Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:14 AM GMT

PDB ID	:	3HQ8
Title	:	CcpA from G. sulfurreducens S134P/V135K variant
Authors	:	Hoffmann, M.; Seidel, J.; Einsle, O.
Deposited on	:	2009-06-05
Resolution	:	2.40 Å(reported)

The following versions of software and data (see references (1)) 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
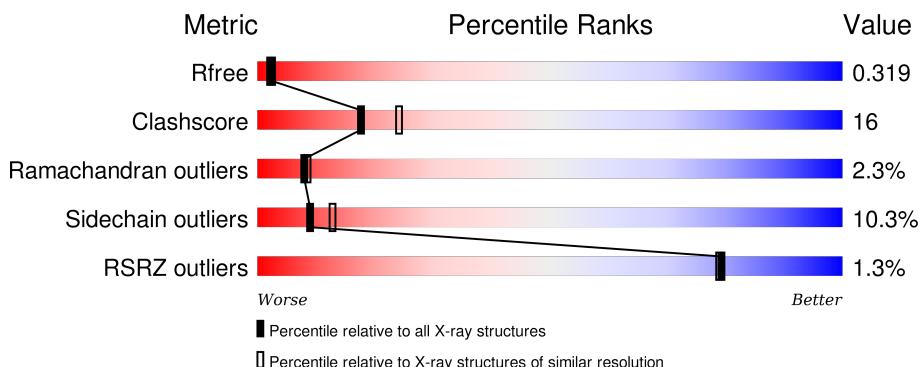
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
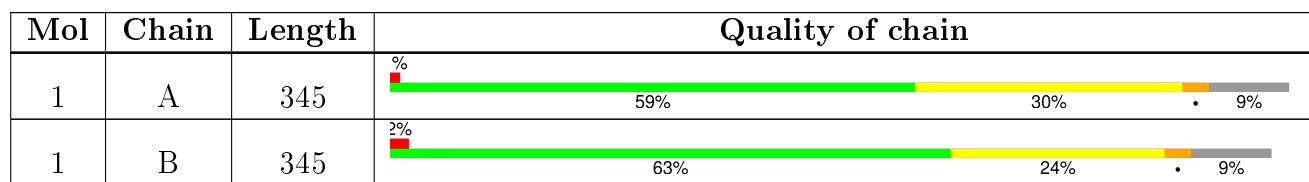
The reported resolution of this entry is 2.40 Å.

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	Percentile Ranks	Value
Rfree		0.319
Clashscore		16
Ramachandran outliers		2.3%
Sidechain outliers		10.3%
RSRZ outliers		1.3%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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.

