Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 01:59 PM EST

PDB ID	:	2KII
Title	:	NMR structure of the SO2144 H-NOX domain from Shewanella oneidensis in the Fe(II)CO ligation state
Authors	:	Erbil, W.K.
Deposited on	:	2009-05-05

This is a Full wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

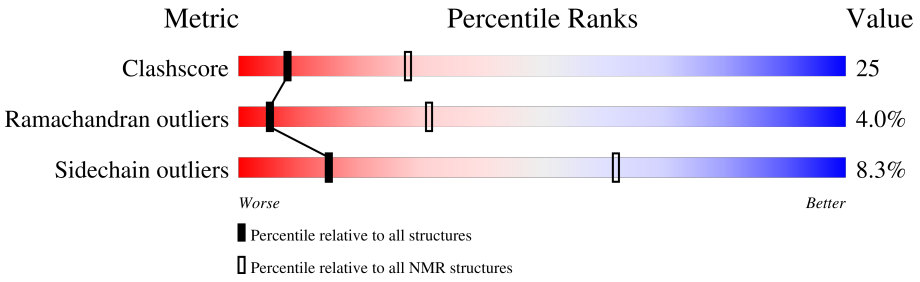
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain
1	A	181	49% 33% • 15%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:3-A:29, A:36-A:38, A:45-A:108, A:116-A:134, A:139-A:179 (154)	0.21	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 10, 11, 13, 16, 17, 19, 20
2	8, 9, 12, 14, 15, 18

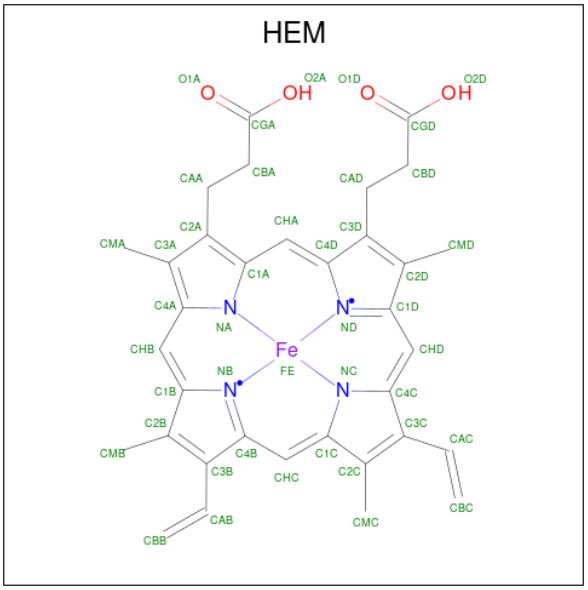
3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2941 atoms, of which 1457 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative uncharacterized protein.

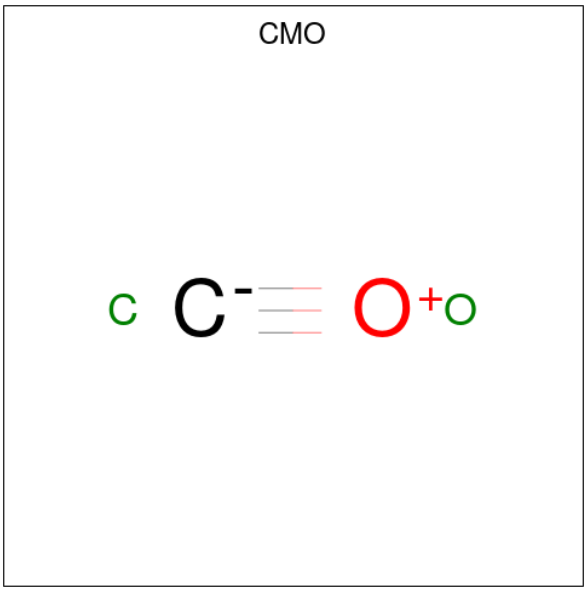
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	181	2866	914	1427	249	264	12	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					
			Total	C	Fe	H	N	O
2	A	1	73	34	1	30	4	4

- Molecule 3 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



Mol	Chain	Residues	Atoms		
			Total	C	O
3	A	1	2	1	1

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Putative uncharacterized protein

Chain A: 49% 33% • 15%

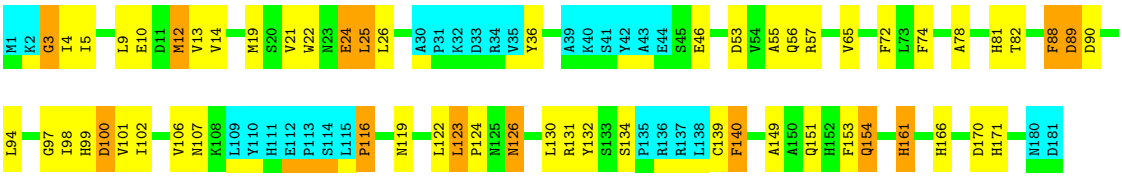
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Putative uncharacterized protein

Chain A: 53% 25% 7% 15%



4.2.2 Score per residue for model 2

• Molecule 1: Putative uncharacterized protein

Chain A: 51% 30% • 15%

M1 K2 G3 I4 I5 L9 E10 D11 M12 V13 V14 M19 S20 V21 W22 L25 L26 E27 K28 H29 A30 P31 K32 D33 R34 V35 Y36 V37 S38 A39 K40 S41 Y42 A43 E44 D53 V54 A55 Q56 R57 D64 V65 F72 L73 F74 A78 H81 T82 D83 D86 K87

F88 D89 D90 F91 T92 S93 L94 V95 M96 G97 I98 H99 D100 V101 I102 V106 N107 K108 L109 Y110 H111 E112 P113 S114 L115 P116 L122 L123 P124 Y132 S133 S134 P135 R136 R137 L138 C139 F140 A149 H152 F153 H161 D162 T163 C164 M165 A169 L174 N180 D181

4.2.3 Score per residue for model 3

- Molecule 1: Putative uncharacterized protein

Chain A: 52% 26% 7% 15%

M1 K2 G3 I4 I5 L9 E10 D11 M12 V13 V14 M19 S20 V21 W22 N23 E24 L25 L26 A30 P31 K32 D33 R34 V35 Y36 A39 K40 S41 Y42 A43 E44 D53 V54 A55 Q56 R57 V65 F72 L73 F74 L77 A78 S79 R80 H81 T82 V85 D86 K87 F88

D89 D90 L94 V95 M96 G97 I98 H99 D100 V101 I102 E105 V106 N107 K108 L109 Y110 H111 E112 P113 S114 L115 P116 H117 I118 L123 P124 N125 A129 L130 S133 S134 P135 R136 R137 L138 A149 H152 F153 H161 D162 T163 D170 H171 C172 M173 L174 N180 D181

