



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 12:50 pm GMT

PDB ID : 2D2N  
Title : Structure of an extracellular giant hemoglobin of the gutless beard worm *Oligobrachia mashikoi*  
Authors : Numoto, N.; Nakagawa, T.; Kita, A.; Sasayama, Y.; Fukumori, Y.; Miki, K.  
Deposited on : 2005-09-12  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

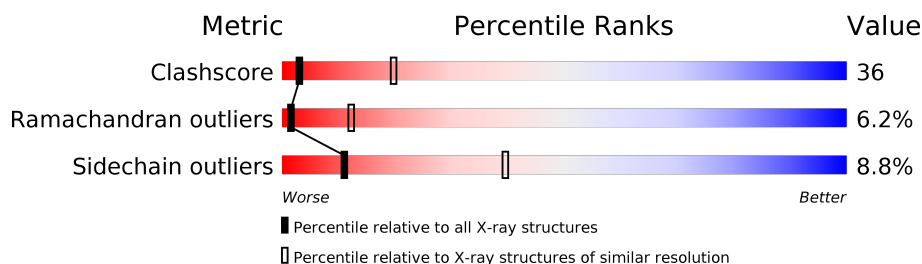
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	122078	1092 (3.20-3.20)
Ramachandran outliers	120005	1075 (3.20-3.20)
Sidechain outliers	119972	1074 (3.20-3.20)

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  $\geq 3$ , 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	140	
2	B	142	
3	C	147	
4	D	145	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4452 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 Giant hemoglobin, A1(b) globin chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1065	656	196	206	7			

- Molecule 2 is a protein called Giant hemoglobin, A2(a5) globin chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	142	Total	C	N	O	S	0	0	0
			1075	662	198	209	6			

- Molecule 3 is a protein called Giant hemoglobin, B2(c) globin chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	146	Total	C	N	O	S	0	0	0
			1088	668	201	210	9			

- Molecule 4 is a protein called Giant hemoglobin, B1(d) globin chain.

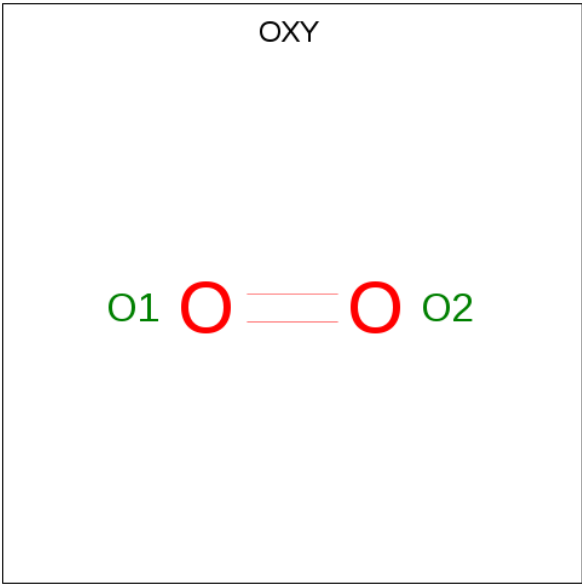
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	145	Total	C	N	O	S	0	0	0
			1036	642	178	209	7			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



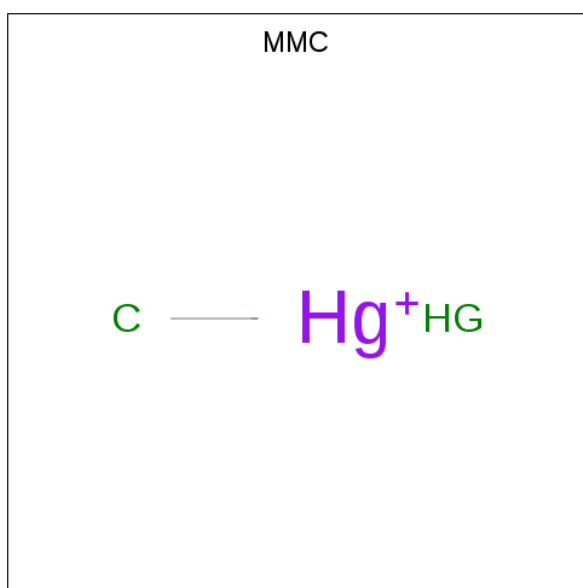
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



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

- Molecule 7 is METHYL MERCURY ION (three-letter code: MMC) (formula: CH<sub>3</sub>Hg).



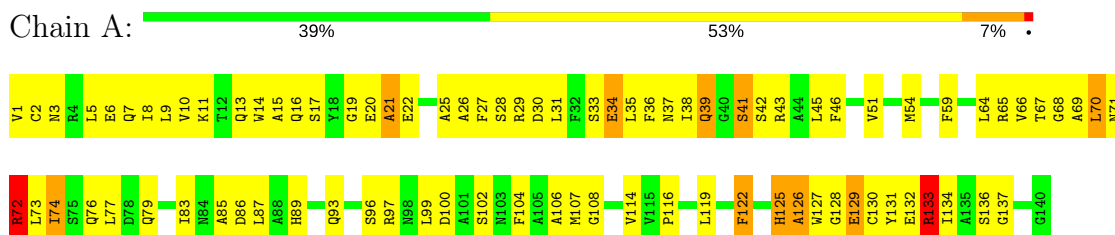
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C Hg 2 1 1	0	0
7	B	1	Total C Hg 2 1 1	0	0
7	C	1	Total C Hg 2 1 1	0	0
7	D	1	Total C Hg 2 1 1	0	0