Mol	Chain	Length	Quality of chain
1	A	345	% 59% 30% · 9%
1	B	345	2% 63% 24% · 9%

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
3	CA	B	402	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5094 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.
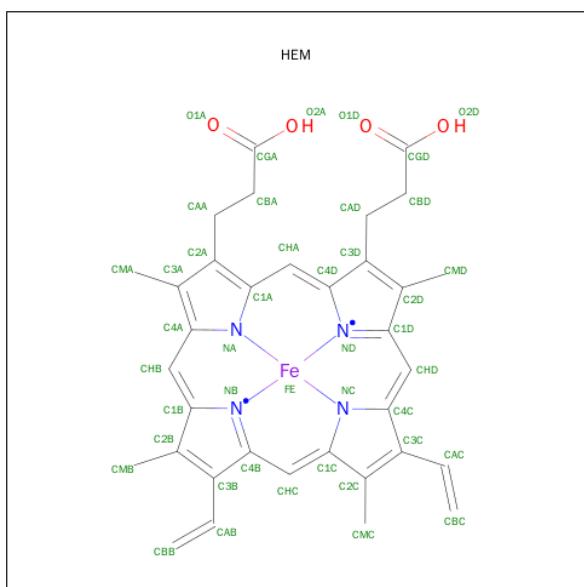
- Molecule 1 is a protein called Cytochrome c551 peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total 2385	C 1525	N 408	O 443	S 9	0	0	0
1	B	313	Total 2381	C 1521	N 408	O 443	S 9	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	PRO	SER	ENGINEERED	UNP Q749D0
A	135	LYS	VAL	ENGINEERED	UNP Q749D0
B	134	PRO	SER	ENGINEERED	UNP Q749D0
B	135	LYS	VAL	ENGINEERED	UNP Q749D0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
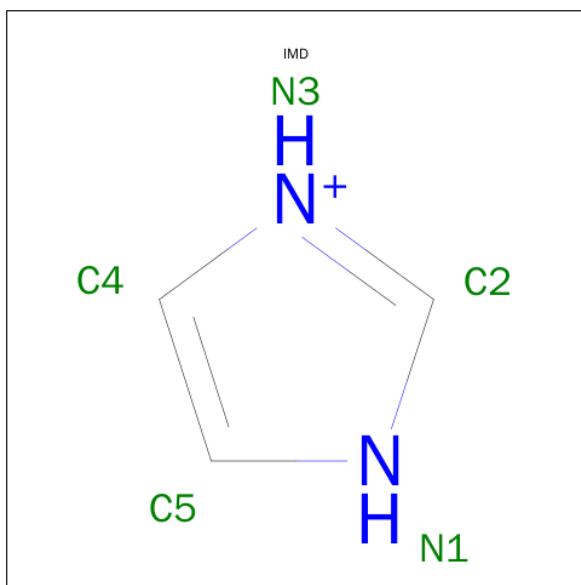
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		
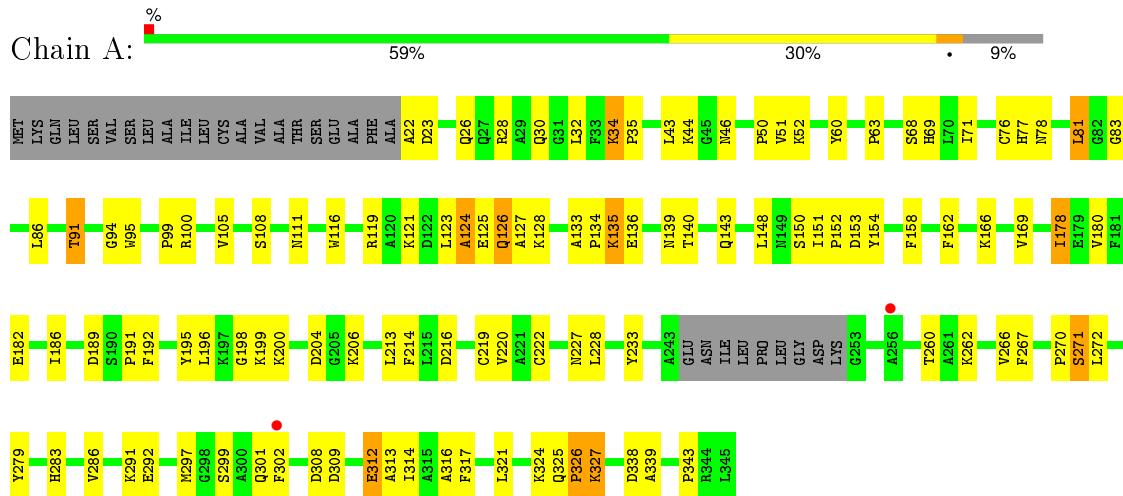
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total 70	O 70	0	0
5	B	74	Total 74	O 74	0	0
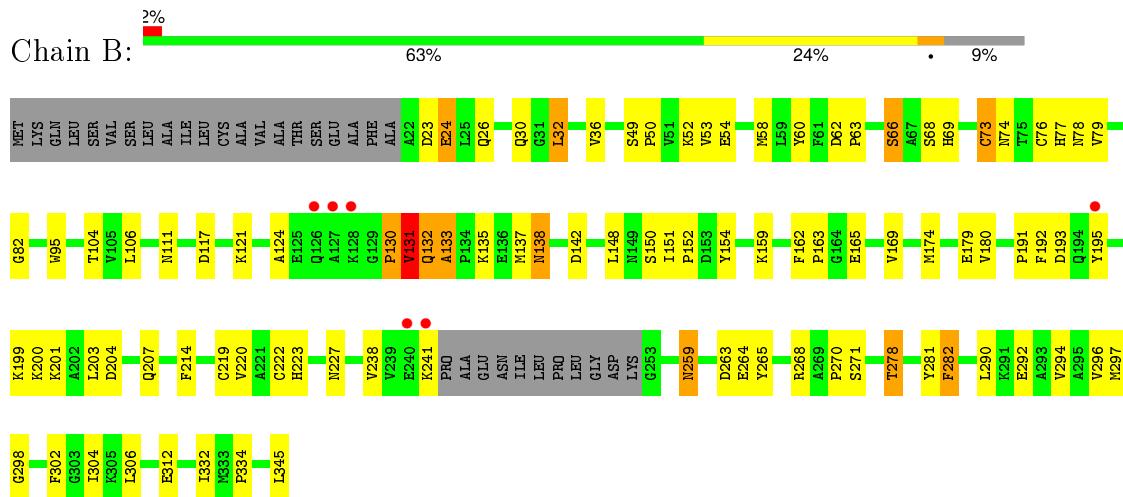
3 Residue-property plots (i)

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.