4.2.4 Score per residue for model 4

- Molecule 1: Putative uncharacterized protein

Chain A: 50% 29% 6% 15%

M1 K2 G3 I4 I5 F6 N7 V8 L9 E10 D11 M12 V13 V14 M19 S20 V21 W22 L25 L26 H29 A30 P31 K32 D33 R34 V35 Y36 V37 S38 A39 K40 S41 Y42 A43 E44 D53 V54 A55 Q56 R57 V65 F72 L73 F74 S79 R80 H81 V85 D86 K87 F88

D89 D90 L94 G97 I98 H99 D100 V101 I102 V106 N107 K108 L109 Y110 H111 E112 P113 S114 L115 P116 H117 I118 L123 P124 Y132 S133 S134 P135 R136 R137 L138 C139 F140 F147 G148 A149 A150 Q151 H152 F153 Q154 H161 D162 T163 C164 M165 H166 T167 L174 N180 D181

4.2.5 Score per residue for model 5

- Molecule 1: Putative uncharacterized protein

Chain A: 47% 30% 8% 15%

M1 K2 G3 I4 I5 L9 E10 D11 M12 V13 V14 M19 S20 V21 W22 N23 E24 L25 L26 E27 A30 P31 K32 D33 R34 V35 Y36 V37 S38 A39 K40 S41 Y42 A43 E44 D53 V54 A55 Q56 R57 V65 F72 L73 F74 L77 A78 S79 R80 H81 T82 D86 K87

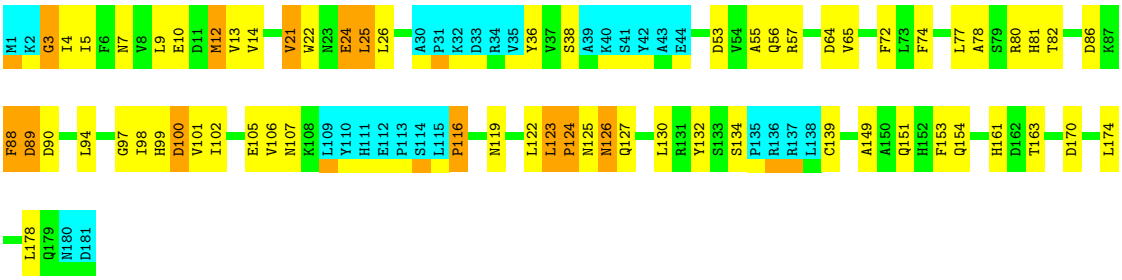
F88 D89 D90 L94 G97 I98 H99 D100 V101 I102 V106 N107 K108 L109 Y110 H111 E112 P113 S114 L115 P116 H117 I118 L122 L123 P124 N125 N126 L130 R131 Y132 S133 S134 P135 R136 R137 L138 C139 F140 C141 A142 A149 A150 Q151 H152 F153 Q154 H161 C164 M165 H166 T167

D170 H171 N180 D181

4.2.6 Score per residue for model 6

• Molecule 1: Putative uncharacterized protein

Chain A: 50% 29% 7% 15%



4.2.7 Score per residue for model 7

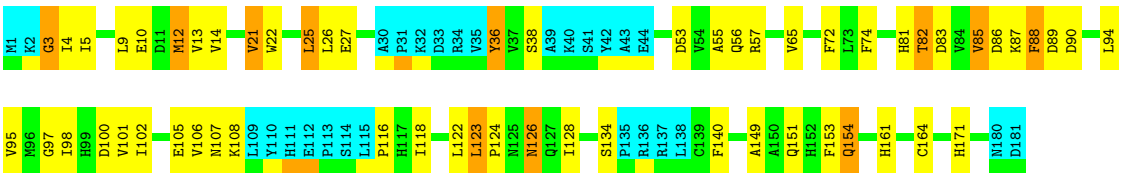
• Molecule 1: Putative uncharacterized protein

Chain A: 49% 28% 8% 15%

4.2.8 Score per residue for model 8

• Molecule 1: Putative uncharacterized protein

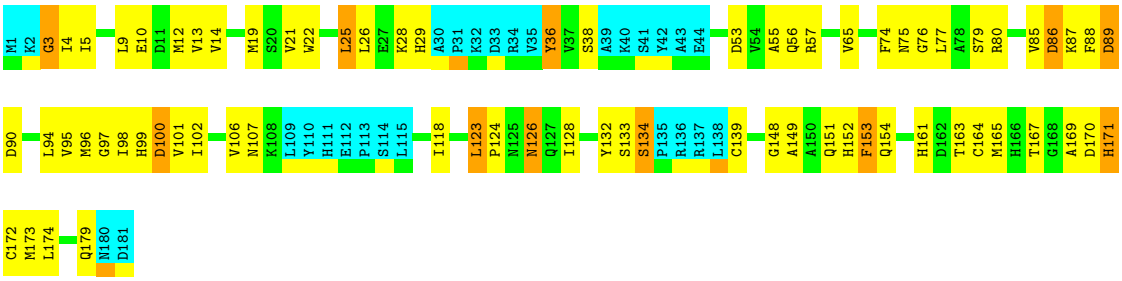
Chain A: 53% 26% 6% 15%



4.2.9 Score per residue for model 9

• Molecule 1: Putative uncharacterized protein

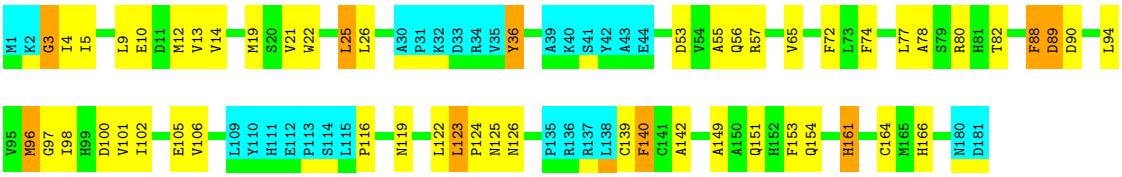
Chain A: 45% 34% 6% 15%



4.2.10 Score per residue for model 10

- Molecule 1: Putative uncharacterized protein

Chain A: 55% 25% 5% 15%



4.2.11 Score per residue for model 11

- Molecule 1: Putative uncharacterized protein

Chain A: 52% 27% 6% 15%

4.2.12 Score per residue for model 12

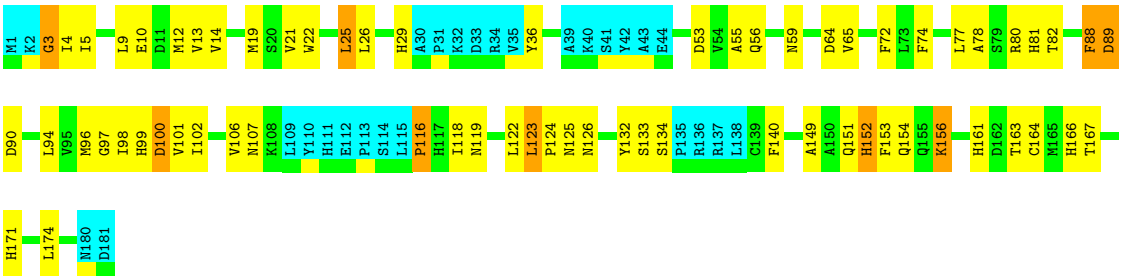
- Molecule 1: Putative uncharacterized protein

