



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:14 PM GMT

PDB ID : 1WNW
Title : D136N mutant of Heme Oxygenase from *Corynebacterium diphtheriae* (HmuO)
Authors : Unno, M.; Matsui, T.; Ikeda-Saito, M.
Deposited on : 2004-08-10
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

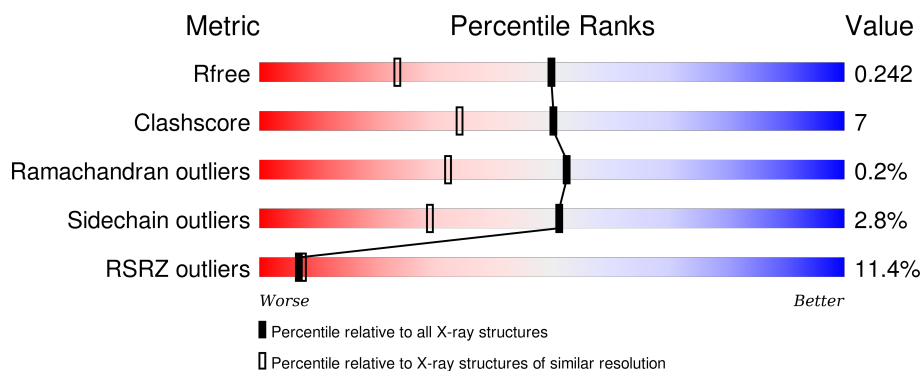
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	215	<div> <div>7%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>
1	B	215	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	C	215	<div> <div>24%</div> <div>75%</div> <div>18%</div> <div>.</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IOD	A	1006	-	-	X	-
2	IOD	A	1007	-	-	X	-
2	IOD	B	1002	-	-	X	-
4	SO4	A	2007	-	-	-	X
4	SO4	B	2003	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5538 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 Heme oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1653	1042	298	310	3			
1	B	210	Total	C	N	O	S	0	1	0
			1668	1050	300	315	3			
1	C	206	Total	C	N	O	S	0	0	0
			1635	1031	291	310	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	LYS	GLU	SEE REMARK 999	UNP P71119
A	60	VAL	ALA	SEE REMARK 999	UNP P71119
A	92	GLY	ASP	SEE REMARK 999	UNP P71119
A	93	SER	GLY	SEE REMARK 999	UNP P71119
A	136	ASN	ASP	ENGINEERED	UNP P71119
A	192	HIS	ASN	SEE REMARK 999	UNP P71119
B	34	LYS	GLU	SEE REMARK 999	UNP P71119
B	60	VAL	ALA	SEE REMARK 999	UNP P71119
B	92	GLY	ASP	SEE REMARK 999	UNP P71119
B	93	SER	GLY	SEE REMARK 999	UNP P71119
B	136	ASN	ASP	ENGINEERED	UNP P71119
B	192	HIS	ASN	SEE REMARK 999	UNP P71119
C	34	LYS	GLU	SEE REMARK 999	UNP P71119
C	60	VAL	ALA	SEE REMARK 999	UNP P71119
C	92	GLY	ASP	SEE REMARK 999	UNP P71119
C	93	SER	GLY	SEE REMARK 999	UNP P71119
C	136	ASN	ASP	ENGINEERED	UNP P71119
C	192	HIS	ASN	SEE REMARK 999	UNP P71119