- Molecule 1: Cytochrome c551 peroxidase

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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.16Å 89.51Å 75.11Å 90.00° 107.57° 90.00°	Depositor
Resolution (Å)	44.77 – 2.40 44.23 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.77-2.40) 98.7 (44.23-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$<I/\sigma(I)>$ [1]	1.35 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.229 , 0.324 0.225 , 0.319	Depositor DCC
R_{free} test set	1370 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Outliers	0 of 27472 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5094	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.64	0/2444	0.75	1/3315 (0.0%)
1	B	0.60	0/2439	0.72	0/3307
All	All	0.62	0/4883	0.74	1/6622 (0.0%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	81	LEU	CA-CB-CG	5.87	128.81	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	GLN	Peptide
1	B	130	PRO	Peptide

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	2385	0	2388	89	0
1	B	2381	0	2382	71	0
2	A	86	0	60	22	0
2	B	86	0	60	23	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	4	0	0
4	B	5	0	4	0	0
5	A	70	0	0	3	0
5	B	74	0	0	0	0
All	All	5094	0	4898	157	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 16.

All (157) 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:219:CYS:SG	2:B:401:HEM:HAB	1.56	1.43
1:A:219:CYS:SG	2:A:401:HEM:HAB	1.63	1.37
1:A:76:CYS:SG	2:A:400:HEM:CAC	2.12	1.36
1:A:219:CYS:SG	2:A:401:HEM:CAB	2.22	1.28
1:A:219:CYS:HG	2:A:401:HEM:CAB	1.47	1.27
1:B:219:CYS:SG	2:B:401:HEM:CAB	2.23	1.25
1:B:76:CYS:SG	2:B:400:HEM:CBC	2.31	1.18
1:A:222:CYS:SG	2:A:401:HEM:CAC	2.32	1.16
1:A:76:CYS:SG	2:A:400:HEM:HAC	1.89	1.08
1:B:73:CYS:SG	2:B:400:HEM:CAB	2.42	1.06
1:B:76:CYS:SG	2:B:400:HEM:CAC	2.47	1.02
1:B:222:CYS:SG	2:B:401:HEM:CAC	2.47	1.01
1:B:222:CYS:HG	2:B:401:HEM:CAC	1.73	1.00
1:B:219:CYS:HG	2:B:401:HEM:CAB	1.70	1.00
1:A:134:PRO:O	1:A:135:LYS:HB2	1.58	0.99
1:A:222:CYS:SG	2:A:401:HEM:HAC	2.12	0.89
1:B:131:VAL:HA	1:B:132:GLN:HB2	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ALA:HB1	1:A:128:LYS:HA	1.56	0.86
1:B:73:CYS:SG	2:B:400:HEM:HAB	2.16	0.86
1:B:297:MET:HG2	2:B:401:HEM:C4B	2.17	0.79
1:A:76:CYS:SG	2:A:400:HEM:CBC	2.70	0.79
1:A:150:SER:HB2	1:A:339:ALA:O	1.85	0.76
1:B:298:GLY:HA3	1:B:306:LEU:HD12	1.68	0.74
1:A:76:CYS:HG	2:A:400:HEM:HAC	1.51	0.73
1:A:108:SER:HA	1:A:111:ASN:ND2	2.05	0.72
1:A:206:LYS:NZ	1:A:312:GLU:HG2	2.05	0.70
1:A:140:THR:H	1:A:143:GLN:NE2	1.89	0.69
1:B:117:ASP:HB2	1:B:265:TYR:HE2	1.59	0.66
1:A:297:MET:HE3	2:A:401:HEM:C4D	2.30	0.66
1:A:95:TRP:HB2	1:B:95:TRP:HB2	1.78	0.66
1:B:60:TYR:CE1	1:B:73:CYS:HB2	2.31	0.65
1:A:108:SER:HA	1:A:111:ASN:HD21	1.62	0.64
1:A:127:ALA:CB	1:A:128:LYS:HA	2.26	0.64