### 3 Residue-property plots

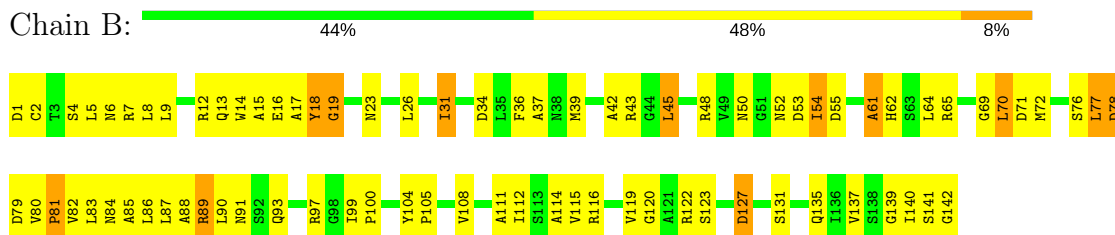
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

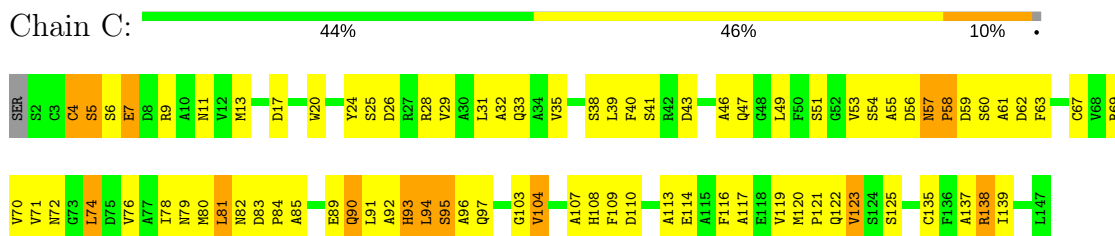
- Molecule 1: Giant hemoglobin, A1(b) globin chain



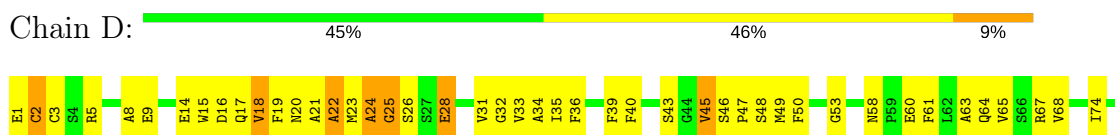
- Molecule 2: Giant hemoglobin, A2(a5) globin chain



- Molecule 3: Giant hemoglobin, B2(c) globin chain



- Molecule 4: Giant hemoglobin, B1(d) globin chain



T80	N81	
T84		
L88		
L89		
S90		
H91		
L92		
N93		
R97		
V102		
T103		
V107		
T108		
H109		
L110		
S111		
Q112		
A113		
I114		
S115		
S116		
V117		
V118		
A119		
Q120		
S124		
A125		
H126		
I127		
D128		
A129		
W130		
M134		
A138		
A139		
G140		
A143		
G144		
L145		

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.75Å 111.75Å 276.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20	Depositor
% Data completeness (in resolution range)	97.6 (50.00-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.242 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.46	0/1083	0.71	0/1464
2	B	0.48	0/1093	0.67	1/1481 (0.1%)
3	C	0.46	0/1110	0.66	0/1507
4	D	0.45	0/1055	0.68	0/1436
All	All	0.46	0/4341	0.68	1/5888 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	45	LEU	CA-CB-CG	5.24	127.35	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1065	0	1014	98	0
2	B	1075	0	1038	65	0
3	C	1088	0	1012	84	0
4	D	1036	0	986	76	0
5	A	43	0	30	3	0
5	B	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	43	0	30	1	0
5	D	43	0	30	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
All	All	4452	0	4170	311	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 36.

