



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:04 PM GMT

PDB ID : 4NOS
Title : HUMAN INDUCIBLE NITRIC OXIDE SYNTHASE WITH INHIBITOR
Authors : Fischmann, T.O.; Weber, P.C.
Deposited on : 1999-02-03
Resolution : 2.25 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

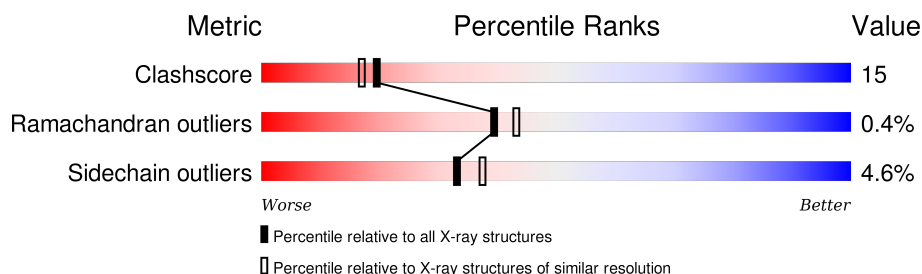
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	427	
1	B	427	
1	C	427	
1	D	427	

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
5	ITU	B	1012	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15317 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
1	A	421	Total	C	N	O	S	0	0	1
			3420	2186	600	612	22			
1	B	421	Total	C	N	O	S	0	0	1
			3420	2186	600	612	22			
1	C	421	Total	C	N	O	S	0	0	1
			3420	2186	600	612	22			
1	D	421	Total	C	N	O	S	0	0	1
			3420	2186	600	612	22			

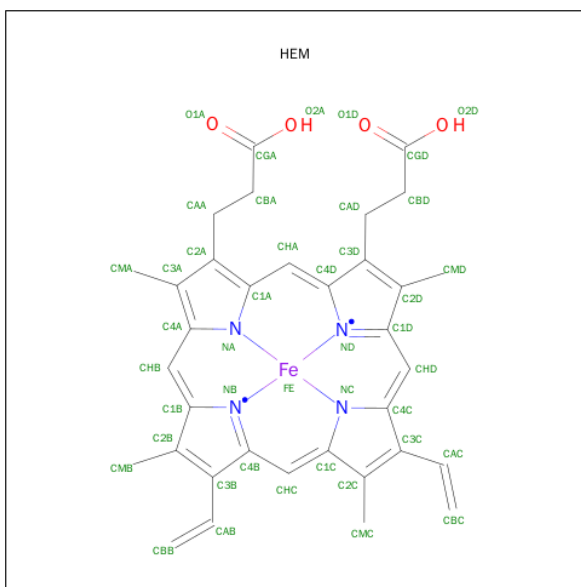
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	423	ILE	LEU	CONFLICT	UNP P35228
B	423	ILE	LEU	CONFLICT	UNP P35228
C	423	ILE	LEU	CONFLICT	UNP P35228
D	423	ILE	LEU	CONFLICT	UNP P35228

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

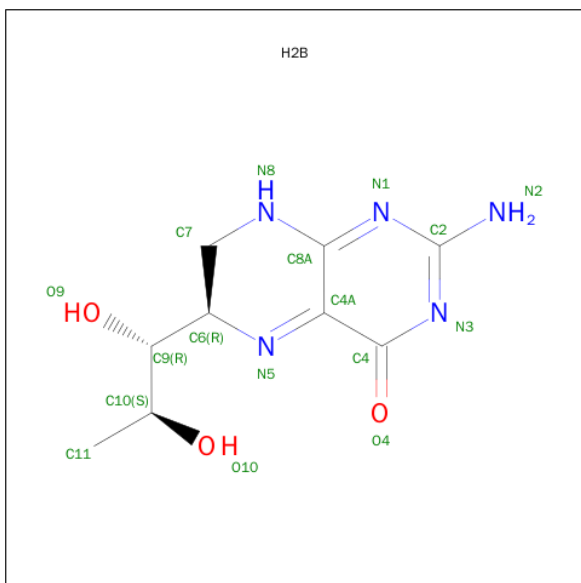
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



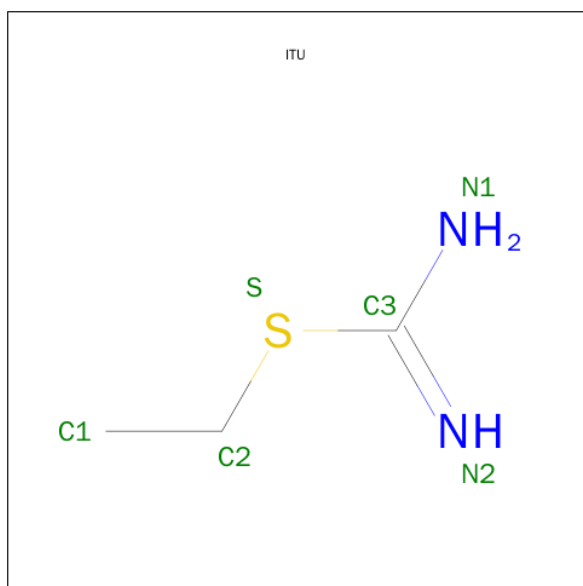
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is 2-AMINO-6-(1,2-DIHYDROXY-PROPYL)-7,8-DIHYDRO-6H-PTERIDIN-4-ONE (three-letter code: H2B) (formula: $C_9H_{13}N_5O_3$).



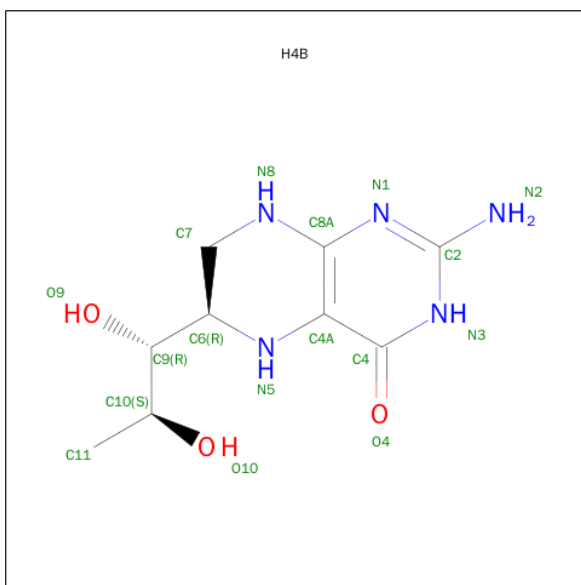
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is ETHYLISOTHIOUREA (three-letter code: ITU) (formula: $C_3H_8N_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	S	0	0
			6	3	2	1		
5	B	1	Total	C	N	S	0	0
			6	3	2	1		
5	C	1	Total	C	N	S	0	0
			6	3	2	1		
5	D	1	Total	C	N	S	0	0
			6	3	2	1		

- 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
6	B	1	Total	C	N	O	0	0
			17	9	5	3		
6	C	1	Total	C	N	O	0	0
			17	9	5	3		
6	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 7 is water.

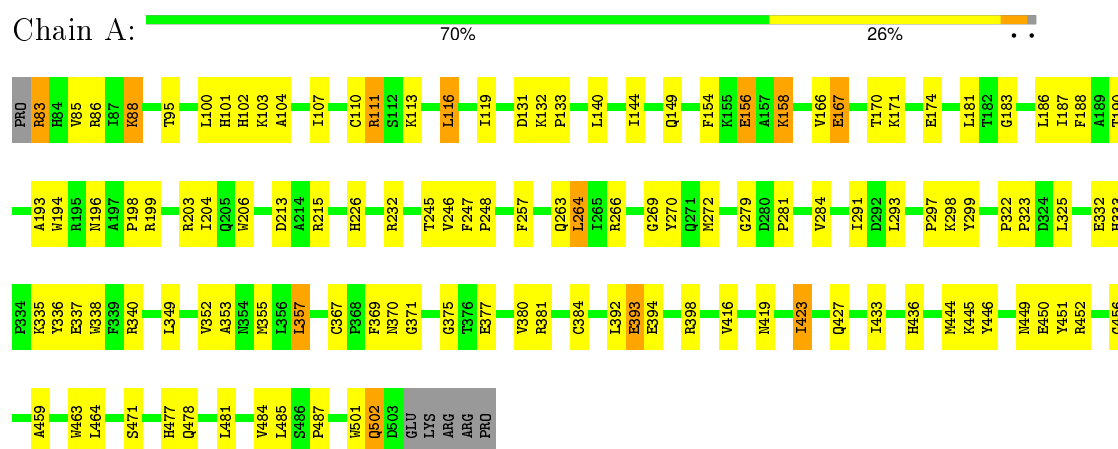
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	336	Total	O	0	0
			336	336		
7	B	335	Total	O	0	0
			335	335		
7	C	339	Total	O	0	0
			339	339		
7	D	361	Total	O	0	0
			361	361		