1:A:68:SER:O	1:A:69:HIS:HB2	1.98	0.64
1:B:222:CYS:SG	2:B:401:HEM:C3C	2.89	0.63
1:A:136:GLU:HB2	2:A:400:HEM:HBC2	1.80	0.63
1:A:313:ALA:O	1:A:316:ALA:HB3	1.99	0.62
1:A:63:PRO:O	1:A:69:HIS:HA	1.99	0.62
1:B:292:GLU:O	1:B:296:VAL:HG23	1.99	0.62
1:B:151:ILE:HG21	1:B:334:PRO:HG2	1.83	0.61
1:B:214:PHE:O	1:B:219:CYS:HB2	2.01	0.61
1:A:52:LYS:HE2	1:A:162:PHE:CE1	2.35	0.61
1:A:22:ALA:HB1	5:A:347:HOH:O	2.01	0.61
1:A:297:MET:HE3	2:A:401:HEM:CHA	2.31	0.60
1:A:76:CYS:SG	2:A:400:HEM:C3C	2.92	0.59
1:A:297:MET:CE	2:A:401:HEM:C4D	2.85	0.59
1:A:228:LEU:HD22	1:A:321:LEU:HD11	1.85	0.58
1:A:178:ILE:O	1:A:182:GLU:HG3	2.03	0.58
1:B:58:MET:O	1:B:62:ASP:HB2	2.02	0.58
1:A:105:VAL:O	1:A:105:VAL:HG22	2.03	0.58
1:A:206:LYS:HZ1	1:A:312:GLU:HG2	1.66	0.58
1:B:282:PHE:CD1	2:B:401:HEM:HBD1	2.39	0.57
1:A:52:LYS:HE2	1:A:162:PHE:CZ	2.40	0.57
1:B:53:VAL:HG22	1:B:180:VAL:HG12	1.86	0.57
1:B:290:LEU:HG	1:B:290:LEU:O	2.03	0.57
1:A:222:CYS:SG	2:A:401:HEM:CBC	2.91	0.57
1:A:60:TYR:OH	1:A:105:VAL:HG11	2.05	0.57
1:A:299:SER:HA	5:A:390:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:CYS:HB3	2:B:400:HEM:C3B	2.41	0.55
1:A:228:LEU:HD22	1:A:321:LEU:CD1	2.37	0.55
1:B:204:ASP:OD1	1:B:207:GLN:HG3	2.07	0.55
1:B:297:MET:HG2	2:B:401:HEM:C3B	2.42	0.54
1:A:69:HIS:CD2	1:A:343:PRO:HG3	2.43	0.54
1:A:28:ARG:O	1:A:32:LEU:HD12	2.07	0.54
1:A:297:MET:O	1:A:299:SER:N	2.41	0.53
1:A:126:GLN:HB3	1:A:127:ALA:CA	2.39	0.53
1:A:192:PHE:CD1	1:A:317:PHE:HE1	2.26	0.53
1:A:169:VAL:HG12	1:A:169:VAL:O	2.08	0.53
1:A:28:ARG:NH2	1:A:216:ASP:OD1	2.33	0.52
1:B:203:LEU:HB3	1:B:207:GLN:HB2	1.91	0.52
1:A:23:ASP:HB2	1:A:200:LYS:NZ	2.25	0.52
1:A:127:ALA:CB	1:A:128:LYS:CA	2.88	0.52
1:B:117:ASP:HB2	1:B:265:TYR:CE2	2.44	0.52
1:A:91:THR:HG21	1:B:345:LEU:HD22	1.91	0.52
1:B:238:VAL:HG21	1:B:282:PHE:CE1	2.45	0.52
1:A:139:ASN:OD1	1:A:143:GLN:NE2	2.43	0.52
1:A:134:PRO:O	1:A:135:LYS:CB	2.42	0.51
1:B:137:MET:HE3	2:B:400:HEM:HHC	1.92	0.51
1:A:297:MET:HG3	2:A:401:HEM:C4A	2.45	0.51
1:B:26:GLN:HE21	1:B:30:GLN:NE2	2.09	0.51
1:A:195:TYR:HA	1:A:199:LYS:O	2.10	0.51
1:B:26:GLN:HE21	1:B:30:GLN:HE22	1.59	0.50
1:B:282:PHE:HD1	2:B:401:HEM:HBD1	1.76	0.50
1:B:222:CYS:SG	2:B:401:HEM:HAC	2.46	0.50
1:A:126:GLN:HB3	1:A:127:ALA:HA	1.94	0.50
1:B:302:PHE:HB2	1:B:304:ILE:HG13	1.94	0.50
1:B:223:HIS:HE1	1:B:270:PRO:HD2	1.77	0.50
1:A:214:PHE:O	1:A:219:CYS:HB2	2.11	0.50
1:A:99:PRO:O	1:A:100:ARG:HD3	2.12	0.50
1:B:214:PHE:CE1	1:B:219:CYS:HB3	2.47	0.49
1:B:73:CYS:SG	2:B:400:HEM:C3B	3.03	0.49
1:A:46:ASN:ND2	1:A:180:VAL:HG23	2.28	0.49
1:A:325:GLN:HB2	1:B:332:ILE:HD13	1.94	0.49
1:B:82:GLY:HA2	1:B:106:LEU:HD11	1.95	0.49
1:A:222:CYS:SG	2:A:401:HEM:C3C	3.03	0.49
1:A:23:ASP:HB2	1:A:200:LYS:HZ3	1.78	0.48
1:A:204:ASP:C	1:A:204:ASP:OD1	2.51	0.48
1:B:270:PRO:HG2	2:B:401:HEM:HBA1	1.95	0.48
1:B:77:HIS:CD2	2:B:400:HEM:NB	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:SER:O	1:B:152:PRO:HD3	2.13	0.47
1:A:78:ASN:HB3	1:A:81:LEU:HB2	1.95	0.47
1:A:119:ARG:HE	1:A:121:LYS:HE3	1.79	0.47
1:B:60:TYR:CD1	1:B:73:CYS:HB2	2.50	0.47
1:A:270:PRO:HD3	2:A:401:HEM:C3D	2.50	0.47
1:B:76:CYS:SG	2:B:400:HEM:C3C	3.07	0.46
1:B:204:ASP:OD1	1:B:204:ASP:C	2.53	0.46
1:B:52:LYS:HE2	1:B:162:PHE:CE1	2.51	0.46
1:A:26:GLN:O	1:A:30:GLN:HG3	2.15	0.46
1:B:259[B]:ASN:ND2	1:B:259[B]:ASN:C	2.68	0.46
1:B:297:MET:HG2	2:B:401:HEM:NB	2.30	0.46
1:B:32:LEU:HG	1:B:220:VAL:HG21	1.98	0.46
1:A:116:TRP:CE3	1:A:283:HIS:HB3	2.51	0.46
1:A:297:MET:HG3	2:A:401:HEM:NA	2.32	0.45
1:B:74:ASN:OD1	1:B:78:ASN:HA	2.15	0.45
1:B:24:GLU:HG2	1:B:24:GLU:O	2.17	0.45
1:B:54:GLU:O	1:B:58:MET:HG3	2.17	0.45
1:B:192:PHE:O	1:B:195:TYR:HB3	2.17	0.45
1:A:123:LEU:HA	1:A:126:GLN:NE2	2.32	0.44
1:B:131:VAL:CA	1:B:132:GLN:HB2	2.36	0.44
1:A:260:THR:HG21	1:A:267:PHE:HE2	1.83	0.44
1:B:104:THR:HB	1:B:278:THR:HG21	2.00	0.44
1:B:238:VAL:HG21	1:B:282:PHE:CZ	2.53	0.44
1:A:227:ASN:HB3	1:A:271:SER:HB2	1.99	0.44
1:A:34:LYS:HD3	1:A:35:PRO:HD2	1.99	0.44
1:A:123:LEU:O	1:A:124:ALA:C	2.56	0.43
1:A:151:ILE:HA	1:A:152:PRO:HD2	1.81	0.43
1:A:327:LYS:HA	1:A:327:LYS:HD2	1.94	0.43
1:A:94:GLY:O	1:A:95:TRP:CB	2.67	0.42
1:B:259[B]:ASN:C	1:B:259[B]:ASN:HD22	2.22	0.42
1:B:63:PRO:O	1:B:66:SER:OG	2.37	0.42
1:A:63:PRO:HA	1:A:71:ILE:O	2.19	0.42
1:A:272:LEU:HA	1:A:272:LEU:HD23	1.66	0.42
1:B:132:GLN:HG3	1:B:133:ALA:N	2.34	0.42
1:A:192:PHE:CE1	1:A:317:PHE:HE1	2.36	0.42
1:B:111:ASN:OD1	1:B:227:ASN:ND2	2.34	0.42
1:A:213:LEU:HB3	1:A:314:ILE:HD11	2.02	0.42
1:B:138:ASN:O	1:B:138:ASN:ND2	2.43	0.42
1:A:272:LEU:HD11	2:A:401:HEM:CHB	2.50	0.42
1:A:220:VAL:HG22	1:A:220:VAL:O	2.20	0.42
1:B:49:SER:O	1:B:50:PRO:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:SER:O	1:A:343:PRO:HB3	2.20	0.41
1:A:233:TYR:HB3	1:A:266:VAL:HB	2.02	0.41
1:B:159:LYS:O	1:B:163:PRO:HA	2.20	0.41
1:A:270:PRO:HG2	2:A:401:HEM:CBA	2.51	0.41
1:B:76:CYS:SG	2:B:400:HEM:HBC2	2.47	0.41
1:B:281:TYR:O	1:B:282:PHE:HB2	2.21	0.41
1:A:297:MET:HB3	2:A:401:HEM:C4B	2.56	0.41
1:A:133:ALA:HB1	1:A:136:GLU:HG2	2.03	0.41
1:A:192:PHE:CE2	1:A:196:LEU:HD11	2.56	0.41
1:A:148:LEU:HD22	1:A:158:PHE:HE2	1.86	0.41
1:B:36:VAL:HG23	1:B:193:ASP:OD2	2.21	0.41
1:A:77:HIS:HA	1:A:83:GLY:O	2.20	0.41
1:A:325:GLN:HA	1:A:326:PRO:HD3	1.94	0.41
1:A:200:LYS:HE3	5:A:348:HOH:O	2.21	0.40
1:B:68:SER:O	1:B:69:HIS:HB2	2.21	0.40
1:B:290:LEU:O	1:B:294:VAL:HG23	2.21	0.40
1:B:263:ASP:O	1:B:264:GLU:HB2	2.22	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	311/345 (90%)	271 (87%)	34 (11%)	6 (2%)	10	12
1	B	310/345 (90%)	277 (89%)	25 (8%)	8 (3%)	7	6
All	All	621/690 (90%)	548 (88%)	59 (10%)	14 (2%)	8	8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ALA

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Mol	Chain	Res	Type
1	A	135	LYS
1	B	130	PRO
1	B	131	VAL
1	B	132	GLN
1	A	198	GLY
1	B	124	ALA
1	B	169	VAL
1	B	282	PHE
1	B	191	PRO
1	A	191	PRO
1	A	50	PRO
1	A	279	TYR
1	B	133	ALA

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	252/276 (91%)	225 (89%)	27 (11%)	8	11
1	B	252/276 (91%)	226 (90%)	26 (10%)	9	13
All	All	504/552 (91%)	451 (90%)	53 (10%)	9	12

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	43	LEU
1	A	44	LYS
1	A	51	VAL
1	A	86	LEU
1	A	91	THR
1	A	125	GLU
1	A	153	ASP
1	A	154	TYR
1	A	166	LYS

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Mol	Chain	Res	Type
1	A	178	ILE
1	A	186	ILE
1	A	189	ASP
1	A	262	LYS
1	A	271	SER
1	A	286	VAL
1	A	291	LYS
1	A	292	GLU
1	A	301	GLN
1	A	302	PHE
1	A	308	ASP
1	A	309	ASP
1	A	312	GLU
1	A	324	LYS
1	A	326	PRO
1	A	327	LYS
1	A	338	ASP
1	B	23	ASP
1	B	24	GLU
1	B	32	LEU
1	B	66	SER
1	B	73	CYS
1	B	79	VAL
1	B	121	LYS
1	B	131	VAL
1	B	135	LYS
1	B	138	ASN
1	B	142	ASP
1	B	148	LEU
1	B	154	TYR
1	B	165	GLU
1	B	174	MET
1	B	179	GLU
1	B	199	LYS
1	B	200	LYS
1	B	201	LYS
1	B	241	LYS
1	B	259[A]	ASN
1	B	259[B]	ASN
1	B	268	ARG
1	B	271	SER
1	B	278	THR

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Mol	Chain	Res	Type
1	B	312	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	107	ASN
1	A	139	ASN
1	A	143	GLN
1	A	301	GLN
1	B	26	GLN
1	B	107	ASN
1	B	173	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)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	IMD	A	346	2	3,5,5	0.38	0	4,5,5	0.50	0
2	HEM	A	400	1,4	30,50,50	2.26	11 (36%)	24,82,82	2.95	13 (54%)
2	HEM	A	401	1	30,50,50	1.85	9 (30%)	24,82,82	2.78	14 (58%)
4	IMD	B	346	2	3,5,5	0.50	0	4,5,5	0.62	0
2	HEM	B	400	1,4	30,50,50	2.31	7 (23%)	24,82,82	2.55	8 (33%)
2	HEM	B	401	1	30,50,50	2.36	8 (26%)	24,82,82	2.43	9 (37%)

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	IMD	A	346	2	-	0/0/0/0	0/1/1/1
2	HEM	A	400	1,4	-	0/10/54/54	0/0/8/8
2	HEM	A	401	1	-	0/10/54/54	0/0/8/8
4	IMD	B	346	2	-	0/0/0/0	0/1/1/1
2	HEM	B	400	1,4	-	0/10/54/54	0/0/8/8
2	HEM	B	401	1	-	0/10/54/54	0/0/8/8

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	HEM	C3B-C4B	-8.98	1.43	1.51
2	B	400	HEM	C3B-C4B	-7.78	1.44	1.51
2	A	400	HEM	C3B-C4B	-6.87	1.45	1.51
2	A	401	HEM	C3B-C4B	-5.35	1.47	1.51
2	B	400	HEM	C3D-C4D	-5.12	1.45	1.51
2	A	400	HEM	C3D-C4D	-5.00	1.45	1.51
2	A	400	HEM	C2C-C1C	-4.44	1.44	1.52
2	B	401	HEM	C3D-C4D	-4.37	1.46	1.51
2	B	400	HEM	C2C-C1C	-4.28	1.44	1.52
2	A	401	HEM	C3D-C4D	-3.67	1.46	1.51
2	B	401	HEM	C2C-C1C	-3.38	1.46	1.52
2	A	401	HEM	C2C-C1C	-3.00	1.46	1.52
2	A	401	HEM	C2D-C1D	-2.63	1.43	1.51
2	A	400	HEM	C2D-C1D	-2.41	1.44	1.51
2	A	401	HEM	C2B-C1B	-2.35	1.44	1.51
2	B	401	HEM	C2B-C1B	-2.30	1.44	1.51
2	A	400	HEM	C2B-C1B	-2.12	1.44	1.51
2	B	400	HEM	C2D-C1D	-2.12	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	HEM	CAA-C2A	2.05	1.55	1.52
2	B	401	HEM	CAA-C2A	2.17	1.55	1.52
2	A	401	HEM	C3B-CAB	2.19	1.55	1.51
2	A	401	HEM	CMA-C3A	2.22	1.56	1.51
2	B	401	HEM	C1C-NC	2.26	1.38	1.36
2	A	400	HEM	CMA-C3A	2.34	1.56	1.51
2	A	401	HEM	C1C-NC	2.36	1.38	1.36
2	B	400	HEM	FE-ND	2.44	2.10	1.97
2	A	400	HEM	C3B-CAB	2.45	1.55	1.51
2	A	401	HEM	C3C-CAC	2.50	1.56	1.51
2	A	400	HEM	FE-ND	2.55	2.11	1.97
2	A	400	HEM	C3C-CAC	2.69	1.56	1.51
2	B	401	HEM	C3C-CAC	2.71	1.56	1.51
2	B	400	HEM	C3C-CAC	2.77	1.56	1.51
2	A	400	HEM	C1C-NC	2.92	1.39	1.36
2	B	400	HEM	C3B-CAB	3.17	1.57	1.51
2	B	401	HEM	FE-ND	3.23	2.14	1.97

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	HEM	CAA-CBA-CGA	-5.73	102.25	112.75
2	A	401	HEM	CBD-CAD-C3D	-4.88	99.36	113.55
2	B	400	HEM	CAA-C2A-C1A	-4.78	121.82	127.01
2	A	400	HEM	C4B-CHC-C1C	-4.53	118.25	125.82
2	B	401	HEM	CBA-CAA-C2A	-3.89	105.55	112.53
2	A	401	HEM	C3B-CAB-CBB	-3.21	119.54	124.46
2	A	400	HEM	CBD-CAD-C3D	-3.01	104.81	113.55
2	A	400	HEM	CAA-C2A-C1A	-2.94	123.81	127.01
2	A	401	HEM	CBA-CAA-C2A	-2.53	108.00	112.53
2	A	400	HEM	CBA-CAA-C2A	-2.26	108.49	112.53
2	A	400	HEM	CMA-C3A-C4A	-2.19	124.73	128.36
2	B	400	HEM	CMA-C3A-C4A	-2.19	124.74	128.36
2	A	401	HEM	CAA-C2A-C3A	-2.11	122.98	129.00
2	B	401	HEM	CAA-C2A-C1A	-2.07	124.76	127.01
2	A	401	HEM	C1D-CHD-C4C	-2.07	122.36	125.82
2	A	401	HEM	CMA-C3A-C4A	-2.02	125.02	128.36
2	A	400	HEM	C2C-C1C-CHC	2.33	127.23	123.68
2	B	401	HEM	C2C-C1C-CHC	2.50	127.48	123.68
2	A	401	HEM	C2C-C1C-CHC	2.56	127.58	123.68
2	B	401	HEM	C3B-C4B-CHC	2.63	126.87	123.16
2	B	401	HEM	CMD-C2D-C3D	2.69	126.23	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	HEM	CMD-C2D-C3D	3.05	127.83	114.35
2	A	401	HEM	C2D-C3D-C4D	3.06	106.68	101.50
2	A	400	HEM	CMD-C2D-C3D	3.10	128.06	114.35
2	B	400	HEM	C3B-C4B-CHC	3.22	127.70	123.16
2	A	401	HEM	CMD-C2D-C3D	3.57	130.15	114.35
2	B	400	HEM	CMB-C2B-C3B	3.62	125.58	116.53
2	A	400	HEM	C3B-C4B-CHC	3.70	128.38	123.16
2	A	401	HEM	C3B-C4B-CHC	3.79	128.50	123.16
2	A	401	HEM	CMC-C2C-C3C	4.06	126.66	116.53
2	A	400	HEM	CMC-C2C-C3C	4.08	126.71	116.53
2	A	401	HEM	CAD-C3D-C2D	4.17	125.21	113.22
2	B	401	HEM	CAD-C3D-C2D	4.28	125.53	113.22
2	B	401	HEM	CMC-C2C-C3C	4.29	127.23	116.53
2	A	401	HEM	CAD-C3D-C4D	4.42	128.06	112.47
2	B	401	HEM	CMB-C2B-C3B	4.44	127.62	116.53
2	B	400	HEM	CAD-C3D-C4D	4.53	128.46	112.47
2	A	400	HEM	CAD-C3D-C4D	4.57	128.59	112.47
2	A	400	HEM	CAD-C3D-C2D	4.65	126.58	113.22
2	A	401	HEM	CMB-C2B-C3B	4.88	128.70	116.53
2	B	400	HEM	CAD-C3D-C2D	4.90	127.30	113.22
2	B	401	HEM	CAD-C3D-C4D	4.96	129.95	112.47
2	A	400	HEM	CMB-C2B-C3B	5.09	129.22	116.53
2	B	400	HEM	CMC-C2C-C3C	5.40	130.02	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	HEM	6	0
2	A	401	HEM	16	0
2	B	400	HEM	10	0
2	B	401	HEM	13	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	315/345 (91%)	-0.09	2 (0%)	90	90	19, 40, 59, 74	0
1	B	313/345 (90%)	0.20	6 (1%)	70	69	22, 40, 72, 83	0
All	All	628/690 (91%)	0.05	8 (1%)	79	79	19, 40, 66, 83	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	ALA	6.4
1	B	195	TYR	4.4
1	B	241	LYS	4.1
1	B	128	LYS	3.7
1	A	256	ALA	2.7
1	A	302	PHE	2.4
1	B	126	GLN	2.1
1	B	240	GLU	2.1

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
3	CA	B	402	1/1	0.95	0.17	2.19	37,37,37,37	0
3	CA	A	402	1/1	0.98	0.16	1.54	31,31,31,31	0
2	HEM	B	401	43/43	0.96	0.16	0.11	27,38,40,40	0
2	HEM	B	400	43/43	0.97	0.16	0.09	24,34,43,48	0
2	HEM	A	400	43/43	0.97	0.14	-0.02	15,25,31,33	0
2	HEM	A	401	43/43	0.96	0.14	-0.28	20,31,33,33	0
4	IMD	B	346	5/5	0.99	0.12	-	40,40,42,42	0
4	IMD	A	346	5/5	0.97	0.19	-	26,26,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.