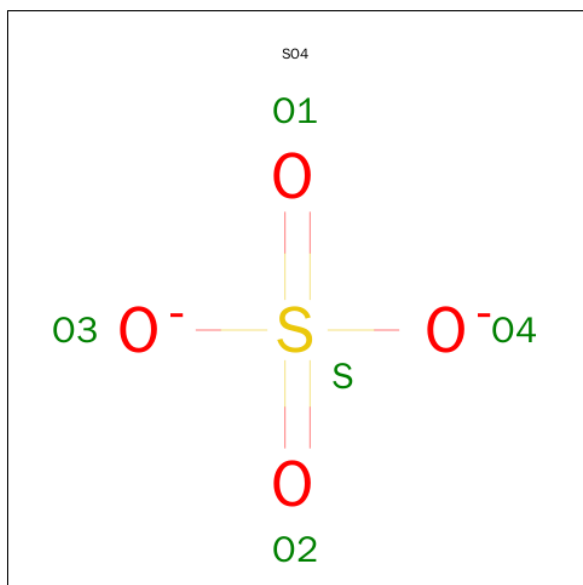
- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total I 4 4	0	0
2	A	4	Total I 4 4	0	0
2	C	1	Total I 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Na 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



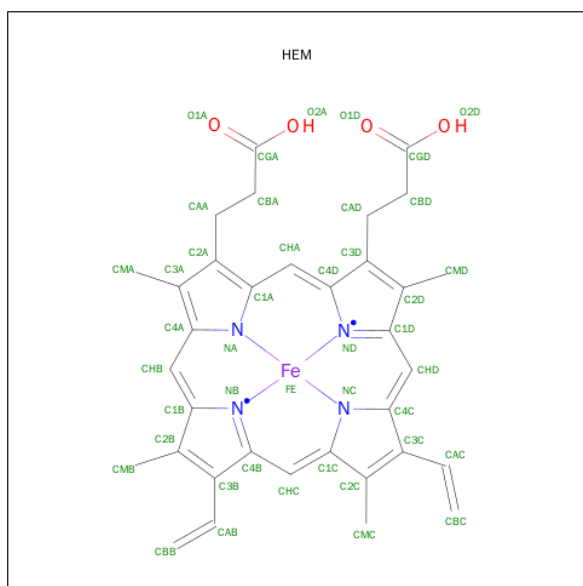
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

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

- 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		

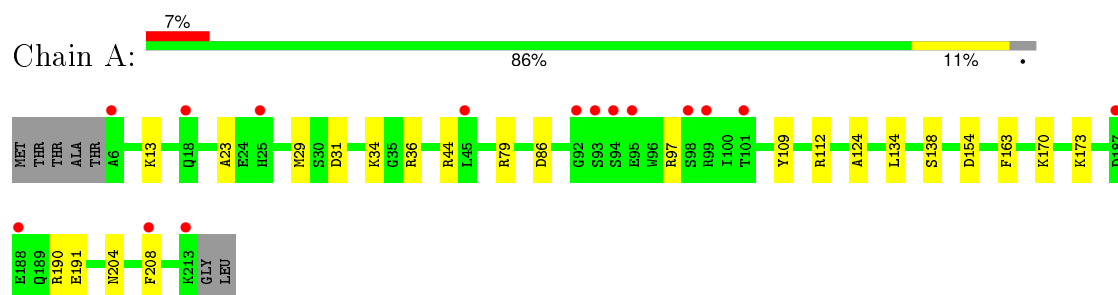
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total 128	O 128	0	0
6	B	157	Total 157	O 157	0	0
6	C	97	Total 97	O 97	0	0

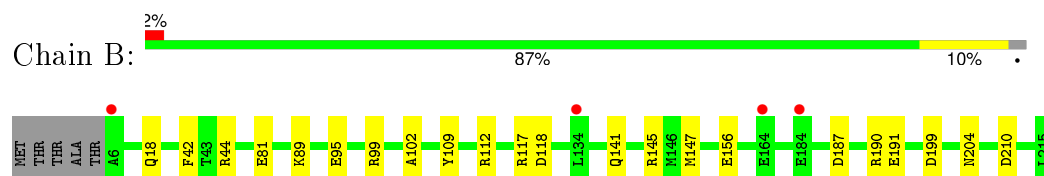
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