3 Residue-property plots

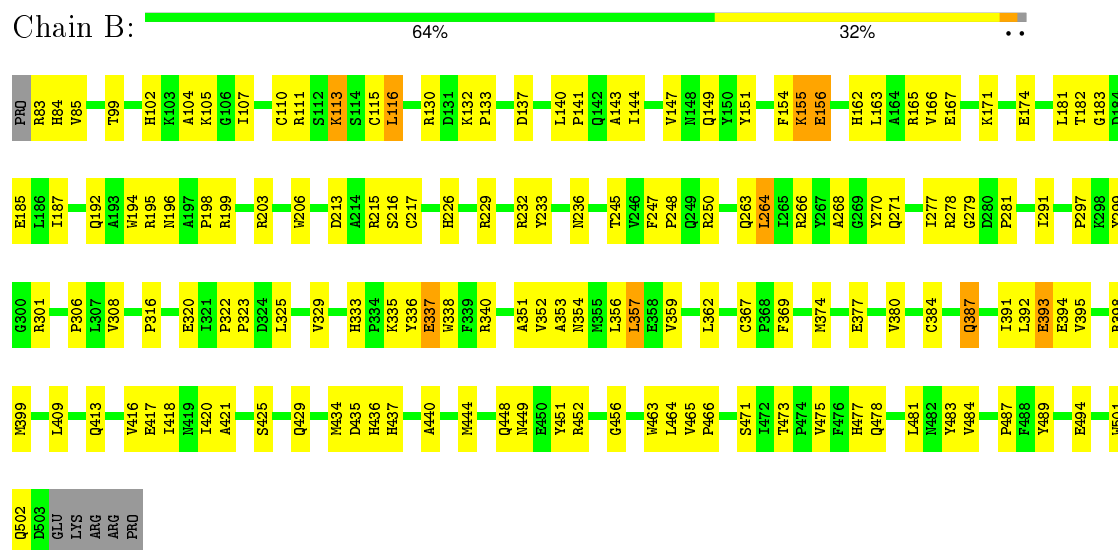
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: INDUCIBLE NITRIC OXIDE SYNTHASE

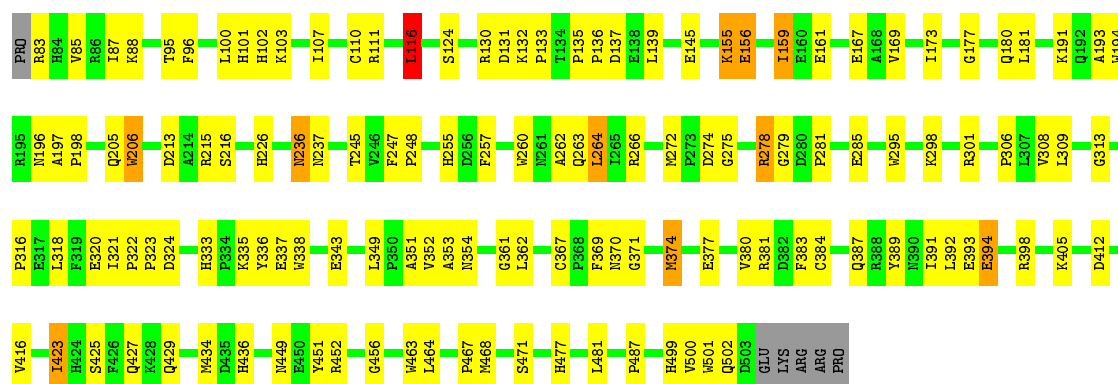


• Molecule 1: INDUCIBLE NITRIC OXIDE SYNTHASE



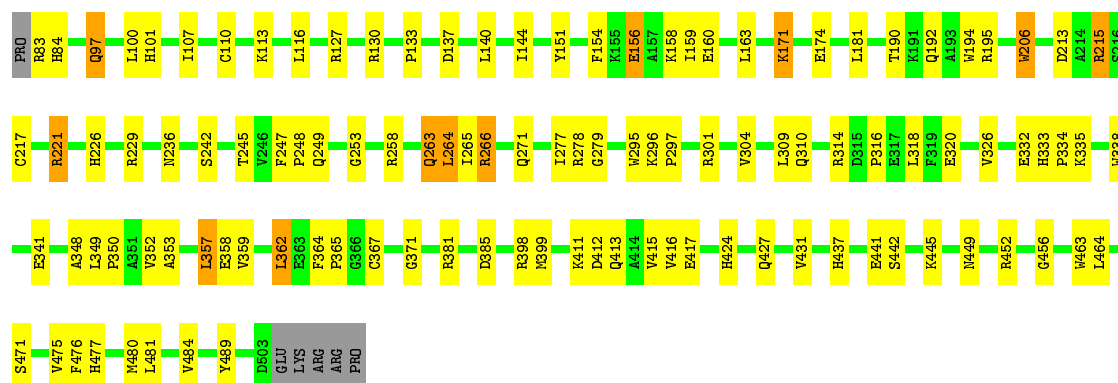
• Molecule 1: INDUCIBLE NITRIC OXIDE SYNTHASE





• Molecule 1: INDUCIBLE NITRIC OXIDE SYNTHASE

Chain D: 72% 24% . .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.76 Å 156.67 Å 190.04 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.25	Depositor
% Data completeness (in resolution range)	88.7 (8.00-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.199 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15317	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, ITU, H4B, H2B

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	0.51	0/3519	0.70	1/4776 (0.0%)
1	B	0.53	0/3519	0.71	1/4776 (0.0%)
1	C	0.53	0/3519	0.74	3/4776 (0.1%)
1	D	0.54	0/3519	0.75	4/4776 (0.1%)
All	All	0.53	0/14076	0.72	9/19104 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	221	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	D	221	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	371	GLY	N-CA-C	-5.91	98.32	113.10
1	C	371	GLY	N-CA-C	-5.68	98.89	113.10
1	C	374	MET	N-CA-C	-5.64	95.78	111.00
1	C	116	LEU	CA-CB-CG	5.56	128.08	115.30
1	A	371	GLY	N-CA-C	-5.49	99.37	113.10
1	D	215	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	374	MET	N-CA-C	-5.33	96.60	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3420	0	3326	101	0
1	B	3420	0	3326	124	0
1	C	3420	0	3326	100	1
1	D	3420	0	3326	89	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	43	0	30	9	0
3	B	43	0	30	4	0
3	C	43	0	30	8	0
3	D	43	0	30	9	0
4	A	17	0	13	0	0
5	A	6	0	7	2	0
5	B	6	0	7	4	0
5	C	6	0	7	3	0
5	D	6	0	7	2	0
6	B	17	0	15	1	0
6	C	17	0	15	2	0
6	D	17	0	15	1	0
7	A	336	0	0	10	0
7	B	335	0	0	15	1
7	C	339	0	0	16	0
7	D	361	0	0	9	0
All	All	15317	0	13510	412	1

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 15.

