



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:56 pm GMT

PDB ID : 4M05
Title : Crystal Structure of Mutant Chlorite Dismutase from Candidatus Nitrospira defluvii R173E
Authors : Gysel, K.; Hagmueller, A.; Djinovic-Carugo, K.
Deposited on : 2013-08-01
Resolution : 2.28 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

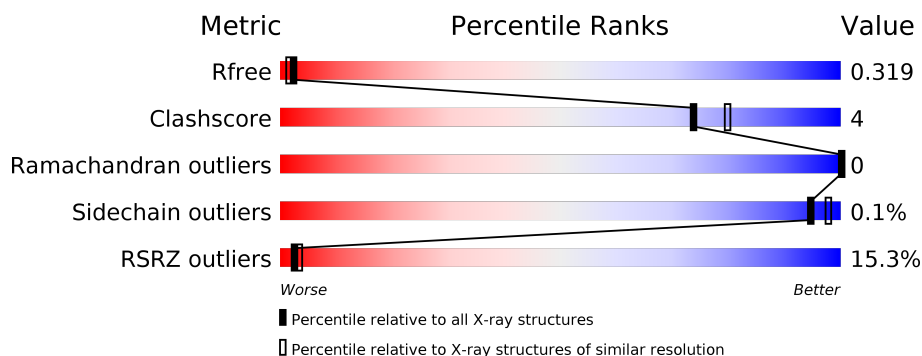
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	100719	5609 (2.30-2.26)
Clashscore	112137	6364 (2.30-2.26)
Ramachandran outliers	110173	6281 (2.30-2.26)
Sidechain outliers	110143	6281 (2.30-2.26)
RSRZ outliers	101464	5639 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	241	<div> <div>17%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div></div> </div> </div>
1	B	241	<div> <div>15%</div> <div> <div></div> <div>91%</div> <div>9%</div> <div></div> </div> </div>
1	C	241	<div> <div>13%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div></div> </div> </div>
1	D	241	<div> <div>17%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div></div> </div> </div>
1	E	241	<div> <div>14%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div></div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9948 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 Chlorite dismutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1917	1222	332	357	6			
1	B	240	Total	C	N	O	S	0	0	0
			1930	1230	334	359	7			
1	C	237	Total	C	N	O	S	0	0	0
			1912	1219	331	356	6			
1	D	238	Total	C	N	O	S	0	0	0
			1917	1222	332	357	6			
1	E	237	Total	C	N	O	S	0	0	0
			1912	1219	331	356	6			

There are 20 discrepancies between the modelled and reference sequences:

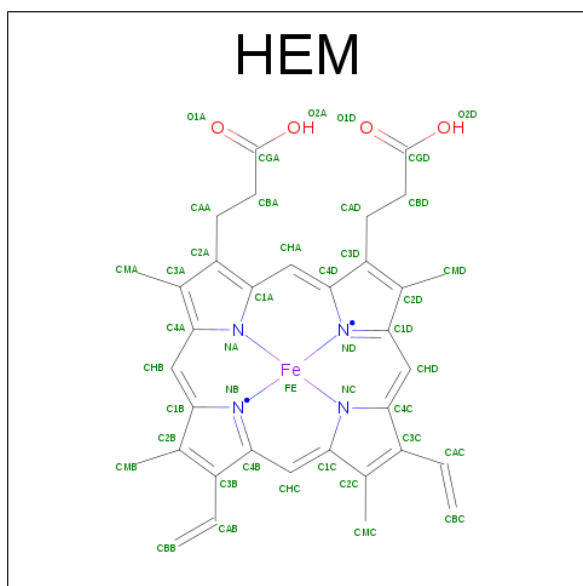
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP B3U4H7
A	-1	ALA	-	EXPRESSION TAG	UNP B3U4H7
A	0	MET	-	EXPRESSION TAG	UNP B3U4H7
A	173	GLU	ARG	ENGINEERED MUTATION	UNP B3U4H7
B	-2	GLY	-	EXPRESSION TAG	UNP B3U4H7
B	-1	ALA	-	EXPRESSION TAG	UNP B3U4H7
B	0	MET	-	EXPRESSION TAG	UNP B3U4H7
B	173	GLU	ARG	ENGINEERED MUTATION	UNP B3U4H7
C	-2	GLY	-	EXPRESSION TAG	UNP B3U4H7
C	-1	ALA	-	EXPRESSION TAG	UNP B3U4H7
C	0	MET	-	EXPRESSION TAG	UNP B3U4H7
C	173	GLU	ARG	ENGINEERED MUTATION	UNP B3U4H7
D	-2	GLY	-	EXPRESSION TAG	UNP B3U4H7
D	-1	ALA	-	EXPRESSION TAG	UNP B3U4H7
D	0	MET	-	EXPRESSION TAG	UNP B3U4H7
D	173	GLU	ARG	ENGINEERED MUTATION	UNP B3U4H7
E	-2	GLY	-	EXPRESSION TAG	UNP B3U4H7
E	-1	ALA	-	EXPRESSION TAG	UNP B3U4H7
E	0	MET	-	EXPRESSION TAG	UNP B3U4H7