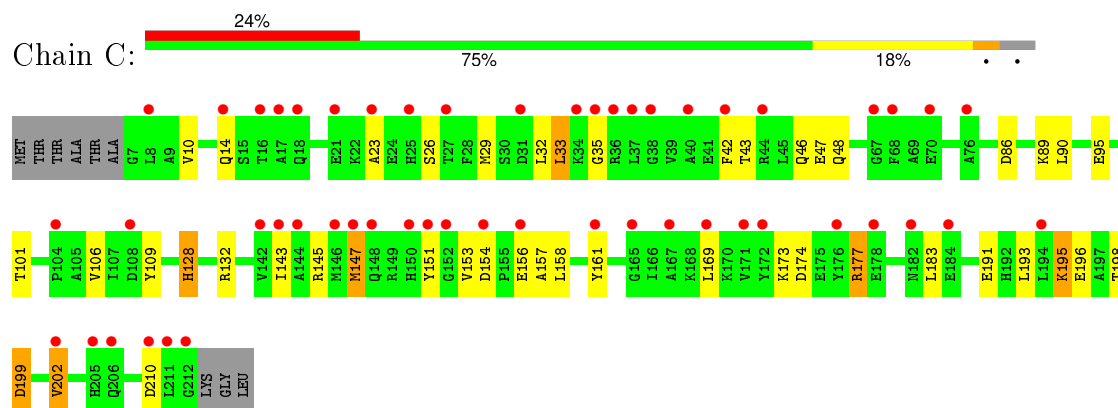
• Molecule 1: Heme oxygenase



• Molecule 1: Heme oxygenase



• Molecule 1: Heme oxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.06 Å 63.10 Å 107.16 Å 90.00° 101.03° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 23.84 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-1.70) 97.2 (23.84-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.71 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.196 , 0.233 0.208 , 0.242	Depositor DCC
R_{free} test set	7615 reflections (11.22%)	DCC
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 57.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 75503 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5538	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, IOD, SO4, NA

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	1.09	1/1692 (0.1%)	1.11	12/2285 (0.5%)
1	B	1.05	2/1707 (0.1%)	1.04	7/2303 (0.3%)
1	C	1.09	4/1667 (0.2%)	1.06	6/2254 (0.3%)
All	All	1.07	7/5066 (0.1%)	1.07	25/6842 (0.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	TYR	CD1-CE1	-6.46	1.29	1.39
1	C	128	HIS	C-O	-6.46	1.11	1.23
1	B	109	TYR	CD1-CE1	5.92	1.48	1.39
1	C	145	ARG	C-O	5.89	1.34	1.23
1	A	124	ALA	CA-CB	-5.80	1.40	1.52
1	B	102	ALA	CA-CB	-5.58	1.40	1.52
1	C	161	TYR	CE1-CZ	5.26	1.45	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	ASP	CB-CG-OD2	9.53	126.88	118.30
1	C	177	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	B	109	TYR	CB-CG-CD2	-7.95	116.23	121.00
1	A	86	ASP	CB-CG-OD2	7.51	125.06	118.30
1	A	79	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	44	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	109	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	C	210	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	31	ASP	CB-CG-OD1	6.28	123.96	118.30
1	A	109	TYR	CB-CG-CD1	6.16	124.70	121.00
1	C	86	ASP	CB-CG-OD2	6.09	123.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	154	ASP	CB-CG-OD2	6.06	123.75	118.30
1	B	118	ASP	CB-CG-OD1	5.92	123.62	118.30
1	C	199	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	210	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	190	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	97	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	97	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	199	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	112[A]	ARG	CG-CD-NE	5.28	122.88	111.80
1	A	112[B]	ARG	CG-CD-NE	5.28	122.88	111.80
1	B	117	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	C	177	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	109	TYR	CB-CG-CD1	5.04	124.02	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1653	0	1611	14	0
1	B	1668	0	1622	11	0
1	C	1635	0	1585	31	0
2	A	4	0	0	6	0
2	B	4	0	0	3	0
2	C	1	0	0	0	0
3	B	2	0	0	0	0
4	A	15	0	0	0	0
4	B	25	0	0	0	0
4	C	20	0	0	0	0
5	A	43	0	30	14	0
5	B	43	0	30	4	0
5	C	43	0	30	2	0
6	A	128	0	0	5	0
6	B	157	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	97	0	0	4	0
All	All	5538	0	4908	70	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 7.