All (412) 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:C:481:LEU:HD22	1:D:116:LEU:HD22	1.52	0.90
3:C:2010:HEM:HMC2	3:C:2010:HEM:HBC2	1.56	0.88
1:A:88:LYS:HB2	1:A:95:THR:HG22	1.57	0.84
3:D:3010:HEM:HBC2	3:D:3010:HEM:HMC2	1.61	0.82
1:D:217:CYS:SG	7:D:3344:HOH:O	2.28	0.81
3:B:1010:HEM:HMC2	3:B:1010:HEM:HBC2	1.63	0.81
1:B:155:LYS:H	1:B:155:LYS:HD3	1.45	0.80
1:A:111:ARG:NH1	1:A:113:LYS:HB3	2.00	0.77
1:A:110:CYS:HB3	1:B:110:CYS:HB3	1.66	0.77
1:B:194:TRP:CE3	1:B:206:TRP:HA	2.21	0.76
1:C:194:TRP:CE3	1:C:206:TRP:HA	2.21	0.75
1:D:213:ASP:OD1	1:D:215:ARG:HD3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LYS:HE3	1:B:336:TYR:CZ	2.22	0.75
1:C:110:CYS:HB3	1:D:110:CYS:HB3	1.67	0.75
1:D:194:TRP:CE3	1:D:206:TRP:HA	2.21	0.74
1:D:314:ARG:HD2	7:D:3271:HOH:O	1.88	0.73
1:A:111:ARG:HB2	1:A:111:ARG:HH11	1.53	0.71
1:D:83:ARG:HE	1:D:84:HIS:HB3	1.55	0.71
1:D:226:HIS:HD2	7:D:3070:HOH:O	1.73	0.71
1:D:333:HIS:HD2	1:D:335:LYS:H	1.38	0.71
1:B:155:LYS:N	1:B:155:LYS:HD3	2.04	0.71
1:C:159:ILE:HD13	1:C:159:ILE:H	1.56	0.71
1:D:192:GLN:HE22	1:D:195:ARG:HH11	1.39	0.71
1:B:144:ILE:HD12	1:B:166:VAL:HG13	1.72	0.70
1:A:449:ASN:HA	1:A:452:ARG:NH1	2.07	0.70
1:C:369:PHE:HE1	5:C:2012:ITU:H11	1.57	0.69
1:D:113:LYS:HZ3	1:D:113:LYS:HB3	1.57	0.69
1:A:352:VAL:HG11	1:A:355:MET:SD	2.32	0.69
1:B:268:ALA:HB2	7:B:1019:HOH:O	1.91	0.68
1:C:338:TRP:CE3	1:C:398:ARG:HD3	2.29	0.67
1:B:434:MET:SD	7:B:1217:HOH:O	2.52	0.67
1:C:194:TRP:CH2	3:C:2010:HEM:HMC1	2.29	0.67
1:A:298:LYS:HE2	7:A:3088:HOH:O	1.94	0.67
1:A:471:SER:O	1:A:477:HIS:HE1	1.77	0.67
1:A:226:HIS:HD2	7:A:3057:HOH:O	1.79	0.66
1:C:213:ASP:OD1	1:C:215:ARG:HD3	1.96	0.66
1:A:481:LEU:HD22	1:B:116:LEU:HD22	1.78	0.66
1:B:333:HIS:HD2	1:B:335:LYS:H	1.45	0.65
1:D:442:SER:HA	1:D:445:LYS:HE3	1.79	0.65
1:D:171:LYS:HA	1:D:171:LYS:HE2	1.78	0.64
1:B:213:ASP:OD1	1:B:215:ARG:HD3	1.98	0.64
1:B:264:LEU:HD13	1:B:353:ALA:HB2	1.80	0.64
1:B:329:VAL:HG13	1:B:429:GLN:HG3	1.80	0.63
1:D:140:LEU:O	1:D:144:ILE:HG12	1.98	0.63
1:D:271:GLN:HA	1:D:277:ILE:HD13	1.80	0.63
1:A:194:TRP:CE3	1:A:206:TRP:HA	2.34	0.62
1:A:213:ASP:OD1	1:A:215:ARG:HD3	2.00	0.62
1:C:264:LEU:HD13	1:C:353:ALA:HB2	1.81	0.62
1:C:226:HIS:HD2	7:C:2069:HOH:O	1.82	0.62
1:C:369:PHE:CE1	5:C:2012:ITU:H11	2.34	0.62
1:B:333:HIS:HD2	1:B:336:TYR:H	1.46	0.62
1:D:113:LYS:NZ	1:D:113:LYS:HB3	2.14	0.62
1:B:183:GLY:O	1:B:187:ILE:HG13	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LYS:HB2	1:B:107:ILE:HG12	1.82	0.62
1:D:352:VAL:HG23	5:D:3012:ITU:H11	1.81	0.61
1:A:83:ARG:O	1:A:102:HIS:HE1	1.83	0.61
1:B:393:GLU:HB2	7:B:1207:HOH:O	2.01	0.61
1:C:333:HIS:HD2	1:C:335:LYS:H	1.48	0.61
1:B:392:LEU:HB2	7:B:1103:HOH:O	1.99	0.61
1:B:83:ARG:O	1:B:102:HIS:HE1	1.83	0.61
1:D:194:TRP:CZ3	1:D:206:TRP:HA	2.35	0.61
1:C:264:LEU:HB2	1:C:351:ALA:HB3	1.81	0.61
1:A:369:PHE:CE1	5:A:512:ITU:H11	2.35	0.61
1:B:449:ASN:ND2	1:B:452:ARG:HH12	1.99	0.61
1:B:84:HIS:HB3	1:B:99:THR:HG23	1.83	0.61
1:B:130:ARG:NH1	1:B:133:PRO:HA	2.16	0.60
1:B:369:PHE:CD1	5:B:1012:ITU:H11	2.36	0.60
1:A:101:HIS:CD2	1:B:111:ARG:HH21	2.18	0.60
1:B:333:HIS:CD2	1:B:335:LYS:H	2.19	0.60
1:B:369:PHE:CE1	5:B:1012:ITU:H11	2.37	0.60
1:A:419:ASN:O	1:A:423:ILE:HG12	2.00	0.60
1:C:139:LEU:HD12	1:C:361:GLY:HA3	1.83	0.60
1:A:272:MET:HE3	1:A:299:TYR:HD1	1.65	0.60
1:B:156:GLU:H	1:B:156:GLU:CD	2.04	0.60
3:A:510:HEM:HBC2	3:A:510:HEM:HMC2	1.83	0.59
1:A:245:THR:O	1:A:367:CYS:HA	2.02	0.59
1:A:144:ILE:HD12	1:A:166:VAL:HG13	1.85	0.59
1:B:163:LEU:O	1:B:167:GLU:HG3	2.03	0.59
1:C:381:ARG:HH21	6:C:2011:H4B:C4	2.15	0.59
1:A:333:HIS:HD2	1:A:336:TYR:H	1.50	0.59
1:A:264:LEU:HD13	1:A:353:ALA:HB2	1.85	0.58
1:B:151:TYR:CD1	1:B:154:PHE:HE2	2.21	0.58
1:D:309:LEU:O	1:D:316:PRO:HA	2.04	0.58
1:C:83:ARG:HH21	1:C:102:HIS:CE1	2.22	0.57
1:A:199:ARG:HD3	1:A:463:TRP:CD2	2.38	0.57
1:A:449:ASN:HA	1:A:452:ARG:HH12	1.69	0.57
1:A:156:GLU:CD	1:A:156:GLU:H	2.07	0.57
1:B:195:ARG:HD2	1:B:206:TRP:CE3	2.39	0.57
1:A:291:ILE:HD11	1:A:297:PRO:HB3	1.86	0.57
1:C:263:GLN:OE1	1:C:266:ARG:HD3	2.05	0.57
1:D:359:VAL:O	1:D:362:LEU:HB2	2.05	0.57
3:C:2010:HEM:CMC	3:C:2010:HEM:HBC2	2.33	0.56
3:B:1010:HEM:HBC2	3:B:1010:HEM:CMC	2.34	0.56
1:A:263:GLN:CD	1:A:266:ARG:HD3	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:SER:O	1:C:477:HIS:HE1	1.87	0.56
1:D:100:LEU:CB	1:D:456:GLY:HA3	2.35	0.56
1:C:380:VAL:O	1:C:384:CYS:HB2	2.06	0.56
1:B:333:HIS:CD2	1:B:336:TYR:H	2.23	0.56
1:B:194:TRP:CZ3	1:B:206:TRP:HA	2.41	0.56
1:D:130:ARG:NH1	1:D:133:PRO:HA	2.21	0.56
1:A:100:LEU:HD12	1:A:103:LYS:HD2	1.88	0.56
1:B:466:PRO:HG2	1:B:473:THR:HG21	1.88	0.56
1:D:352:VAL:CG2	5:D:3012:ITU:H11	2.35	0.55
1:C:194:TRP:CZ2	3:C:2010:HEM:HMC1	2.41	0.55
