
1:A:165:LYS:NZ	6:A:1040:HOH:O	2.24	0.41
1:B:215:GLN:HG3	1:B:219:GLN:NE2	2.34	0.41
1:B:488:GLU:HA	1:B:489:PRO:HD2	1.67	0.41
1:B:211:CYS:O	1:B:212:SER:HB3	2.20	0.41
1:B:332:TRP:HE3	1:B:392:ARG:HH12	1.68	0.41
1:B:258:LEU:HB2	1:B:345:ALA:HB3	2.02	0.41
1:A:297:ASP:HB3	6:A:1048:HOH:O	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:TRP:CZ2	4:A:901:HEM:HBB1	2.56	0.41
1:A:375:ARG:NE	6:A:1001:HOH:O	1.93	0.41
1:B:123:PRO:HG3	1:B:492:THR:HG21	2.02	0.41
1:B:188:HIS:HD2	4:B:901:HEM:C4C	2.38	0.41
1:B:348:ASN:H	1:B:348:ASN:ND2	2.18	0.41
1:A:353:VAL:HB	1:A:481:PRO:HB3	2.03	0.41
1:B:268:ASP:HB2	1:B:270:THR:HG23	2.03	0.41
1:B:325:MET:CE	1:B:416:VAL:HA	2.51	0.41
1:B:393:MET:HB2	6:B:1037:HOH:O	2.21	0.41
1:B:138:ILE:HG23	1:B:160:LEU:CD2	2.51	0.41
1:A:228:ALA:O	1:A:234:ILE:HA	2.21	0.40
1:A:249:HIS:HB3	1:A:306:ASP:OD1	2.20	0.40
1:A:258:LEU:HD12	1:A:258:LEU:HA	1.89	0.40
1:B:348:ASN:N	1:B:348:ASN:ND2	2.69	0.40
1:B:111:GLY:O	1:B:112:SER:CB	2.68	0.40
1:A:374:VAL:HG11	1:A:462:VAL:HG13	2.04	0.40
1:A:454:ASP:OD1	1:A:454:ASP:C	2.59	0.40
1:A:488:GLU:HB2	1:A:491:LYS:HD2	2.04	0.40
1:A:239:THR:O	1:A:361:CYS:HA	2.20	0.40
1:B:200:TRP:CG	1:B:201:SER:N	2.90	0.40
1:B:300:PRO:HB2	1:B:312:VAL:HG13	2.04	0.40

All (15) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1028:HOH:O	6:A:1030:HOH:O[10_554]	0.33	1.87
1:B:407:ARG:NH1	6:B:1050:HOH:O[8_556]	0.44	1.76
6:B:1156:HOH:O	6:B:1156:HOH:O[8_556]	0.80	1.40
1:B:407:ARG:CZ	6:B:1050:HOH:O[8_556]	1.12	1.08
6:B:1136:HOH:O	6:B:1172:HOH:O[8_556]	1.24	0.96
6:B:1100:HOH:O	6:B:1159:HOH:O[10_555]	1.28	0.92
1:B:411:GLU:OE1	6:B:1183:HOH:O[8_556]	1.65	0.55
1:B:231:ASN:ND2	6:B:1166:HOH:O[10_555]	1.70	0.50
6:B:1100:HOH:O	6:B:1158:HOH:O[10_555]	1.74	0.46
6:B:1050:HOH:O	6:B:1183:HOH:O[8_556]	1.82	0.38
1:B:473:GLU:OE1	6:B:1144:HOH:O[8_556]	1.83	0.37
1:B:407:ARG:NE	6:B:1050:HOH:O[8_556]	1.93	0.27
6:B:1137:HOH:O	6:B:1137:HOH:O[8_556]	2.02	0.18
6:B:1141:HOH:O	6:B:1148:HOH:O[8_556]	2.05	0.15
1:A:462:VAL:CB	6:A:1030:HOH:O[10_554]	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	404/431 (94%)	365 (90%)	38 (9%)	1 (0%)	47	69
1	B	408/431 (95%)	366 (90%)	40 (10%)	2 (0%)	29	47
All	All	812/862 (94%)	731 (90%)	78 (10%)	3 (0%)	34	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	GLY
1	B	464	GLY
1	B	335	GLU

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	357/379 (94%)	321 (90%)	36 (10%)	7	12
1	B	357/379 (94%)	319 (89%)	38 (11%)	6	11
All	All	714/758 (94%)	640 (90%)	74 (10%)	7	11