All (70) 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)
2:A:1006:IOD:I	6:A:2132:HOH:O	2.23	1.23
5:B:902:HEM:HHD	5:B:902:HEM:HBC2	1.31	1.07
1:A:204:ASN:HD21	5:A:901:HEM:CBB	1.76	0.99
2:B:1002:IOD:I	6:B:4097:HOH:O	2.50	0.98
1:A:204:ASN:HD21	5:A:901:HEM:HBB1	1.26	0.97
5:A:901:HEM:HBD2	6:A:2126:HOH:O	1.66	0.94
2:A:1008:IOD:I	6:A:2127:HOH:O	2.57	0.92
1:A:204:ASN:ND2	5:A:901:HEM:CBB	2.38	0.85
1:A:204:ASN:ND2	5:A:901:HEM:HBB1	1.94	0.81
2:A:1007:IOD:I	5:A:901:HEM:HAB	2.52	0.80
5:B:902:HEM:CHD	5:B:902:HEM:HBC2	2.04	0.79
1:C:191:GLU:O	1:C:195:LYS:HD3	1.87	0.73
5:B:902:HEM:HHD	5:B:902:HEM:CBC	2.16	0.72
2:A:1006:IOD:I	2:A:1007:IOD:I	3.47	0.72
1:A:23:ALA:HB1	5:A:901:HEM:HBB2	1.72	0.72
1:A:23:ALA:HB1	5:A:901:HEM:CBB	2.20	0.72
2:A:1006:IOD:I	6:A:2083:HOH:O	2.81	0.69
1:C:199:ASP:O	1:C:202:VAL:HG13	1.93	0.67
1:C:128:HIS:HE1	1:C:196:GLU:OE2	1.77	0.67
2:A:1007:IOD:I	6:A:2032:HOH:O	2.84	0.65
1:B:99:ARG:HG2	1:B:99:ARG:O	1.97	0.64
1:B:190:ARG:NH1	6:B:4092:HOH:O	2.33	0.61
1:C:35:GLY:HA2	1:C:151:TYR:CZ	2.36	0.61
1:C:199:ASP:HA	1:C:202:VAL:CG1	2.32	0.60
1:C:32:LEU:HD21	1:C:147:MET:HE1	1.84	0.60
1:C:169:LEU:HG	1:C:173:LYS:HE2	1.85	0.59
5:A:901:HEM:HHA	5:A:901:HEM:CGD	2.34	0.58
1:C:154:ASP:OD2	1:C:156:GLU:HG2	2.03	0.58
1:A:138:SER:HB3	5:A:901:HEM:HAD1	1.85	0.58
1:C:32:LEU:HG	1:C:147:MET:HE3	1.86	0.57
1:C:89:LYS:HD2	1:C:156:GLU:O	2.04	0.57
1:B:99:ARG:NH2	6:B:4140:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ARG:NH1	6:C:2078:HOH:O	2.38	0.56
1:B:141:GLN:NE2	6:B:4119:HOH:O	2.40	0.55
1:C:95:GLU:HG2	6:C:2030:HOH:O	2.07	0.54
1:C:89:LYS:HD3	1:C:156:GLU:HG3	1.90	0.52
1:B:187:ASP:O	1:B:191:GLU:HG3	2.09	0.52