All (311) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PHE:HB2	1:A:51:VAL:HG11	1.24	1.08
2:B:9:LEU:HD21	2:B:13:GLN:HE21	1.42	0.84
3:C:25:SER:HA	3:C:28:ARG:CD	2.10	0.81
1:A:14:TRP:HE1	1:A:71:ASN:ND2	1.79	0.80
3:C:25:SER:HA	3:C:28:ARG:HD3	1.64	0.79
1:A:46:PHE:CB	1:A:51:VAL:HG11	2.10	0.79
1:A:1:VAL:HG12	1:A:129:GLU:HG3	1.65	0.77
3:C:90:GLN:HA	3:C:90:GLN:HE21	1.48	0.77
3:C:82:ASN:O	3:C:84:PRO:HD3	1.85	0.76
1:A:65:ARG:CZ	4:D:91:HIS:ND1	2.50	0.75
4:D:97:ARG:HA	4:D:145:LEU:HD21	1.69	0.74
1:A:46:PHE:HB2	1:A:51:VAL:CG1	2.10	0.74
4:D:1:GLU:HG3	4:D:2:CYS:H	1.53	0.73
1:A:3:ASN:ND2	1:A:6:GLU:HG3	2.03	0.73
1:A:108:GLY:HA3	1:A:131:TYR:CE2	2.24	0.72
4:D:19:PHE:HB3	4:D:24:ALA:HB2	1.70	0.72
2:B:16:GLU:HG2	2:B:119:VAL:HG12	1.71	0.72
3:C:31:LEU:HD13	3:C:123:VAL:HG21	1.71	0.72
1:A:43:ARG:HH11	1:A:43:ARG:HG2	1.54	0.71
1:A:97:ARG:H	1:A:97:ARG:HD2	1.53	0.70
1:A:5:LEU:HD12	3:C:122:GLN:NE2	2.05	0.70
1:A:129:GLU:O	1:A:132:GLU:HB3	1.92	0.70
4:D:14:GLU:OE1	4:D:125:ALA:HA	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LEU:HA	1:A:8:ILE:CD1	2.22	0.70
4:D:115:SER:OG	4:D:134:MET:HG3	1.92	0.68
1:A:29:ARG:HD3	1:A:54:MET:O	1.94	0.67
4:D:36:PHE:HZ	4:D:68:VAL:HG21	1.60	0.67
1:A:8:ILE:CD1	3:C:123:VAL:HG13	2.25	0.67
1:A:116:PRO:HB3	1:A:122:PHE:CD2	2.30	0.66
2:B:1:ASP:CG	2:B:2:CYS:H	1.98	0.65
2:B:89:ARG:O	2:B:93:GLN:HG3	1.96	0.65
2:B:99:ILE:HD12	5:B:200:HEM:HAC	1.79	0.65
1:A:83:ILE:HG12	1:A:87:LEU:HD12	1.78	0.64
3:C:49:LEU:HD11	3:C:108:HIS:CE1	2.33	0.64
3:C:32:ALA:CB	3:C:67:CYS:HB3	2.27	0.64
2:B:43:ARG:HD3	2:B:52:ASN:HA	1.79	0.64
3:C:25:SER:HA	3:C:28:ARG:HD2	1.79	0.64
1:A:99:LEU:HD22	5:A:200:HEM:HAC	1.79	0.63
1:A:3:ASN:HD21	1:A:6:GLU:HG3	1.62	0.63
1:A:133:ARG:HD2	1:A:133:ARG:O	1.98	0.63
4:D:90:SER:O	4:D:93:ASN:HB3	1.99	0.63
3:C:9:ARG:O	3:C:13:MET:HG3	1.99	0.62
1:A:97:ARG:HG2	5:A:200:HEM:HMD1	1.80	0.62
4:D:31:VAL:O	4:D:35:ILE:HG12	1.98	0.62
4:D:110:LEU:O	4:D:110:LEU:HD13	1.99	0.62
3:C:82:ASN:C	3:C:84:PRO:HD3	2.19	0.62
4:D:14:GLU:HA	4:D:17:GLN:CB	2.29	0.62
2:B:9:LEU:HD23	2:B:9:LEU:C	2.20	0.61
3:C:43:ASP:OD1	3:C:46:ALA:HB2	2.01	0.61
4:D:47:PRO:C	4:D:49:MET:H	2.04	0.61
2:B:115:VAL:O	2:B:119:VAL:HG22	2.00	0.61
2:B:76:SER:O	2:B:78:ASP:N	2.33	0.61
1:A:38:ILE:HD11	1:A:106:ALA:O	2.00	0.61
3:C:93:HIS:O	3:C:95:SER:N	2.34	0.61
4:D:49:MET:O	4:D:49:MET:HG2	1.99	0.60
2:B:5:LEU:O	2:B:8:LEU:HB2	2.01	0.60
1:A:34:GLU:OE1	1:A:34:GLU:HA	2.02	0.60
1:A:99:LEU:HD13	1:A:104:PHE:HE1	1.66	0.59
4:D:14:GLU:HA	4:D:17:GLN:HB2	1.85	0.59
1:A:34:GLU:O	1:A:37:ASN:N	2.36	0.59
2:B:43:ARG:HH21	2:B:54:ILE:HD11	1.67	0.59
3:C:53:VAL:O	3:C:55:ALA:N	2.33	0.59
1:A:8:ILE:HD13	3:C:123:VAL:HG13	1.83	0.59
3:C:91:LEU:HD21	3:C:139:ILE:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:108:THR:O	4:D:112:GLN:HG3	2.02	0.59
3:C:32:ALA:HB2	3:C:71:VAL:CG2	2.33	0.58
1:A:83:ILE:HG12	1:A:87:LEU:CD1	2.33	0.58
1:A:42:SER:O	1:A:45:LEU:N	2.36	0.58
2:B:104:TYR:HB2	2:B:105:PRO:HD3	1.86	0.58
3:C:35:VAL:HA	3:C:119:VAL:HG21	1.86	0.58
2:B:89:ARG:NH2	3:C:69:ARG:NH1	2.51	0.58
1:A:66:VAL:O	1:A:70:LEU:HB2	2.04	0.57
1:A:86:ASP:OD2	4:D:67:ARG:HD3	2.04	0.57
3:C:90:GLN:HA	3:C:90:GLN:NE2	2.19	0.57
3:C:76:VAL:O	3:C:80:MET:HG3	2.05	0.57
1:A:130:CYS:O	1:A:134:ILE:HG13	2.05	0.57
1:A:5:LEU:HA	1:A:8:ILE:HD11	1.87	0.57