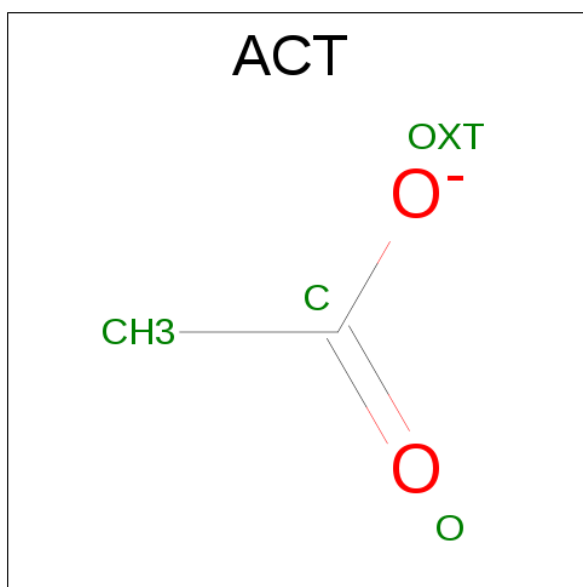
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Chain	Residue	Modelled	Actual	Comment	Reference
E	173	GLU	ARG	ENGINEERED MUTATION	UNP B3U4H7

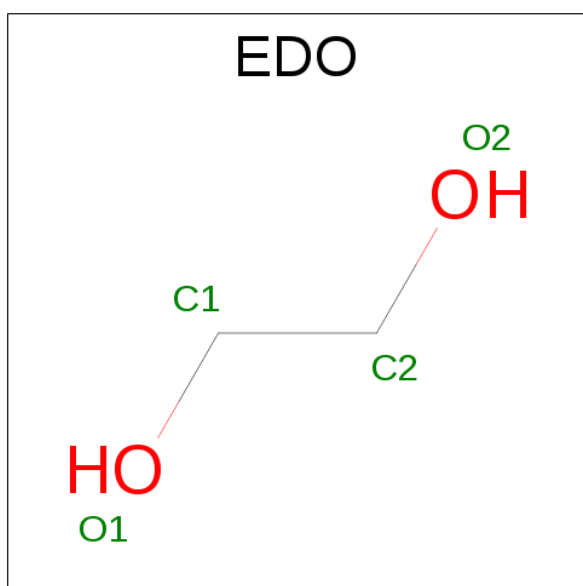
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		

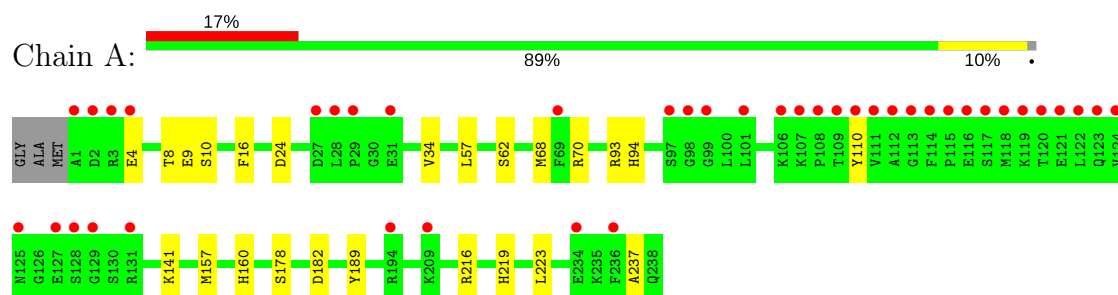
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total 32	O 32	0	0
5	B	25	Total 25	O 25	0	0
5	C	27	Total 27	O 27	0	0
5	D	25	Total 25	O 25	0	0
5	E	24	Total 24	O 24	0	0