1:C:153:VAL:HG11	1:C:158:LEU:HD21	1.92	0.52
1:A:34:LYS:HG3	1:A:36:ARG:HG3	1.92	0.51
1:A:23:ALA:CB	5:A:901:HEM:HBB2	2.41	0.50
1:C:33:LEU:HD11	1:C:143:ILE:HD13	1.95	0.49
2:B:1002:IOD:I	5:B:902:HEM:HAB	2.84	0.48
1:C:95:GLU:CD	6:C:2069:HOH:O	2.52	0.48
1:B:81:GLU:HG3	6:B:4071:HOH:O	2.14	0.47
1:B:44:ARG:NH2	6:B:4124:HOH:O	2.46	0.47
1:C:193:LEU:HD23	1:C:193:LEU:O	2.15	0.47
1:C:35:GLY:HA2	1:C:151:TYR:OH	2.15	0.46
1:C:42:PHE:HB2	1:C:147:MET:HE2	1.98	0.46
1:C:23:ALA:HB1	5:C:903:HEM:CBB	2.47	0.45
1:C:42:PHE:HB2	1:C:147:MET:CE	2.46	0.45
1:C:193:LEU:C	1:C:193:LEU:HD23	2.37	0.44
1:C:33:LEU:HD11	5:C:903:HEM:HBC2	2.00	0.44
1:C:33:LEU:HD23	1:C:33:LEU:N	2.33	0.43
1:A:138:SER:OG	1:A:173:LYS:HE3	2.18	0.43
1:B:42:PHE:CG	1:B:147:MET:HE2	2.52	0.43
1:C:199:ASP:HA	1:C:202:VAL:HG12	1.99	0.43
1:C:90:LEU:HG	1:C:157:ALA:HB1	1.99	0.43
1:C:48:GLN:OE1	1:C:106:VAL:HG21	2.19	0.43
1:B:145:ARG:HD2	2:B:1005:IOD:I	2.89	0.43
1:C:183:LEU:O	6:C:2057:HOH:O	2.21	0.42
1:B:89:LYS:HD2	1:B:156:GLU:O	2.19	0.42
1:C:43:THR:O	1:C:47:GLU:HG3	2.19	0.42
1:A:29:MET:HA	1:A:29:MET:HE2	2.01	0.42
1:C:46:GLN:HA	1:C:46:GLN:OE1	2.20	0.41
5:A:901:HEM:HA	5:A:901:HEM:O1D	2.20	0.41
1:A:208:PHE:CE2	5:A:901:HEM:HBB1	2.56	0.41
1:B:81:GLU:OE1	6:B:4057:HOH:O	2.22	0.41
1:C:10:VAL:O	1:C:14:GLN:HG3	2.20	0.41
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.92	0.41
1:A:13:LYS:HE3	5:A:901:HEM:O2D	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	34	15
1	B	209/215 (97%)	205 (98%)	4 (2%)	0	100	100
1	C	204/215 (95%)	201 (98%)	3 (2%)	0	100	100
All	All	620/645 (96%)	607 (98%)	12 (2%)	1 (0%)	52	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	PHE