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	80	ARG
1	A	81	ILE

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Mol	Chain	Res	Type
1	A	88	GLU
1	A	89	ILE
1	A	97	LYS
1	A	115	ASN
1	A	119	LEU
1	A	124	ARG
1	A	141	ILE
1	A	169	THR
1	A	180	LEU
1	A	195	ILE
1	A	201	SER
1	A	235	ARG
1	A	256	SER
1	A	258	LEU
1	A	260	ARG
1	A	264	TYR
1	A	272	ARG
1	A	303	LEU
1	A	338	LEU
1	A	346	VAL
1	A	348	ASN
1	A	370	THR
1	A	381	GLN
1	A	384	ASN
1	A	386	LEU
1	A	387	GLU
1	A	391	ARG
1	A	397	THR
1	A	421	GLN
1	A	422	LYS
1	A	446	ARG
1	A	456	ILE
1	A	475	LEU
1	B	81	ILE
1	B	94	LEU
1	B	96	HIS
1	B	113	ILE
1	B	119	LEU
1	B	121	ARG
1	B	126	LYS
1	B	133	LEU
1	B	164	THR

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Mol	Chain	Res	Type
1	B	172	THR
1	B	180	LEU
1	B	203	LEU
1	B	211	CYS
1	B	233	ASN
1	B	236	SER
1	B	239	THR
1	B	258	LEU
1	B	301	LEU
1	B	303	LEU
1	B	324	THR
1	B	325	MET
1	B	334	GLN
1	B	338	LEU
1	B	339	LYS
1	B	348	ASN
1	B	381	GLN
1	B	386	LEU
1	B	388	GLU
1	B	391	ARG
1	B	395	LEU
1	B	402	SER
1	B	409	VAL
1	B	414	VAL
1	B	417	LEU
1	B	442	GLN
1	B	475	LEU
1	B	486	GLN
1	B	494	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	91	HIS
1	A	95	HIS
1	A	174	GLN
1	A	188	HIS
1	A	199	GLN
1	A	219	GLN
1	A	220	HIS
1	A	233	ASN

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Mol	Chain	Res	Type
1	A	257	GLN
1	A	348	ASN
1	A	381	GLN
1	A	384	ASN
1	A	398	HIS
1	A	471	HIS
1	B	95	HIS
1	B	143	GLN
1	B	219	GLN
1	B	231	ASN
1	B	233	ASN
1	B	257	GLN
1	B	265	GLN
1	B	334	GLN
1	B	348	ASN
1	B	364	ASN
1	B	381	GLN
1	B	471	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are modelled with single atom - leaving 5 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	$\#\|Z\| > 2$
4	HEM	B	901	-	41,50,50	2.01	6 (14%)	45,82,82	1.81	10 (22%)
2	SO4	A	1	-	4,4,4	0.12	0	6,6,6	0.15	0
5	H4B	B	902	-	16,18,18	3.94	8 (50%)	11,26,26	2.80	5 (45%)
4	HEM	A	901	1	41,50,50	1.94	8 (19%)	45,82,82	1.70	9 (20%)
5	H4B	A	902	-	16,18,18	4.03	7 (43%)	11,26,26	2.97	7 (63%)