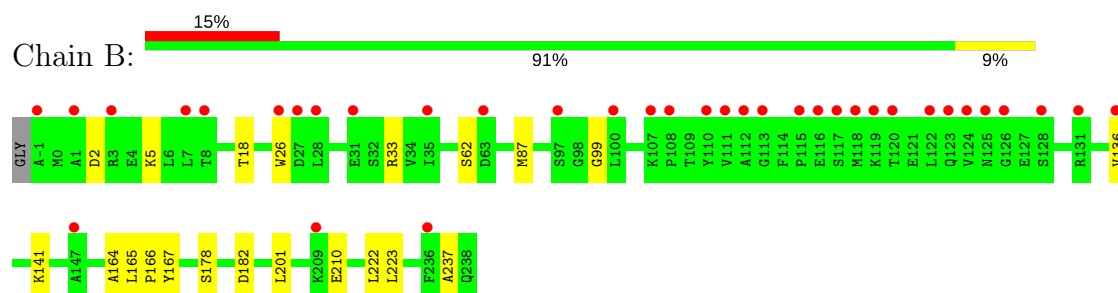
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

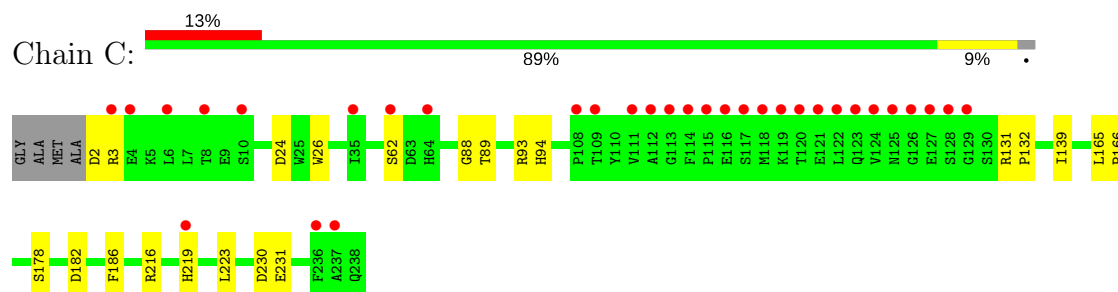
● Molecule 1: Chlorite dismutase



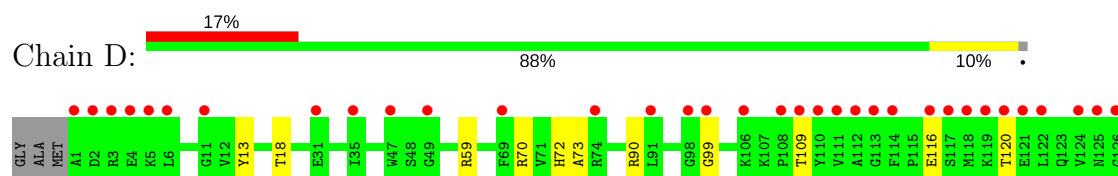
● Molecule 1: Chlorite dismutase

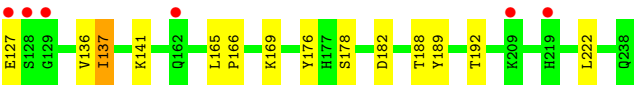


● Molecule 1: Chlorite dismutase

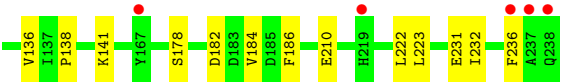
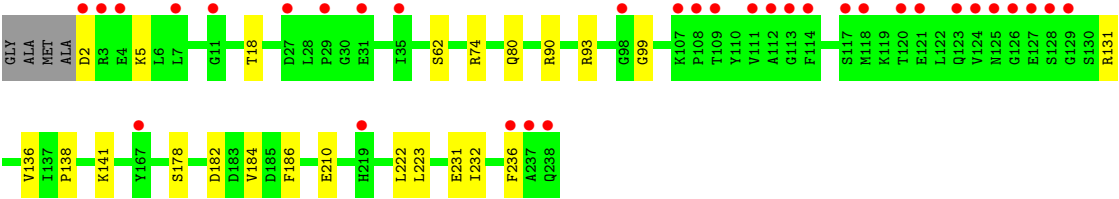
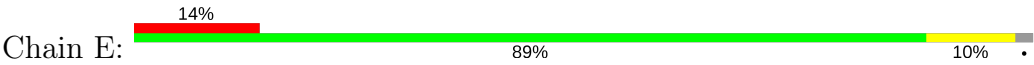