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	169/175 (97%)	167 (99%)	2 (1%)	78	65
1	B	170/175 (97%)	167 (98%)	3 (2%)	66	49
1	C	167/175 (95%)	158 (95%)	9 (5%)	27	9
All	All	506/525 (96%)	492 (97%)	14 (3%)	51	29

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	A	191	GLU

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Mol	Chain	Res	Type
1	B	18	GLN
1	B	95	GLU
1	B	204	ASN
1	C	26	SER
1	C	29	MET
1	C	33	LEU
1	C	101	THR
1	C	132	ARG
1	C	147	MET
1	C	195	LYS
1	C	198	THR
1	C	202	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	78	ASN
1	A	182	ASN
1	A	204	ASN
1	B	78	ASN
1	B	150	HIS
1	B	162	HIS
1	B	182	ASN
1	C	25	HIS
1	C	78	ASN
1	C	128	HIS
1	C	150	HIS
1	C	162	HIS
1	C	205	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 11 are monoatomic - leaving 15 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	SO4	A	2007	-	4,4,4	0.21	0	6,6,6	0.29	0
4	SO4	A	2009	-	4,4,4	0.25	0	6,6,6	0.42	0
4	SO4	A	2011	-	4,4,4	0.33	0	6,6,6	0.37	0
5	HEM	A	901	1,6	30,50,50	2.68	4 (13%)	24,82,82	3.55	10 (41%)
4	SO4	B	2003	-	4,4,4	0.32	0	6,6,6	0.95	1 (16%)
4	SO4	B	2004	-	4,4,4	0.41	0	6,6,6	0.44	0
4	SO4	B	2005	-	4,4,4	0.14	0	6,6,6	0.51	0
4	SO4	B	2006	-	4,4,4	0.16	0	6,6,6	0.46	0
4	SO4	B	2008	-	4,4,4	0.17	0	6,6,6	0.18	0
5	HEM	B	902	1,6	30,50,50	2.20	6 (20%)	24,82,82	2.89	10 (41%)
4	SO4	C	2001	-	4,4,4	0.24	0	6,6,6	0.82	0
4	SO4	C	2002	-	4,4,4	0.39	0	6,6,6	0.93	1 (16%)
4	SO4	C	2010	-	4,4,4	0.65	0	6,6,6	0.52	0
4	SO4	C	2012	-	4,4,4	0.09	0	6,6,6	0.09	0
5	HEM	C	903	1,6	30,50,50	1.92	8 (26%)	24,82,82	2.53	8 (33%)

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	SO4	A	2007	-	-	0/0/0/0	0/0/0/0
4	SO4	A	2009	-	-	0/0/0/0	0/0/0/0
4	SO4	A	2011	-	-	0/0/0/0	0/0/0/0
5	HEM	A	901	1,6	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	B	2003	-	-	0/0/0/0	0/0/0/0
4	SO4	B	2004	-	-	0/0/0/0	0/0/0/0
4	SO4	B	2005	-	-	0/0/0/0	0/0/0/0
4	SO4	B	2006	-	-	0/0/0/0	0/0/0/0
4	SO4	B	2008	-	-	0/0/0/0	0/0/0/0
5	HEM	B	902	1,6	-	0/10/54/54	0/0/8/8
4	SO4	C	2001	-	-	0/0/0/0	0/0/0/0
4	SO4	C	2002	-	-	0/0/0/0	0/0/0/0
4	SO4	C	2010	-	-	0/0/0/0	0/0/0/0
4	SO4	C	2012	-	-	0/0/0/0	0/0/0/0
5	HEM	C	903	1,6	-	0/10/54/54	0/0/8/8

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	HEM	C3B-C4B	-11.41	1.41	1.51
5	B	902	HEM	C3B-C4B	-6.96	1.45	1.51
5	A	901	HEM	C3D-C4D	-6.18	1.43	1.51
5	C	903	HEM	C3B-C4B	-5.64	1.46	1.51
5	B	902	HEM	C3D-C4D	-4.84	1.45	1.51
5	B	902	HEM	C2C-C1C	-4.45	1.44	1.52
5	C	903	HEM	C3D-C4D	-4.19	1.46	1.51
5	A	901	HEM	C2C-C1C	-3.76	1.45	1.52
5	B	902	HEM	C2D-C1D	-3.33	1.40	1.51
5	C	903	HEM	C2C-C1C	-3.18	1.46	1.52
5	A	901	HEM	C2D-C1D	-3.04	1.41	1.51
5	C	903	HEM	C2B-C1B	-2.32	1.44	1.51
5	C	903	HEM	CMB-C2B	2.13	1.58	1.53
5	C	903	HEM	C4C-NC	2.27	1.38	1.36
5	C	903	HEM	FE-NC	2.42	2.05	1.95
5	C	903	HEM	C3C-CAC	2.43	1.55	1.51
5	B	902	HEM	CAA-C2A	2.47	1.56	1.52
5	B	902	HEM	C1C-NC	3.55	1.40	1.36