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
4	HEM	A	901	1	-	2/12/54/54	-
5	H4B	B	902	-	-	0/8/17/17	0/2/2/2
4	HEM	B	901	-	-	5/12/54/54	-
5	H4B	A	902	-	-	0/8/17/17	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	902	H4B	C4A-C8A	-7.80	1.26	1.41
5	A	902	H4B	C4A-C8A	-7.48	1.27	1.41
5	A	902	H4B	C8A-N1	7.34	1.48	1.34
4	B	901	HEM	C3D-C2D	7.23	1.52	1.36
4	A	901	HEM	C3D-C2D	7.20	1.52	1.36
5	B	902	H4B	O4-C4	7.19	1.42	1.24
5	A	902	H4B	O4-C4	7.13	1.42	1.24
5	B	902	H4B	C8A-N1	6.28	1.46	1.34
5	A	902	H4B	C7-C6	5.74	1.57	1.52
5	A	902	H4B	C2-N2	4.98	1.43	1.33
5	B	902	H4B	C7-C6	4.95	1.57	1.52
5	B	902	H4B	C2-N2	4.93	1.43	1.33
5	B	902	H4B	C4A-N5	4.69	1.47	1.38
4	B	901	HEM	FE-ND	4.53	2.19	1.96
5	A	902	H4B	C4A-N5	4.46	1.47	1.38
4	B	901	HEM	C3C-C2C	-4.07	1.34	1.40
4	A	901	HEM	C3C-C2C	-4.05	1.34	1.40
4	A	901	HEM	FE-ND	3.80	2.15	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	HEM	C3C-CAC	3.79	1.55	1.47
5	B	902	H4B	C4A-C4	3.61	1.46	1.41
4	B	901	HEM	C3C-CAC	3.17	1.54	1.47
4	B	901	HEM	CAB-C3B	3.05	1.55	1.47
5	A	902	H4B	C4A-C4	3.02	1.45	1.41
4	A	901	HEM	CAB-C3B	3.02	1.55	1.47
4	B	901	HEM	CAA-C2A	2.82	1.56	1.52
4	A	901	HEM	C4A-NA	2.09	1.40	1.36
4	A	901	HEM	FE-NB	2.08	2.07	1.96
4	A	901	HEM	CMB-C2B	2.03	1.55	1.50
5	B	902	H4B	C2-N1	2.01	1.39	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	902	H4B	C8A-C4A-C4	7.35	121.10	114.57
5	A	902	H4B	C8A-C4A-C4	7.05	120.83	114.57
4	A	901	HEM	C4D-ND-C1D	5.41	110.66	105.07
4	B	901	HEM	C4D-ND-C1D	5.29	110.53	105.07
4	B	901	HEM	CAD-C3D-C4D	5.06	133.50	124.66
4	A	901	HEM	CBA-CAA-C2A	-3.48	106.69	112.62
5	A	902	H4B	N1-C2-N3	-3.43	120.05	125.42
4	B	901	HEM	CAD-C3D-C2D	-3.19	121.93	127.88
4	B	901	HEM	C4A-C3A-C2A	3.15	109.19	107.00
4	A	901	HEM	CAD-CBD-CGD	-3.14	106.84	113.60
4	B	901	HEM	C4B-CHC-C1C	2.79	126.24	122.56
4	A	901	HEM	C1B-NB-C4B	2.75	107.91	105.07
5	B	902	H4B	N1-C2-N3	-2.70	121.18	125.42
5	A	902	H4B	O10-C10-C11	2.70	117.73	109.74
4	B	901	HEM	CMC-C2C-C3C	2.63	129.60	124.68
4	B	901	HEM	C1B-NB-C4B	2.62	107.78	105.07
5	A	902	H4B	C2-N3-C4	2.58	120.03	115.93
5	A	902	H4B	N2-C2-N1	2.58	121.26	117.25
5	A	902	H4B	C2-N1-C8A	2.46	120.05	114.54
4	A	901	HEM	CMD-C2D-C1D	2.42	128.73	125.04
4	B	901	HEM	CMD-C2D-C1D	2.41	128.71	125.04
4	A	901	HEM	CAD-C3D-C4D	2.39	128.84	124.66
5	B	902	H4B	O10-C10-C11	2.34	116.69	109.74
4	A	901	HEM	C4C-CHD-C1D	2.31	125.60	122.56
4	A	901	HEM	C1D-C2D-C3D	-2.29	104.55	106.96
5	B	902	H4B	C2-N1-C8A	2.27	119.62	114.54
5	A	902	H4B	C4-C4A-N5	-2.17	117.30	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	902	H4B	N2-C2-N1	2.15	120.60	117.25
4	A	901	HEM	C4A-C3A-C2A	2.13	108.48	107.00
4	B	901	HEM	C2B-C1B-NB	-2.13	107.32	109.84
4	B	901	HEM	C3B-C2B-C1B	2.05	108.01	106.49

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	901	HEM	C2D-C3D-CAD-CBD
4	B	901	HEM	C4D-C3D-CAD-CBD
4	B	901	HEM	C3D-CAD-CBD-CGD
4	B	901	HEM	CAD-CBD-CGD-O1D
4	A	901	HEM	CAA-CBA-CGA-O1A
4	B	901	HEM	CAD-CBD-CGD-O2D
4	A	901	HEM	CAA-CBA-CGA-O2A

