Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:05 PM GMT

PDB ID	:	1IQC
Title	:	Crystal structure of Di-Heme Peroxidase from Nitrosomonas europaea
Authors	:	Shimizu, H.
Deposited on	:	2001-07-20
Resolution	:	1.80 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 (i) symbol.

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

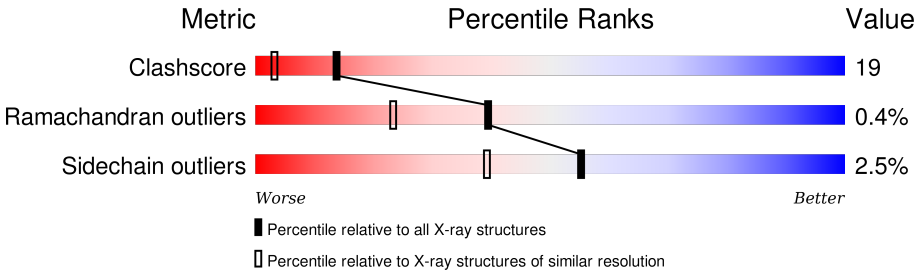
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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 <=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	308	83% 16%
1	B	308	74% 23%
1	C	308	88% 11%
1	D	308	52% 44%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10767 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 di-heme peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	B	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	C	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			
1	D	308	Total	C	N	O	S	0	0	0
			2388	1497	411	467	13			

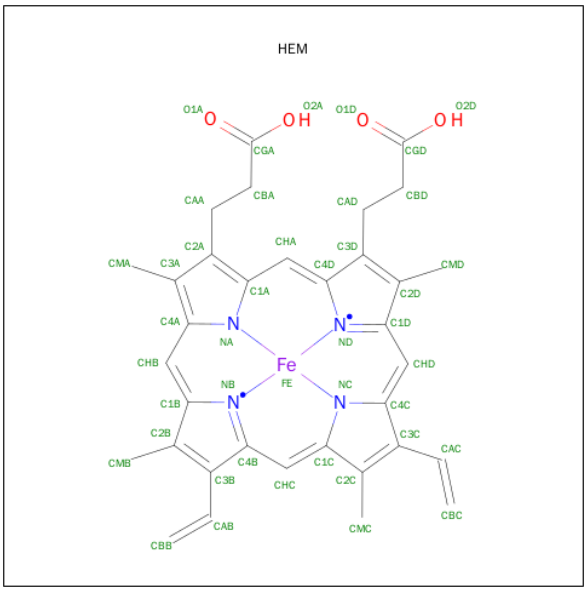
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	2	Total	Ca	0	0
			2	2		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

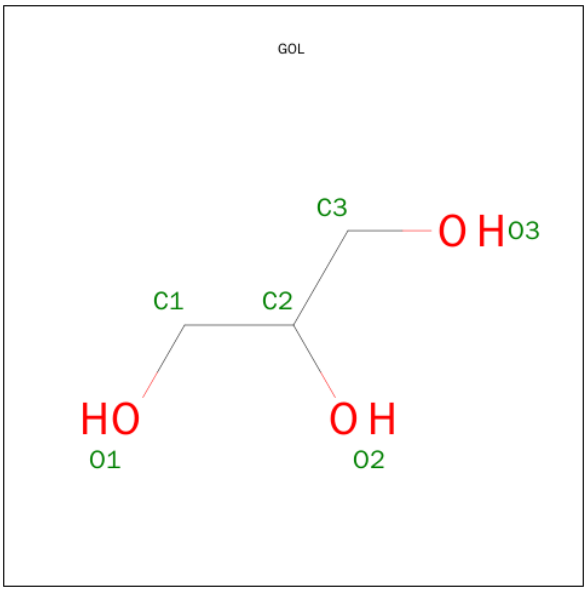
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- 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
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	260	Total O 260 260	0	0
6	B	199	Total O 199 199	0	0
6	C	279	Total O 279 279	0	0
6	D	120	Total O 120 120	0	0

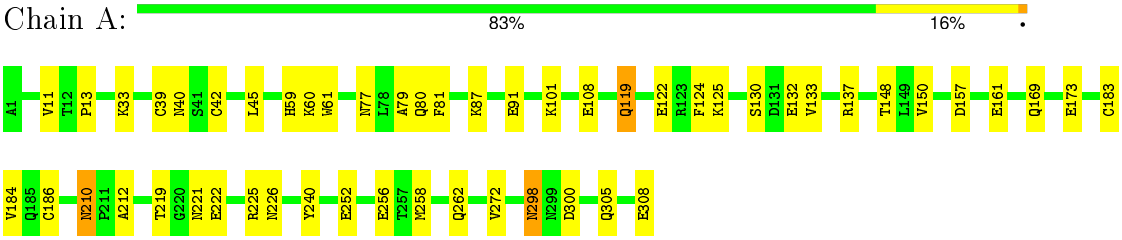
3 Residue-property plots (i)

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.

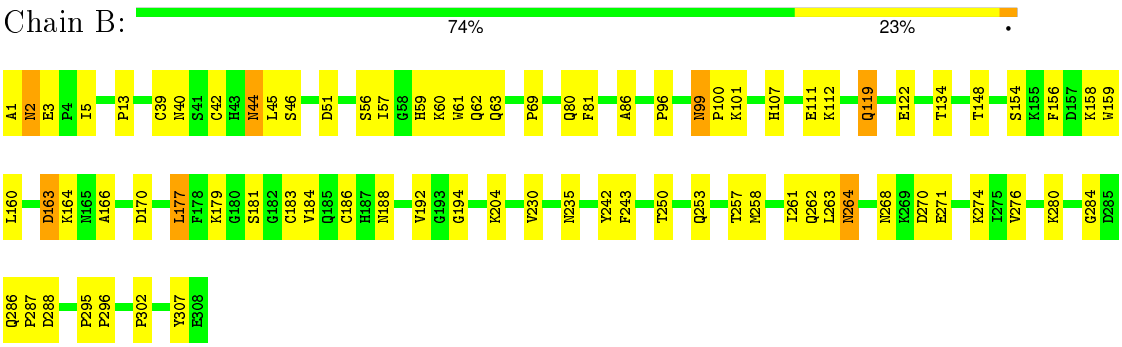
- Molecule 1: di-heme peroxidase

Chain A:



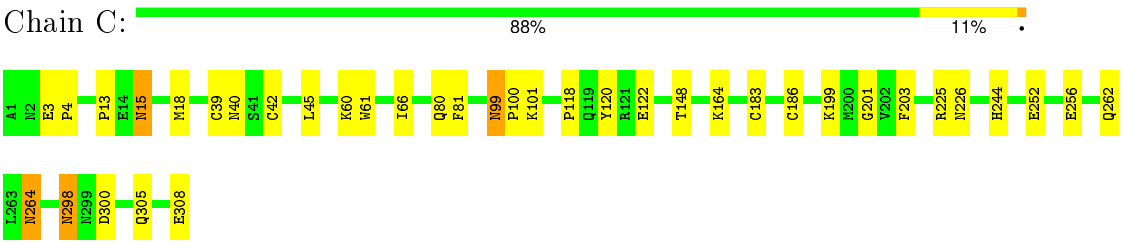
- Molecule 1: di-heme peroxidase

Chain B:



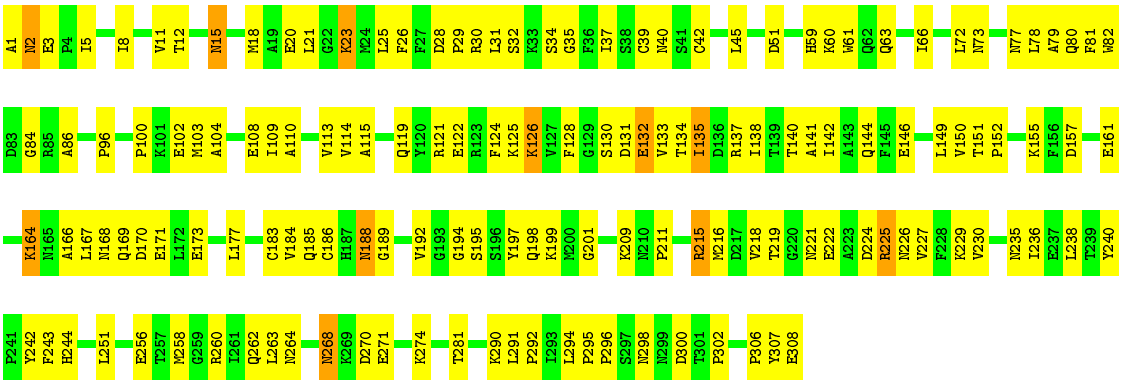
- Molecule 1: di-heme peroxidase

Chain C:



- Molecule 1: di-heme peroxidase

Chain D:


A1 M2 E3 P4 I5 I8 V11 T12 N15 M18 A19 E20 L21 G22 K23 M24 L25 F26 F27 D28 P29 R30 I31 S32 K33 S34 G35 F36 I37 S38 C39 N40 S41 C42 L45 D51 H59 K60 W61 Q62 Q63 I66 L72 N73 N77 L78 A79 Q80 F81 W82
D83 G84 R85 A86 P96 P100 K101 E102 M103 A104 E108 I109 A110 V113 V114 A115 Q119 Y120 R121 E122 R123 F124 K125 K126 V127 F128 G129 S130 D131 E132 V133 T134 I135 D136 R137 I138 T139 T140 A141 I142 A143 Q144 F145 E146 L149 V150 T151 P152 K155 F156 D157 E161
K164 N165 A166 L167 N168 Q169 D170 E171 L172 E173 L177 C183 V184 Q185 C186 H187 N188 G189 V192 G193 G194 S195 S196 Y197 Q198 K199 M200 G201 K209 N210 P211 R215 M216 D217 V218 T219 G220 N221 E222 A223 D224 R225 N226 V227 F228 K229 V230 N235 I236 E237 L238 T239 Y240
P241 Y242 F243 H244 L251 E256 T257 M258 G259 R260 I261 Q262 I263 N264 N268 K269 D270 E271 K274 T281 K290 L291 P292 I293 L294 P295 P296 S297 N298 N299 D300 T301 P302 P306 Y307 E308

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.13Å 55.11Å 144.00Å 90.00° 103.60° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	95.9 (30.00-1.80)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10767	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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: GOL, CA, MG, 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	0.32	0/2441	0.58	0/3304
1	B	0.29	0/2441	0.56	0/3304
1	C	0.32	0/2441	0.58	0/3304
1	D	0.29	0/2441	0.52	0/3304
All	All	0.30	0/9764	0.56	0/13216