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	HEM	C3B-CAB-CBB	-9.82	109.39	124.46
5	B	902	HEM	C3C-CAC-CBC	-4.61	117.38	124.46
5	B	902	HEM	CAA-CBA-CGA	-4.59	104.34	112.75
5	C	903	HEM	CAA-CBA-CGA	-4.46	104.56	112.75
5	B	902	HEM	C3B-CAB-CBB	-4.17	118.06	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	HEM	CAA-CBA-CGA	-4.15	105.15	112.75
5	B	902	HEM	CBD-CAD-C3D	-3.69	102.81	113.55
5	A	901	HEM	C3B-C4B-NB	-3.52	104.90	111.63
5	A	901	HEM	C3C-CAC-CBC	-3.31	119.38	124.46
5	B	902	HEM	CMA-C3A-C4A	-3.31	122.88	128.36
5	C	903	HEM	CMA-C3A-C4A	-2.80	123.72	128.36
5	A	901	HEM	CMA-C3A-C4A	-2.68	123.94	128.36
4	C	2002	SO4	O4-S-O3	2.10	117.52	108.98
4	B	2003	SO4	O2-S-O1	2.26	116.66	109.50
5	C	903	HEM	CMD-C2D-C3D	2.87	127.05	114.35
5	B	902	HEM	CMD-C2D-C3D	3.42	129.46	114.35
5	C	903	HEM	CMB-C2B-C3B	3.79	125.99	116.53
5	C	903	HEM	C3B-C4B-CHC	3.97	128.76	123.16
5	C	903	HEM	CAD-C3D-C4D	4.11	126.95	112.47
5	B	902	HEM	CMB-C2B-C3B	4.18	126.96	116.53
5	C	903	HEM	CMC-C2C-C3C	4.28	127.22	116.53
5	A	901	HEM	CAD-C3D-C4D	4.29	127.61	112.47
5	A	901	HEM	C3B-C4B-CHC	4.33	129.27	123.16
5	B	902	HEM	CMC-C2C-C3C	4.47	127.69	116.53
5	A	901	HEM	CMC-C2C-C3C	4.49	127.73	116.53
5	B	902	HEM	CAD-C3D-C4D	4.67	128.94	112.47
5	B	902	HEM	CAD-C3D-C2D	4.95	127.44	113.22
5	A	901	HEM	CAD-C3D-C2D	5.67	129.53	113.22
5	C	903	HEM	CAD-C3D-C2D	6.10	130.77	113.22
5	A	901	HEM	CMB-C2B-C3B	6.69	133.24	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	HEM	14	0
5	B	902	HEM	4	0
5	C	903	HEM	2	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	208/215 (96%)	0.37	15 (7%) 18 20	17, 27, 45, 51	0
1	B	210/215 (97%)	0.28	4 (1%) 70 74	16, 26, 38, 43	0
1	C	206/215 (95%)	1.43	52 (25%) 1 1	19, 40, 61, 78	0
All	All	624/645 (96%)	0.69	71 (11%) 7 7	16, 29, 53, 78	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	6.5
1	C	212	GLY	6.4
1	C	36	ARG	6.2
1	C	206	GLN	5.3
1	C	150	HIS	5.2
1	B	6	ALA	5.1
1	C	35	GLY	5.0
1	C	152	GLY	4.9
1	C	27	THR	4.4
1	C	21	GLU	4.3
1	C	151	TYR	4.2
1	C	210	ASP	4.0
1	C	143	ILE	4.0
1	A	101	THR	3.9
1	C	17	ALA	3.9
1	C	34	LYS	3.9
1	C	202	VAL	3.8
1	C	38	GLY	3.8
1	C	184	GLU	3.7
1	C	147	MET	3.6
1	C	37	LEU	3.5
1	C	18	GLN	3.5