Chain A: 51% 28% 6% • 15%

4.2.13 Score per residue for model 13

• Molecule 1: Putative uncharacterized protein

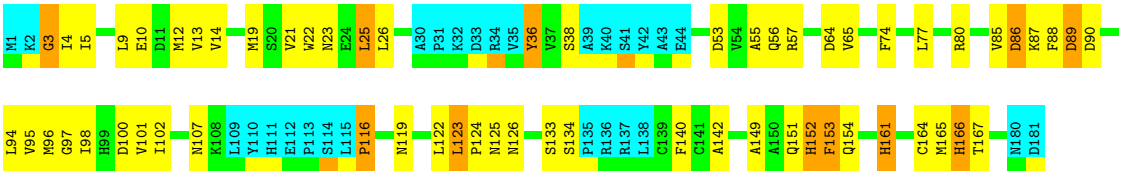
Chain A: 49% 31% 5% 15%



4.2.14 Score per residue for model 14

• Molecule 1: Putative uncharacterized protein

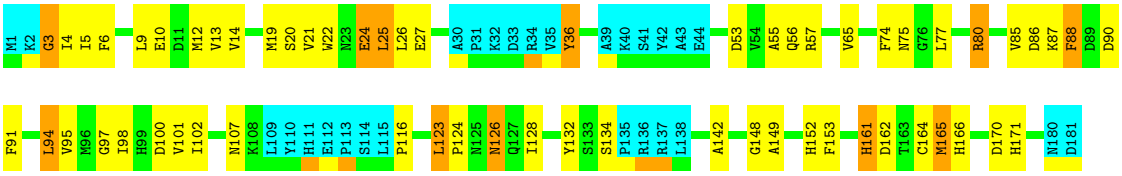
Chain A: 51% 28% 6% 15%



4.2.15 Score per residue for model 15

• Molecule 1: Putative uncharacterized protein

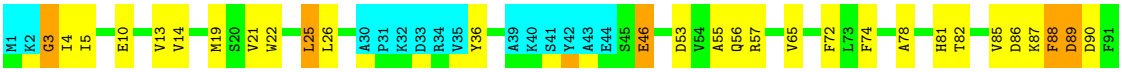
Chain A: 52% 27% 6% 15%

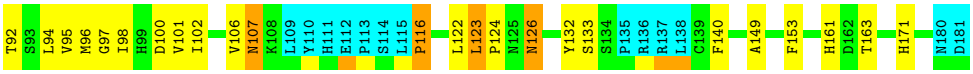


4.2.16 Score per residue for model 16

• Molecule 1: Putative uncharacterized protein

Chain A: 56% 24% 5% 15%

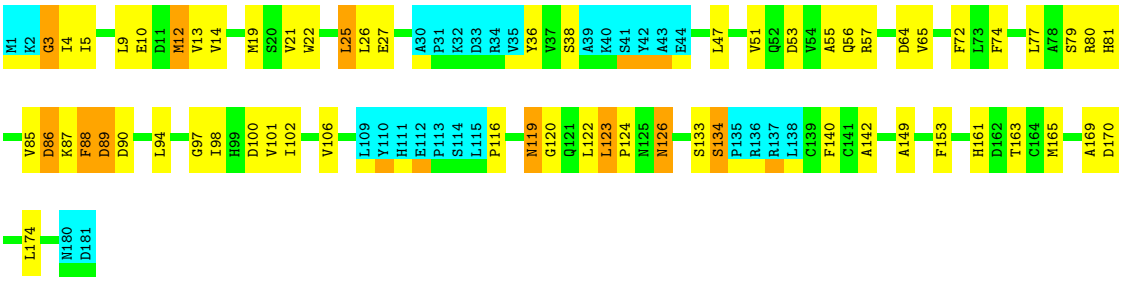




4.2.17 Score per residue for model 17

• Molecule 1: Putative uncharacterized protein

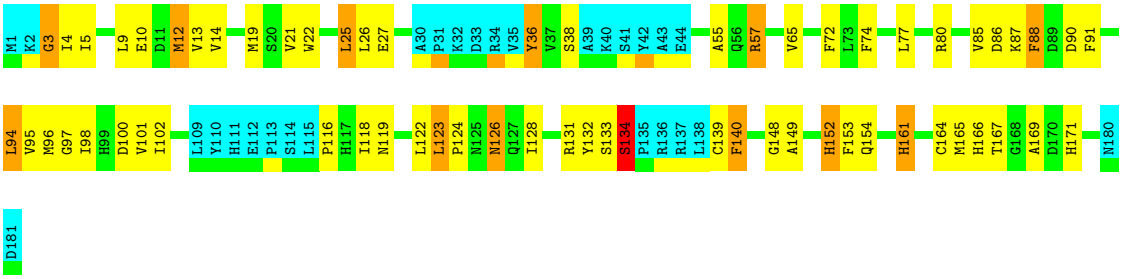
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Putative uncharacterized protein

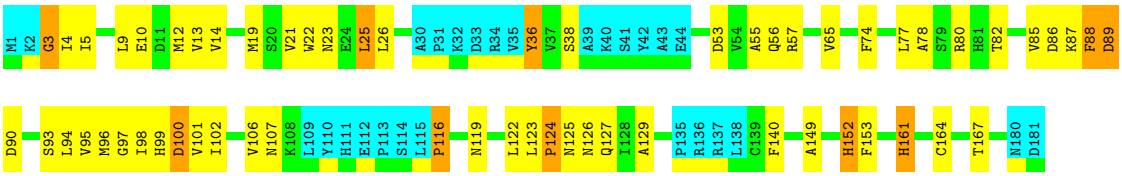
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Putative uncharacterized protein

Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Putative uncharacterized protein

Chain A: 48% 33% • 15%

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1215	1198	1190	61±6
2	A	43	30	30	2±2
All	All	25200	24560	24400	1232