1:A:154:PHE:CD2	1:A:158:LYS:HD3	2.41	0.55
3:A:510:HEM:HHC	3:A:510:HEM:HBB2	1.89	0.55
1:B:354:ASN:HB2	7:B:1173:HOH:O	2.06	0.55
1:A:104:ALA:O	1:B:113:LYS:HD2	2.07	0.55
1:D:226:HIS:ND1	7:D:3344:HOH:O	2.32	0.55
1:B:105:LYS:HG2	1:B:484:VAL:O	2.08	0.54
1:B:357:LEU:HD22	1:B:359:VAL:HG22	1.88	0.54
1:B:387:GLN:NE2	1:B:387:GLN:HA	2.21	0.54
1:B:229:ARG:NH2	7:B:1031:HOH:O	2.40	0.54
1:A:104:ALA:HA	1:A:485:LEU:HD23	1.88	0.54
1:C:264:LEU:HD22	1:C:351:ALA:HB1	1.90	0.54
1:B:192:GLN:HB3	1:B:487:PRO:HG2	1.90	0.54
1:D:194:TRP:CZ2	3:D:3010:HEM:HBB2	2.43	0.54
1:C:194:TRP:CZ3	1:C:206:TRP:HA	2.43	0.54
7:A:3063:HOH:O	1:B:409:LEU:HA	2.07	0.54
1:A:196:ASN:O	1:A:198:PRO:HD3	2.08	0.54
1:B:226:HIS:HD2	7:B:1069:HOH:O	1.89	0.53
1:D:190:THR:HG22	1:D:357:LEU:HD11	1.88	0.53
1:B:194:TRP:CZ2	3:B:1010:HEM:HBB2	2.43	0.53
1:A:263:GLN:NE2	1:A:266:ARG:HD3	2.22	0.53
1:B:143:ALA:O	1:B:147:VAL:HG23	2.09	0.53
1:C:381:ARG:NH2	6:C:2011:H4B:C4	2.71	0.53
1:D:156:GLU:HG2	1:D:158:LYS:HE2	1.90	0.53
1:A:194:TRP:CH2	3:A:510:HEM:HMC1	2.44	0.53
1:A:369:PHE:CD1	5:A:512:ITU:H11	2.43	0.53
1:D:130:ARG:O	1:D:253:GLY:HA3	2.08	0.53
1:D:263:GLN:HE22	1:D:266:ARG:NE	2.07	0.53
1:C:262:ALA:HA	1:C:354:ASN:ND2	2.24	0.52
1:B:232:ARG:HD2	7:B:1304:HOH:O	2.09	0.52
1:D:194:TRP:CH2	3:D:3010:HEM:HMC1	2.44	0.52
1:B:226:HIS:HE1	7:B:1118:HOH:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:HIS:O	1:D:441:GLU:HG3	2.10	0.52
1:C:449:ASN:ND2	1:C:452:ARG:HH12	2.07	0.52
1:B:436:HIS:CD2	1:B:436:HIS:H	2.27	0.52
1:C:205:GLN:HG3	3:C:2010:HEM:HBB1	1.90	0.52
1:B:352:VAL:HB	1:B:369:PHE:CE1	2.45	0.52
1:B:440:ALA:HB1	1:B:475:VAL:HG23	1.92	0.52
1:D:381:ARG:O	1:D:385:ASP:HB2	2.10	0.52
1:A:167:GLU:O	1:A:171:LYS:HG2	2.09	0.52
1:A:193:ALA:HB2	1:A:487:PRO:HB2	1.91	0.52
1:A:204:ILE:HD11	1:A:445:LYS:HD3	1.92	0.52
1:A:83:ARG:O	1:A:102:HIS:CE1	2.62	0.52
1:A:86:ARG:NH2	1:A:95:THR:HG21	2.24	0.51
1:B:270:TYR:CE2	1:B:299:TYR:HA	2.46	0.51
3:D:3010:HEM:HBB2	3:D:3010:HEM:HHC	1.92	0.51
1:A:110:CYS:HB3	1:B:110:CYS:CB	2.39	0.51
1:B:263:GLN:HE21	1:B:266:ARG:HD3	1.76	0.51
1:B:425:SER:O	1:B:429:GLN:HG2	2.11	0.51
1:D:247:PHE:HB3	1:D:248:PRO:CD	2.41	0.50
1:B:194:TRP:HZ2	3:B:1010:HEM:HBB2	1.76	0.50
1:B:279:GLY:O	1:B:281:PRO:HD3	2.11	0.50
1:D:194:TRP:HZ2	3:D:3010:HEM:HBB2	1.76	0.50
1:B:162:HIS:O	1:B:166:VAL:HG23	2.12	0.50
1:B:151:TYR:HA	1:B:154:PHE:CD2	2.46	0.50
1:B:357:LEU:HG	1:B:489:TYR:CE1	2.47	0.50
1:B:271:GLN:HA	1:B:277:ILE:HD13	1.94	0.50
1:B:316:PRO:HD2	1:B:501:TRP:CZ3	2.47	0.50
1:D:130:ARG:HH12	1:D:133:PRO:HA	1.77	0.50
1:B:165:ARG:HA	7:B:1309:HOH:O	2.11	0.50
1:A:394:GLU:HB2	7:A:3330:HOH:O	2.10	0.50
1:B:264:LEU:HB2	1:B:351:ALA:HB3	1.94	0.50
1:B:333:HIS:NE2	1:B:335:LYS:HG2	2.27	0.50
3:A:510:HEM:CMC	3:A:510:HEM:HBC2	2.42	0.50
1:C:451:TYR:CE1	1:C:456:GLY:HA2	2.46	0.50
1:D:449:ASN:HD22	1:D:452:ARG:HH12	1.59	0.49
1:C:88:LYS:HG3	1:C:95:THR:HG22	1.93	0.49
1:D:245:THR:O	1:D:367:CYS:HA	2.12	0.49
1:D:264:LEU:HD13	1:D:353:ALA:HB2	1.94	0.49
1:A:170:THR:O	1:A:174:GLU:HG3	2.12	0.49
1:A:194:TRP:CZ3	1:A:206:TRP:HA	2.47	0.49
1:C:279:GLY:O	1:C:281:PRO:HD3	2.13	0.49
1:B:377:GLU:HB3	7:B:1129:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:LEU:HB3	1:D:456:GLY:HA3	1.95	0.49
1:B:192:GLN:HB3	1:B:487:PRO:CG	2.42	0.49
1:B:338:TRP:CE3	1:B:398:ARG:HD3	2.48	0.49
1:A:194:TRP:HZ2	3:A:510:HEM:HBB2	1.78	0.49
1:C:436:HIS:HD2	7:C:2061:HOH:O	1.94	0.49
1:B:151:TYR:CD1	1:B:154:PHE:CE2	3.00	0.49
1:C:412:ASP:O	1:C:416:VAL:HG23	2.13	0.49
1:D:350:PRO:HG2	1:D:350:PRO:O	2.13	0.49
3:A:510:HEM:HHC	3:A:510:HEM:CBB	2.43	0.49
1:A:186:LEU:HD22	1:A:215:ARG:HD2	1.95	0.49
1:C:352:VAL:HB	1:C:369:PHE:CE1	2.48	0.48
1:D:217:CYS:CB	7:D:3344:HOH:O	2.60	0.48
1:D:338:TRP:CE3	1:D:398:ARG:HD3	2.48	0.48
1:A:393:GLU:HB2	7:A:3289:HOH:O	2.13	0.48
1:A:204:ILE:CD1	1:A:445:LYS:HD3	2.44	0.48
1:C:500:VAL:HA	7:C:2218:HOH:O	2.14	0.48
1:A:194:TRP:CZ2	3:A:510:HEM:HMC1	2.47	0.48
1:C:377:GLU:HB3	7:C:2131:HOH:O	2.14	0.48
1:D:304:VAL:HG21	1:D:326:VAL:HG11	1.95	0.48
1:A:436:HIS:CD2	1:A:436:HIS:H	2.32	0.48
1:A:333:HIS:CD2	1:A:336:TYR:H	2.31	0.48
1:D:107:ILE:HD11	1:D:484:VAL:HB	1.96	0.48
1:A:423:ILE:O	1:A:427:GLN:HG3	2.13	0.48
1:D:399:MET:CE	1:D:417:GLU:HG3	2.44	0.48
1:A:132:LYS:HG3	1:A:133:PRO:HD2	1.95	0.48
1:A:416:VAL:HG11	1:B:413:GLN:HG2	1.96	0.48
1:C:111:ARG:HH21	1:D:101:HIS:CD2	2.31	0.48
1:B:416:VAL:O	1:B:420:ILE:HG13	2.13	0.48
1:B:182:THR:OG1	1:B:185:GLU:HG3	2.13	0.48
1:A:194:TRP:CZ2	3:A:510:HEM:HBB2	2.49	0.47
1:D:411:LYS:O	1:D:415:VAL:HG12	2.14	0.47
1:C:248:PRO:HD2	1:C:257:PHE:CG	2.49	0.47
1:D:310:GLN:HG3	1:D:314:ARG:O	2.14	0.47
1:C:100:LEU:HD12	1:C:103:LYS:HD2	1.97	0.47