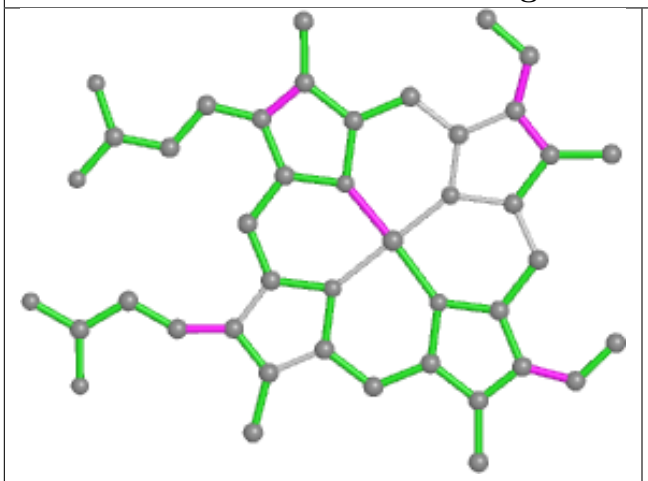
There are no ring outliers.

4 monomers are involved in 17 short contacts:

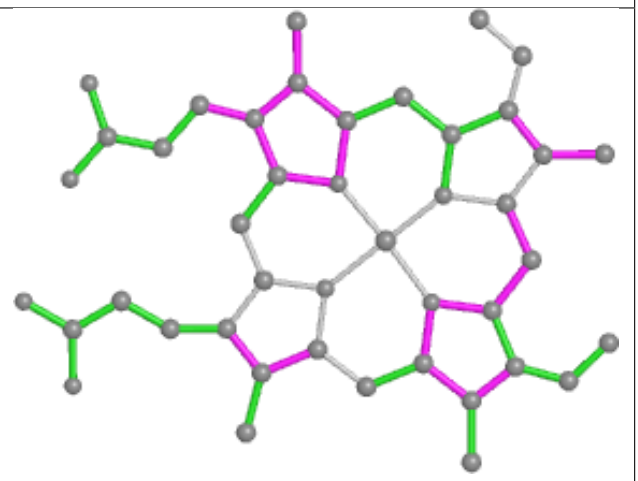
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	901	HEM	7	0
5	B	902	H4B	1	0
4	A	901	HEM	7	0
5	A	902	H4B	2	0

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.