1:A:74:ILE:HA	1:A:77:LEU:HG	1.87	0.56
2:B:17:ALA:HB2	2:B:119:VAL:HG13	1.87	0.56
3:C:103:GLY:O	3:C:104:VAL:C	2.42	0.56
1:A:72:ARG:NE	4:D:67:ARG:HG2	2.19	0.56
3:C:58:PRO:O	3:C:60:SER:N	2.38	0.56
1:A:15:ALA:O	1:A:19:GLY:HA3	2.06	0.56
1:A:65:ARG:NE	4:D:91:HIS:ND1	2.54	0.56
1:A:35:LEU:HD13	1:A:107:MET:HA	1.87	0.56
3:C:74:LEU:HD22	3:C:78:ILE:HG13	1.87	0.56
4:D:32:GLY:O	4:D:35:ILE:HB	2.06	0.56
4:D:108:THR:HA	4:D:111:SER:OG	2.06	0.55
3:C:120:MET:HB2	3:C:121:PRO:HD3	1.88	0.55
4:D:16:ASP:O	4:D:19:PHE:N	2.39	0.55
4:D:61:PHE:O	4:D:65:VAL:HG23	2.06	0.55
2:B:87:LEU:HA	2:B:90:LEU:HD12	1.87	0.55
1:A:34:GLU:O	1:A:35:LEU:C	2.44	0.55
1:A:99:LEU:HD13	1:A:104:PHE:CE1	2.42	0.55
3:C:72:ASN:O	3:C:76:VAL:HG23	2.07	0.55
3:C:38:SER:O	3:C:39:LEU:C	2.45	0.54
3:C:84:PRO:O	3:C:85:ALA:C	2.45	0.54
4:D:36:PHE:CZ	4:D:68:VAL:HG21	2.40	0.54
2:B:14:TRP:CH2	2:B:70:LEU:HD23	2.43	0.54
2:B:97:ARG:H	2:B:97:ARG:HD2	1.71	0.54
2:B:53:ASP:O	2:B:55:ASP:N	2.40	0.54
1:A:13:GLN:OE1	1:A:122:PHE:HA	2.08	0.54
3:C:40:PHE:CE1	3:C:47:GLN:HA	2.42	0.54
1:A:42:SER:O	1:A:45:LEU:HB3	2.08	0.54
2:B:9:LEU:HD21	2:B:13:GLN:NE2	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:ASP:O	3:C:114:GLU:HG2	2.07	0.54
3:C:53:VAL:CG1	3:C:63:PHE:HA	2.37	0.54
4:D:114:ILE:HB	4:D:134:MET:HE2	1.89	0.54
1:A:2:CYS:HB2	1:A:130:CYS:HA	1.90	0.54
1:A:17:SER:HB2	1:A:119:LEU:HD21	1.90	0.53
1:A:39:GLN:HG2	1:A:41:SER:OG	2.09	0.53
1:A:43:ARG:NH1	1:A:43:ARG:HG2	2.23	0.53
3:C:58:PRO:HA	3:C:63:PHE:CD1	2.44	0.53
2:B:26:LEU:C	2:B:26:LEU:HD13	2.29	0.53
4:D:113:ALA:O	4:D:117:VAL:HG23	2.09	0.53
2:B:23:ASN:O	2:B:26:LEU:HB3	2.09	0.52
2:B:99:ILE:HG23	5:B:200:HEM:HAC	1.90	0.52
4:D:18:VAL:HG12	4:D:19:PHE:N	2.23	0.52
2:B:4:SER:HA	2:B:7:ARG:HH21	1.75	0.52
1:A:125:HIS:O	1:A:127:TRP:N	2.43	0.52
4:D:16:ASP:O	4:D:19:PHE:C	2.47	0.52
2:B:69:GLY:HA2	2:B:72:MET:CE	2.40	0.52
4:D:61:PHE:O	4:D:64:GLN:HB3	2.10	0.51
1:A:69:ALA:HA	1:A:72:ARG:HG2	1.93	0.51
4:D:5:ARG:NH1	4:D:80:THR:HB	2.25	0.51
2:B:76:SER:O	2:B:77:LEU:C	2.48	0.51
3:C:32:ALA:HB3	3:C:67:CYS:HB3	1.92	0.51
3:C:32:ALA:HB2	3:C:71:VAL:HG21	1.93	0.51
1:A:15:ALA:O	1:A:19:GLY:CA	2.58	0.51
1:A:20:GLU:O	1:A:21:ALA:O	2.28	0.51
1:A:36:PHE:CG	1:A:43:ARG:HG3	2.46	0.51
1:A:8:ILE:HD12	3:C:123:VAL:HG13	1.91	0.51
3:C:9:ARG:HD3	3:C:81:LEU:O	2.10	0.51
1:A:133:ARG:CD	1:A:133:ARG:O	2.59	0.51
1:A:7:GLN:O	1:A:11:LYS:HG3	2.10	0.51
3:C:31:LEU:O	3:C:35:VAL:HG23	2.10	0.51
2:B:91:ASN:HB2	2:B:139:GLY:O	2.10	0.50
4:D:118:VAL:HG12	4:D:119:ALA:N	2.26	0.50
3:C:29:VAL:O	3:C:33:GLN:HG3	2.12	0.50
1:A:14:TRP:NE1	1:A:71:ASN:ND2	2.55	0.50
3:C:31:LEU:HD12	3:C:119:VAL:HG11	1.93	0.50
4:D:14:GLU:HA	4:D:17:GLN:HB3	1.93	0.49
4:D:64:GLN:HE21	4:D:68:VAL:CG2	2.24	0.49
4:D:21:ALA:O	4:D:22:ALA:HB2	2.12	0.49
1:A:54:MET:HA	1:A:59:PHE:CD2	2.46	0.49
1:A:8:ILE:O	1:A:9:LEU:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ASP:O	2:B:131:SER:HB2	2.12	0.49
3:C:28:ARG:HB3	3:C:71:VAL:HG11	1.92	0.49
4:D:33:VAL:HG23	4:D:34:ALA:N	2.26	0.49
1:A:125:HIS:O	1:A:128:GLY:N	2.46	0.49
2:B:97:ARG:HG2	5:B:200:HEM:HMD3	1.93	0.49
4:D:39:PHE:HZ	5:D:200:HEM:HBC2	1.77	0.49
4:D:43:SER:HA	4:D:109:HIS:CD2	2.48	0.49
2:B:69:GLY:HA2	2:B:72:MET:HE2	1.94	0.48
2:B:69:GLY:O	2:B:72:MET:N	2.46	0.48
2:B:2:CYS:HA	2:B:6:ASN:HD22	1.78	0.48
3:C:78:ILE:O	3:C:81:LEU:HB2	2.14	0.48