1:A:110:CYS:CB	1:B:110:CYS:HB3	2.39	0.47
1:B:270:TYR:CD2	1:B:299:TYR:HA	2.50	0.47
1:B:435:ASP:OD2	1:B:437:HIS:HB2	2.14	0.47
1:A:263:GLN:HE22	1:A:266:ARG:NH1	2.13	0.47
1:C:298:LYS:HE2	7:C:2100:HOH:O	2.14	0.47
7:A:3017:HOH:O	1:B:477:HIS:HD2	1.96	0.47
1:B:337:GLU:O	1:B:340:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ARG:HD3	1:B:463:TRP:CD2	2.49	0.47
3:D:3010:HEM:HHC	3:D:3010:HEM:CBB	2.44	0.47
1:C:449:ASN:HD22	1:C:452:ARG:HH12	1.61	0.47
1:B:316:PRO:HD2	1:B:501:TRP:CH2	2.49	0.47
1:C:100:LEU:HB3	1:C:456:GLY:HA3	1.95	0.47
1:D:295:TRP:HB2	1:D:318:LEU:HD23	1.95	0.47
1:C:131:ASP:OD1	1:C:132:LYS:HG3	2.15	0.47
1:C:463:TRP:HZ3	3:C:2010:HEM:HBA2	1.79	0.47
1:A:322:PRO:HD2	1:A:325:LEU:HD12	1.97	0.47
1:C:130:ARG:NH1	1:C:133:PRO:HA	2.30	0.47
1:A:423:ILE:HD11	1:B:409:LEU:HG	1.97	0.47
1:A:333:HIS:HD2	1:A:335:LYS:H	1.63	0.47
1:A:156:GLU:HG2	1:A:156:GLU:O	2.14	0.47
1:A:107:ILE:HD11	1:A:484:VAL:HG11	1.97	0.47
1:B:335:LYS:HE3	1:B:336:TYR:CE1	2.50	0.47
1:A:338:TRP:CE3	1:A:398:ARG:HD3	2.50	0.47
1:A:247:PHE:HB3	1:A:248:PRO:CD	2.44	0.47
1:C:236:ASN:O	1:C:237:ASN:HB2	2.15	0.46
1:A:140:LEU:O	1:A:144:ILE:HG12	2.15	0.46
1:B:149:GLN:NE2	7:B:1122:HOH:O	2.48	0.46
1:C:245:THR:O	1:C:367:CYS:HA	2.15	0.46
1:B:394:GLU:HG3	7:B:1337:HOH:O	2.16	0.46
1:C:191:LYS:O	1:C:194:TRP:HB3	2.16	0.46
1:C:130:ARG:HD3	7:C:2269:HOH:O	2.15	0.46
1:A:88:LYS:CB	1:A:95:THR:HG22	2.39	0.46
1:B:463:TRP:HA	6:B:1011:H4B:N1	2.31	0.46
1:A:272:MET:HE3	1:A:299:TYR:CD1	2.49	0.46
1:A:380:VAL:O	1:A:384:CYS:HB2	2.16	0.46
1:B:391:ILE:O	1:B:395:VAL:HG23	2.15	0.46
1:A:263:GLN:HG2	7:A:3122:HOH:O	2.15	0.46
1:D:159:ILE:HG22	1:D:163:LEU:HD12	1.98	0.46
1:B:140:LEU:O	1:B:144:ILE:HG12	2.15	0.46
1:A:471:SER:O	1:A:477:HIS:CE1	2.64	0.46
1:A:333:HIS:CD2	1:A:335:LYS:H	2.34	0.46
1:C:247:PHE:HB3	1:C:248:PRO:CD	2.45	0.46
3:D:3010:HEM:HBC2	3:D:3010:HEM:CMC	2.37	0.45
1:C:101:HIS:O	1:D:113:LYS:NZ	2.49	0.45
1:A:85:VAL:HG11	1:A:481:LEU:HD21	1.98	0.45
1:C:156:GLU:H	1:C:156:GLU:CD	2.18	0.45
1:C:467:PRO:HB2	1:D:471:SER:OG	2.15	0.45
1:C:255:HIS:HA	1:C:313:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:HIS:CE1	7:D:3344:HOH:O	2.70	0.45
1:A:446:TYR:CZ	1:A:450:GLU:HG3	2.50	0.45
1:C:322:PRO:HA	1:C:323:PRO:HD3	1.75	0.45
1:A:269:GLY:O	1:A:284:VAL:HA	2.16	0.45
1:D:332:GLU:O	1:D:424:HIS:HD2	1.99	0.45
1:C:194:TRP:CE2	3:C:2010:HEM:C2C	3.05	0.45
1:A:204:ILE:HG13	1:A:446:TYR:HB2	1.97	0.45
1:D:463:TRP:HA	6:D:3011:H4B:N1	2.32	0.45
1:C:338:TRP:CZ3	1:C:398:ARG:HD3	2.52	0.45
1:A:158:LYS:NZ	1:A:158:LYS:HB3	2.31	0.45
1:B:308:VAL:HG12	1:B:316:PRO:HB2	1.99	0.45
1:C:193:ALA:HB2	1:C:487:PRO:HB2	1.99	0.45
1:C:394:GLU:HB2	7:C:2048:HOH:O	2.16	0.45
1:C:335:LYS:HE2	7:C:2240:HOH:O	2.16	0.45
1:B:151:TYR:HA	1:B:154:PHE:CE2	2.51	0.45
1:B:85:VAL:HB	1:B:481:LEU:HD11	1.98	0.45
1:A:375:GLY:HA2	1:A:433:ILE:HD11	1.99	0.45
1:B:263:GLN:HE22	1:B:266:ARG:NH1	2.15	0.45
1:B:449:ASN:HD22	1:B:452:ARG:NH1	2.15	0.45
1:D:107:ILE:HD11	1:D:484:VAL:CB	2.47	0.45
1:C:155:LYS:HB2	1:C:156:GLU:OE1	2.17	0.45
1:B:451:TYR:CE1	1:B:456:GLY:HA2	2.52	0.45
1:B:137:ASP:O	1:B:141:PRO:HD2	2.17	0.44
1:D:217:CYS:HB2	7:D:3344:HOH:O	2.16	0.44
1:B:116:LEU:HD23	1:B:116:LEU:N	2.32	0.44
1:A:183:GLY:O	1:A:187:ILE:HG13	2.17	0.44
1:D:151:TYR:CD1	1:D:154:PHE:CE2	3.06	0.44
1:A:116:LEU:O	1:A:119:ILE:HG12	2.17	0.44
1:C:423:ILE:O	1:C:427:GLN:HG3	2.18	0.44
1:A:190:THR:HG22	1:A:357:LEU:HD11	2.00	0.44
1:D:412:ASP:O	1:D:416:VAL:HG23	2.18	0.44
1:B:245:THR:O	1:B:367:CYS:HA	2.18	0.44
7:C:2056:HOH:O	1:D:477:HIS:HD2	2.00	0.44
1:C:159:ILE:H	1:C:159:ILE:CD1	2.27	0.44
1:B:471:SER:O	1:B:477:HIS:HE1	2.00	0.44
1:C:374:MET:HA	1:C:434:MET:O	2.18	0.44
1:A:502:GLN:HG2	1:A:502:GLN:O	2.18	0.44
1:D:338:TRP:O	1:D:341:GLU:HB2	2.18	0.44
1:B:196:ASN:O	1:B:198:PRO:HD3	2.18	0.44
1:B:232:ARG:CZ	1:B:325:LEU:HD21	2.48	0.43
1:A:279:GLY:O	1:A:281:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:MET:HE3	1:B:417:GLU:HG3	2.00	0.43
1:C:260:TRP:HB2	1:C:308:VAL:HB	1.99	0.43
1:C:405:LYS:HB3	1:C:405:LYS:HE2	1.78	0.43
1:A:111:ARG:HH12	1:A:113:LYS:HB3	1.80	0.43
1:C:159:ILE:HD13	1:C:159:ILE:N	2.27	0.43
1:B:263:GLN:NE2	1:B:266:ARG:HD3	2.32	0.43
1:D:348:ALA:HB1	1:D:431:VAL:HG11	2.00	0.43
1:C:135:PRO:HA	1:C:136:PRO:HD3	1.81	0.43
1:D:194:TRP:CZ2	3:D:3010:HEM:HMC1	2.53	0.43
1:B:448:GLN:HG2	1:B:452:ARG:NH2	2.33	0.43
1:D:107:ILE:HD11	1:D:484:VAL:HG11	2.00	0.43
1:A:116:LEU:HD23	1:A:116:LEU:N	2.33	0.43
1:A:444:MET:HE1	1:A:478:GLN:OE1	2.18	0.43
1:B:130:ARG:HB2	1:B:250:ARG:HD3	1.99	0.43
1:C:499:HIS:HD2	1:C:501:TRP:CE2	2.36	0.43
1:C:321:ILE:HG13	7:C:2026:HOH:O	2.18	0.43
1:D:357:LEU:HG	1:D:489:TYR:CE1	2.54	0.43
1:C:87:ILE:HG13	1:C:96:PHE:HB2	1.99	0.43