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 25.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:PHE:O	1:A:90:ASP:N	0.94	2.00	14	16
1:A:25:LEU:HD13	1:A:26:LEU:N	0.93	1.78	12	20
1:A:125:ASN:O	1:A:127:GLN:N	0.80	2.14	6	2
1:A:118:ILE:HD12	1:A:119:ASN:N	0.77	1.93	7	1
1:A:25:LEU:HD22	1:A:25:LEU:O	0.75	1.81	16	20
1:A:161:HIS:O	1:A:161:HIS:CG	0.72	2.42	18	9
1:A:88:PHE:CD1	1:A:89:ASP:N	0.71	2.58	20	14
1:A:25:LEU:C	1:A:25:LEU:HD22	0.70	2.07	12	2
1:A:25:LEU:HD22	1:A:25:LEU:C	0.68	2.08	14	18
1:A:85:VAL:O	1:A:88:PHE:CD1	0.68	2.47	8	4
1:A:118:ILE:H	1:A:118:ILE:HD13	0.65	1.52	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:VAL:O	1:A:87:LYS:N	0.64	2.30	14	13
1:A:118:ILE:HD13	1:A:118:ILE:N	0.63	2.08	4	1
1:A:88:PHE:CE1	1:A:153:PHE:CZ	0.63	2.87	9	2
1:A:161:HIS:CD2	1:A:172:CYS:SG	0.63	2.92	3	2
1:A:3:GLY:H	1:A:38:SER:N	0.62	1.92	9	11
1:A:88:PHE:CZ	1:A:153:PHE:CE1	0.62	2.87	14	2
1:A:36:TYR:CD1	1:A:36:TYR:N	0.62	2.68	11	8
1:A:6:PHE:CD2	1:A:36:TYR:CD2	0.62	2.88	15	2
1:A:131:ARG:NH2	1:A:171:HIS:CD2	0.61	2.68	18	1
1:A:28:LYS:NZ	1:A:29:HIS:NE2	0.61	2.48	9	1
1:A:74:PHE:CE1	1:A:149:ALA:HB2	0.61	2.30	16	14
1:A:132:TYR:CD1	1:A:133:SER:N	0.61	2.68	9	4
1:A:74:PHE:CZ	1:A:149:ALA:HB2	0.60	2.31	10	20
1:A:165:MET:SD	1:A:166:HIS:N	0.60	2.74	15	1
1:A:12:MET:SD	1:A:72:PHE:CD2	0.60	2.94	11	9
1:A:88:PHE:C	1:A:90:ASP:H	0.60	1.99	17	14
1:A:28:LYS:NZ	1:A:29:HIS:CD2	0.60	2.68	9	1
1:A:161:HIS:NE2	1:A:172:CYS:SG	0.60	2.75	3	2
1:A:12:MET:SD	1:A:72:PHE:CG	0.59	2.95	8	9
1:A:131:ARG:NH2	1:A:171:HIS:CG	0.59	2.70	18	2
1:A:3:GLY:N	1:A:36:TYR:O	0.59	2.35	19	16
1:A:81:HIS:CD2	2:A:182:HEM:CBC	0.59	2.86	16	3
1:A:99:HIS:CG	1:A:100:ASP:N	0.59	2.69	13	4
1:A:25:LEU:HD13	1:A:26:LEU:H	0.59	1.56	12	12
1:A:131:ARG:HH21	1:A:171:HIS:CG	0.58	2.16	1	3
1:A:123:LEU:O	1:A:124:PRO:O	0.58	2.20	6	7
1:A:10:GLU:O	1:A:14:VAL:HG23	0.58	1.98	14	20
1:A:88:PHE:CG	1:A:88:PHE:O	0.58	2.55	18	3
1:A:172:CYS:SG	1:A:174:LEU:CD1	0.58	2.91	9	2
1:A:161:HIS:O	1:A:161:HIS:ND1	0.58	2.37	10	7
1:A:101:VAL:HG23	1:A:102:ILE:N	0.57	2.14	13	20
1:A:149:ALA:O	1:A:153:PHE:CD2	0.57	2.58	10	19
1:A:156:LYS:NZ	1:A:179:GLN:NE2	0.57	2.53	7	2
1:A:118:ILE:N	1:A:118:ILE:CD1	0.57	2.68	4	1
1:A:118:ILE:HD12	1:A:118:ILE:C	0.57	2.19	7	1
1:A:94:LEU:O	1:A:97:GLY:N	0.57	2.37	15	20
1:A:78:ALA:O	1:A:82:THR:N	0.56	2.38	3	12
1:A:166:HIS:CE1	1:A:167:THR:OG1	0.56	2.59	14	3
1:A:125:ASN:ND2	1:A:126:ASN:H	0.56	1.98	19	1
1:A:99:HIS:ND1	1:A:100:ASP:N	0.56	2.54	13	2
1:A:3:GLY:H	1:A:38:SER:H	0.55	1.43	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:ASN:ND2	1:A:152:HIS:NE2	0.55	2.54	9	2
1:A:81:HIS:NE2	1:A:85:VAL:CG2	0.55	2.70	17	3
1:A:126:ASN:O	1:A:126:ASN:OD1	0.55	2.25	13	4
1:A:25:LEU:HD13	1:A:25:LEU:C	0.54	2.22	19	19
1:A:101:VAL:CG2	1:A:102:ILE:N	0.54	2.70	7	20
1:A:28:LYS:NZ	1:A:29:HIS:CE1	0.54	2.76	2	1
1:A:161:HIS:NE2	1:A:163:THR:O	0.54	2.40	6	9
1:A:88:PHE:CD1	1:A:88:PHE:O	0.54	2.61	12	3
1:A:75:ASN:OD1	1:A:152:HIS:CE1	0.54	2.61	15	2
1:A:27:GLU:N	1:A:27:GLU:OE1	0.54	2.41	5	1
1:A:88:PHE:O	1:A:88:PHE:CD1	0.54	2.61	18	1
1:A:105:GLU:OE1	1:A:106:VAL:N	0.53	2.41	10	2
1:A:7:ASN:ND2	1:A:80:ARG:NH2	0.53	2.56	11	1
1:A:21:VAL:CG2	1:A:57:ARG:NE	0.53	2.71	8	17
1:A:148:GLY:O	1:A:152:HIS:CE1	0.53	2.61	15	2
1:A:46:GLU:N	1:A:46:GLU:OE1	0.53	2.42	20	3
1:A:142:ALA:N	2:A:182:HEM:O1A	0.53	2.42	15	1
1:A:4:ILE:HG23	1:A:5:ILE:N	0.53	2.17	14	20
1:A:149:ALA:O	1:A:153:PHE:CE2	0.53	2.62	7	13
1:A:166:HIS:O	1:A:166:HIS:ND1	0.53	2.42	1	6
1:A:147:PHE:O	1:A:151:GLN:NE2	0.53	2.42	4	1
1:A:132:TYR:CE1	2:A:182:HEM:HMA1	0.53	2.39	15	1
1:A:163:THR:O	1:A:172:CYS:SG	0.53	2.67	3	2
1:A:126:ASN:ND2	1:A:178:LEU:O	0.53	2.42	6	2
1:A:166:HIS:ND1	1:A:166:HIS:C	0.53	2.61	11	3
1:A:170:ASP:O	1:A:171:HIS:ND1	0.53	2.42	1	3
1:A:161:HIS:CD2	1:A:172:CYS:HG	0.53	2.22	9	2
1:A:132:TYR:CE1	1:A:139:CYS:SG	0.53	2.96	4	2
1:A:99:HIS:NE2	1:A:100:ASP:OD1	0.53	2.42	7	2
1:A:81:HIS:O	1:A:83:ASP:N	0.53	2.42	8	1
1:A:132:TYR:CZ	1:A:134:SER:OG	0.52	2.62	5	5
1:A:164:CYS:SG	1:A:164:CYS:O	0.52	2.67	9	3
1:A:21:VAL:CG2	1:A:57:ARG:HE	0.52	2.17	5	1
1:A:148:GLY:O	1:A:152:HIS:ND1	0.52	2.42	18	2
1:A:170:ASP:OD1	1:A:171:HIS:CD2	0.52	2.62	1	1
1:A:88:PHE:CD1	1:A:88:PHE:C	0.52	2.83	12	6
1:A:126:ASN:N	1:A:126:ASN:OD1	0.52	2.42	1	8
1:A:161:HIS:CG	1:A:174:LEU:HD11	0.52	2.39	7	8
1:A:99:HIS:CE1	1:A:100:ASP:OD1	0.52	2.62	6	1
1:A:28:LYS:HZ2	1:A:29:HIS:CD2	0.52	2.22	9	1
1:A:99:HIS:CE1	1:A:100:ASP:OD2	0.52	2.62	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:ASN:HD22	1:A:126:ASN:H	0.52	1.45	19	1
1:A:99:HIS:CD2	1:A:100:ASP:OD1	0.52	2.62	3	2