2:B:18:TYR:O	2:B:19:GLY:O	2.31	0.48
3:C:43:ASP:CG	3:C:46:ALA:HB2	2.33	0.48
1:A:96:SER:OG	1:A:97:ARG:HD2	2.13	0.48
2:B:39:MET:HG2	2:B:39:MET:O	2.14	0.48
3:C:57:ASN:O	3:C:58:PRO:C	2.51	0.48
1:A:100:ASP:OD1	1:A:102:SER:OG	2.30	0.48
1:A:71:ASN:C	1:A:73:LEU:H	2.17	0.48
3:C:51:SER:C	3:C:53:VAL:H	2.17	0.48
1:A:132:GLU:O	1:A:134:ILE:N	2.47	0.47
1:A:46:PHE:CB	1:A:51:VAL:CG1	2.82	0.47
2:B:31:ILE:HG22	2:B:114:ALA:CB	2.44	0.47
2:B:9:LEU:HD23	2:B:9:LEU:O	2.14	0.47
3:C:4:CYS:HB2	3:C:135:CYS:HA	1.96	0.47
1:A:36:PHE:CD1	1:A:43:ARG:HG3	2.49	0.47
3:C:74:LEU:O	3:C:78:ILE:HG13	2.14	0.47
4:D:102:VAL:CG1	4:D:145:LEU:HD13	2.44	0.47
1:A:31:LEU:HA	1:A:114:VAL:HG21	1.97	0.47
1:A:66:VAL:C	1:A:68:GLY:N	2.66	0.47
4:D:97:ARG:HG2	4:D:97:ARG:HH11	1.80	0.47
2:B:1:ASP:CG	2:B:2:CYS:N	2.66	0.47
4:D:2:CYS:O	4:D:3:CYS:HB3	2.14	0.47
1:A:13:GLN:HA	1:A:16:GLN:HB2	1.97	0.47
2:B:104:TYR:O	2:B:108:VAL:HG23	2.14	0.47
1:A:5:LEU:HD13	3:C:122:GLN:HB2	1.95	0.47
4:D:103:THR:O	4:D:107:VAL:HG23	2.14	0.47
4:D:39:PHE:CZ	5:D:200:HEM:HBC2	2.49	0.47
2:B:141:SER:OG	2:B:142:GLY:N	2.49	0.46
1:A:30:ASP:O	1:A:33:SER:HB3	2.15	0.46
1:A:3:ASN:CG	1:A:6:GLU:HG3	2.35	0.46
2:B:64:LEU:HD12	3:C:80:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:VAL:HA	3:C:108:HIS:ND1	2.29	0.46
3:C:137:ALA:O	3:C:138:ARG:C	2.53	0.46
4:D:89:LEU:HB3	4:D:140:GLY:HA3	1.97	0.46
1:A:27:PHE:O	1:A:30:ASP:HB2	2.15	0.46
1:A:64:LEU:O	1:A:68:GLY:N	2.46	0.46
3:C:32:ALA:HB2	3:C:71:VAL:HG23	1.98	0.46
3:C:70:VAL:HG12	3:C:71:VAL:N	2.30	0.46
1:A:125:HIS:O	1:A:126:ALA:C	2.54	0.46
1:A:45:LEU:HD21	1:A:99:LEU:CD2	2.46	0.46
2:B:43:ARG:NH2	2:B:54:ILE:HD11	2.30	0.46
3:C:32:ALA:O	3:C:35:VAL:N	2.48	0.46
3:C:49:LEU:HD13	3:C:104:VAL:HB	1.97	0.46
3:C:74:LEU:HD12	3:C:116:PHE:CZ	2.50	0.46
4:D:35:ILE:HD13	4:D:117:VAL:HG21	1.97	0.46
1:A:15:ALA:O	1:A:19:GLY:N	2.49	0.45
2:B:34:ASP:O	2:B:37:ALA:N	2.45	0.45
2:B:69:GLY:O	2:B:71:ASP:N	2.50	0.45
4:D:23:MET:O	4:D:24:ALA:C	2.53	0.45
4:D:16:ASP:C	4:D:18:VAL:N	2.69	0.45
2:B:83:LEU:O	2:B:84:ASN:C	2.54	0.45
3:C:109:PHE:O	3:C:113:ALA:HB2	2.16	0.45
3:C:137:ALA:O	3:C:139:ILE:N	2.49	0.45
4:D:97:ARG:HG2	4:D:97:ARG:NH1	2.32	0.45
4:D:16:ASP:O	4:D:18:VAL:N	2.49	0.45
1:A:36:PHE:CE2	1:A:43:ARG:HA	2.51	0.45
2:B:104:TYR:N	2:B:105:PRO:CD	2.79	0.45
2:B:61:ALA:O	2:B:64:LEU:HB2	2.17	0.45
3:C:7:GLU:CD	3:C:7:GLU:H	2.20	0.45
4:D:47:PRO:O	4:D:49:MET:N	2.49	0.45
3:C:90:GLN:CA	3:C:90:GLN:NE2	2.80	0.45
4:D:23:MET:O	4:D:25:GLY:N	2.50	0.45
2:B:97:ARG:CD	2:B:97:ARG:H	2.30	0.45
1:A:100:ASP:OD1	1:A:102:SER:N	2.46	0.45
3:C:58:PRO:C	3:C:60:SER:H	2.20	0.45
3:C:4:CYS:SG	3:C:9:ARG:HG2	2.56	0.44
4:D:1:GLU:O	4:D:3:CYS:N	2.50	0.44
1:A:64:LEU:O	1:A:65:ARG:C	2.56	0.44
3:C:5:SER:O	3:C:9:ARG:HG3	2.18	0.44
1:A:3:ASN:ND2	1:A:6:GLU:CG	2.76	0.44
2:B:31:ILE:O	2:B:31:ILE:HD12	2.17	0.44
3:C:38:SER:O	3:C:41:SER:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:LEU:O	3:C:92:ALA:C	2.56	0.44
1:A:89:HIS:O	1:A:93:GLN:HG3	2.18	0.44
3:C:53:VAL:HA	3:C:62:ASP:OD2	2.17	0.44
3:C:95:SER:O	3:C:97:GLN:N	2.51	0.44
4:D:39:PHE:CE1	4:D:110:LEU:HB2	2.53	0.44
4:D:58:ASN:OD1	4:D:60:GLU:HB2	2.18	0.44
1:A:99:LEU:CD1	1:A:104:PHE:HE1	2.31	0.44
1:A:132:GLU:C	1:A:134:ILE:N	2.72	0.44
2:B:6:ASN:O	2:B:7:ARG:C	2.54	0.44
3:C:109:PHE:CD1	5:C:200:HEM:HMC3	2.53	0.44