1:B:291:ILE:HD11	1:B:297:PRO:HB3	2.00	0.43
1:C:387:GLN:HB3	7:C:2259:HOH:O	2.18	0.43
1:C:295:TRP:HB2	1:C:318:LEU:HD23	2.00	0.43
1:B:130:ARG:HD2	1:B:132:LYS:O	2.18	0.43
1:B:357:LEU:HD22	1:B:359:VAL:CG2	2.47	0.43
1:B:380:VAL:O	1:B:384:CYS:HB2	2.19	0.43
1:B:356:LEU:HD23	1:B:356:LEU:C	2.39	0.43
1:D:427:GLN:HA	7:D:3089:HOH:O	2.18	0.43
1:B:444:MET:HE1	1:B:478:GLN:OE1	2.19	0.43
1:D:358:GLU:HA	1:D:362:LEU:O	2.19	0.43
1:B:306:PRO:HB3	1:B:320:GLU:HG2	2.00	0.43
3:C:2010:HEM:C4C	5:C:2012:ITU:H13	2.54	0.43
1:B:270:TYR:O	1:B:277:ILE:HA	2.18	0.42
1:B:278:ARG:NH1	1:B:301:ARG:HG3	2.33	0.42
1:C:349:LEU:HD11	1:C:370:ASN:ND2	2.33	0.42
1:A:111:ARG:CB	1:A:111:ARG:HH11	2.26	0.42
1:A:451:TYR:CE1	1:A:456:GLY:HA2	2.54	0.42
1:D:84:HIS:CE1	1:D:97:GLN:HG2	2.54	0.42
1:D:357:LEU:HB3	1:D:364:PHE:HB2	2.00	0.42
1:A:291:ILE:CD1	1:A:297:PRO:HB3	2.49	0.42
1:D:127:ARG:NH1	1:D:358:GLU:HG3	2.34	0.42
1:D:266:ARG:HD3	7:D:3040:HOH:O	2.18	0.42
1:C:116:LEU:HD12	7:C:2222:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:HD11	1:A:246:VAL:HG21	2.01	0.42
1:B:369:PHE:CD1	5:B:1012:ITU:C1	3.02	0.42
1:D:190:THR:HG22	1:D:357:LEU:CD1	2.49	0.42
1:A:232:ARG:HD3	7:A:3211:HOH:O	2.19	0.42
1:A:349:LEU:HD11	1:A:370:ASN:ND2	2.35	0.42
1:B:247:PHE:HB3	1:B:248:PRO:CD	2.50	0.42
1:C:425:SER:O	1:C:429:GLN:HG2	2.19	0.42
1:C:169:VAL:O	1:C:173:ILE:HG13	2.19	0.42
1:B:233:TYR:O	1:B:236:ASN:HB2	2.19	0.42
1:C:156:GLU:CD	1:C:156:GLU:N	2.73	0.42
1:D:258:ARG:HG2	1:D:365:PRO:HB2	2.01	0.42
1:C:107:ILE:HD12	1:C:124:SER:O	2.19	0.42
1:D:264:LEU:HA	1:D:264:LEU:HD12	1.90	0.42
1:C:301:ARG:HH22	1:C:343:GLU:HB3	1.84	0.42
1:B:369:PHE:HD1	5:B:1012:ITU:C1	2.33	0.42
1:A:199:ARG:HD3	1:A:463:TRP:CE2	2.55	0.42
1:B:181:LEU:O	1:B:215:ARG:NH2	2.47	0.41
1:B:263:GLN:HA	1:B:351:ALA:O	2.20	0.41
1:A:270:TYR:CE2	1:A:299:TYR:HA	2.55	0.41
1:C:416:VAL:HG22	1:C:468:MET:CE	2.50	0.41
1:D:265:ILE:HD12	1:D:349:LEU:HB3	2.02	0.41
1:B:203:ARG:O	1:B:206:TRP:HD1	2.02	0.41
1:B:263:GLN:HG2	7:B:1130:HOH:O	2.19	0.41
1:C:308:VAL:HG12	1:C:316:PRO:HB2	2.02	0.41
1:A:459:ALA:HB1	1:A:464:LEU:CD1	2.50	0.41
1:C:180:GLN:NE2	7:C:2210:HOH:O	2.53	0.41
1:C:383:PHE:O	1:C:391:ILE:HG12	2.20	0.41
1:D:475:VAL:HG13	1:D:480:MET:CE	2.51	0.41
1:C:216:SER:HB2	7:C:2311:HOH:O	2.18	0.41
3:A:510:HEM:CHC	3:A:510:HEM:HBB2	2.50	0.41
1:B:449:ASN:ND2	1:B:452:ARG:NH1	2.67	0.41
1:C:116:LEU:HB3	1:D:481:LEU:CD2	2.51	0.41
1:C:301:ARG:HH22	1:C:343:GLU:CB	2.33	0.41
1:A:392:LEU:HB2	7:A:3092:HOH:O	2.20	0.41
1:A:149:GLN:HG2	1:A:188:PHE:HZ	1.84	0.41
1:D:194:TRP:CE2	3:D:3010:HEM:C2C	3.08	0.41
1:B:465:VAL:HA	1:B:466:PRO:HD3	1.96	0.41
1:B:322:PRO:HA	1:B:323:PRO:HD2	1.69	0.41
1:B:418:ILE:O	1:B:421:ALA:HB3	2.20	0.41
1:A:158:LYS:HB2	7:A:3115:HOH:O	2.20	0.41
1:C:197:ALA:HA	1:C:198:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:PHE:HA	1:C:389:TYR:HB2	2.03	0.41
1:A:352:VAL:HB	1:A:369:PHE:CE1	2.55	0.41
1:C:336:TYR:HB3	1:C:338:TRP:CE2	2.56	0.41
1:D:381:ARG:NH1	1:D:385:ASP:OD2	2.53	0.41
1:C:316:PRO:HD2	1:C:501:TRP:CH2	2.56	0.41
1:C:173:ILE:O	1:C:177:GLY:N	2.52	0.41
1:C:85:VAL:HB	1:C:481:LEU:HD11	2.03	0.41
1:B:104:ALA:CB	1:B:483:TYR:HB2	2.51	0.41
1:C:161:GLU:HG3	7:C:2128:HOH:O	2.20	0.41
1:D:83:ARG:HH21	1:D:84:HIS:HB3	1.86	0.41
1:D:263:GLN:NE2	1:D:266:ARG:HG2	2.36	0.41
1:D:471:SER:HA	1:D:476:PHE:CG	2.56	0.41
1:C:481:LEU:CD2	1:D:116:LEU:HD22	2.38	0.40
1:C:309:LEU:O	1:C:316:PRO:HA	2.21	0.40
1:D:279:GLY:HA2	1:D:301:ARG:HA	2.01	0.40
1:D:296:LYS:HA	1:D:297:PRO:HD2	1.90	0.40
1:A:332:GLU:HG2	1:A:340:ARG:HD3	2.02	0.40
1:D:333:HIS:CD2	1:D:334:PRO:HD2	2.56	0.40
1:D:249:GLN:HB3	1:D:364:PHE:CE2	2.56	0.40
1:C:306:PRO:HB3	1:C:320:GLU:HG2	2.04	0.40
1:A:377:GLU:O	1:A:381:ARG:HB2	2.20	0.40
1:A:248:PRO:HD2	1:A:257:PHE:CG	2.57	0.40
1:C:196:ASN:O	1:C:198:PRO:HD3	2.20	0.40
1:A:293:LEU:HD21	1:A:501:TRP:CH2	2.57	0.40
1:C:392:LEU:HB2	7:C:2104:HOH:O	2.21	0.40
1:C:436:HIS:H	1:C:436:HIS:CD2	2.39	0.40
1:C:416:VAL:HG11	1:D:413:GLN:HG2	2.04	0.40
1:B:171:LYS:O	1:B:174:GLU:HB3	2.21	0.40
1:D:333:HIS:CD2	1:D:335:LYS:HG3	2.57	0.40
1:C:272:MET:HE2	1:C:278:ARG:HB2	2.03	0.40
1:B:115:CYS:SG	7:B:1220:HOH:O	2.63	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ASP:O	7:B:1165:HOH:O[4_455]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/427 (98%)	390 (93%)	28 (7%)	1 (0%)	52	61
1	B	419/427 (98%)	395 (94%)	24 (6%)	0	100	100
1	C	419/427 (98%)	390 (93%)	26 (6%)	3 (1%)	26	26
1	D	419/427 (98%)	398 (95%)	19 (4%)	2 (0%)	34	34
All	All	1676/1708 (98%)	1573 (94%)	97 (6%)	6 (0%)	39	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	236	ASN
1	D	206	TRP
1	C	206	TRP
1	A	203	ARG
1	D	236	ASN
1	C	275	GLY