1:A:165:MET:SD	1:A:169:ALA:O	0.52	2.68	2	4
1:A:29:HIS:NE2	1:A:53:ASP:OD2	0.52	2.42	13	2
1:A:170:ASP:OD1	1:A:171:HIS:ND1	0.52	2.42	5	3
1:A:24:GLU:OE1	1:A:24:GLU:N	0.52	2.42	5	5
1:A:79:SER:OG	1:A:80:ARG:NH1	0.52	2.42	4	2
1:A:148:GLY:O	1:A:152:HIS:CG	0.52	2.62	9	2
1:A:139:CYS:SG	1:A:140:PHE:N	0.52	2.83	18	3
1:A:170:ASP:O	1:A:171:HIS:CG	0.52	2.63	15	1
1:A:132:TYR:CE1	1:A:134:SER:OG	0.52	2.62	13	1
1:A:151:GLN:O	1:A:154:GLN:N	0.52	2.43	6	11
1:A:152:HIS:O	1:A:152:HIS:ND1	0.52	2.42	7	7
1:A:139:CYS:SG	1:A:164:CYS:SG	0.52	3.04	2	1
1:A:81:HIS:CE1	1:A:105:GLU:OE2	0.52	2.62	20	1
1:A:88:PHE:C	1:A:90:ASP:N	0.51	2.64	17	14
1:A:81:HIS:CG	2:A:182:HEM:HBC1	0.51	2.40	16	2
1:A:94:LEU:HD23	1:A:94:LEU:C	0.51	2.26	8	3
2:A:182:HEM:CGA	2:A:182:HEM:CMA	0.51	2.88	14	3
2:A:182:HEM:CGA	2:A:182:HEM:C3A	0.51	2.93	19	1
1:A:124:PRO:O	1:A:125:ASN:C	0.51	2.48	12	2
1:A:161:HIS:NE2	1:A:164:CYS:SG	0.51	2.84	8	1
1:A:132:TYR:CE2	1:A:134:SER:OG	0.51	2.63	18	1
1:A:85:VAL:O	1:A:88:PHE:N	0.51	2.41	8	3
1:A:125:ASN:O	1:A:126:ASN:CG	0.51	2.48	10	3
1:A:25:LEU:C	1:A:25:LEU:CD2	0.51	2.79	12	20
1:A:90:ASP:OD1	1:A:91:PHE:N	0.51	2.43	15	2
1:A:134:SER:O	1:A:165:MET:SD	0.51	2.69	14	4
1:A:81:HIS:CD2	2:A:182:HEM:HBC1	0.51	2.40	16	1
1:A:165:MET:SD	1:A:165:MET:O	0.50	2.69	18	3
1:A:164:CYS:SG	1:A:167:THR:OG1	0.50	2.69	9	6
1:A:89:ASP:OD1	1:A:90:ASP:N	0.50	2.45	12	2
1:A:96:MET:SD	1:A:96:MET:O	0.50	2.69	11	6
2:A:182:HEM:HMA2	2:A:182:HEM:O1A	0.50	2.07	12	1
1:A:161:HIS:CE1	1:A:164:CYS:HG	0.50	2.24	8	1
1:A:88:PHE:CE2	1:A:153:PHE:CE2	0.50	3.00	4	11
1:A:161:HIS:CD2	1:A:163:THR:O	0.50	2.65	2	10
1:A:55:ALA:CB	1:A:65:VAL:HG21	0.49	2.37	6	20
1:A:77:LEU:O	1:A:80:ARG:N	0.49	2.43	11	15
1:A:81:HIS:NE2	2:A:182:HEM:HMC3	0.49	2.22	17	1
1:A:81:HIS:CE1	2:A:182:HEM:CBC	0.49	2.95	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:VAL:C	1:A:87:LYS:N	0.49	2.66	8	11
1:A:88:PHE:CZ	1:A:153:PHE:CE2	0.49	3.01	4	9
1:A:3:GLY:N	1:A:38:SER:N	0.49	2.61	9	5
1:A:74:PHE:CE1	1:A:149:ALA:CB	0.49	2.96	16	10
1:A:88:PHE:O	1:A:88:PHE:CG	0.49	2.65	8	1
1:A:156:LYS:NZ	1:A:156:LYS:CB	0.49	2.76	11	1
1:A:12:MET:SD	1:A:72:PHE:CB	0.49	3.01	2	8
1:A:13:VAL:HG23	1:A:14:VAL:N	0.49	2.23	14	20
1:A:21:VAL:CG2	1:A:57:ARG:NH1	0.49	2.75	18	1
1:A:4:ILE:HD11	1:A:80:ARG:HD3	0.48	1.86	6	1
1:A:4:ILE:CG2	1:A:5:ILE:N	0.48	2.77	10	16
1:A:132:TYR:CD1	1:A:132:TYR:C	0.48	2.86	4	3
1:A:125:ASN:O	1:A:126:ASN:OD1	0.48	2.32	13	4
1:A:132:TYR:CD2	1:A:139:CYS:SG	0.48	3.07	12	1
1:A:81:HIS:CD2	2:A:182:HEM:CAC	0.48	2.96	16	1
1:A:107:ASN:O	1:A:107:ASN:ND2	0.48	2.45	16	1
1:A:92:THR:O	1:A:96:MET:CE	0.48	2.61	16	2
2:A:182:HEM:O1A	2:A:182:HEM:C2A	0.48	2.66	16	1
1:A:164:CYS:C	1:A:166:HIS:N	0.48	2.67	4	6
1:A:88:PHE:CZ	1:A:153:PHE:CZ	0.48	3.01	9	2
1:A:156:LYS:HZ1	1:A:179:GLN:HE22	0.48	1.52	11	1
2:A:182:HEM:CGA	2:A:182:HEM:HMA3	0.48	2.39	19	2
1:A:21:VAL:CG1	1:A:22:TRP:N	0.47	2.77	18	15
1:A:88:PHE:CD2	1:A:90:ASP:C	0.47	2.88	17	12
1:A:123:LEU:CB	1:A:124:PRO:CD	0.47	2.93	9	12
1:A:27:GLU:OE1	1:A:27:GLU:CA	0.47	2.62	5	1
1:A:153:PHE:CD1	1:A:153:PHE:N	0.47	2.80	9	12
1:A:161:HIS:CD2	1:A:161:HIS:C	0.47	2.87	19	1
1:A:83:ASP:O	1:A:86:ASP:OD1	0.47	2.32	2	1
1:A:116:PRO:CG	2:A:182:HEM:O2A	0.47	2.62	3	2
1:A:133:SER:O	1:A:134:SER:CB	0.47	2.62	9	5
1:A:125:ASN:ND2	1:A:126:ASN:N	0.47	2.63	19	1
1:A:24:GLU:OE1	1:A:24:GLU:CA	0.47	2.62	5	5
1:A:172:CYS:SG	1:A:173:MET:N	0.47	2.88	9	2
1:A:131:ARG:NH2	1:A:171:HIS:ND1	0.47	2.62	1	1
1:A:132:TYR:CE1	2:A:182:HEM:HMA3	0.47	2.45	5	1
2:A:182:HEM:C3A	2:A:182:HEM:O1A	0.47	2.68	5	1
1:A:81:HIS:C	1:A:83:ASP:N	0.47	2.69	8	1
1:A:156:LYS:NZ	1:A:179:GLN:CD	0.47	2.68	7	1
1:A:9:LEU:O	1:A:12:MET:N	0.47	2.46	18	18
1:A:107:ASN:ND2	1:A:107:ASN:C	0.47	2.68	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:HIS:CG	1:A:100:ASP:H	0.46	2.27	7	2
1:A:81:HIS:NE2	2:A:182:HEM:CBC	0.46	2.79	8	1
1:A:105:GLU:O	1:A:108:LYS:N	0.46	2.48	8	2
1:A:164:CYS:SG	1:A:166:HIS:CD2	0.46	3.08	14	1
1:A:170:ASP:C	1:A:171:HIS:CG	0.46	2.88	20	2
1:A:81:HIS:CE1	1:A:85:VAL:CG2	0.46	2.97	4	3
1:A:75:ASN:CG	1:A:152:HIS:NE2	0.46	2.69	9	2
1:A:6:PHE:CG	1:A:36:TYR:CD2	0.46	3.04	15	1
1:A:85:VAL:C	1:A:87:LYS:H	0.46	2.13	15	11
1:A:116:PRO:CG	2:A:182:HEM:O1A	0.46	2.63	7	2
1:A:156:LYS:NZ	1:A:179:GLN:HE22	0.46	2.09	11	1
1:A:55:ALA:HB2	1:A:65:VAL:HG21	0.46	1.87	8	20
1:A:119:ASN:HD22	1:A:120:GLY:N	0.46	2.07	17	1
1:A:96:MET:C	1:A:96:MET:SD	0.46	2.95	10	4
1:A:165:MET:SD	1:A:165:MET:C	0.45	2.93	15	1
1:A:132:TYR:HH	2:A:182:HEM:CGA	0.45	2.23	16	1
1:A:106:VAL:HG23	1:A:107:ASN:N	0.45	2.26	19	5
1:A:151:GLN:OE1	1:A:151:GLN:N	0.45	2.49	4	1