1:A:45:LEU:HD21	1:A:99:LEU:HD23	2.00	0.43
2:B:122:ARG:O	2:B:123:SER:HB2	2.18	0.43
2:B:61:ALA:CB	2:B:65:ARG:HH21	2.31	0.43
3:C:24:TYR:HB3	3:C:26:ASP:OD2	2.17	0.43
3:C:93:HIS:C	3:C:95:SER:N	2.71	0.43
1:A:85:ALA:O	1:A:86:ASP:C	2.56	0.43
1:A:10:VAL:O	1:A:11:LYS:C	2.57	0.43
4:D:45:VAL:CG1	4:D:46:SER:N	2.80	0.43
2:B:12:ARG:O	2:B:15:ALA:N	2.52	0.43
4:D:47:PRO:C	4:D:49:MET:N	2.69	0.43
1:A:6:GLU:OE1	1:A:129:GLU:HG2	2.18	0.43
1:A:34:GLU:O	1:A:36:PHE:N	2.51	0.43
4:D:81:ASN:OD1	4:D:84:THR:HG23	2.19	0.43
2:B:116:ARG:O	2:B:120:GLY:N	2.50	0.43
2:B:80:VAL:HB	2:B:81:PRO:HD3	2.01	0.43
4:D:108:THR:HG23	4:D:138:ALA:HB1	2.00	0.43
1:A:79:GLN:OE1	1:A:79:GLN:HA	2.18	0.43
1:A:28:SER:HA	1:A:67:THR:HG21	2.00	0.43
4:D:93:ASN:OD1	4:D:143:ALA:HB3	2.19	0.43
3:C:35:VAL:CA	3:C:119:VAL:HG21	2.49	0.42
4:D:145:LEU:HA	4:D:145:LEU:HD23	1.91	0.42
1:A:20:GLU:O	1:A:21:ALA:C	2.57	0.42
2:B:99:ILE:HA	2:B:100:PRO:HD3	1.83	0.42
3:C:58:PRO:HA	3:C:63:PHE:CE1	2.54	0.42
3:C:49:LEU:HD11	3:C:108:HIS:HE1	1.82	0.42
1:A:108:GLY:HA3	1:A:131:TYR:CD2	2.54	0.42
3:C:79:ASN:HD22	3:C:79:ASN:HA	1.64	0.42
4:D:15:TRP:HE3	4:D:130:TRP:HH2	1.68	0.42
3:C:114:GLU:HA	3:C:117:ALA:HB3	2.02	0.42
2:B:111:ALA:O	2:B:112:ILE:C	2.55	0.42
2:B:5:LEU:HD12	4:D:120:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:HIS:HA	2:B:65:ARG:CZ	2.49	0.42
2:B:80:VAL:O	2:B:81:PRO:C	2.53	0.42
4:D:91:HIS:HD2	4:D:91:HIS:O	2.02	0.41
4:D:45:VAL:HG11	5:D:200:HEM:HBC1	2.02	0.41
4:D:74:ILE:HG22	4:D:88:LEU:HD13	2.02	0.41
1:A:68:GLY:O	1:A:71:ASN:HB3	2.20	0.41
1:A:64:LEU:O	1:A:66:VAL:N	2.53	0.41
2:B:82:VAL:O	2:B:83:LEU:C	2.57	0.41
2:B:85:ALA:O	2:B:88:ALA:HB3	2.20	0.41
3:C:38:SER:OG	3:C:39:LEU:N	2.54	0.41
3:C:61:ALA:O	3:C:62:ASP:C	2.59	0.41
4:D:124:SER:O	4:D:125:ALA:C	2.58	0.41
4:D:40:PHE:CE1	4:D:47:PRO:HB3	2.56	0.41
2:B:137:VAL:O	2:B:140:ILE:N	2.50	0.41
4:D:125:ALA:O	4:D:127:ILE:N	2.54	0.41
4:D:15:TRP:HB2	4:D:130:TRP:CH2	2.56	0.41
1:A:66:VAL:HG22	5:A:200:HEM:CHB	2.51	0.41
1:A:8:ILE:H	1:A:8:ILE:HG13	1.54	0.41
3:C:17:ASP:O	3:C:20:TRP:HB3	2.20	0.41
3:C:93:HIS:O	3:C:94:LEU:C	2.58	0.41
4:D:118:VAL:HG21	4:D:130:TRP:CH2	2.55	0.41
4:D:45:VAL:HG12	4:D:46:SER:N	2.36	0.41
3:C:32:ALA:O	3:C:33:GLN:C	2.59	0.41
4:D:118:VAL:CG1	4:D:119:ALA:N	2.83	0.41
4:D:20:ASN:OD1	4:D:23:MET:HG2	2.21	0.41
1:A:34:GLU:CA	1:A:34:GLU:OE1	2.68	0.41
2:B:83:LEU:O	2:B:86:LEU:N	2.54	0.41
3:C:70:VAL:O	3:C:71:VAL:C	2.58	0.41
4:D:28:GLU:O	4:D:32:GLY:N	2.45	0.41
4:D:63:ALA:O	4:D:67:ARG:HG3	2.21	0.41
1:A:26:ALA:O	1:A:27:PHE:C	2.59	0.40
3:C:25:SER:O	3:C:29:VAL:HG23	2.21	0.40
1:A:97:ARG:N	1:A:97:ARG:HD2	2.28	0.40
3:C:55:ALA:HA	3:C:63:PHE:CD2	2.56	0.40
3:C:80:MET:O	3:C:82:ASN:N	2.55	0.40
4:D:91:HIS:C	4:D:91:HIS:CD2	2.95	0.40
1:A:25:ALA:O	1:A:29:ARG:HG3	2.21	0.40
2:B:104:TYR:CG	2:B:141:SER:HB3	2.57	0.40
2:B:36:PHE:HB3	2:B:43:ARG:NH1	2.37	0.40
2:B:42:ALA:O	2:B:45:LEU:HD23	2.21	0.40
4:D:50:PHE:O	4:D:53:GLY:N	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:8:ALA:O	4:D:9:GLU:C	2.60	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	138/140 (99%)	102 (74%)	27 (20%)	9 (6%)	1	11
2	B	140/142 (99%)	103 (74%)	32 (23%)	5 (4%)	4	26
3	C	144/147 (98%)	107 (74%)	25 (17%)	12 (8%)	1	5
4	D	143/145 (99%)	110 (77%)	24 (17%)	9 (6%)	1	11
All	All	565/574 (98%)	422 (75%)	108 (19%)	35 (6%)	1	12