5.3.2 Protein sidechains

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	366/373 (98%)	350 (96%)	16 (4%)	35	40
1	B	366/373 (98%)	351 (96%)	15 (4%)	37	44
1	C	366/373 (98%)	347 (95%)	19 (5%)	29	31
1	D	366/373 (98%)	348 (95%)	18 (5%)	31	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1464/1492 (98%)	1396 (95%)	68 (5%)	33 37

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	A	88	LYS
1	A	111	ARG
1	A	116	LEU
1	A	131	ASP
1	A	156	GLU
1	A	158	LYS
1	A	167	GLU
1	A	181	LEU
1	A	264	LEU
1	A	323	PRO
1	A	337	GLU
1	A	357	LEU
1	A	393	GLU
1	A	423	ILE
1	A	502	GLN
1	B	113	LYS
1	B	116	LEU
1	B	155	LYS
1	B	156	GLU
1	B	216	SER
1	B	217	CYS
1	B	264	LEU
1	B	337	GLU
1	B	357	LEU
1	B	362	LEU
1	B	387	GLN
1	B	393	GLU
1	B	464	LEU
1	B	494	GLU
1	B	502	GLN
1	C	116	LEU
1	C	145	GLU
1	C	155	LYS
1	C	156	GLU
1	C	159	ILE
1	C	167	GLU

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Mol	Chain	Res	Type
1	C	181	LEU
1	C	264	LEU
1	C	274	ASP
1	C	278	ARG
1	C	285	GLU
1	C	324	ASP
1	C	337	GLU
1	C	362	LEU
1	C	393	GLU
1	C	394	GLU
1	C	423	ILE
1	C	464	LEU
1	C	502	GLN
1	D	97	GLN
1	D	137	ASP
1	D	156	GLU
1	D	160	GLU
1	D	171	LYS
1	D	174	GLU
1	D	181	LEU
1	D	221	ARG
1	D	229	ARG
1	D	242	SER
1	D	263	GLN
1	D	264	LEU
1	D	266	ARG
1	D	278	ARG
1	D	320	GLU
1	D	357	LEU
1	D	362	LEU
1	D	464	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	180	GLN
1	A	205	GLN
1	A	208	ASN
1	A	226	HIS
1	A	312	ASN
1	A	333	HIS

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Mol	Chain	Res	Type
1	A	390	ASN
1	A	404	HIS
1	A	424	HIS
1	A	436	HIS
1	A	448	GLN
1	A	449	ASN
1	A	477	HIS
1	B	102	HIS
1	B	149	GLN
1	B	205	GLN
1	B	208	ASN
1	B	226	HIS
1	B	239	ASN
1	B	263	GLN
1	B	271	GLN
1	B	333	HIS
1	B	387	GLN
1	B	390	ASN
1	B	436	HIS
1	B	448	GLN
1	B	449	ASN
1	B	477	HIS
1	C	97	GLN
1	C	180	GLN
1	C	205	GLN
1	C	208	ASN
1	C	226	HIS
1	C	333	HIS
1	C	436	HIS
1	C	448	GLN
1	C	449	ASN
1	C	477	HIS
1	C	492	GLN
1	D	102	HIS
1	D	192	GLN
1	D	205	GLN
1	D	263	GLN
1	D	310	GLN
1	D	333	HIS
1	D	390	ASN
1	D	436	HIS
1	D	448	GLN

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Mol	Chain	Res	Type
1	D	449	ASN
1	D	477	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\# Z > 2$
3	HEM	A	510	1	30,50,50	2.61	12 (40%)	24,82,82	3.12	14 (58%)
4	H2B	A	511	-	10,18,18	3.35	3 (30%)	12,26,26	2.86	6 (50%)
5	ITU	A	512	-	4,5,5	0.75	0	4,5,5	0.79	0
3	HEM	B	1010	1	30,50,50	2.57	9 (30%)	24,82,82	3.16	14 (58%)
6	H4B	B	1011	-	13,18,18	1.88	3 (23%)	11,26,26	4.40	7 (63%)
5	ITU	B	1012	-	4,5,5	0.94	0	4,5,5	0.93	0
3	HEM	C	2010	1	30,50,50	2.64	13 (43%)	24,82,82	3.14	14 (58%)
6	H4B	C	2011	-	13,18,18	1.76	2 (15%)	11,26,26	4.34	7 (63%)
5	ITU	C	2012	-	4,5,5	1.00	0	4,5,5	0.94	0
3	HEM	D	3010	1	30,50,50	2.55	12 (40%)	24,82,82	3.10	13 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	H4B	D	3011	-	13,18,18	2.00	4 (30%)	11,26,26	4.39	7 (63%)
5	ITU	D	3012	-	4,5,5	1.00	0	4,5,5	0.88	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
3	HEM	A	510	1	-	0/10/54/54	0/0/8/8
4	H2B	A	511	-	-	0/8/33/33	0/2/2/2
5	ITU	A	512	-	-	0/3/3/3	0/0/0/0
3	HEM	B	1010	1	-	0/10/54/54	0/0/8/8
6	H4B	B	1011	-	-	0/8/17/17	0/2/2/2
5	ITU	B	1012	-	-	0/3/3/3	0/0/0/0
3	HEM	C	2010	1	-	0/10/54/54	0/0/8/8
6	H4B	C	2011	-	-	0/8/17/17	0/2/2/2
5	ITU	C	2012	-	-	0/3/3/3	0/0/0/0
3	HEM	D	3010	1	-	0/10/54/54	0/0/8/8
6	H4B	D	3011	-	-	0/8/17/17	0/2/2/2
5	ITU	D	3012	-	-	0/3/3/3	0/0/0/0

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2010	HEM	C2D-C3D	-6.74	1.34	1.54
3	D	3010	HEM	C2D-C3D	-6.73	1.34	1.54
3	D	3010	HEM	C3B-C4B	-6.50	1.46	1.51
3	B	1010	HEM	C3B-C4B	-6.41	1.46	1.51
3	B	1010	HEM	C2D-C3D	-6.24	1.35	1.54
3	A	510	HEM	C2D-C3D	-6.16	1.36	1.54
3	C	2010	HEM	C3B-C4B	-6.15	1.46	1.51
3	A	510	HEM	C3B-C4B	-6.03	1.46	1.51
3	B	1010	HEM	C3D-C4D	-5.33	1.44	1.51
3	A	510	HEM	C3D-C4D	-5.16	1.45	1.51
3	D	3010	HEM	C3D-C4D	-4.88	1.45	1.51
3	C	2010	HEM	C3D-C4D	-4.18	1.46	1.51
3	C	2010	HEM	C2C-C1C	-2.97	1.46	1.52
3	A	510	HEM	C2D-C1D	-2.61	1.43	1.51
3	C	2010	HEM	C2B-C1B	-2.48	1.43	1.51
3	A	510	HEM	C2B-C1B	-2.47	1.43	1.51
3	B	1010	HEM	C2B-C1B	-2.19	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3010	HEM	C2D-C1D	-2.18	1.44	1.51
3	B	1010	HEM	C2D-C1D	-2.18	1.44	1.51
3	D	3010	HEM	C2B-C1B	-2.16	1.44	1.51
3	D	3010	HEM	C2C-C1C	-2.16	1.48	1.52
3	C	2010	HEM	C3B-CAB	2.01	1.55	1.51
3	D	3010	HEM	C4C-NC	2.08	1.38	1.36
3	A	510	HEM	FE-NB	2.09	2.08	1.97
6	D	3011	H4B	C8A-N1	2.10	1.38	1.34
3	D	3010	HEM	FE-NB	2.17	2.09	1.97
3	D	3010	HEM	C3C-CAC	2.23	1.55	1.51
3	A	510	HEM	CHC-C1C	2.24	1.41	1.36
3	C	2010	HEM	FE-ND	2.31	2.09	1.97
6	D	3011	H4B	C4A-C8A	2.32	1.46	1.41
6	B	1011	H4B	C8A-N1	2.33	1.38	1.34
3	A	510	HEM	FE-ND	2.38	2.10	1.97
3	C	2010	HEM	C1C-NC	2.39	1.39	1.36
3	C	2010	HEM	C4C-NC	2.42	1.39	1.36
6	B	1011	H4B	C6-N5	2.53	1.50	1.45
3	B	1010	HEM	C4C-NC	2.59	1.39	1.36
6	C	2011	H4B	C6-N5	2.69	1.51	1.45
3	A	510	HEM	C4C-NC	2.70	1.39	1.36
3	D	3010	HEM	FE-NC	2.76	2.06	1.95
3	C	2010	HEM	FE-NC	2.78	2.06	1.95
4	A	511	H2B	C4-N3	2.87	1.43	1.38
6	D	3011	H4B	C6-N5	3.27	1.52	1.45
3	C	2010	HEM	FE-NB	3.51	2.16	1.97
3	A	510	HEM	FE-NC	3.72	2.10	1.95
4	A	511	H2B	C4A-N5	4.05	1.39	1.28
3	C	2010	HEM	CBC-CAC	4.07	1.52	1.29
3	B	1010	HEM	FE-NC	4.13	2.12	1.95
3	B	1010	HEM	CBC-CAC	4.14	1.53	1.29
3	A	510	HEM	CBC-CAC	4.16	1.53	1.29
3	D	3010	HEM	CBB-CAB	4.17	1.53	1.29
3	C	2010	HEM	CBB-CAB	4.17	1.53	1.29
3	B	1010	HEM	CBB-CAB	4.18	1.53	1.29
3	A	510	HEM	CBB-CAB	4.27	1.53	1.29
3	D	3010	HEM	CBC-CAC	4.33	1.54	1.29
6	C	2011	H4B	C4-N3	4.83	1.42	1.33
6	B	1011	H4B	C4-N3	4.86	1.42	1.33
6	D	3011	H4B	C4-N3	5.25	1.42	1.33
4	A	511	H2B	C8A-N1	8.79	1.39	1.28