1:A:123:LEU:HD11	1:A:129:ALA:HB2	0.45	1.86	19	1
1:A:53:ASP:O	1:A:56:GLN:N	0.45	2.49	10	19
1:A:96:MET:SD	1:A:122:LEU:HD13	0.45	2.52	2	2
1:A:148:GLY:O	1:A:152:HIS:CD2	0.45	2.69	15	2
1:A:94:LEU:CD2	1:A:94:LEU:C	0.45	2.85	12	3
1:A:22:TRP:O	1:A:26:LEU:CB	0.45	2.65	12	12
1:A:94:LEU:C	1:A:94:LEU:CD2	0.45	2.86	8	3
1:A:164:CYS:SG	1:A:165:MET:CE	0.45	3.05	15	1
1:A:161:HIS:O	1:A:161:HIS:CD2	0.45	2.70	19	1
1:A:164:CYS:O	1:A:166:HIS:N	0.44	2.50	4	4
1:A:78:ALA:O	1:A:82:THR:CA	0.44	2.65	20	6
1:A:88:PHE:O	1:A:93:SER:OG	0.44	2.27	20	2
1:A:125:ASN:ND2	1:A:127:GLN:OE1	0.44	2.50	19	1
1:A:102:ILE:O	1:A:106:VAL:HG13	0.44	2.13	6	5
1:A:106:VAL:HG11	2:A:182:HEM:CAC	0.44	2.42	11	3
1:A:125:ASN:N	1:A:125:ASN:OD1	0.44	2.50	10	2
1:A:75:ASN:ND2	1:A:152:HIS:CE1	0.44	2.85	9	2
1:A:118:ILE:HG23	1:A:118:ILE:O	0.44	2.11	12	2
1:A:90:ASP:O	1:A:90:ASP:OD1	0.43	2.36	3	4
1:A:106:VAL:CG1	2:A:182:HEM:CBC	0.43	2.95	4	1
1:A:152:HIS:CG	1:A:153:PHE:CE1	0.43	3.06	19	2
1:A:164:CYS:C	1:A:166:HIS:H	0.43	2.16	13	5
1:A:88:PHE:O	1:A:90:ASP:OD1	0.43	2.36	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:ASN:HD21	1:A:152:HIS:CE1	0.43	2.30	15	2
1:A:125:ASN:HD21	1:A:127:GLN:CG	0.43	2.26	19	1
1:A:23:ASN:O	1:A:27:GLU:OE2	0.43	2.36	5	1
1:A:133:SER:O	1:A:134:SER:OG	0.43	2.37	14	2
1:A:165:MET:HA	1:A:169:ALA:HB3	0.43	1.89	9	1
1:A:170:ASP:OD1	1:A:171:HIS:N	0.43	2.52	1	1
1:A:86:ASP:O	1:A:86:ASP:OD1	0.43	2.37	6	9
1:A:88:PHE:CE1	1:A:153:PHE:CE2	0.43	3.07	14	2
2:A:182:HEM:HMA1	2:A:182:HEM:CGA	0.43	2.43	10	1
1:A:162:ASP:OD1	1:A:162:ASP:N	0.43	2.42	15	1
1:A:75:ASN:OD1	1:A:152:HIS:ND1	0.43	2.48	20	1
1:A:102:ILE:CG2	2:A:182:HEM:C2C	0.43	3.01	6	8
1:A:64:ASP:O	1:A:64:ASP:OD1	0.43	2.37	6	4
1:A:20:SER:O	1:A:24:GLU:OE1	0.43	2.37	5	2
1:A:89:ASP:O	1:A:90:ASP:OD1	0.43	2.37	8	7
1:A:156:LYS:NZ	1:A:179:GLN:OE1	0.43	2.50	7	1
1:A:95:VAL:CG1	1:A:128:ILE:HG21	0.43	2.44	8	5
1:A:142:ALA:HB2	2:A:182:HEM:CMA	0.43	2.44	5	2
1:A:96:MET:O	1:A:100:ASP:OD2	0.43	2.37	7	1
1:A:132:TYR:CD1	1:A:139:CYS:SG	0.43	3.03	9	1
1:A:7:ASN:ND2	1:A:80:ARG:HH21	0.43	2.12	4	1
1:A:85:VAL:HG12	1:A:88:PHE:CE1	0.43	2.49	15	2
1:A:46:GLU:N	1:A:46:GLU:CD	0.43	2.72	20	2
1:A:94:LEU:O	1:A:95:VAL:C	0.42	2.57	16	8
1:A:118:ILE:C	1:A:118:ILE:CD1	0.42	2.85	7	1
1:A:161:HIS:CE1	1:A:164:CYS:SG	0.42	3.12	8	1
1:A:88:PHE:CG	1:A:89:ASP:N	0.42	2.87	19	1
1:A:125:ASN:O	1:A:126:ASN:C	0.42	2.57	12	2
1:A:132:TYR:CG	1:A:133:SER:N	0.42	2.88	11	3
1:A:3:GLY:CA	1:A:36:TYR:O	0.42	2.67	15	1
1:A:170:ASP:OD1	1:A:170:ASP:O	0.42	2.38	3	5
1:A:3:GLY:N	1:A:38:SER:H	0.42	2.10	19	2
1:A:88:PHE:O	1:A:89:ASP:C	0.42	2.56	9	2
1:A:106:VAL:CG1	2:A:182:HEM:HAC	0.42	2.45	20	2
1:A:132:TYR:OH	2:A:182:HEM:CGA	0.42	2.67	16	1
1:A:171:HIS:CD2	1:A:171:HIS:N	0.42	2.87	8	2
1:A:76:GLY:O	1:A:79:SER:OG	0.42	2.36	12	2
1:A:86:ASP:OD1	1:A:86:ASP:C	0.42	2.57	2	1
1:A:126:ASN:OD1	1:A:126:ASN:N	0.42	2.53	9	1
1:A:132:TYR:OH	2:A:182:HEM:O2A	0.42	2.37	9	2
1:A:132:TYR:CD2	1:A:133:SER:N	0.42	2.88	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:HIS:ND1	1:A:99:HIS:N	0.41	2.67	3	1
1:A:88:PHE:CE1	1:A:153:PHE:CE1	0.41	3.08	14	1
1:A:170:ASP:CG	1:A:171:HIS:CD2	0.41	2.93	1	1
1:A:106:VAL:CG2	1:A:107:ASN:N	0.41	2.84	19	3
1:A:124:PRO:O	1:A:125:ASN:CG	0.41	2.58	19	1
1:A:151:GLN:O	1:A:153:PHE:N	0.41	2.53	6	2
1:A:3:GLY:H	1:A:37:VAL:C	0.41	2.19	5	1
1:A:64:ASP:OD1	1:A:64:ASP:O	0.41	2.39	17	2
1:A:89:ASP:O	1:A:89:ASP:OD1	0.41	2.38	7	1
1:A:85:VAL:CG1	1:A:88:PHE:CZ	0.41	3.02	15	2
1:A:6:PHE:CG	1:A:36:TYR:CG	0.41	3.08	15	1
1:A:126:ASN:O	1:A:126:ASN:CG	0.41	2.58	6	1
1:A:171:HIS:N	1:A:171:HIS:ND1	0.41	2.67	9	1
1:A:150:ALA:HB1	1:A:155:GLN:O	0.41	2.15	20	1
1:A:86:ASP:OD1	1:A:86:ASP:O	0.41	2.39	3	1
1:A:156:LYS:CD	1:A:156:LYS:H	0.41	2.28	13	1
1:A:170:ASP:OD1	1:A:170:ASP:N	0.41	2.54	5	1
1:A:118:ILE:O	1:A:118:ILE:HG23	0.41	2.15	9	1
1:A:153:PHE:O	1:A:154:GLN:C	0.41	2.58	18	1
1:A:23:ASN:O	1:A:27:GLU:CD	0.40	2.59	5	1
1:A:139:CYS:O	1:A:142:ALA:N	0.40	2.54	10	1
1:A:81:HIS:CE1	2:A:182:HEM:HMC3	0.40	2.52	4	1
1:A:47:LEU:O	1:A:51:VAL:HG23	0.40	2.16	17	1
1:A:81:HIS:O	1:A:81:HIS:CG	0.40	2.75	17	1
1:A:7:ASN:HD21	1:A:80:ARG:NH2	0.40	2.12	11	1
1:A:94:LEU:C	1:A:94:LEU:HD23	0.40	2.35	18	1
1:A:88:PHE:CD2	1:A:90:ASP:O	0.40	2.75	2	1
1:A:123:LEU:HD21	1:A:129:ALA:CB	0.40	2.46	3	1
1:A:81:HIS:CE1	1:A:85:VAL:HG23	0.40	2.51	4	1
1:A:142:ALA:CA	2:A:182:HEM:O1A	0.40	2.70	14	1
1:A:151:GLN:N	1:A:151:GLN:CD	0.40	2.75	4	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	154/181 (85%)	135±2 (88±2%)	13±2 (8±2%)	6±1 (4±0%)	5 31
All	All	3080/3620 (85%)	2701 (88%)	256 (8%)	123 (4%)	5 31