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ALA
1	A	22	GLU
3	C	54	SER
3	C	59	ASP
3	C	94	LEU
3	C	104	VAL
4	D	2	CYS
4	D	22	ALA
4	D	24	ALA
1	A	133	ARG
2	B	19	GLY
2	B	54	ILE
2	B	70	LEU
2	B	77	LEU

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Mol	Chain	Res	Type
3	C	95	SER
3	C	96	ALA
4	D	48	SER
1	A	126	ALA
1	A	136	SER
3	C	138	ARG
4	D	125	ALA
1	A	72	ARG
2	B	61	ALA
3	C	93	HIS
3	C	107	ALA
4	D	25	GLY
4	D	126	HIS
1	A	39	GLN
1	A	125	HIS
1	A	137	GLY
3	C	81	LEU
4	D	26	SER
3	C	5	SER
4	D	45	VAL
3	C	83	ASP

### 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	110/110 (100%)	101 (92%)	9 (8%)	12	44
2	B	113/113 (100%)	103 (91%)	10 (9%)	11	39
3	C	110/111 (99%)	98 (89%)	12 (11%)	7	29
4	D	108/108 (100%)	100 (93%)	8 (7%)	15	50
All	All	441/442 (100%)	402 (91%)	39 (9%)	11	39

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	41	SER
1	A	70	LEU
1	A	72	ARG
1	A	74	ILE
1	A	76	GLN
1	A	122	PHE
1	A	129	GLU
1	A	133	ARG
2	B	18	TYR
2	B	31	ILE
2	B	48	ARG
2	B	50	ASN
2	B	78	ASP
2	B	79	ASP
2	B	81	PRO
2	B	89	ARG
2	B	127	ASP
2	B	135	GLN
3	C	4	CYS
3	C	6	SER
3	C	7	GLU
3	C	11	ASN
3	C	56	ASP
3	C	57	ASN
3	C	58	PRO
3	C	74	LEU
3	C	89	GLU
3	C	90	GLN
3	C	123	VAL
3	C	125	SER
4	D	18	VAL
4	D	28	GLU
4	D	93	ASN
4	D	103	THR
4	D	108	THR
4	D	118	VAL
4	D	124	SER
4	D	128	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	62	HIS
1	A	71	ASN
1	A	76	GLN
2	B	6	ASN
2	B	13	GLN
2	B	23	ASN
2	B	50	ASN
2	B	52	ASN
2	B	84	ASN
2	B	134	ASN
3	C	11	ASN
3	C	47	GLN
3	C	57	ASN
3	C	79	ASN
3	C	82	ASN
3	C	90	GLN
3	C	99	GLN
3	C	122	GLN
3	C	133	ASN
3	C	141	ASN
4	D	93	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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
5	HEM	A	200	1,6	27,50,50	0.90	1 (3%)	17,82,82	1.54	4 (23%)
6	OXY	A	201	5	1,1,1	0.00	0	0,0,0	0.00	-
7	MMC	A	500	1	0,1,1	0.00	-	0,0,0	0.00	-
6	OXY	B	1201	5	1,1,1	0.02	0	0,0,0	0.00	-
7	MMC	B	1500	2	0,1,1	0.00	-	0,0,0	0.00	-
5	HEM	B	200	2,6	27,50,50	0.91	1 (3%)	17,82,82	1.56	4 (23%)
5	HEM	C	200	3,6	27,50,50	0.85	1 (3%)	17,82,82	1.69	4 (23%)
6	OXY	C	2201	5	1,1,1	0.03	0	0,0,0	0.00	-
7	MMC	C	2500	3	0,1,1	0.00	-	0,0,0	0.00	-
5	HEM	D	200	4,6	27,50,50	0.91	1 (3%)	17,82,82	1.45	3 (17%)
6	OXY	D	3201	5	1,1,1	0.00	0	0,0,0	0.00	-
7	MMC	D	3500	4	0,1,1	0.00	-	0,0,0	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	A	200	1,6	-	0/6/54/54	0/0/8/8
6	OXY	A	201	5	-	0/0/0/0	0/0/0/0
7	MMC	A	500	1	-	0/0/0/0	0/0/0/0
6	OXY	B	1201	5	-	0/0/0/0	0/0/0/0
7	MMC	B	1500	2	-	0/0/0/0	0/0/0/0
5	HEM	B	200	2,6	-	0/6/54/54	0/0/8/8
5	HEM	C	200	3,6	-	0/6/54/54	0/0/8/8
6	OXY	C	2201	5	-	0/0/0/0	0/0/0/0
7	MMC	C	2500	3	-	0/0/0/0	0/0/0/0
5	HEM	D	200	4,6	-	0/6/54/54	0/0/8/8
6	OXY	D	3201	5	-	0/0/0/0	0/0/0/0
7	MMC	D	3500	4	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	200	HEM	C3B-C2B	-2.49	1.36	1.40