● Molecule 1: Chlorite dismutase





● Molecule 1: Chlorite dismutase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.47Å 112.39Å 119.25Å 90.00° 117.84° 90.00°	Depositor
Resolution (Å)	44.22 – 2.28 44.22 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.22-2.28) 99.6 (44.22-2.28)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.268 , 0.320 0.266 , 0.319	Depositor DCC
R_{free} test set	7110 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9948	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, EDO, ACT

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	0.41	0/1963	0.56	0/2655
1	B	0.44	0/1976	0.59	0/2672
1	C	0.43	0/1958	0.62	0/2648
1	D	0.42	0/1963	0.59	0/2655
1	E	0.40	0/1958	0.57	0/2648
All	All	0.42	0/9818	0.59	0/13278

There are no bond length outliers.

There are no bond angle outliers.

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	1917	0	1886	14	0
1	B	1930	0	1900	12	0
1	C	1912	0	1878	16	0
1	D	1917	0	1886	16	0
1	E	1912	0	1878	13	0
2	A	43	0	30	5	0
2	B	43	0	30	2	0
2	C	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	43	0	30	3	0
2	E	43	0	30	1	0
3	B	4	0	3	0	0
3	D	4	0	3	0	0
4	C	4	0	6	0	0
5	A	32	0	0	0	0
5	B	25	0	0	0	0
5	C	27	0	0	0	0
5	D	25	0	0	1	0
5	E	24	0	0	0	0
All	All	9948	0	9590	74	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 4.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ARG:NH2	1:C:219:HIS:O	2.23	0.71
1:C:131:ARG:NH1	1:C:231:GLU:OE1	2.26	0.69
2:D:301:HEM:HHC	2:D:301:HEM:HBB2	1.76	0.68
2:A:301:HEM:HBB2	2:A:301:HEM:HHC	1.76	0.67
1:E:131:ARG:NH2	1:E:231:GLU:OE2	2.28	0.66
1:A:216:ARG:NH1	1:A:219:HIS:O	2.29	0.65
2:B:301:HEM:HHC	2:B:301:HEM:HBB2	1.81	0.63
1:E:62:SER:OG	1:E:223:LEU:O	2.16	0.62
1:E:141:LYS:NZ	1:E:210:GLU:OE2	2.34	0.61
1:D:178:SER:OG	1:D:182:ASP:OD1	2.19	0.60
1:B:33:ARG:HD2	1:B:237:ALA:HA	1.84	0.60
1:C:88:GLY:O	1:C:93:ARG:NH2	2.35	0.60
1:D:166:PRO:O	1:D:169:LYS:HG2	2.02	0.59
1:B:62:SER:OG	1:B:223:LEU:O	2.19	0.59
1:C:62:SER:OG	1:C:223:LEU:O	2.21	0.59
1:C:178:SER:OG	1:C:182:ASP:OD1	2.21	0.58
1:B:18:THR:OG1	1:B:99:GLY:N	2.37	0.57
1:A:4:GLU:O	1:A:8:THR:OG1	2.11	0.57
1:C:230:ASP:OD1	1:C:231:GLU:N	2.39	0.56
1:D:70:ARG:NH1	1:D:189:TYR:CE2	2.75	0.55
1:B:141:LYS:NZ	1:B:210:GLU:OE2	2.40	0.55
1:E:18:THR:OG1	1:E:99:GLY:N	2.40	0.55
1:A:178:SER:OG	1:A:182:ASP:OD1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:HEM:CBA	2:A:301:HEM:HHA	2.39	0.52
1:E:186:PHE:CE1	2:E:301:HEM:HAD1	2.43	0.52
2:A:301:HEM:HBA1	2:A:301:HEM:HHA	1.93	0.50
1:B:178:SER:OG	1:B:182:ASP:OD1	2.28	0.50
1:D:127:GLU:OE2	1:D:192:THR:HA	2.12	0.49
1:A:62:SER:OG	1:A:223:LEU:O	2.31	0.49
1:D:109:THR:N	2:D:301:HEM:O1A	2.42	0.48
1:A:16:PHE:HD2	1:A:68:MET:HE3	1.78	0.48
2:C:301:HEM:HHA	2:C:301:HEM:HBA1	1.95	0.48
1:E:90:ARG:HA	1:E:93:ARG:HE	1.77	0.48
1:A:160:HIS:CE1	2:A:301:HEM:NC	2.81	0.47
1:C:24:ASP:OD1	1:C:94:HIS:ND1	2.47	0.47
1:E:2:ASP:HB3	1:E:5:LYS:HB3	1.96	0.46
1:A:110:TYR:CD2	1:A:157:MET:HG3	2.50	0.46
1:D:18:THR:OG1	1:D:99:GLY:N	2.48	0.46
1:C:139:ILE:HD13	2:C:301:HEM:HMD2	1.97	0.46
1:A:93:ARG:HD3	1:C:26:TRP:HB3	1.98	0.45
1:A:24:ASP:OD1	1:A:94:HIS:ND1	2.49	0.45
1:A:57:LEU:O	1:E:80:GLN:NE2	2.50	0.45
1:E:2:ASP:OD2	1:E:74:ARG:NH2	2.48	0.45
1:B:167:TYR:CE2	1:B:201:LEU:HA	2.53	0.44
1:B:165:LEU:N	1:B:166:PRO:HD2	2.33	0.44
1:D:137:ILE:HB	1:D:188:THR:OG1	2.16	0.44
1:D:90:ARG:N	5:D:406:HOH:O	2.51	0.44
1:C:131:ARG:N	1:C:132:PRO:CD	2.81	0.44
1:D:165:LEU:N	1:D:166:PRO:HD2	2.32	0.44
1:D:116:GLU:O	1:D:120:THR:HG23	2.17	0.43
1:A:9:GLU:HG2	1:A:10:SER:N	2.33	0.43
2:B:301:HEM:HHA	2:B:301:HEM:HBA1	2.00	0.43
1:E:178:SER:OG	1:E:182:ASP:OD1	2.36	0.43
1:C:89:THR:O	1:C:93:ARG:HG3	2.19	0.43
1:A:34:VAL:HG12	1:A:237:ALA:HB1	2.01	0.42
1:D:70:ARG:NH1	1:D:189:TYR:CZ	2.88	0.42
1:E:232:ILE:HG22	1:E:236:PHE:CE2	2.54	0.42
1:E:136:VAL:HB	1:E:222:LEU:HB2	2.01	0.41
1:B:2:ASP:HA	1:B:5:LYS:HB2	2.01	0.41
1:E:138:PRO:HB2	1:E:184:VAL:HG11	2.02	0.41
1:D:136:VAL:HB	1:D:222:LEU:HB2	2.02	0.41
1:B:136:VAL:HB	1:B:222:LEU:HB2	2.02	0.41
1:C:2:ASP:OD2	1:C:3:ARG:N	2.53	0.41
1:B:26:TRP:HB3	1:C:93:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:TYR:N	1:D:73:ALA:O	2.54	0.41
1:D:72:HIS:CE1	1:D:176:TYR:HH	2.31	0.41
1:C:165:LEU:N	1:C:166:PRO:HD2	2.36	0.41
1:C:186:PHE:CE1	2:C:301:HEM:HAD1	2.56	0.41
1:D:141:LYS:HZ1	2:D:301:HEM:HBD2	1.86	0.41
1:B:164:ALA:C	1:B:166:PRO:HD2	2.41	0.41
1:A:70:ARG:NH1	1:A:189:TYR:CE2	2.90	0.40
1:C:131:ARG:N	1:C:132:PRO:HD3	2.36	0.40
1:A:141:LYS:NZ	2:A:301:HEM:HBD2	2.35	0.40
1:B:87:MET:HB3	1:D:59:ARG:NH2	2.37	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	236/241 (98%)	230 (98%)	6 (2%)	0	100	100
1	B	238/241 (99%)	228 (96%)	10 (4%)	0	100	100
1	C	235/241 (98%)	228 (97%)	7 (3%)	0	100	100
1	D	236/241 (98%)	231 (98%)	5 (2%)	0	100	100
1	E	235/241 (98%)	229 (97%)	6 (3%)	0	100	100
All	All	1180/1205 (98%)	1146 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	205/206 (100%)	205 (100%)	0	100	100
1	B	206/206 (100%)	206 (100%)	0	100	100
1	C	205/206 (100%)	205 (100%)	0	100	100
1	D	205/206 (100%)	204 (100%)	1 (0%)	91	95
1	E	205/206 (100%)	205 (100%)	0	100	100
All	All	1026/1030 (100%)	1025 (100%)	1 (0%)	94	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	137	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

8 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	$\# Z > 2$
2	HEM	A	301	1	28,50,50	2.16	7 (25%)	17,82,82	1.88	6 (35%)
2	HEM	B	301	1	28,50,50	2.17	7 (25%)	17,82,82	1.71	3 (17%)
3	ACT	B	302	-	1,3,3	1.31	0	0,3,3	0.00	-
2	HEM	C	301	1	28,50,50	2.11	6 (21%)	17,82,82	2.27	6 (35%)
4	EDO	C	302	-	3,3,3	0.53	0	2,2,2	0.11	0
2	HEM	D	301	1	28,50,50	2.19	6 (21%)	17,82,82	1.96	6 (35%)
3	ACT	D	302	-	1,3,3	1.27	0	0,3,3	0.00	-
2	HEM	E	301	1	28,50,50	2.19	8 (28%)	17,82,82	2.02	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	301	1	-	0/6/54/54	0/0/8/8
2	HEM	B	301	1	-	0/6/54/54	0/0/8/8
3	ACT	B	302	-	-	0/0/0/0	0/0/0/0
2	HEM	C	301	1	-	0/6/54/54	0/0/8/8
4	EDO	C	302	-	-	0/1/1/1	0/0/0/0
2	HEM	D	301	1	-	0/6/54/54	0/0/8/8
3	ACT	D	302	-	-	0/0/0/0	0/0/0/0
2	HEM	E	301	1	-	0/6/54/54	0/0/8/8

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	HEM	C3B-C2B	-4.88	1.33	1.40
2	D	301	HEM	C3B-C2B	-4.32	1.34	1.40
2	A	301	HEM	C3B-C2B	-4.29	1.34	1.40
2	C	301	HEM	C3B-C2B	-4.14	1.34	1.40
2	C	301	HEM	C3C-C2C	-3.99	1.35	1.40
2	B	301	HEM	C3C-C2C	-3.76	1.35	1.40
2	E	301	HEM	C3B-C2B	-3.73	1.35	1.40
2	D	301	HEM	C3C-C2C	-3.66	1.35	1.40
2	E	301	HEM	C3C-C2C	-3.64	1.35	1.40
2	A	301	HEM	C3C-C2C	-3.48	1.35	1.40
2	E	301	HEM	CAA-C2A	2.00	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	HEM	CMB-C2B	2.02	1.55	1.51
2	C	301	HEM	CAA-C2A	2.05	1.55	1.52
2	A	301	HEM	CMC-C2C	2.12	1.56	1.51
2	B	301	HEM	CMA-C3A	2.12	1.56	1.51
2	A	301	HEM	C4D-ND	2.17	1.39	1.36
2	D	301	HEM	C4D-ND	2.33	1.39	1.36
2	B	301	HEM	C4D-ND	2.51	1.39	1.36
2	E	301	HEM	C4D-ND	2.84	1.40	1.36
2	B	301	HEM	C3C-CAC	3.67	1.55	1.47
2	C	301	HEM	C3C-CAC	3.84	1.55	1.47
2	A	301	HEM	C3B-CAB	3.88	1.55	1.47
2	B	301	HEM	C3B-CAB	3.90	1.55	1.47
2	E	301	HEM	C3C-CAC	3.92	1.55	1.47
2	C	301	HEM	C3B-CAB	4.03	1.55	1.47
2	D	301	HEM	C3C-CAC	4.11	1.55	1.47
2	D	301	HEM	C3B-CAB	4.11	1.56	1.47
2	E	301	HEM	C3B-CAB	4.23	1.56	1.47
2	A	301	HEM	C3C-CAC	4.35	1.56	1.47
2	C	301	HEM	C3D-C2D	4.85	1.52	1.37
2	B	301	HEM	C3D-C2D	5.27	1.53	1.37
2	D	301	HEM	C3D-C2D	5.33	1.53	1.37
2	A	301	HEM	C3D-C2D	5.34	1.53	1.37
2	E	301	HEM	C3D-C2D	5.68	1.54	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	HEM	CBD-CAD-C3D	-4.75	103.40	112.47
2	D	301	HEM	CAA-CBA-CGA	-4.38	105.18	112.66
2	C	301	HEM	C1D-C2D-C3D	-3.66	104.45	107.00
2	E	301	HEM	C1D-C2D-C3D	-3.38	104.64	107.00
2	A	301	HEM	CBD-CAD-C3D	-3.05	106.65	112.47
2	D	301	HEM	C1D-C2D-C3D	-2.83	105.02	107.00
2	B	301	HEM	CAA-CBA-CGA	-2.82	107.84	112.66
2	C	301	HEM	CAA-CBA-CGA	-2.61	108.19	112.66
2	A	301	HEM	CAA-C2A-C3A	-2.53	121.77	129.00
2	D	301	HEM	CAD-CBD-CGD	-2.33	108.68	112.66
2	E	301	HEM	CAA-CBA-CGA	-2.31	108.70	112.66
2	C	301	HEM	CAA-C2A-C3A	-2.21	122.70	129.00
2	A	301	HEM	CMA-C3A-C4A	-2.20	125.08	128.46
2	D	301	HEM	CBD-CAD-C3D	-2.18	108.31	112.47
2	B	301	HEM	CAD-CBD-CGD	-2.08	109.11	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	HEM	CMB-C2B-C3B	2.01	128.62	124.89
2	A	301	HEM	CMB-C2B-C3B	2.03	128.67	124.89
2	A	301	HEM	C4A-C3A-C2A	2.70	108.87	107.00
2	D	301	HEM	CMC-C2C-C3C	3.40	131.20	124.89
2	A	301	HEM	CMC-C2C-C3C	3.76	131.87	124.89
2	C	301	HEM	CMB-C2B-C3B	3.78	131.90	124.89
2	E	301	HEM	CMB-C2B-C3B	3.89	132.12	124.89
2	C	301	HEM	CMC-C2C-C3C	3.91	132.15	124.89
2	E	301	HEM	CMC-C2C-C3C	3.95	132.22	124.89
2	B	301	HEM	CMC-C2C-C3C	4.39	133.05	124.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	HEM	5	0
2	B	301	HEM	2	0
2	C	301	HEM	3	0
2	D	301	HEM	3	0
2	E	301	HEM	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	238/241 (98%)	1.05	41 (17%)	2 2	44, 72, 131, 155	2 (0%)
1	B	240/241 (99%)	0.89	36 (15%)	3 3	39, 62, 118, 157	1 (0%)
1	C	237/241 (98%)	0.92	32 (13%)	3 5	38, 61, 118, 159	2 (0%)
1	D	238/241 (98%)	1.13	40 (16%)	2 2	39, 72, 132, 164	0
1	E	237/241 (98%)	0.95	33 (13%)	3 4	42, 67, 123, 162	1 (0%)
All	All	1190/1205 (98%)	0.99	182 (15%)	2 3	38, 67, 125, 164	6 (0%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	13.3
1	D	129	GLY	9.0
1	C	124	VAL	8.8
1	D	1	ALA	8.5
1	E	128	SER	8.5
1	A	129	GLY	8.2
1	C	127	GLU	7.7
1	D	6	LEU	7.6
1	A	111	VAL	7.5
1	B	3	ARG	7.5
1	D	111	VAL	7.4
1	B	120	THR	6.9
1	D	109	THR	6.8
1	A	110	TYR	6.8
1	E	124	VAL	6.7
1	B	125	ASN	6.5
1	C	128	SER	6.3
1	A	128	SER	6.2
1	A	120	THR	5.9
1	E	126	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	110	TYR	5.8
1	E	129	GLY	5.8
1	D	116	GLU	5.7
1	D	127	GLU	5.7
1	C	126	GLY	5.7
1	D	74	ARG	5.7
1	D	3	ARG	5.6
1	A	122	LEU	5.6
1	D	117	SER	5.5
1	E	4	GLU	5.5
1	D	128	SER	5.4
1	D	49	GLY	5.3
1	C	119	LYS	5.3
1	C	237	ALA	5.2
1	E	125	ASN	5.2
1	A	28	LEU	5.2
1	C	129	GLY	5.2
1	C	122	LEU	5.1
1	A	113	GLY	5.1
1	A	108	PRO	5.1
1	C	123	GLN	5.0
1	E	7	LEU	4.9
1	E	123	GLN	4.7
1	C	113	GLY	4.7
1	E	118	MET	4.6
1	E	98	GLY	4.6
1	E	121	GLU	4.5
1	D	120	THR	4.5
1	B	236	PHE	4.5
1	A	4	GLU	4.5
1	B	27	ASP	4.5
1	D	125	ASN	4.5
1	E	237	ALA	4.5
1	D	126	GLY	4.3
1	A	117	SER	4.2
1	D	4	GLU	4.2
1	D	47	TRP	4.2
1	D	31	GLU	4.2
1	E	236	PHE	4.1
1	A	112	ALA	4.1
1	E	35	ILE	4.1
1	A	3	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	27	ASP	4.1
1	D	124	VAL	4.1
1	D	2	ASP	4.0
1	C	108	PRO	3.9
1	E	3	ARG	3.9
1	C	125	ASN	3.9
1	B	107	LYS	3.8
1	A	236	PHE	3.8
1	A	116	GLU	3.8
1	D	118	MET	3.8
1	A	123	GLN	3.8
1	D	209	LYS	3.8
1	A	131	ARG	3.8
1	B	113	GLY	3.7
1	D	5	LYS	3.7
1	B	26	TRP	3.7
1	D	113	GLY	3.7
1	B	124	VAL	3.7
1	E	117	SER	3.6
1	C	4	GLU	3.6
1	C	112	ALA	3.5
1	E	120	THR	3.5
1	B	123	GLN	3.4
1	B	-1	ALA	3.4
1	D	112	ALA	3.4
1	C	111	VAL	3.4
1	A	106	LYS	3.4
1	D	11	GLY	3.4
1	B	108	PRO	3.4
1	B	35	ILE	3.4
1	A	124	VAL	3.3
1	B	111	VAL	3.3
1	D	119	LYS	3.3
1	E	112	ALA	3.3
1	B	116	GLU	3.3
1	B	7	LEU	3.3
1	E	108	PRO	3.2
1	E	11	GLY	3.2
1	E	113	GLY	3.2
1	A	29	PRO	3.2
1	A	98	GLY	3.2
1	D	114	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	125	ASN	3.1
1	C	6	LEU	3.0
1	B	117	SER	3.0
1	C	114	PHE	3.0
1	C	120	THR	3.0
1	B	126	GLY	2.9
1	C	117	SER	2.9
1	D	122	LEU	2.9
1	E	127	GLU	2.9
1	B	131	ARG	2.9
1	A	99	GLY	2.8
1	C	118	MET	2.7
1	A	109	THR	2.7
1	C	115	PRO	2.7
1	B	1	ALA	2.7
1	A	114	PHE	2.7
1	A	2	ASP	2.7
1	E	238	GLN	2.7
1	B	119	LYS	2.7
1	D	35	ILE	2.7
1	A	127	GLU	2.7
1	B	8	THR	2.7
1	A	97	SER	2.6
1	B	97	SER	2.6
1	A	121	GLU	2.6
1	C	116	GLU	2.6
1	A	118	MET	2.6
1	B	110	TYR	2.6
1	E	219	HIS	2.6
1	E	27	ASP	2.5
1	A	115	PRO	2.5
1	A	69	PHE	2.5
1	C	10	SER	2.5
1	B	122	LEU	2.5
1	A	31	GLU	2.4
1	B	31	GLU	2.4
1	E	31	GLU	2.4
1	B	112	ALA	2.4
1	E	111	VAL	2.4
1	D	106	LYS	2.4
1	B	100	LEU	2.4
1	B	118	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	121	GLU	2.4
1	E	114	PHE	2.4
1	D	162	GLN	2.3
1	B	63	ASP	2.3
1	D	99	GLY	2.3
1	D	98	GLY	2.3
1	C	121	GLU	2.3
1	C	236	PHE	2.3
1	C	3	ARG	2.3
1	B	147	ALA	2.3
1	C	219	HIS	2.3
1	A	107	LYS	2.3
1	C	109	THR	2.2
1	A	119	LYS	2.2
1	B	136	VAL	2.2
1	A	234	GLU	2.2
1	D	108	PRO	2.2
1	E	2	ASP	2.1
1	B	28	LEU	2.1
1	E	107	LYS	2.1
1	E	167	TYR	2.1
1	A	101	LEU	2.1
1	C	64	HIS	2.1
1	A	194	ARG	2.1
1	B	128	SER	2.1
1	C	62	SER	2.1
1	D	69	PHE	2.1
1	B	115	PRO	2.1
1	D	91	LEU	2.0
1	A	209	LYS	2.0
1	C	35	ILE	2.0
1	C	8	THR	2.0
1	E	29	PRO	2.0
1	B	209	LYS	2.0
1	D	219	HIS	2.0
1	E	109	THR	2.0

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

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
2	HEM	E	301	43/43	0.97	0.18	0.03	40,44,74,97	0
2	HEM	C	301	43/43	0.96	0.18	-0.23	37,43,68,84	0
2	HEM	B	301	43/43	0.97	0.17	-0.33	37,42,84,117	0
2	HEM	D	301	43/43	0.97	0.16	-0.37	40,57,97,109	0
2	HEM	A	301	43/43	0.97	0.17	-0.37	40,50,86,152	0
3	ACT	B	302	4/4	0.93	0.32	-	50,54,55,59	0
3	ACT	D	302	4/4	0.83	0.32	-	51,65,78,85	0
4	EDO	C	302	4/4	0.83	0.27	-	54,56,108,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.