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	TYR	Sidechain

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	2388	0	2331	59	0
1	B	2388	0	2331	85	0
1	C	2388	0	2331	43	0
1	D	2388	0	2331	185	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	86	0	60	18	0
4	B	86	0	60	18	0
4	C	86	0	60	15	0
4	D	86	0	60	22	0
5	B	6	0	8	0	0
6	A	260	0	0	4	0
6	B	199	0	0	4	0
6	C	279	0	0	0	0
6	D	120	0	0	6	0
All	All	10767	0	9572	360	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (360) 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:186:CYS:SG	4:B:402:HEM:HAC	1.50	1.50
1:A:39:CYS:SG	4:A:401:HEM:CAB	2.12	1.38
1:B:39:CYS:SG	4:B:401:HEM:CAB	2.13	1.37
1:A:42:CYS:SG	4:A:401:HEM:CAC	2.14	1.36
1:C:183:CYS:SG	4:C:402:HEM:CAB	2.13	1.36
1:C:42:CYS:SG	4:C:401:HEM:CAC	2.12	1.36
1:A:183:CYS:SG	4:A:402:HEM:CAB	2.13	1.36
1:C:186:CYS:SG	4:C:402:HEM:CAC	2.15	1.35
1:A:186:CYS:SG	4:A:402:HEM:CAC	2.14	1.34
1:A:183:CYS:HG	4:A:402:HEM:CAB	1.39	1.34
1:B:42:CYS:SG	4:B:401:HEM:CAC	2.17	1.33
1:B:186:CYS:SG	4:B:402:HEM:CAC	2.16	1.32
1:B:183:CYS:SG	4:B:402:HEM:CAB	2.18	1.31
1:D:42:CYS:SG	4:D:401:HEM:HAC	1.70	1.31
1:D:183:CYS:SG	4:D:402:HEM:CAB	2.19	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:CYS:SG	4:D:401:HEM:CAB	2.19	1.30
1:D:186:CYS:SG	4:D:402:HEM:CAC	2.19	1.30
1:D:42:CYS:SG	4:D:401:HEM:CAC	2.20	1.29
1:D:42:CYS:HG	4:D:401:HEM:CAC	1.48	1.26
1:C:39:CYS:SG	4:C:401:HEM:HAB	1.72	1.25
1:A:183:CYS:SG	4:A:402:HEM:HAB	1.75	1.21
1:A:39:CYS:SG	4:A:401:HEM:HAB	1.77	1.15
1:B:183:CYS:SG	4:B:402:HEM:HAB	1.79	1.15
1:D:183:CYS:SG	4:D:402:HEM:HAB	1.86	1.13
1:B:39:CYS:SG	4:B:401:HEM:HAB	1.86	1.07
1:C:186:CYS:SG	4:C:402:HEM:HAC	1.90	1.06
1:B:186:CYS:HG	4:B:402:HEM:CAC	1.61	1.05
1:A:42:CYS:SG	4:A:401:HEM:HAC	1.87	1.05
1:D:39:CYS:SG	4:D:401:HEM:HAB	1.91	1.04
1:C:42:CYS:SG	4:C:401:HEM:HAC	1.97	1.03
1:C:183:CYS:SG	4:C:402:HEM:HAB	1.95	1.03
1:A:186:CYS:SG	4:A:402:HEM:HAC	1.98	1.01
1:D:151:THR:HG21	1:D:235:ASN:HD21	1.23	1.00
1:D:125:LYS:HE2	1:D:131:ASP:HB3	1.42	1.00
1:D:73:ASN:HD21	1:D:151:THR:HG22	1.25	0.98
1:D:186:CYS:SG	4:D:402:HEM:HAC	2.02	0.97
1:B:119:GLN:H	1:B:119:GLN:HE21	0.97	0.95
1:A:298:ASN:HD22	1:A:300:ASP:H	1.19	0.90
1:B:42:CYS:SG	4:B:401:HEM:HAC	2.10	0.90
1:D:225:ARG:HH11	1:D:225:ARG:HB2	1.38	0.88
1:B:119:GLN:H	1:B:119:GLN:NE2	1.70	0.88
1:D:224:ASP:O	1:D:227:VAL:HG12	1.74	0.88
1:D:201:GLY:H	1:D:262:GLN:HE22	1.20	0.87
1:D:268:ASN:ND2	1:D:271:GLU:H	1.72	0.87
1:D:201:GLY:H	1:D:262:GLN:NE2	1.72	0.87
1:D:40:ASN:HD21	1:D:45:LEU:H	1.22	0.86
1:A:33:LYS:HD3	6:A:1640:HOH:O	1.74	0.85
1:C:201:GLY:H	1:C:262:GLN:HE22	1.27	0.83
1:B:119:GLN:N	1:B:119:GLN:HE21	1.77	0.82
1:D:122:GLU:O	1:D:126:LYS:HD3	1.79	0.82
1:C:298:ASN:HD22	1:C:300:ASP:H	1.24	0.81
1:D:164:LYS:HA	1:D:164:LYS:HE3	1.61	0.81
1:D:151:THR:HG21	1:D:235:ASN:ND2	1.98	0.79
1:C:42:CYS:SG	4:C:401:HEM:CBC	2.70	0.79
1:B:42:CYS:SG	4:B:401:HEM:C3C	2.75	0.79
1:C:183:CYS:SG	4:C:402:HEM:CBB	2.71	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:ASN:HD21	1:D:271:GLU:H	1.32	0.78
1:D:113:VAL:HG22	1:D:302:PRO:HG2	1.66	0.78
1:A:42:CYS:SG	4:A:401:HEM:C3C	2.76	0.78
1:B:5:ILE:HD12	1:B:192:VAL:HG22	1.67	0.77
1:C:39:CYS:SG	4:C:401:HEM:CBB	2.71	0.77
1:B:39:CYS:SG	4:B:401:HEM:CBB	2.73	0.77
1:D:31:LEU:HB2	6:D:2502:HOH:O	1.84	0.76
1:A:210:ASN:HD22	1:A:212:ALA:H	1.33	0.76
1:D:186:CYS:SG	4:D:402:HEM:C3C	2.79	0.75
1:D:40:ASN:ND2	1:D:45:LEU:H	1.83	0.75
1:B:44:ASN:HD22	1:B:46:SER:H	1.33	0.75
1:B:204:LYS:HB2	1:B:261:ILE:HG22	1.69	0.75
1:B:186:CYS:SG	4:B:402:HEM:C3C	2.80	0.74
1:D:73:ASN:ND2	1:D:151:THR:HG22	2.01	0.74
1:D:298:ASN:HD22	1:D:300:ASP:H	1.35	0.74
1:B:42:CYS:SG	4:B:401:HEM:CBC	2.75	0.74
1:C:42:CYS:SG	4:C:401:HEM:C3C	2.81	0.74
1:A:186:CYS:SG	4:A:402:HEM:C3C	2.81	0.74
1:A:119:GLN:NE2	1:A:119:GLN:H	1.84	0.74
1:C:186:CYS:SG	4:C:402:HEM:C3C	2.81	0.74
1:D:66:ILE:HD11	1:D:244:HIS:HB2	1.69	0.73
1:A:186:CYS:SG	4:A:402:HEM:CBC	2.75	0.73
1:D:130:SER:HB2	1:D:137:ARG:HH12	1.54	0.73
1:D:103:MET:HE1	6:D:2502:HOH:O	1.88	0.73
1:B:46:SER:OG	1:D:291:LEU:HD21	1.89	0.73
1:D:125:LYS:CE	1:D:131:ASP:HB3	2.19	0.72
1:A:252:GLU:O	1:A:256:GLU:HG3	1.90	0.72
1:D:3:GLU:O	1:D:188:ASN:HB2	1.89	0.71
1:B:13:PRO:HG3	1:B:148:THR:CG2	2.19	0.71
1:D:73:ASN:HD21	1:D:151:THR:CG2	2.00	0.71
1:D:42:CYS:SG	4:D:401:HEM:C3C	2.80	0.71
1:B:44:ASN:ND2	1:B:46:SER:H	1.88	0.71
1:D:130:SER:HB2	1:D:137:ARG:HH22	1.54	0.70
1:D:221:ASN:HB2	1:D:224:ASP:OD2	1.91	0.70
1:D:216:MET:SD	1:D:225:ARG:NH1	2.65	0.70
1:A:308:GLU:HG3	1:A:308:GLU:OXT	1.92	0.70
1:A:39:CYS:SG	4:A:401:HEM:CBB	2.79	0.69
1:D:215:ARG:HB3	1:D:227:VAL:HG13	1.73	0.69
1:A:308:GLU:CG	1:A:308:GLU:OXT	2.40	0.69
1:D:169:GLN:HG3	1:D:170:ASP:N	2.08	0.69
1:C:183:CYS:SG	4:C:402:HEM:C3B	2.85	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ASP:OD1	1:B:274:LYS:HE3	1.93	0.69
1:D:183:CYS:SG	4:D:402:HEM:CBB	2.81	0.68
1:D:108:GLU:OE1	1:D:109:ILE:HG13	1.94	0.68
1:C:80:GLN:O	1:C:81:PHE:HB2	1.93	0.68
1:D:298:ASN:HD21	1:D:300:ASP:HB2	1.59	0.67
1:D:3:GLU:HG3	1:D:189:GLY:HA2	1.77	0.67
1:D:114:VAL:HG21	1:D:133:VAL:HG11	1.77	0.67
1:A:184:VAL:HG22	6:A:1464:HOH:O	1.95	0.67
1:B:13:PRO:HG3	1:B:148:THR:HG21	1.77	0.67
1:A:169:GLN:O	1:A:173:GLU:HG3	1.95	0.67
1:C:201:GLY:H	1:C:262:GLN:NE2	1.93	0.66
1:D:215:ARG:HB3	1:D:227:VAL:CG1	2.26	0.66
1:A:80:GLN:O	1:A:81:PHE:HB2	1.96	0.66
1:B:96:PRO:HG3	6:B:1609:HOH:O	1.96	0.66
1:D:18:MET:HB3	1:D:144:GLN:HG2	1.77	0.66
1:D:110:ALA:O	1:D:114:VAL:HG22	1.96	0.65
1:D:1:ALA:O	1:D:2:ASN:HB2	1.96	0.65
1:D:186:CYS:SG	4:D:402:HEM:CBC	2.86	0.64
1:D:20:GLU:O	1:D:23:LYS:HG2	1.97	0.64