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	3	GLY	20
1	A	98	ILE	20
1	A	100	ASP	20
1	A	116	PRO	18
1	A	89	ASP	16
1	A	86	ASP	15
1	A	124	PRO	8
1	A	134	SER	3
1	A	126	ASN	2
1	A	82	THR	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	136/160 (85%)	125±2 (92±2%)	11±2 (8±2%)	15 62
All	All	2720/3200 (85%)	2495 (92%)	225 (8%)	15 62

All 39 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	25	LEU	20
1	A	88	PHE	18
1	A	123	LEU	18
1	A	19	MET	15
1	A	140	PHE	15
1	A	122	LEU	12
1	A	126	ASN	10
1	A	36	TYR	10

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Mol	Chain	Res	Type	Models (Total)
1	A	12	MET	9
1	A	119	ASN	9
1	A	161	HIS	8
1	A	152	HIS	7
1	A	81	HIS	6
1	A	72	PHE	6
1	A	118	ILE	6
1	A	24	GLU	5
1	A	130	LEU	5
1	A	134	SER	5
1	A	153	PHE	5
1	A	21	VAL	5
1	A	154	GLN	3
1	A	23	ASN	3
1	A	166	HIS	3
1	A	94	LEU	3
1	A	96	MET	2
1	A	82	THR	2
1	A	171	HIS	2
1	A	59	ASN	2
1	A	108	LYS	1
1	A	125	ASN	1
1	A	27	GLU	1
1	A	133	SER	1
1	A	85	VAL	1
1	A	156	LYS	1
1	A	80	ARG	1
1	A	165	MET	1
1	A	46	GLU	1
1	A	107	ASN	1
1	A	57	ARG	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	CMO	A	183	2	0,1,1	0.00±0.00	-
2	HEM	A	182	1,3	27,50,50	1.92±0.02	4±0 (15±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	CMO	A	183	2	-	-	-
2	HEM	A	182	1,3	17,82,82	1.13±0.04	0±0 (0±1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	182	1,3	-	0±0,6,54,54	-