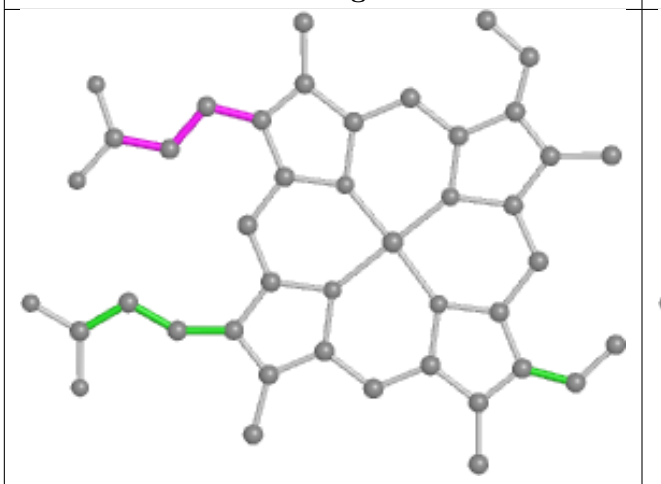
Ligand HEM B 901



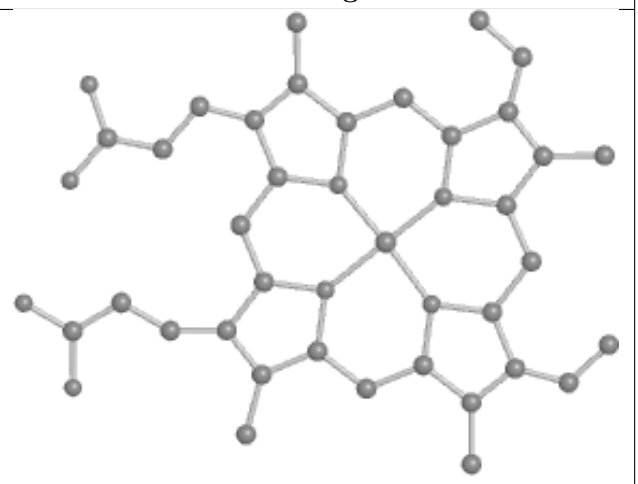
Bond lengths



Bond angles

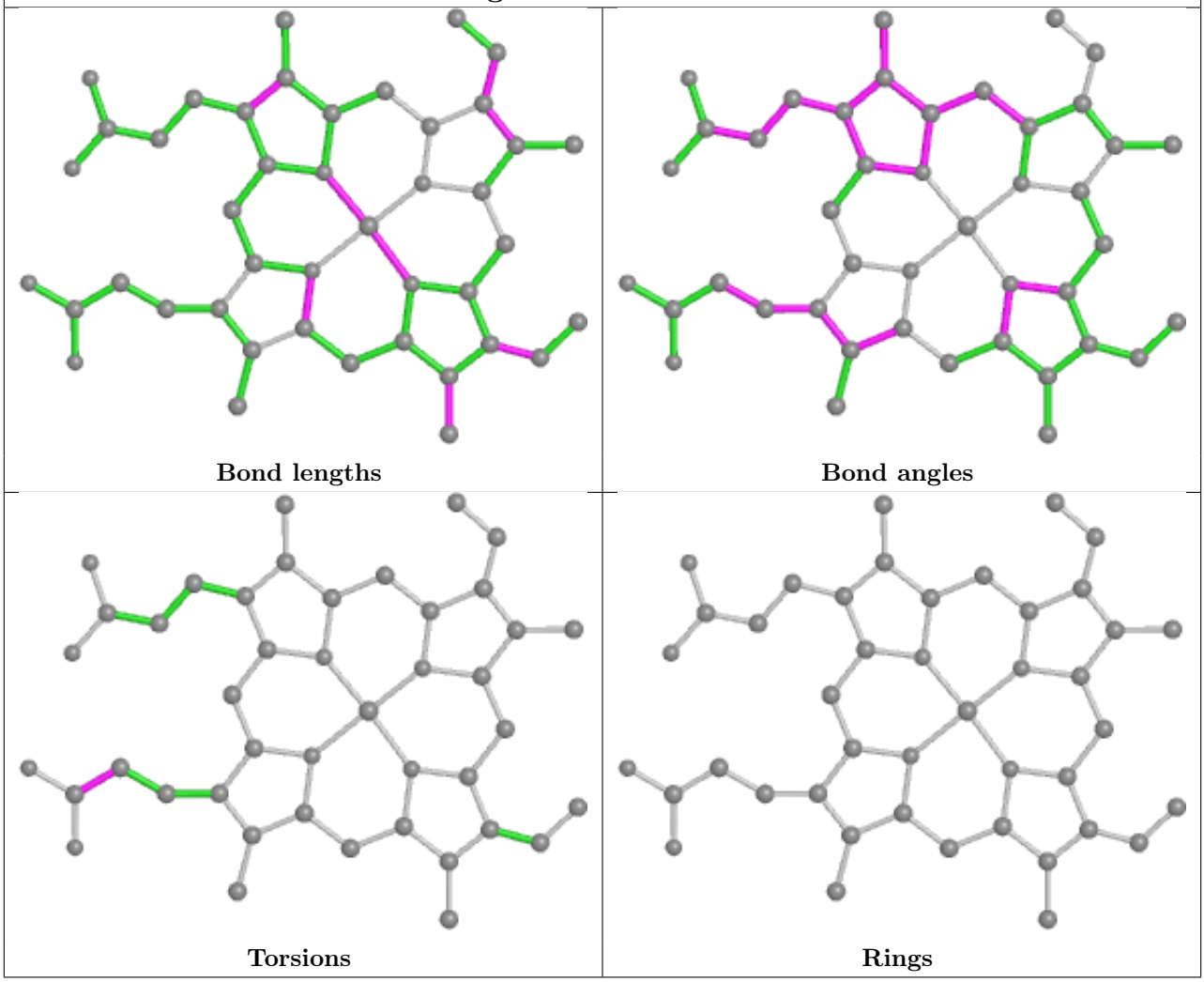


Torsions



Rings

Ligand HEM A 901



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	408/431 (94%)	0.05	10 (2%)	57	66	43, 69, 113, 161	0
1	B	412/431 (95%)	-0.03	9 (2%)	62	70	38, 68, 110, 160	0
All	All	820/862 (95%)	0.01	19 (2%)	60	69	38, 69, 112, 161	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	TYR	4.6
1	A	495	TRP	4.0
1	A	90	LEU	3.6
1	A	267	PRO	3.5
1	B	270	THR	3.5
1	A	91	HIS	3.2
1	A	89	ILE	3.0
1	A	295	ARG	2.9
1	B	77	GLN	2.8
1	B	459	VAL	2.7
1	A	268	ASP	2.5
1	B	267	PRO	2.5
1	A	269	GLY	2.4
1	A	77	GLN	2.3
1	B	78	TYR	2.3
1	B	494	ILE	2.3
1	B	495	TRP	2.2
1	B	152	LYS	2.1
1	B	91	HIS	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)

