Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:14 AM GMT

PDB ID	:	3HQ6
Title	:	Cytochrome c peroxidase from G. sulfurreducens, wild type
Authors	:	Hoffmann, M.; Seidel, J.; Einsle, O.
Deposited on	:	2009-06-05
Resolution	:	2.00 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

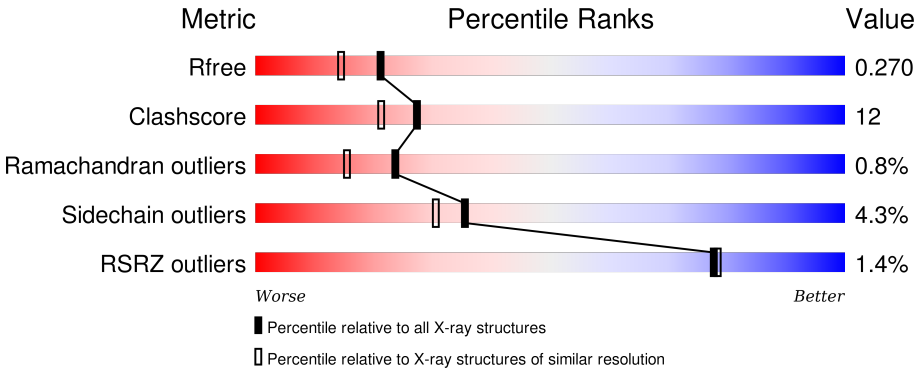
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	2% 73% 17% 6%
1	B	345	% 73% 16% 9%

2 Entry composition

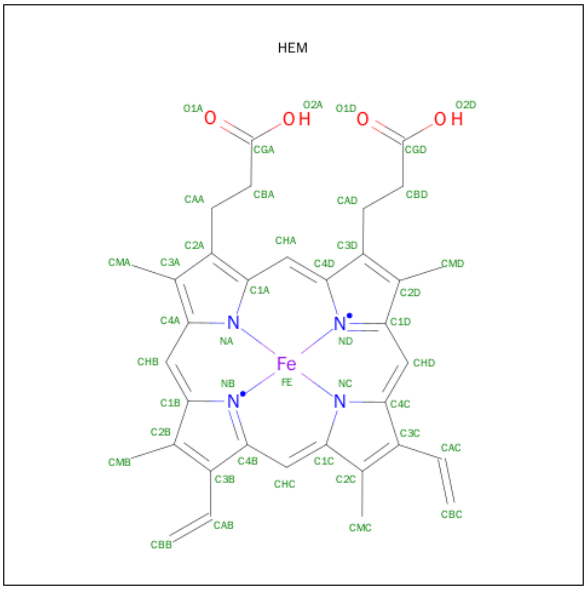
There are 4 unique types of molecules in this entry. The entry contains 5716 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	324	Total	C	N	O	S	0	0	0
			2451	1566	418	458	9			
1	B	313	Total	C	N	O	S	0	0	0
			2370	1514	405	442	9			

- 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 1 1	0	0
3	A	1	Total Ca 1 1	0	0

- Molecule 4 is water.

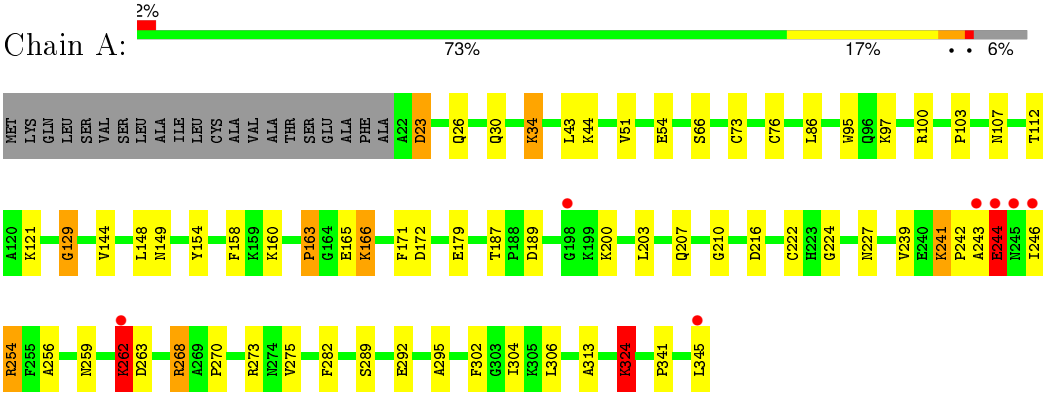
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	342	Total O 342 342	0	0
4	B	379	Total O 379 379	0	0

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.

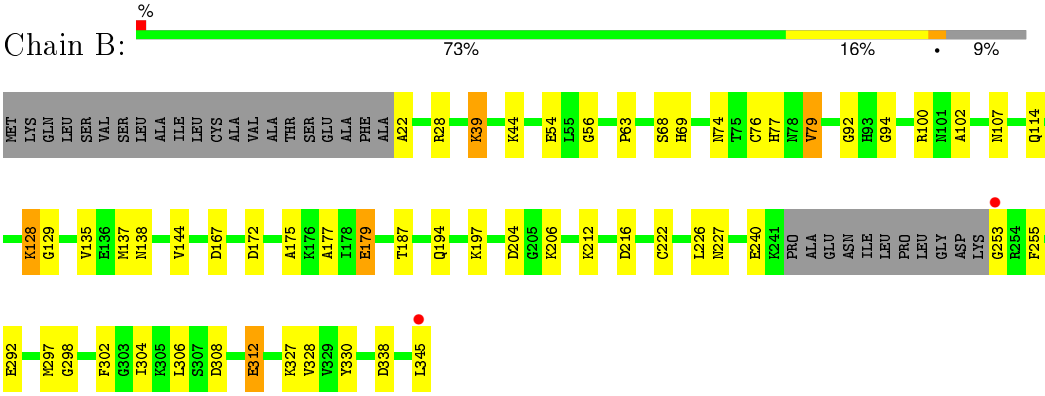
- Molecule 1: Cytochrome c551 peroxidase

Chain A:



- Molecule 1: Cytochrome c551 peroxidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.24Å 55.78Å 78.64Å 68.69° 71.84° 57.76°	Depositor
Resolution (Å)	70.00 – 2.00 36.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.6 (70.00-2.00) 86.1 (36.22-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.266 0.192 , 0.270	Depositor DCC
R_{free} test set	2319 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	19.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.9	EDS
Estimated twinning fraction	0.010 for -h+k,k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 45908 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5716	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	1.28	10/2511 (0.4%)	1.06	6/3408 (0.2%)
1	B	1.33	8/2427 (0.3%)	1.08	8/3291 (0.2%)
All	All	1.30	18/4938 (0.4%)	1.07	14/6699 (0.2%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	292	GLU	CG-CD	7.84	1.63	1.51
1	A	275	VAL	CB-CG2	6.25	1.66	1.52
1	B	94	GLY	N-CA	6.06	1.55	1.46
1	A	282	PHE	CE2-CZ	5.86	1.48	1.37
1	A	66	SER	CB-OG	5.83	1.49	1.42
1	A	179	GLU	CD-OE1	5.81	1.32	1.25
1	B	54	GLU	CG-CD	5.77	1.60	1.51
1	A	171	PHE	CD1-CE1	5.72	1.50	1.39
1	B	102	ALA	CA-CB	5.63	1.64	1.52
1	B	79	VAL	CB-CG2	5.62	1.64	1.52
1	A	54	GLU	CG-CD	5.58	1.60	1.51
1	B	125	GLU	CG-CD	5.52	1.60	1.51
1	A	295	ALA	CA-CB	-5.47	1.41	1.52
1	B	330	TYR	CD2-CE2	5.39	1.47	1.39
1	B	179	GLU	CB-CG	5.11	1.61	1.52
1	A	224	GLY	N-CA	5.09	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	LYS	CD-CE	5.07	1.64	1.51
1	A	112	THR	CB-CG2	5.06	1.69	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	338	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	298	GLY	N-CA-C	-6.33	97.28	113.10
1	A	216	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	306	LEU	CB-CG-CD1	-5.66	101.38	111.00
1	B	119	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	A	86	LEU	CA-CB-CG	5.64	128.28	115.30
1	B	338	ASP	CB-CG-OD2	-5.48	113.36	118.30
1	A	306	LEU	CB-CG-CD2	5.45	120.27	111.00
1	B	345	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	100	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	226	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	A	172	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	163	PRO	C-N-CA	-5.17	111.44	122.30
1	B	100	ARG	NE-CZ-NH1	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ASP	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	2451	0	2454	68	0
1	B	2370	0	2369	50	0
2	A	86	0	60	18	0
2	B	86	0	60	16	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	342	0	0	10	4
4	B	379	0	0	13	4
All	All	5716	0	4943	118	4

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 12.

All (118) 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:73:CYS:SG	2:A:400:HEM:CAB	2.03	1.47
1:A:73:CYS:SG	2:A:400:HEM:HAB	1.62	1.40
1:A:76:CYS:SG	2:A:400:HEM:CAC	2.10	1.39
1:A:222:CYS:HG	2:A:401:HEM:CAC	1.47	1.26
1:B:222:CYS:SG	2:B:401:HEM:CAC	2.25	1.25
1:A:222:CYS:SG	2:A:401:HEM:CAC	2.25	1.24
1:B:76:CYS:SG	2:B:400:HEM:CAC	2.29	1.21
1:B:44:LYS:HD3	4:B:660:HOH:O	1.53	1.09
1:B:222:CYS:HG	2:B:401:HEM:CAC	1.61	1.08
1:B:28:ARG:HD2	4:B:653:HOH:O	1.52	1.07
1:A:304:ILE:O	4:A:509:HOH:O	1.76	1.03
1:A:76:CYS:SG	2:A:400:HEM:HAC	2.00	1.01
1:A:166:LYS:HE3	1:A:166:LYS:H	1.31	0.95
1:B:172:ASP:HB2	4:B:584:HOH:O	1.66	0.95
1:A:246:ILE:HG22	1:A:246:ILE:O	1.66	0.92
1:B:76:CYS:HG	2:B:400:HEM:CAC	1.77	0.90
1:A:254:ARG:HG2	1:A:254:ARG:HH21	1.36	0.88
1:A:243:ALA:O	1:A:244:GLU:HG3	1.76	0.85
1:B:222:CYS:SG	2:B:401:HEM:CBC	2.66	0.84
1:A:222:CYS:HG	2:A:401:HEM:CBC	1.92	0.83
1:A:51:VAL:HG23	4:A:592:HOH:O	1.79	0.83
1:A:254:ARG:HH21	1:A:254:ARG:CG	1.92	0.83
1:A:165:GLU:HA	1:A:166:LYS:HE3	1.61	0.81
1:A:222:CYS:SG	2:A:401:HEM:CBC	2.69	0.80
1:B:259:ASN:HB2	4:B:535:HOH:O	1.81	0.79
1:A:76:CYS:SG	2:A:400:HEM:CBC	2.70	0.79
1:A:166:LYS:HD2	4:A:659:HOH:O	1.82	0.78
1:A:166:LYS:CE	1:A:166:LYS:H	1.98	0.76
1:B:76:CYS:SG	2:B:400:HEM:CBC	2.73	0.76
1:A:76:CYS:SG	2:A:400:HEM:C3C	2.79	0.76
1:A:166:LYS:N	1:A:166:LYS:HE3	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLN:O	1:A:30:GLN:HG3	1.88	0.74
1:B:222:CYS:HG	2:B:401:HEM:CBC	2.02	0.72
1:A:73:CYS:SG	2:A:400:HEM:CBB	2.78	0.71
1:A:302:PHE:HB2	1:A:304:ILE:HG13	1.73	0.70
1:A:241:LYS:HG3	1:A:254:ARG:O	1.92	0.70
1:B:222:CYS:SG	2:B:401:HEM:C3C	2.80	0.68
1:A:254:ARG:HG2	1:A:254:ARG:NH2	2.07	0.68
1:B:240:GLU:HG2	1:B:255:PHE:CE1	2.28	0.68
1:B:175:ALA:O	1:B:179:GLU:HG3	1.93	0.68
1:A:222:CYS:SG	2:A:401:HEM:C3C	2.82	0.67
1:B:135:VAL:CG1	1:B:144:VAL:HG21	2.26	0.66
1:B:39:LYS:HG2	4:B:657:HOH:O	1.96	0.66
1:B:76:CYS:SG	2:B:400:HEM:HAC	2.34	0.65
1:A:246:ILE:CG2	1:A:246:ILE:O	2.39	0.65
1:A:34:LYS:HD2	4:A:599:HOH:O	1.96	0.65
1:B:114:GLN:HE22	1:B:128:LYS:HB2	1.63	0.64
1:A:324:LYS:HD3	4:A:424:HOH:O	1.97	0.64
1:A:222:CYS:SG	2:A:401:HEM:HAC	2.31	0.63
1:A:73:CYS:CB	2:A:400:HEM:HAB	2.29	0.62
1:B:206:LYS:HE2	4:B:534:HOH:O	2.00	0.62
1:B:22:ALA:N	4:B:477:HOH:O	2.34	0.60
1:A:243:ALA:O	1:A:244:GLU:CG	2.48	0.60
1:B:76:CYS:SG	2:B:400:HEM:C3C	2.88	0.60
1:A:252:LYS:HB3	1:A:292:GLU:HG3	1.84	0.59
1:A:268:ARG:O	1:A:270:PRO:HD3	2.03	0.58
1:A:289:SER:HB3	1:A:292:GLU:HB2	1.86	0.58
1:B:114:GLN:HE22	1:B:128:LYS:CB	2.15	0.58
1:A:114:GLN:HE22	1:A:129:GLY:H	1.52	0.57
1:B:138:ASN:C	4:B:460:HOH:O	2.42	0.57
1:A:23:ASP:HB2	1:A:200:LYS:NZ	2.20	0.57
1:B:253:GLY:N	4:B:573:HOH:O	2.37	0.56
1:A:246:ILE:O	1:A:247:LEU:HG	2.05	0.56
1:A:121:LYS:NZ	4:A:626:HOH:O	2.39	0.55
1:B:222:CYS:SG	2:B:401:HEM:HAC	2.37	0.54
1:A:241:LYS:HD2	1:A:256:ALA:HB2	1.89	0.54
1:A:259:ASN:ND2	4:A:503:HOH:O	2.19	0.53
1:B:56:GLY:HA3	1:B:177:ALA:O	2.09	0.53
1:A:73:CYS:CB	2:A:400:HEM:CAB	2.87	0.53
1:A:73:CYS:SG	2:A:400:HEM:C3B	2.99	0.52
1:B:114:GLN:HE22	1:B:129:GLY:H	1.58	0.51
1:A:107:ASN:HD21	1:A:187:THR:H	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLY:HA3	2:B:400:HEM:C3C	2.46	0.50
1:B:259:ASN:CB	4:B:535:HOH:O	2.51	0.49
1:A:165:GLU:CA	1:A:166:LYS:HE3	2.38	0.49
1:B:328:VAL:HG22	4:B:551:HOH:O	2.11	0.49
1:A:154:TYR:O	1:A:158:PHE:HD2	1.95	0.49
1:A:149:ASN:ND2	4:A:554:HOH:O	2.46	0.48
1:A:210:GLY:HA3	1:A:313:ALA:O	2.13	0.48
1:A:95:TRP:CD1	1:A:95:TRP:C	2.87	0.48
1:B:63:PRO:O	1:B:69:HIS:HA	2.15	0.46
1:B:327:LYS:HD3	4:B:537:HOH:O	2.15	0.46
1:A:203:LEU:HD22	1:A:207:GLN:HB3	1.98	0.46
1:A:254:ARG:NH2	1:A:254:ARG:CG	2.62	0.45
1:B:212:LYS:HE2	1:B:216:ASP:OD2	2.15	0.45
1:A:76:CYS:HG	2:A:400:HEM:HAC	1.73	0.45
1:B:297:MET:HG3	2:B:401:HEM:C4A	2.51	0.45
1:B:74:ASN:OD1	1:B:79:VAL:HG22	2.17	0.45
1:B:194:GLN:OE1	1:B:197:LYS:NZ	2.40	0.45
1:A:103:PRO:HD2	2:A:400:HEM:C3D	2.52	0.45
1:A:189:ASP:HB2	1:A:324:LYS:HD2	1.99	0.45
1:B:204:ASP:OD1	1:B:206:LYS:N	2.50	0.45
1:A:241:LYS:HG3	1:A:254:ARG:C	2.37	0.44
1:B:92:GLY:HA3	2:B:400:HEM:C4C	2.52	0.44
1:B:77:HIS:CD2	2:B:400:HEM:NB	2.85	0.44
1:A:262:LYS:HD2	1:A:263:ASP:OD2	2.19	0.43
1:A:324:LYS:NZ	4:A:513:HOH:O	2.45	0.43
1:A:23:ASP:OD1	1:A:23:ASP:C	2.57	0.43
1:B:167:ASP:OD1	4:B:478:HOH:O	2.21	0.43
1:B:114:GLN:NE2	1:B:128:LYS:HB2	2.31	0.42
1:B:204:ASP:OD1	1:B:204:ASP:C	2.58	0.42
1:A:166:LYS:CD	1:A:166:LYS:H	2.28	0.42
1:B:68:SER:O	1:B:69:HIS:HB2	2.19	0.42
1:B:302:PHE:HB2	1:B:304:ILE:HG13	2.01	0.42
1:A:34:LYS:HB3	1:A:34:LYS:HE2	1.77	0.42
1:A:163:PRO:O	4:A:493:HOH:O	2.22	0.42
1:B:259:ASN:OD1	1:B:259:ASN:N	2.52	0.42
1:B:76:CYS:HG	2:B:400:HEM:CBC	2.28	0.42
1:A:144:VAL:O	1:A:148:LEU:HG	2.20	0.42
1:B:128:LYS:H	1:B:128:LYS:HG2	1.71	0.42
1:A:119:ARG:HE	1:A:119:ARG:HB3	1.59	0.41
1:A:165:GLU:HA	1:A:166:LYS:CE	2.42	0.41
1:A:227:ASN:OD1	1:A:273:ARG:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LYS:HZ2	1:B:312:GLU:HG3	1.85	0.41
1:A:51:VAL:HG21	1:A:160:LYS:HE2	2.03	0.41
1:B:114:GLN:NE2	1:B:128:LYS:CB	2.84	0.40
1:A:97:LYS:HA	1:A:97:LYS:HD3	1.86	0.40
1:B:107:ASN:HD21	1:B:187:THR:H	1.69	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:669:HOH:O	4:B:414:HOH:O[1_655]	1.76	0.44
4:A:669:HOH:O	4:B:416:HOH:O[1_655]	1.94	0.26
4:A:463:HOH:O	4:B:690:HOH:O[1_556]	2.15	0.05
4:A:462:HOH:O	4:B:380:HOH:O[1_556]	2.16	0.04

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	322/345 (93%)	304 (94%)	13 (4%)	5 (2%)	12 5
1	B	309/345 (90%)	294 (95%)	15 (5%)	0	100 100
All	All	631/690 (91%)	598 (95%)	28 (4%)	5 (1%)	24 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	GLU
1	A	242	PRO
1	A	253	GLY
1	A	129	GLY
1	A	262	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/276 (94%)	245 (94%)	15 (6%)	25	19
1	B	251/276 (91%)	244 (97%)	7 (3%)	51	50
All	All	511/552 (93%)	489 (96%)	22 (4%)	35	30

All (22) 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	119	ARG
1	A	166	LYS
1	A	239	VAL
1	A	241	LYS
1	A	244	GLU
1	A	252	LYS
1	A	254	ARG
1	A	262	LYS
1	A	268	ARG
1	A	324	LYS
1	A	341	PRO
1	A	345	LEU
1	B	39	LYS
1	B	128	LYS
1	B	137	MET
1	B	227	ASN
1	B	291	LYS
1	B	308	ASP
1	B	312	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	114	GLN
1	A	149	ASN
1	B	107	ASN
1	B	114	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	HEM	A	400	1	30,50,50	2.75	12 (40%)	24,82,82	2.77	13 (54%)
2	HEM	A	401	1	30,50,50	2.68	11 (36%)	24,82,82	3.04	11 (45%)
2	HEM	B	400	1	30,50,50	3.30	11 (36%)	24,82,82	2.99	13 (54%)
2	HEM	B	401	1	30,50,50	2.18	9 (30%)	24,82,82	2.88	10 (41%)

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	400	1	-	0/10/54/54	0/0/8/8
2	HEM	A	401	1	-	0/10/54/54	0/0/8/8
2	HEM	B	400	1	-	0/10/54/54	0/0/8/8
2	HEM	B	401	1	-	0/10/54/54	0/0/8/8

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	HEM	C3B-C4B	-12.07	1.41	1.51
2	A	400	HEM	C3B-C4B	-9.71	1.43	1.51
2	A	401	HEM	C3B-C4B	-9.21	1.43	1.51
2	B	401	HEM	C3B-C4B	-6.92	1.45	1.51
2	A	401	HEM	C3D-C4D	-5.87	1.44	1.51
2	B	400	HEM	C3D-C4D	-5.27	1.44	1.51
2	A	400	HEM	C3D-C4D	-5.17	1.44	1.51
2	A	400	HEM	C2C-C1C	-4.59	1.43	1.52
2	A	401	HEM	C2C-C1C	-4.19	1.44	1.52
2	B	400	HEM	C2C-C1C	-3.87	1.45	1.52
2	B	401	HEM	C2C-C1C	-3.76	1.45	1.52
2	A	401	HEM	C2D-C1D	-2.85	1.42	1.51
2	B	400	HEM	C2D-C1D	-2.53	1.43	1.51
2	B	400	HEM	C2B-C1B	-2.40	1.44	1.51
2	B	401	HEM	C3D-C4D	-2.22	1.48	1.51
2	A	400	HEM	C2A-C3A	-2.08	1.31	1.37
2	A	400	HEM	C2D-C1D	-2.01	1.45	1.51
2	A	401	HEM	C3C-CAC	2.01	1.55	1.51
2	A	400	HEM	CBB-CAB	2.06	1.41	1.29
2	B	401	HEM	CMC-C2C	2.07	1.57	1.53
2	A	400	HEM	C1C-NC	2.10	1.38	1.36
2	A	400	HEM	CAA-C2A	2.16	1.55	1.52
2	A	401	HEM	CMA-C3A	2.27	1.56	1.51
2	B	401	HEM	C1C-NC	2.40	1.39	1.36
2	A	401	HEM	FE-NC	2.45	2.05	1.95
2	A	401	HEM	CAA-C2A	2.57	1.56	1.52
2	A	400	HEM	FE-NC	2.61	2.06	1.95
2	B	401	HEM	C3B-CAB	2.69	1.56	1.51
2	A	400	HEM	C4C-NC	2.75	1.39	1.36
2	A	401	HEM	C3B-CAB	2.79	1.56	1.51
2	A	401	HEM	FE-NB	3.03	2.13	1.97
2	B	401	HEM	C3C-CAC	3.03	1.57	1.51
2	B	401	HEM	FE-ND	3.19	2.14	1.97
2	B	400	HEM	CAA-C2A	3.35	1.57	1.52
2	A	400	HEM	C3B-CAB	3.44	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	HEM	C1C-NC	3.54	1.40	1.36
2	B	401	HEM	CAA-C2A	3.63	1.58	1.52
2	B	400	HEM	C3B-CAB	3.63	1.58	1.51
2	B	400	HEM	CMA-C3A	3.79	1.59	1.51
2	B	400	HEM	C3C-CAC	3.80	1.58	1.51
2	A	400	HEM	C3C-CAC	4.23	1.59	1.51
2	B	400	HEM	C1C-NC	4.96	1.42	1.36
2	B	400	HEM	C4C-NC	5.57	1.42	1.36

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	HEM	C3B-CAB-CBB	-6.40	114.64	124.46
2	A	401	HEM	C3B-CAB-CBB	-5.58	115.89	124.46
2	A	400	HEM	C3B-CAB-CBB	-5.26	116.39	124.46
2	B	401	HEM	C3B-CAB-CBB	-5.08	116.66	124.46
2	A	401	HEM	CBA-CAA-C2A	-4.80	103.93	112.53
2	A	401	HEM	CAA-C2A-C1A	-4.54	122.08	127.01
2	B	401	HEM	CMA-C3A-C4A	-4.45	121.00	128.36
2	B	400	HEM	CAA-CBA-CGA	-4.07	105.28	112.75
2	B	400	HEM	CBD-CAD-C3D	-3.74	102.66	113.55
2	A	400	HEM	CMA-C3A-C4A	-3.47	122.62	128.36
2	A	400	HEM	CBD-CAD-C3D	-3.42	103.60	113.55
2	A	401	HEM	CMA-C3A-C4A	-3.39	122.76	128.36
2	B	400	HEM	C1D-CHD-C4C	-3.07	120.69	125.82
2	B	400	HEM	C4B-CHC-C1C	-3.05	120.73	125.82
2	B	400	HEM	CAA-C2A-C1A	-2.79	123.98	127.01
2	B	400	HEM	CMA-C3A-C4A	-2.69	123.91	128.36
2	A	400	HEM	C4B-CHC-C1C	-2.68	121.34	125.82
2	B	401	HEM	CBA-CAA-C2A	-2.66	107.76	112.53
2	A	400	HEM	CAA-CBA-CGA	-2.37	108.39	112.75
2	B	400	HEM	CBA-CAA-C2A	-2.36	108.30	112.53
2	A	400	HEM	CAA-C2A-C3A	-2.05	123.15	129.00
2	A	401	HEM	C3B-C4B-CHC	2.15	126.19	123.16
2	B	401	HEM	CMA-C3A-C2A	2.21	129.87	125.24
2	B	401	HEM	C2C-C1C-CHC	2.23	127.07	123.68
2	A	400	HEM	CMD-C2D-C3D	2.29	124.47	114.35
2	A	401	HEM	CMD-C2D-C3D	2.32	124.63	114.35
2	A	400	HEM	C2C-C1C-CHC	2.46	127.42	123.68
2	A	401	HEM	C2D-C3D-C4D	2.67	106.02	101.50
2	B	401	HEM	CMD-C2D-C3D	3.07	127.92	114.35
2	B	400	HEM	CAD-C3D-C2D	3.38	122.93	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	HEM	C2D-C3D-C4D	3.48	107.40	101.50
2	A	400	HEM	CAD-C3D-C2D	3.63	123.67	113.22
2	A	400	HEM	C2D-C3D-C4D	3.68	107.74	101.50
2	A	400	HEM	CMB-C2B-C3B	4.00	126.53	116.53
2	A	401	HEM	CAD-C3D-C2D	4.39	125.84	113.22
2	A	401	HEM	CAD-C3D-C4D	4.42	128.07	112.47
2	B	401	HEM	CAD-C3D-C2D	4.44	125.98	113.22
2	B	400	HEM	CMC-C2C-C3C	4.53	127.84	116.53
2	A	400	HEM	CAD-C3D-C4D	4.55	128.50	112.47
2	B	400	HEM	CMB-C2B-C3B	4.59	127.99	116.53
2	A	400	HEM	CMC-C2C-C3C	4.81	128.53	116.53
2	B	400	HEM	CAD-C3D-C4D	4.87	129.66	112.47
2	B	401	HEM	CAD-C3D-C4D	4.93	129.84	112.47
2	A	401	HEM	CMB-C2B-C3B	5.35	129.89	116.53
2	B	401	HEM	CMC-C2C-C3C	5.51	130.29	116.53
2	A	401	HEM	CMC-C2C-C3C	5.65	130.64	116.53
2	B	401	HEM	CMB-C2B-C3B	6.21	132.02	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	HEM	12	0
2	A	401	HEM	6	0
2	B	400	HEM	9	0
2	B	401	HEM	7	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, 95^{th} 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	324/345 (93%)	-0.22	7 (2%)	65	66	12, 21, 44, 66	0
1	B	313/345 (90%)	-0.31	2 (0%)	90	90	12, 20, 35, 52	0
All	All	637/690 (92%)	-0.26	9 (1%)	78	78	12, 21, 40, 66	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	LEU	7.9
1	A	345	LEU	3.8
1	A	244	GLU	3.7
1	A	246	ILE	3.4
1	A	243	ALA	3.3
1	A	245	ASN	3.2
1	B	253	GLY	2.4
1	A	198	GLY	2.3
1	A	262	LYS	2.2

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

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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	0.99	0.12	0.98	18,18,18,18	0
2	HEM	A	400	43/43	0.98	0.12	0.96	8,14,19,28	0
3	CA	A	402	1/1	1.00	0.10	0.35	17,17,17,17	0
2	HEM	B	400	43/43	0.98	0.11	0.21	4,12,19,26	0
2	HEM	B	401	43/43	0.98	0.10	0.00	11,18,21,21	0
2	HEM	A	401	43/43	0.98	0.10	-0.13	12,19,23,24	0

6.5 Other polymers (i)

There are no such residues in this entry.