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	200	HEM	C3B-C2B	-2.43	1.37	1.40
5	C	200	HEM	C3B-C2B	-2.29	1.37	1.40
5	B	200	HEM	C3B-C2B	-2.22	1.37	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	200	HEM	CAD-CBD-CGD	-3.58	106.55	112.66
5	B	200	HEM	CAD-CBD-CGD	-3.07	107.41	112.66
5	D	200	HEM	CMA-C3A-C4A	-2.28	124.96	128.46
5	A	200	HEM	CMA-C3A-C4A	-2.24	125.01	128.46
5	A	200	HEM	CAD-CBD-CGD	-2.22	108.86	112.66
5	A	200	HEM	CMD-C2D-C1D	-2.18	125.12	128.46
5	B	200	HEM	CMA-C3A-C4A	-2.16	125.15	128.46
5	C	200	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
5	B	200	HEM	CMC-C2C-C3C	2.21	128.91	124.88
5	C	200	HEM	CMB-C2B-C3B	2.34	129.14	124.88
5	C	200	HEM	CMC-C2C-C3C	2.37	129.19	124.88
5	D	200	HEM	CMC-C2C-C3C	2.45	129.34	124.88
5	A	200	HEM	CMC-C2C-C3C	2.63	129.67	124.88
5	B	200	HEM	CMB-C2B-C3B	2.76	129.90	124.88
5	D	200	HEM	CMB-C2B-C3B	2.89	130.14	124.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	200	HEM	3	0
5	B	200	HEM	3	0
5	C	200	HEM	1	0
5	D	200	HEM	3	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.