1	C	25	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	14	GLN	3.3
1	C	165	GLY	3.3
1	A	213	LYS	3.2
1	A	92	GLY	3.2
1	C	154	ASP	3.2
1	B	184	GLU	3.1
1	A	99	ARG	3.1
1	C	16	THR	3.1
1	A	94	SER	3.1
1	A	187	ASP	3.0
1	C	194	LEU	3.0
1	A	93	SER	2.9
1	C	148	GLN	2.8
1	C	31	ASP	2.8
1	C	67	GLY	2.8
1	C	178	GLU	2.7
1	C	23	ALA	2.7
1	C	156	GLU	2.7
1	C	182	ASN	2.7
1	C	104	PRO	2.7
1	C	205	HIS	2.7
1	C	169	LEU	2.6
1	C	146	MET	2.6
1	A	95	GLU	2.6
1	C	8	LEU	2.5
1	A	98	SER	2.5
1	C	211	LEU	2.5
1	C	176	TYR	2.5
1	C	40	ALA	2.5
1	C	108	ASP	2.5
1	C	167	ALA	2.5
1	A	25	HIS	2.4
1	A	45	LEU	2.4
1	A	208	PHE	2.3
1	C	42	PHE	2.3
1	A	188	GLU	2.2
1	C	76	ALA	2.2
1	C	172	TYR	2.2
1	C	70	GLU	2.2
1	C	142	VAL	2.2
1	B	164	GLU	2.1
1	B	134	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	144	ALA	2.1
1	C	161	TYR	2.1
1	C	44	ARG	2.1
1	C	171	VAL	2.0
1	C	68	PHE	2.0
1	A	18	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	B	2003	5/5	0.82	0.29	5.49	63,64,66,67	0
4	SO4	A	2007	5/5	0.88	0.27	2.05	79,79,80,81	0
4	SO4	B	2006	5/5	0.80	0.25	1.94	80,80,81,82	0
4	SO4	C	2010	5/5	0.92	0.32	1.49	40,49,54,54	0
4	SO4	C	2002	5/5	0.83	0.20	0.87	62,62,64,64	0
5	HEM	A	901	43/43	0.96	0.12	0.51	18,28,46,56	0
5	HEM	C	903	43/43	0.89	0.15	0.05	31,38,52,61	0
5	HEM	B	902	43/43	0.96	0.11	-0.02	18,26,41,54	0
2	IOD	A	1006	1/1	0.96	0.13	-0.14	77,77,77,77	0
2	IOD	C	1001	1/1	0.93	0.07	-1.33	41,41,41,41	0
2	IOD	B	1005	1/1	0.96	0.06	-1.73	44,44,44,44	0
2	IOD	B	1004	1/1	0.96	0.07	-2.36	74,74,74,74	0
2	IOD	A	1008	1/1	0.98	0.06	-4.13	56,56,56,56	0
4	SO4	B	2005	5/5	0.87	0.22	-	62,67,68,69	0
4	SO4	B	2008	5/5	0.77	0.25	-	95,95,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	IOD	B	1002	1/1	0.99	0.11	-	45,45,45,45	0
4	SO4	B	2004	5/5	0.95	0.26	-	40,43,45,47	0
4	SO4	A	2011	5/5	0.95	0.13	-	51,55,56,58	0
3	NA	B	4002	1/1	0.75	0.26	-	57,57,57,57	0
2	IOD	A	1009	1/1	0.99	0.17	-	49,49,49,49	0
2	IOD	B	1003	1/1	0.98	0.15	-	64,64,64,64	0
3	NA	B	4001	1/1	0.89	0.15	-	50,50,50,50	0
4	SO4	C	2001	5/5	0.97	0.29	-	53,55,57,57	0
4	SO4	C	2012	5/5	0.90	0.39	-	76,76,77,77	0
2	IOD	A	1007	1/1	0.97	0.12	-	54,54,54,54	0
4	SO4	A	2009	5/5	0.85	0.30	-	62,64,68,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.