1:C:186:CYS:SG	4:C:402:HEM:CBC	2.84	0.64
1:D:263:LEU:HD21	4:D:402:HEM:HMC2	1.78	0.64
1:D:298:ASN:ND2	1:D:300:ASP:HB2	2.13	0.64
1:C:298:ASN:ND2	1:C:300:ASP:H	1.96	0.64
1:B:39:CYS:SG	4:B:401:HEM:C3B	2.89	0.64
1:D:225:ARG:NH1	1:D:225:ARG:HB2	2.12	0.63
1:D:268:ASN:HD22	1:D:268:ASN:C	2.01	0.63
1:A:125:LYS:HA	1:A:130:SER:O	1.98	0.63
1:A:39:CYS:SG	4:A:401:HEM:C3B	2.91	0.63
1:A:298:ASN:ND2	1:A:300:ASP:H	1.94	0.63
1:D:39:CYS:SG	4:D:401:HEM:C3B	2.89	0.63
1:B:286:GLN:HB3	1:B:287:PRO:HD2	1.80	0.63
1:B:270:ASP:O	1:B:274:LYS:HD3	1.99	0.62
1:C:252:GLU:O	1:C:256:GLU:HG3	1.99	0.62
1:D:39:CYS:SG	4:D:401:HEM:CBB	2.87	0.62
1:B:80:GLN:O	1:B:81:PHE:HB2	1.99	0.62
1:B:1:ALA:O	1:B:2:ASN:HB2	1.99	0.62
1:D:66:ILE:HG13	1:D:244:HIS:O	2.00	0.62
1:D:188:ASN:C	1:D:188:ASN:HD22	2.03	0.62
1:B:268:ASN:HB2	1:B:271:GLU:HG3	1.82	0.62
1:D:125:LYS:HA	1:D:130:SER:O	2.00	0.61
1:A:210:ASN:ND2	1:A:212:ALA:H	1.96	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:CYS:SG	4:A:401:HEM:CBC	2.87	0.61
1:D:80:GLN:O	1:D:81:PHE:HB2	1.99	0.61
1:A:130:SER:HB3	1:A:137:ARG:HH12	1.65	0.60
1:A:183:CYS:SG	4:A:402:HEM:CBB	2.86	0.60
1:B:183:CYS:SG	4:B:402:HEM:CBB	2.88	0.60
1:D:135:ILE:HD13	1:D:135:ILE:O	2.01	0.60
1:D:108:GLU:CD	1:D:109:ILE:HG13	2.22	0.60
1:D:96:PRO:HG3	6:D:2540:HOH:O	2.02	0.60
1:C:15:ASN:C	1:C:15:ASN:HD22	2.05	0.60
1:C:13:PRO:HG3	1:C:148:THR:HG22	1.83	0.59
1:C:39:CYS:SG	4:C:401:HEM:C3B	2.91	0.59
1:D:3:GLU:HG3	1:D:189:GLY:CA	2.33	0.59
1:B:107:HIS:O	1:B:111:GLU:HG3	2.03	0.58
1:D:155:LYS:O	1:D:166:ALA:HB1	2.04	0.58
1:D:29:PRO:O	1:D:35:GLY:HA2	2.04	0.58
1:D:78:LEU:C	1:D:78:LEU:HD12	2.23	0.58
1:A:298:ASN:HD21	1:A:300:ASP:HB2	1.68	0.58
1:A:119:GLN:HE21	1:A:119:GLN:H	1.47	0.58
1:D:130:SER:HB2	1:D:137:ARG:NH2	2.18	0.58
1:D:225:ARG:HH11	1:D:225:ARG:CB	2.14	0.58
1:D:130:SER:HB2	1:D:137:ARG:NH1	2.17	0.58
1:C:298:ASN:HD21	1:C:300:ASP:HB2	1.68	0.58
1:D:2:ASN:ND2	1:D:3:GLU:H	2.03	0.57
1:B:163:ASP:OD2	1:B:166:ALA:HB2	2.05	0.57
1:B:61:TRP:HB2	1:D:61:TRP:HB2	1.87	0.57
1:B:183:CYS:SG	4:B:402:HEM:C3B	2.94	0.56
1:A:157:ASP:O	1:A:161:GLU:HG3	2.05	0.56
1:D:198:GLN:C	1:D:227:VAL:HG23	2.25	0.56
1:C:118:PRO:O	1:C:122:GLU:HG3	2.05	0.56
1:B:288:ASP:HA	6:B:1514:HOH:O	2.06	0.56
1:C:13:PRO:HG3	1:C:148:THR:CG2	2.36	0.56
1:B:44:ASN:HD22	1:B:44:ASN:C	2.09	0.56
1:B:13:PRO:HG3	1:B:148:THR:HG22	1.86	0.56
1:D:15:ASN:OD1	1:D:18:MET:HB2	2.06	0.55
1:D:124:PHE:CE2	1:D:133:VAL:HG13	2.41	0.55
1:B:1:ALA:O	1:B:2:ASN:CB	2.54	0.55
1:A:13:PRO:HG3	1:A:148:THR:CG2	2.36	0.55
1:D:21:LEU:O	1:D:25:LEU:HD23	2.06	0.55
1:D:5:ILE:H	1:D:5:ILE:HD12	1.72	0.55
1:D:151:THR:HG23	1:D:151:THR:O	2.06	0.55
1:A:305:GLN:HB3	1:A:308:GLU:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASN:HD22	1:B:264:ASN:C	2.10	0.54
1:B:258:MET:O	1:B:262:GLN:HB2	2.07	0.54
1:D:130:SER:CB	1:D:137:ARG:HH12	2.19	0.54
1:B:242:TYR:O	1:B:243:PHE:HB2	2.08	0.54
1:D:28:ASP:OD1	1:D:30:ARG:HB2	2.08	0.54
1:D:215:ARG:CB	1:D:227:VAL:HG13	2.37	0.54
1:D:298:ASN:ND2	1:D:300:ASP:H	2.02	0.54
1:D:183:CYS:SG	4:D:402:HEM:C3B	2.97	0.53
1:D:5:ILE:N	1:D:5:ILE:HD12	2.22	0.53
1:B:134:THR:HG22	6:B:1575:HOH:O	2.09	0.53
1:D:268:ASN:HD21	1:D:271:GLU:HG3	1.73	0.53
1:D:5:ILE:HA	1:D:189:GLY:O	2.09	0.53
1:B:235:ASN:HD21	1:B:284:GLY:H	1.54	0.53
1:D:209:LYS:O	1:D:211:PRO:HD3	2.09	0.53
1:D:114:VAL:CG2	1:D:133:VAL:HG11	2.38	0.53
1:D:42:CYS:HA	1:D:51:ASP:HB3	1.90	0.53
1:D:135:ILE:HA	1:D:138:ILE:HD12	1.90	0.53
1:A:13:PRO:HG3	1:A:148:THR:HG21	1.91	0.53
1:B:194:GLY:HA2	1:B:230:VAL:O	2.08	0.53
1:C:99:ASN:ND2	1:C:101:LYS:H	2.07	0.53
1:D:134:THR:O	1:D:138:ILE:HG13	2.10	0.52
1:D:37:ILE:N	1:D:37:ILE:HD12	2.23	0.52
1:D:82:TRP:HZ3	4:D:402:HEM:HBD2	1.75	0.52
1:D:268:ASN:C	1:D:268:ASN:ND2	2.62	0.52
1:D:194:GLY:N	1:D:230:VAL:O	2.43	0.52
1:C:40:ASN:HD21	1:C:45:LEU:H	1.57	0.52
1:D:169:GLN:O	1:D:173:GLU:HG3	2.10	0.51
1:D:78:LEU:HD11	1:D:197:TYR:OH	2.10	0.51
1:D:132:GLU:HA	1:D:132:GLU:OE1	2.08	0.51
1:A:130:SER:OG	1:A:132:GLU:HG2	2.10	0.51
1:C:99:ASN:C	1:C:99:ASN:HD22	2.13	0.51
1:D:306:PRO:HG2	1:D:307:TYR:CD1	2.45	0.51
1:B:5:ILE:HD11	1:B:188:ASN:HA	1.93	0.51
1:A:60:LYS:HA	1:C:61:TRP:CD2	2.45	0.51
1:D:229:LYS:NZ	4:D:401:HEM:O1A	2.43	0.51
1:D:291:LEU:HD23	1:D:291:LEU:C	2.31	0.51
1:D:177:LEU:HD21	1:D:271:GLU:HB3	1.92	0.51
1:D:168:ASN:OD1	1:D:171:GLU:HG3	2.11	0.51
1:D:258:MET:O	1:D:262:GLN:HB2	2.10	0.51
1:D:268:ASN:HD21	1:D:271:GLU:N	2.03	0.50
1:D:270:ASP:OD2	1:D:274:LYS:HE2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:TYR:O	1:D:243:PHE:HB2	2.12	0.50
1:D:8:ILE:O	1:D:152:PRO:HB3	2.11	0.50
1:A:40:ASN:HD21	1:A:45:LEU:H	1.60	0.50
1:B:40:ASN:ND2	1:B:45:LEU:H	2.10	0.50
1:B:44:ASN:HD21	1:B:46:SER:HB2	1.76	0.50
1:D:80:GLN:HB2	1:D:86:ALA:HB3	1.94	0.50
1:B:56:SER:HB3	4:B:401:HEM:HAC	1.94	0.50
1:A:61:TRP:HB2	1:C:61:TRP:HB2	1.93	0.49
1:D:201:GLY:N	1:D:262:GLN:HE22	2.00	0.49
1:B:60:LYS:HA	1:D:61:TRP:CD2	2.47	0.49
1:B:5:ILE:CD1	1:B:188:ASN:HA	2.41	0.49
1:D:2:ASN:CG	1:D:3:GLU:H	2.15	0.49
1:D:268:ASN:ND2	1:D:271:GLU:HB2	2.27	0.49
1:D:77:ASN:HB3	1:D:79:ALA:O	2.12	0.49
1:B:59:HIS:O	1:B:62:GLN:HG3	2.12	0.49
1:A:256:GLU:HG2	1:A:272:VAL:HG21	1.95	0.49
1:C:40:ASN:ND2	1:C:45:LEU:H	2.11	0.49
1:D:135:ILE:HD13	1:D:135:ILE:C	2.33	0.49
1:D:215:ARG:O	1:D:218:VAL:HG12	2.13	0.48
1:A:61:TRP:CD2	1:C:60:LYS:HA	2.48	0.48
1:D:183:CYS:CB	4:D:402:HEM:HAB	2.42	0.48
1:D:34:SER:HB3	1:D:59:HIS:CE1	2.47	0.48
1:D:222:GLU:OE2	1:D:225:ARG:NH1	2.46	0.48
1:D:218:VAL:HG13	1:D:219:THR:HG23	1.95	0.48
1:D:78:LEU:HD11	1:D:197:TYR:CZ	2.48	0.48
1:B:112:LYS:HD3	1:B:302:PRO:HG3	1.94	0.48