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3010	HEM	C3B-CAB-CBB	-6.25	114.87	124.46
3	A	510	HEM	C3B-CAB-CBB	-5.93	115.37	124.46
3	B	1010	HEM	C3C-CAC-CBC	-5.90	115.41	124.46
3	C	2010	HEM	C3C-CAC-CBC	-5.76	115.62	124.46
3	B	1010	HEM	C3B-CAB-CBB	-5.55	115.95	124.46
3	D	3010	HEM	C3C-CAC-CBC	-5.39	116.18	124.46
3	C	2010	HEM	C3B-CAB-CBB	-5.01	116.77	124.46
3	A	510	HEM	C3C-CAC-CBC	-4.99	116.81	124.46
3	D	3010	HEM	CAA-C2A-C1A	-4.24	122.41	127.01
4	A	511	H2B	C4A-C4-N3	-3.91	114.46	117.83
4	A	511	H2B	C4A-C8A-N1	-3.74	115.98	124.90
4	A	511	H2B	C8A-C4A-N5	-3.72	115.13	124.42
6	C	2011	H4B	N3-C2-N1	-3.72	119.44	125.53
3	B	1010	HEM	CAA-C2A-C1A	-3.68	123.01	127.01
6	B	1011	H4B	N3-C2-N1	-3.63	119.59	125.53
6	D	3011	H4B	C8A-C4A-N5	-3.51	114.42	118.85
6	D	3011	H4B	N3-C2-N1	-3.50	119.79	125.53
3	C	2010	HEM	CAA-C2A-C1A	-3.47	123.24	127.01
3	A	510	HEM	CAA-C2A-C1A	-3.42	123.29	127.01
3	C	2010	HEM	CBD-CAD-C3D	-3.33	103.85	113.55
3	B	1010	HEM	CBD-CAD-C3D	-3.32	103.88	113.55
6	B	1011	H4B	C8A-C4A-N5	-3.29	114.70	118.85
3	B	1010	HEM	CMA-C3A-C4A	-3.13	123.19	128.36
3	A	510	HEM	CBA-CAA-C2A	-3.09	106.99	112.53
3	A	510	HEM	CMA-C3A-C4A	-3.06	123.30	128.36
6	C	2011	H4B	C8A-C4A-N5	-2.93	115.16	118.85
3	A	510	HEM	CBD-CAD-C3D	-2.92	105.04	113.55
3	C	2010	HEM	CBA-CAA-C2A	-2.86	107.40	112.53
3	C	2010	HEM	CMA-C3A-C4A	-2.85	123.65	128.36
3	D	3010	HEM	CBD-CAD-C3D	-2.73	105.62	113.55
3	D	3010	HEM	CMA-C3A-C4A	-2.49	124.24	128.36
3	D	3010	HEM	CBA-CAA-C2A	-2.40	108.22	112.53
3	B	1010	HEM	CBA-CAA-C2A	-2.21	108.56	112.53
6	B	1011	H4B	N2-C2-N3	2.06	120.62	117.20
3	B	1010	HEM	CAA-CBA-CGA	2.20	116.77	112.75
3	A	510	HEM	CAA-CBA-CGA	2.20	116.78	112.75
3	C	2010	HEM	CAA-CBA-CGA	2.28	116.92	112.75
6	D	3011	H4B	N2-C2-N3	2.45	121.25	117.20
6	C	2011	H4B	N2-C2-N3	2.55	121.42	117.20
3	D	3010	HEM	CMD-C2D-C3D	2.86	127.02	114.35
3	C	2010	HEM	CMD-C2D-C3D	2.93	127.32	114.35
3	A	510	HEM	CMD-C2D-C3D	3.03	127.76	114.35
4	A	511	H2B	C4A-C8A-N8	3.10	125.05	116.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1010	HEM	CMD-C2D-C3D	3.11	128.11	114.35
3	D	3010	HEM	C3B-C4B-CHC	3.11	127.55	123.16
3	A	510	HEM	C3B-C4B-CHC	3.43	128.00	123.16
3	B	1010	HEM	C2D-C3D-C4D	3.44	107.34	101.50
3	A	510	HEM	C2D-C3D-C4D	3.45	107.35	101.50
6	B	1011	H4B	C2-N1-C8A	3.47	122.33	114.54
3	C	2010	HEM	C2D-C3D-C4D	3.56	107.53	101.50
3	B	1010	HEM	C3B-C4B-CHC	3.58	128.21	123.16
6	D	3011	H4B	C2-N1-C8A	3.60	122.64	114.54
3	D	3010	HEM	C2D-C3D-C4D	3.69	107.75	101.50
6	C	2011	H4B	C2-N1-C8A	3.74	122.95	114.54
3	C	2010	HEM	CAD-C3D-C4D	3.80	125.88	112.47
3	B	1010	HEM	CAD-C3D-C4D	3.83	125.97	112.47
3	C	2010	HEM	C3B-C4B-CHC	3.86	128.60	123.16
4	A	511	H2B	C4-C4A-N5	3.96	121.65	117.87
3	D	3010	HEM	CAD-C3D-C4D	3.99	126.53	112.47
3	A	510	HEM	CAD-C3D-C2D	4.16	125.18	113.22
3	A	510	HEM	CAD-C3D-C4D	4.25	127.45	112.47
3	D	3010	HEM	CAD-C3D-C2D	4.35	125.71	113.22
3	D	3010	HEM	CMB-C2B-C3B	4.59	127.98	116.53
3	C	2010	HEM	CAD-C3D-C2D	4.65	126.58	113.22
3	B	1010	HEM	CAD-C3D-C2D	4.68	126.67	113.22
3	B	1010	HEM	CMB-C2B-C3B	4.79	128.49	116.53
4	A	511	H2B	C4-C4A-C8A	5.02	123.21	117.63
3	C	2010	HEM	CMB-C2B-C3B	5.04	129.11	116.53
3	A	510	HEM	CMB-C2B-C3B	5.11	129.29	116.53
3	A	510	HEM	CMC-C2C-C3C	5.20	129.52	116.53
3	C	2010	HEM	CMC-C2C-C3C	5.23	129.58	116.53
3	B	1010	HEM	CMC-C2C-C3C	5.27	129.69	116.53
3	D	3010	HEM	CMC-C2C-C3C	5.30	129.75	116.53
6	B	1011	H4B	C4-N3-C2	5.81	124.01	115.94
6	C	2011	H4B	C4-N3-C2	5.88	124.10	115.94
6	B	1011	H4B	C4A-C8A-N8	5.92	125.40	118.43
6	D	3011	H4B	C4-N3-C2	6.03	124.31	115.94
6	D	3011	H4B	C4A-C8A-N8	6.05	125.55	118.43
6	C	2011	H4B	C4A-C8A-N8	6.17	125.70	118.43
6	C	2011	H4B	C4-C4A-C8A	9.33	123.01	114.56
6	D	3011	H4B	C4-C4A-C8A	9.58	123.23	114.56
6	B	1011	H4B	C4-C4A-C8A	9.85	123.48	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	510	HEM	9	0
5	A	512	ITU	2	0
3	B	1010	HEM	4	0
6	B	1011	H4B	1	0
5	B	1012	ITU	4	0
3	C	2010	HEM	8	0
6	C	2011	H4B	2	0
5	C	2012	ITU	3	0
3	D	3010	HEM	9	0
6	D	3011	H4B	1	0
5	D	3012	ITU	2	0

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](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.