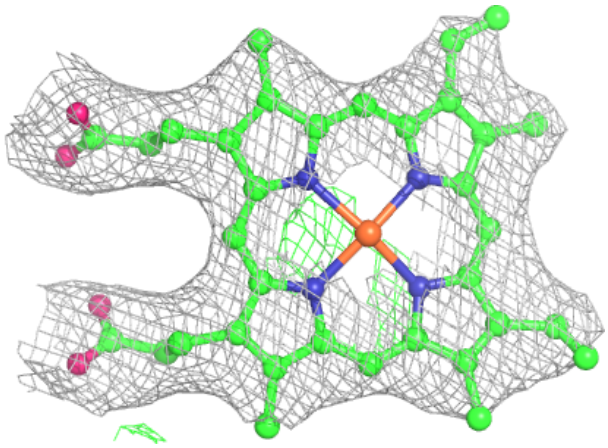
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

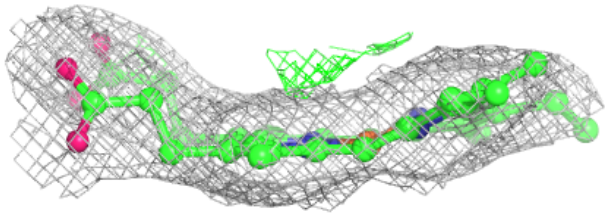
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NH4	A	497	1/1	0.81	1.00	43,43,43,43	0
3	NH4	B	1	1/1	0.81	1.54	57,57,57,57	0
2	SO4	A	1	5/5	0.92	0.22	103,120,127,128	0
4	HEM	A	901	43/43	0.97	0.22	28,54,64,68	0
4	HEM	B	901	43/43	0.97	0.22	33,51,68,75	0
5	H4B	B	902	17/17	0.97	0.18	20,30,49,56	0
5	H4B	A	902	17/17	0.98	0.18	26,36,45,46	0

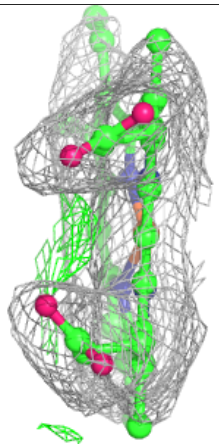
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM A 901:

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

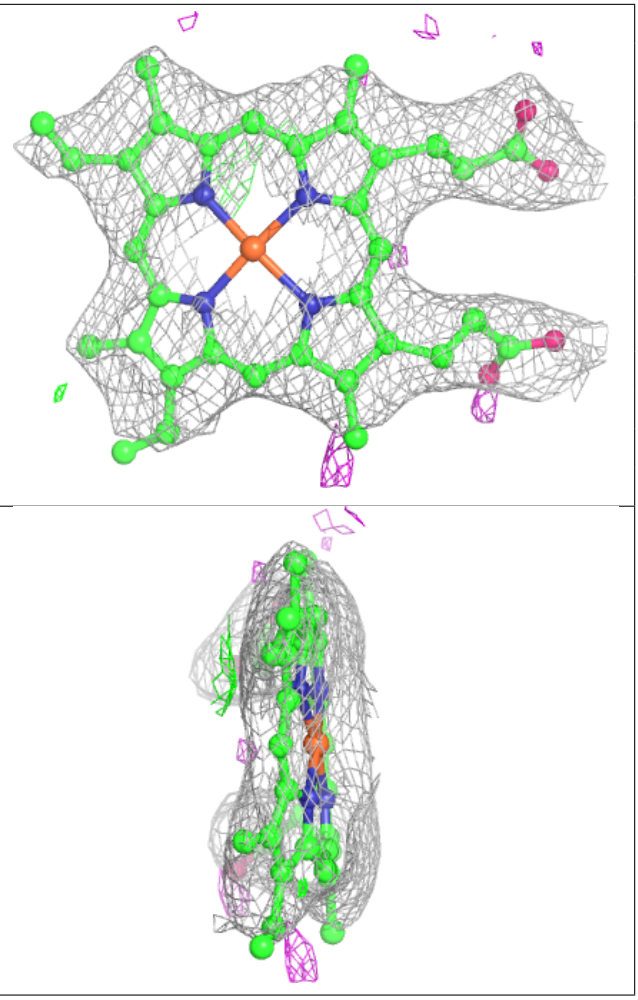






Electron density around HEM B 901:

$2mF_o$-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.