1:A:183:CYS:SG	4:A:402:HEM:C3B	2.89	0.48
1:B:40:ASN:HD21	1:B:45:LEU:H	1.62	0.48
1:D:96:PRO:HA	1:D:102:GLU:OE1	2.14	0.48
1:D:291:LEU:HD23	1:D:292:PRO:N	2.28	0.47
1:C:15:ASN:ND2	1:C:18:MET:H	2.13	0.47
1:B:57:ILE:HD11	1:D:306:PRO:HB2	1.97	0.47
1:A:101:LYS:HD3	6:A:1524:HOH:O	2.12	0.47
1:B:177:LEU:HD23	1:B:181:SER:HG	1.79	0.47
1:D:155:LYS:HD3	1:D:166:ALA:O	2.14	0.47
1:B:57:ILE:HD13	1:D:307:TYR:CZ	2.49	0.47
1:C:66:ILE:HD11	1:C:244:HIS:HB2	1.97	0.47
1:C:308:GLU:HG2	1:C:308:GLU:OXT	2.15	0.47
1:D:1:ALA:HB2	1:D:184:VAL:HG23	1.97	0.47
1:D:80:GLN:HA	1:D:80:GLN:NE2	2.30	0.47
1:D:78:LEU:HD23	1:D:195:SER:C	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:PRO:HB3	1:D:238:LEU:HD22	1.97	0.46
1:D:113:VAL:HG22	1:D:302:PRO:CG	2.41	0.46
1:D:167:LEU:HD22	1:D:281:THR:HG21	1.98	0.46
1:D:80:GLN:O	1:D:84:GLY:HA2	2.15	0.46
1:C:203:PHE:CD2	1:C:264:ASN:HB2	2.51	0.46
1:B:99:ASN:HD22	1:B:100:PRO:N	2.14	0.46
1:B:99:ASN:HD22	1:B:100:PRO:CD	2.27	0.46
1:B:181:SER:O	1:B:263:LEU:HD13	2.16	0.46
1:D:128:PHE:HE2	1:D:140:THR:HG21	1.81	0.46
1:D:134:THR:OG1	1:D:137:ARG:HG3	2.16	0.46
1:D:225:ARG:O	1:D:226:ASN:HB2	2.16	0.46
1:D:188:ASN:C	1:D:188:ASN:ND2	2.69	0.46
1:D:240:TYR:HB2	6:D:2535:HOH:O	2.15	0.46
1:B:288:ASP:OD1	1:D:290:LYS:HD3	2.16	0.46
1:D:256:GLU:CD	1:D:260:ARG:HH12	2.19	0.46
1:C:99:ASN:HD22	1:C:100:PRO:N	2.13	0.45
1:D:100:PRO:HA	1:D:104:ALA:HA	1.98	0.45
1:D:146:GLU:HA	1:D:149:LEU:HG	1.99	0.45
1:D:23:LYS:HB2	1:D:23:LYS:NZ	2.32	0.45
1:B:177:LEU:HD11	1:B:271:GLU:HB3	1.98	0.45
1:B:63:GLN:HG3	1:D:307:TYR:CZ	2.51	0.45
1:B:42:CYS:HA	1:B:51:ASP:HB3	1.99	0.45
1:D:78:LEU:HD12	1:D:79:ALA:HB2	1.99	0.45
1:A:40:ASN:ND2	1:A:45:LEU:H	2.14	0.45
1:D:150:VAL:HG23	1:D:152:PRO:HD3	1.99	0.45
1:D:258:MET:HG3	4:D:402:HEM:C4A	2.52	0.45
1:A:59:HIS:CD2	1:A:60:LYS:HG3	2.52	0.45
1:D:142:ILE:O	1:D:146:GLU:HG3	2.16	0.45
1:D:268:ASN:ND2	1:D:271:GLU:CB	2.80	0.44
1:C:225:ARG:O	1:C:226:ASN:HB2	2.18	0.44
1:D:72:LEU:O	1:D:73:ASN:HB2	2.18	0.44
1:B:99:ASN:HD22	1:B:100:PRO:HD2	1.83	0.44
1:B:99:ASN:C	1:B:99:ASN:HD22	2.19	0.44
1:A:108:GLU:CD	1:A:108:GLU:H	2.20	0.44
1:A:225:ARG:O	1:A:226:ASN:HB2	2.18	0.44
1:B:179:LYS:HG2	1:B:184:VAL:HG11	2.00	0.44
1:D:270:ASP:O	1:D:274:LYS:HG3	2.18	0.44
1:D:260:ARG:O	1:D:264:ASN:HA	2.18	0.44
1:C:305:GLN:HB3	1:C:308:GLU:HB3	1.99	0.44
1:D:183:CYS:C	1:D:185:GLN:H	2.21	0.44
1:B:257:THR:O	1:B:261:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:LYS:HE3	1:C:226:ASN:HB2	2.00	0.44
1:D:194:GLY:HA2	1:D:230:VAL:O	2.18	0.43
1:B:307:TYR:CZ	1:D:63:GLN:HG3	2.53	0.43
1:B:235:ASN:ND2	1:B:284:GLY:H	2.15	0.43
1:B:112:LYS:HE2	6:B:1474:HOH:O	2.18	0.43
1:D:26:PHE:O	1:D:39:CYS:HB2	2.18	0.43
1:B:177:LEU:HD23	1:B:181:SER:OG	2.18	0.43
1:B:99:ASN:ND2	1:B:101:LYS:H	2.16	0.43
1:A:298:ASN:ND2	1:A:300:ASP:HB2	2.32	0.43
1:D:59:HIS:O	1:D:60:LYS:HB2	2.18	0.43
1:D:11:VAL:HG12	1:D:12:THR:N	2.33	0.43
1:D:236:ILE:HA	6:D:2461:HOH:O	2.18	0.43
1:B:44:ASN:ND2	1:B:46:SER:HB2	2.33	0.43
1:B:250:THR:HG23	1:B:253:GLN:H	1.84	0.43
1:D:229:LYS:HE2	1:D:229:LYS:HB3	1.89	0.42
1:D:157:ASP:O	1:D:161:GLU:HG3	2.18	0.42
1:D:164:LYS:HA	1:D:164:LYS:CE	2.42	0.42
1:A:87:LYS:HG2	1:A:91:GLU:OE1	2.19	0.42
1:D:294:LEU:HA	1:D:295:PRO:HD3	1.89	0.42
1:D:199:LYS:HA	1:D:227:VAL:HA	2.02	0.42
1:D:199:LYS:N	1:D:227:VAL:HG23	2.34	0.42
1:B:276:VAL:HG12	1:B:280:LYS:HE3	2.01	0.42
1:B:69:PRO:HG2	4:B:401:HEM:HBA1	2.02	0.42
1:D:258:MET:SD	1:D:262:GLN:HG3	2.60	0.42
1:D:32:SER:HB3	1:D:37:ILE:O	2.20	0.42
1:A:219:THR:HB	1:A:221:ASN:ND2	2.35	0.42
1:D:115:ALA:O	1:D:121:ARG:HD3	2.19	0.42
1:D:198:GLN:HA	1:D:198:GLN:NE2	2.34	0.42
1:D:268:ASN:HD21	1:D:271:GLU:CG	2.32	0.42
1:D:192:VAL:HG12	1:D:192:VAL:O	2.20	0.42
1:D:5:ILE:CD1	1:D:5:ILE:H	2.33	0.41
1:A:77:ASN:HB3	1:A:79:ALA:O	2.20	0.41
1:B:119:GLN:CD	1:B:295:PRO:HB3	2.40	0.41
1:A:11:VAL:HG23	1:A:150:VAL:HG21	2.01	0.41
1:A:258:MET:O	1:A:262:GLN:HB2	2.20	0.41
1:D:183:CYS:CB	4:D:402:HEM:CAB	2.98	0.41
1:D:130:SER:HB2	1:D:137:ARG:CZ	2.50	0.41
1:B:112:LYS:HD3	1:B:302:PRO:CG	2.50	0.41
1:B:154:SER:O	1:B:158:LYS:HG3	2.20	0.41
1:B:80:GLN:HB2	1:B:86:ALA:HB3	2.02	0.41
1:A:87:LYS:HE2	6:A:1550:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:LYS:HA	1:C:164:LYS:HD3	1.87	0.41
1:C:3:GLU:HA	1:C:4:PRO:HD3	1.82	0.41
1:D:119:GLN:NE2	1:D:296:PRO:HD2	2.36	0.41
1:B:156:PHE:CE2	1:B:160:LEU:HD11	2.56	0.41
1:D:141:ALA:O	1:D:144:GLN:HB3	2.21	0.41
1:D:201:GLY:N	1:D:262:GLN:NE2	2.54	0.41
1:D:78:LEU:HD12	1:D:79:ALA:CB	2.51	0.41
1:D:236:ILE:HG13	1:D:251:LEU:HD21	2.03	0.41
1:A:13:PRO:HG3	1:A:148:THR:HG22	2.03	0.41
1:D:21:LEU:O	1:D:25:LEU:CD2	2.69	0.41
1:D:119:GLN:HE22	1:D:296:PRO:HD2	1.86	0.41
1:B:159:TRP:CD1	1:B:164:LYS:HA	2.56	0.41
1:A:80:GLN:O	1:A:81:PHE:CB	2.68	0.40
1:A:124:PHE:CE2	1:A:133:VAL:HG13	2.55	0.40
1:D:80:GLN:HA	1:D:80:GLN:HE21	1.85	0.40
1:A:42:CYS:CB	4:A:401:HEM:C3C	3.04	0.40
1:D:151:THR:HG23	6:D:2519:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	306/308 (99%)	296 (97%)	10 (3%)	0	100 100
1	B	306/308 (99%)	287 (94%)	16 (5%)	3 (1%)	19 5
1	C	306/308 (99%)	298 (97%)	8 (3%)	0	100 100
1	D	306/308 (99%)	285 (93%)	19 (6%)	2 (1%)	26 11
All	All	1224/1232 (99%)	1166 (95%)	53 (4%)	5 (0%)	39 23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ASN
1	D	2	ASN
1	B	163	ASP
1	D	215	ARG
1	B	3	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	260/260 (100%)	255 (98%)	5 (2%)	65	52
1	B	260/260 (100%)	254 (98%)	6 (2%)	58	42
1	C	260/260 (100%)	255 (98%)	5 (2%)	65	52
1	D	260/260 (100%)	250 (96%)	10 (4%)	40	22
All	All	1040/1040 (100%)	1014 (98%)	26 (2%)	55	39

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	122	GLU
1	A	210	ASN
1	A	222	GLU
1	A	298	ASN
1	B	44	ASN
1	B	99	ASN
1	B	119	GLN
1	B	122	GLU
1	B	177	LEU
1	B	264	ASN
1	C	15	ASN
1	C	99	ASN
1	C	120	TYR
1	C	264	ASN
1	C	298	ASN
1	D	15	ASN

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Mol	Chain	Res	Type
1	D	23	LYS
1	D	126	LYS
1	D	132	GLU
1	D	135	ILE
1	D	164	LYS
1	D	188	ASN
1	D	225	ARG
1	D	268	ASN
1	D	308	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	52	ASN
1	A	62	GLN
1	A	119	GLN
1	A	165	ASN
1	A	198	GLN
1	A	210	ASN
1	A	221	ASN
1	A	226	ASN
1	A	253	GLN
1	A	298	ASN
1	A	299	ASN
1	B	40	ASN
1	B	44	ASN
1	B	52	ASN
1	B	59	HIS
1	B	63	GLN
1	B	99	ASN
1	B	119	GLN
1	B	165	ASN
1	B	176	ASN
1	B	198	GLN
1	B	226	ASN
1	B	235	ASN
1	B	264	ASN
1	B	268	ASN
1	B	299	ASN
1	C	2	ASN
1	C	15	ASN

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Mol	Chain	Res	Type
1	C	40	ASN
1	C	52	ASN
1	C	62	GLN
1	C	63	GLN
1	C	99	ASN
1	C	119	GLN
1	C	176	ASN
1	C	185	GLN
1	C	221	ASN
1	C	226	ASN
1	C	253	GLN
1	C	262	GLN
1	C	264	ASN
1	C	298	ASN
1	D	40	ASN
1	D	62	GLN
1	D	63	GLN
1	D	77	ASN
1	D	80	GLN
1	D	119	GLN
1	D	144	GLN
1	D	198	GLN
1	D	226	ASN
1	D	262	GLN
1	D	268	ASN
1	D	298	ASN
1	D	299	ASN

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 (i)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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	A	401	1,6	30,50,50	3.18	11 (36%)	24,82,82	2.13	7 (29%)
4	HEM	A	402	1	30,50,50	2.89	11 (36%)	24,82,82	2.18	8 (33%)
5	GOL	B	1410	-	5,5,5	0.21	0	5,5,5	0.25	0
4	HEM	B	401	1,6	30,50,50	2.86	11 (36%)	24,82,82	2.11	6 (25%)
4	HEM	B	402	1	30,50,50	2.85	10 (33%)	24,82,82	2.06	7 (29%)
4	HEM	C	401	1,6	30,50,50	3.16	11 (36%)	24,82,82	2.13	8 (33%)
4	HEM	C	402	1	30,50,50	2.97	11 (36%)	24,82,82	2.18	7 (29%)
4	HEM	D	401	1,6	30,50,50	2.83	12 (40%)	24,82,82	2.03	6 (25%)
4	HEM	D	402	1	30,50,50	2.93	11 (36%)	24,82,82	2.13	7 (29%)

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	401	1,6	-	0/10/54/54	0/0/8/8
4	HEM	A	402	1	-	0/10/54/54	0/0/8/8
5	GOL	B	1410	-	-	0/4/4/4	0/0/0/0
4	HEM	B	401	1,6	-	0/10/54/54	0/0/8/8
4	HEM	B	402	1	-	0/10/54/54	0/0/8/8
4	HEM	C	401	1,6	-	0/10/54/54	0/0/8/8
4	HEM	C	402	1	-	0/10/54/54	0/0/8/8
4	HEM	D	401	1,6	-	0/10/54/54	0/0/8/8
4	HEM	D	402	1	-	0/10/54/54	0/0/8/8

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	HEM	C3B-C4B	-9.29	1.43	1.51
4	A	401	HEM	C3B-C4B	-8.77	1.44	1.51
4	C	402	HEM	C3B-C4B	-8.08	1.44	1.51
4	B	401	HEM	C3B-C4B	-7.95	1.44	1.51
4	D	402	HEM	C3B-C4B	-7.81	1.44	1.51
4	A	402	HEM	C3B-C4B	-7.28	1.45	1.51
4	A	401	HEM	C3C-CAC	-6.82	1.38	1.51
4	A	402	HEM	C2D-C3D	-6.68	1.34	1.54
4	B	402	HEM	C3B-C4B	-6.58	1.46	1.51
4	D	402	HEM	C3B-CAB	-6.49	1.39	1.51
4	C	401	HEM	C3B-CAB	-6.39	1.39	1.51
4	C	402	HEM	C2D-C3D	-6.36	1.35	1.54
4	B	402	HEM	C3C-CAC	-6.35	1.39	1.51
4	D	402	HEM	C2D-C3D	-6.30	1.35	1.54
4	C	401	HEM	C3D-C4D	-6.27	1.43	1.51
4	C	401	HEM	C2D-C3D	-6.19	1.35	1.54
4	A	401	HEM	C2D-C3D	-6.08	1.36	1.54
4	A	402	HEM	C3C-CAC	-6.06	1.40	1.51
4	D	402	HEM	C3C-CAC	-6.03	1.40	1.51
4	B	401	HEM	C3B-CAB	-6.02	1.40	1.51
4	D	401	HEM	C3B-CAB	-6.00	1.40	1.51
4	D	401	HEM	C3C-CAC	-5.96	1.40	1.51
4	C	402	HEM	C3C-CAC	-5.96	1.40	1.51
4	D	401	HEM	C3B-C4B	-5.94	1.46	1.51
4	D	401	HEM	C2D-C3D	-5.93	1.36	1.54
4	C	402	HEM	C3B-CAB	-5.91	1.40	1.51
4	C	401	HEM	C3C-CAC	-5.90	1.40	1.51
4	B	402	HEM	C3B-CAB	-5.89	1.40	1.51
4	B	402	HEM	C2D-C3D	-5.85	1.37	1.54
4	C	402	HEM	C3D-C4D	-5.78	1.44	1.51
4	A	402	HEM	C3B-CAB	-5.72	1.40	1.51
4	B	401	HEM	C2D-C3D	-5.69	1.37	1.54
4	A	401	HEM	C3B-CAB	-5.61	1.40	1.51
4	B	401	HEM	C3D-C4D	-5.28	1.44	1.51
4	B	401	HEM	C3C-CAC	-5.22	1.41	1.51
4	A	402	HEM	C3D-C4D	-5.06	1.45	1.51
4	A	401	HEM	C3D-C4D	-4.82	1.45	1.51
4	B	402	HEM	C3D-C4D	-4.82	1.45	1.51
4	A	401	HEM	C2C-C1C	-4.64	1.43	1.52
4	D	402	HEM	C3D-C4D	-4.64	1.45	1.51
4	D	401	HEM	C3D-C4D	-4.34	1.46	1.51
4	D	401	HEM	C2C-C1C	-3.97	1.45	1.52
4	A	402	HEM	C2C-C1C	-3.65	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	HEM	C2C-C1C	-3.56	1.45	1.52
4	B	402	HEM	C2C-C1C	-3.26	1.46	1.52
4	C	401	HEM	C2C-C1C	-3.24	1.46	1.52
4	D	402	HEM	C2C-C1C	-3.19	1.46	1.52
4	B	401	HEM	C2C-C1C	-3.11	1.46	1.52
4	A	402	HEM	C2D-C1D	-2.35	1.44	1.51
4	C	401	HEM	C2D-C1D	-2.24	1.44	1.51
4	B	401	HEM	C2D-C1D	-2.17	1.44	1.51
4	C	401	HEM	C2B-C1B	-2.17	1.44	1.51
4	D	401	HEM	C2D-C1D	-2.07	1.45	1.51
4	C	402	HEM	C2D-C1D	-2.05	1.45	1.51
4	D	402	HEM	C2B-C1B	-2.04	1.45	1.51
4	A	401	HEM	CHD-C4C	2.10	1.41	1.36
4	D	401	HEM	CHC-C1C	2.12	1.41	1.36
4	C	402	HEM	C1C-NC	2.16	1.38	1.36
4	A	402	HEM	C4C-NC	2.20	1.38	1.36
4	C	401	HEM	C1C-NC	2.24	1.38	1.36
4	B	401	HEM	C1C-NC	2.36	1.38	1.36
4	A	402	HEM	C1C-NC	2.37	1.38	1.36
4	C	402	HEM	C4C-NC	2.50	1.39	1.36
4	D	402	HEM	C1C-NC	2.65	1.39	1.36
4	B	402	HEM	CBC-CAC	2.75	1.45	1.29
4	D	402	HEM	C4C-NC	2.79	1.39	1.36
4	A	402	HEM	CBC-CAC	2.84	1.45	1.29
4	B	402	HEM	CBB-CAB	2.84	1.45	1.29
4	C	402	HEM	CBB-CAB	2.88	1.45	1.29
4	C	402	HEM	CBC-CAC	2.90	1.46	1.29
4	C	401	HEM	CBC-CAC	2.91	1.46	1.29
4	B	401	HEM	CBC-CAC	2.91	1.46	1.29
4	D	402	HEM	CBB-CAB	2.91	1.46	1.29
4	B	401	HEM	CBB-CAB	2.92	1.46	1.29
4	D	401	HEM	CBC-CAC	2.97	1.46	1.29
4	D	401	HEM	CBB-CAB	2.99	1.46	1.29
4	B	401	HEM	C4C-NC	3.01	1.39	1.36
4	D	402	HEM	CBC-CAC	3.09	1.47	1.29
4	A	402	HEM	CBB-CAB	3.10	1.47	1.29
4	A	401	HEM	CBB-CAB	3.14	1.47	1.29
4	A	401	HEM	CBC-CAC	3.16	1.47	1.29
4	B	402	HEM	C1C-NC	3.23	1.40	1.36
4	C	401	HEM	CBB-CAB	3.32	1.48	1.29
4	D	401	HEM	C4C-NC	3.52	1.40	1.36
4	B	402	HEM	C4C-NC	3.59	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	HEM	C1C-NC	3.61	1.40	1.36
4	A	401	HEM	C1C-NC	3.63	1.40	1.36
4	A	401	HEM	C4C-NC	4.02	1.41	1.36

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	401	HEM	CAA-C2A-C1A	-3.23	123.50	127.01
4	D	402	HEM	CAA-C2A-C1A	-2.76	124.01	127.01
4	B	402	HEM	CAA-C2A-C1A	-2.34	124.47	127.01
4	A	402	HEM	CAA-C2A-C1A	-2.31	124.50	127.01
4	C	402	HEM	CMA-C3A-C4A	-2.26	124.62	128.36
4	C	401	HEM	CBD-CAD-C3D	-2.07	107.52	113.55
4	A	402	HEM	CBD-CAD-C3D	-2.06	107.56	113.55
4	A	401	HEM	CBD-CAD-C3D	-2.02	107.66	113.55
4	C	401	HEM	CMD-C2D-C3D	2.38	124.89	114.35
4	B	401	HEM	CMD-C2D-C3D	2.49	125.34	114.35
4	D	402	HEM	CMD-C2D-C3D	2.51	125.45	114.35
4	D	401	HEM	CMD-C2D-C3D	2.53	125.53	114.35
4	B	402	HEM	CMD-C2D-C3D	2.63	126.00	114.35
4	A	402	HEM	CMD-C2D-C3D	2.82	126.80	114.35
4	C	402	HEM	CMD-C2D-C3D	2.83	126.87	114.35
4	D	402	HEM	CAD-C3D-C4D	2.86	122.56	112.47
4	C	401	HEM	C2D-C3D-C4D	2.86	106.35	101.50
4	A	401	HEM	CMD-C2D-C3D	2.87	127.02	114.35
4	D	401	HEM	C2D-C3D-C4D	3.02	106.61	101.50
4	A	401	HEM	C2D-C3D-C4D	3.02	106.62	101.50
4	B	402	HEM	C2D-C3D-C4D	3.12	106.80	101.50
4	B	401	HEM	C2D-C3D-C4D	3.21	106.95	101.50
4	B	401	HEM	CAD-C3D-C4D	3.33	124.20	112.47
4	C	402	HEM	C2D-C3D-C4D	3.53	107.49	101.50
4	A	401	HEM	CAD-C3D-C4D	3.56	125.01	112.47
4	D	402	HEM	CMC-C2C-C3C	3.68	125.73	116.53
4	C	402	HEM	CAD-C3D-C4D	3.70	125.53	112.47
4	A	402	HEM	C2D-C3D-C4D	3.71	107.78	101.50
4	D	402	HEM	CBD-CAD-C3D	3.76	124.51	113.55
4	D	401	HEM	CAD-C3D-C4D	3.83	125.98	112.47
4	C	401	HEM	CMB-C2B-C3B	3.84	126.11	116.53
4	C	401	HEM	CAD-C3D-C4D	3.91	126.26	112.47
4	B	402	HEM	CAD-C3D-C4D	3.95	126.39	112.47
4	A	401	HEM	CMB-C2B-C3B	4.00	126.53	116.53
4	B	402	HEM	CMC-C2C-C3C	4.00	126.53	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	402	HEM	CAD-C3D-C4D	4.02	126.66	112.47
4	B	402	HEM	CMB-C2B-C3B	4.07	126.70	116.53
4	D	401	HEM	CMC-C2C-C3C	4.07	126.70	116.53
4	B	401	HEM	CMC-C2C-C3C	4.12	126.82	116.53
4	A	401	HEM	CMC-C2C-C3C	4.13	126.85	116.53
4	D	401	HEM	CMB-C2B-C3B	4.13	126.85	116.53
4	B	401	HEM	CMB-C2B-C3B	4.27	127.18	116.53
4	D	402	HEM	CMB-C2B-C3B	4.28	127.20	116.53
4	A	402	HEM	CAD-C3D-C2D	4.28	125.51	113.22
4	A	402	HEM	CMB-C2B-C3B	4.34	127.37	116.53
4	A	402	HEM	CMC-C2C-C3C	4.53	127.84	116.53
4	C	402	HEM	CMB-C2B-C3B	4.57	127.95	116.53
4	C	402	HEM	CMC-C2C-C3C	4.61	128.05	116.53
4	C	402	HEM	CAD-C3D-C2D	4.62	126.50	113.22
4	B	402	HEM	CAD-C3D-C2D	4.70	126.72	113.22
4	C	401	HEM	CMC-C2C-C3C	4.79	128.50	116.53
4	D	401	HEM	CAD-C3D-C2D	4.89	127.29	113.22
4	C	401	HEM	CAD-C3D-C2D	4.91	127.33	113.22
4	A	401	HEM	CAD-C3D-C2D	5.21	128.20	113.22
4	B	401	HEM	CAD-C3D-C2D	5.25	128.32	113.22
4	D	402	HEM	CAD-C3D-C2D	5.42	128.80	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	HEM	9	0
4	A	402	HEM	9	0
4	B	401	HEM	10	0
4	B	402	HEM	8	0
4	C	401	HEM	7	0
4	C	402	HEM	8	0
4	D	401	HEM	9	0
4	D	402	HEM	13	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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