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	182	HEM	C3B-CAB	4.80	1.38	1.47	5	20
2	A	182	HEM	C3C-CAC	4.61	1.38	1.47	5	20
2	A	182	HEM	C3C-C2C	4.34	1.34	1.40	13	20
2	A	182	HEM	C3B-C2B	4.13	1.34	1.40	19	20
2	A	182	HEM	CAA-C2A	2.18	1.48	1.52	5	1

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	182	HEM	C4A-C3A-C2A	2.76	105.08	107.00	6	2

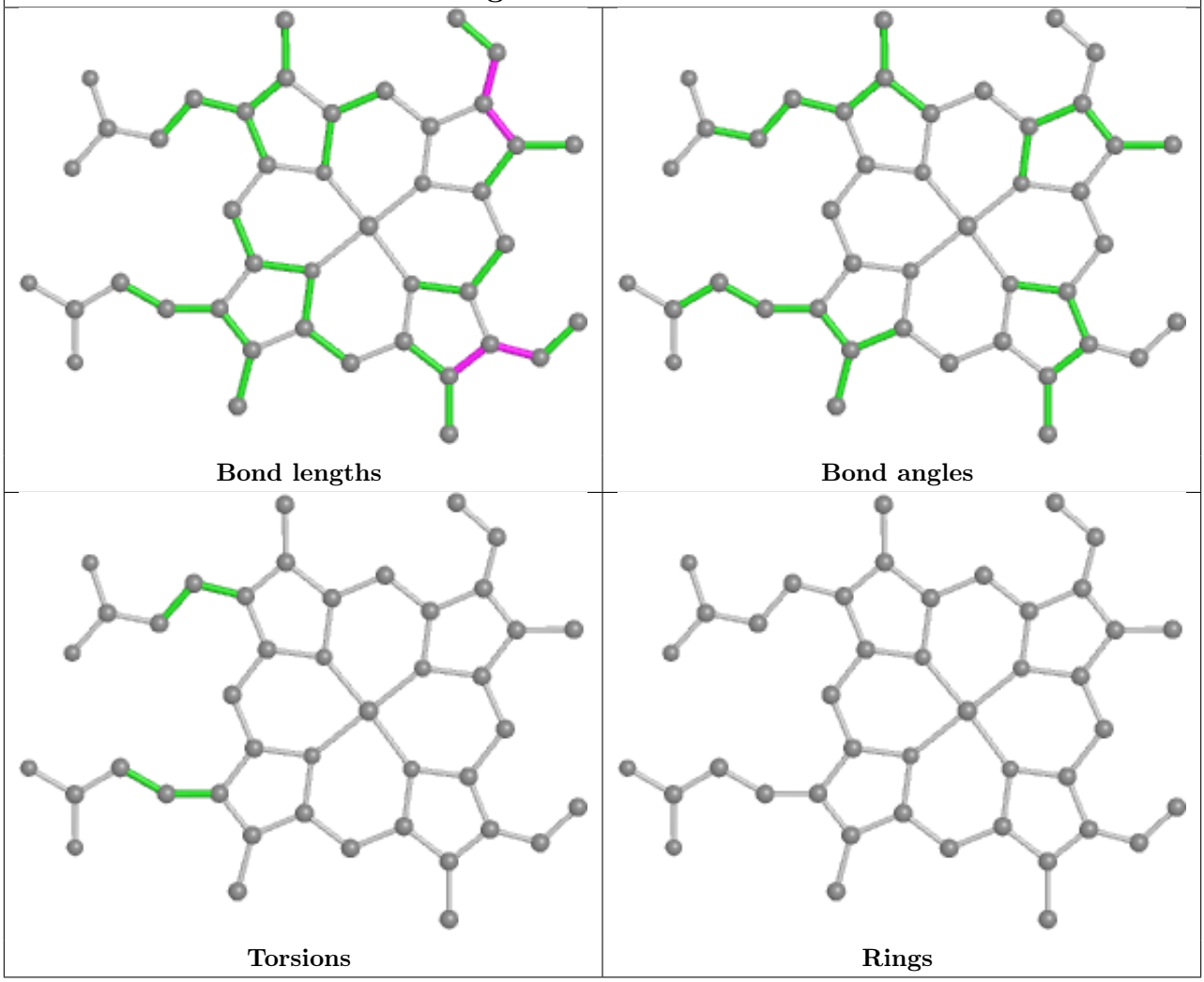
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 A 182



6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided