Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:42 AM GMT

PDB ID	:	3BVD
Title	:	Structure of Surface-engineered Cytochrome ba3 Oxidase from Thermus thermophilus under Xenon Pressure, 100psi 5min
Authors	:	Luna, V.M.; Chen, Y.; Fee, J.A.; Stout, C.D.
Deposited on	:	2008-01-07
Resolution	:	3.37 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:

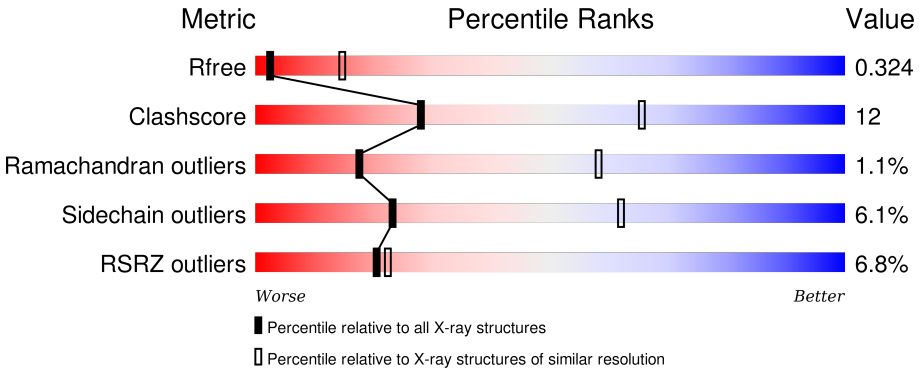
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.37 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	1084 (3.46-3.30)
Clashscore	102246	1158 (3.46-3.30)
Ramachandran outliers	100387	1139 (3.46-3.30)
Sidechain outliers	100360	1138 (3.46-3.30)
RSRZ outliers	91569	1089 (3.46-3.30)

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	568	7%, 70%, 25%
2	B	168	4%, 83%, 15%
3	C	34	9%, 82%, 12%

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
8	XE	A	808	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6025 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4350	2948	699	687	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP Q5SJ79
A	-4	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-3	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-2	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	0	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	258	ARG	LYS	ENGINEERED	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1298	844	217	233	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLN	GLU	ENGINEERED	UNP Q5SJ80

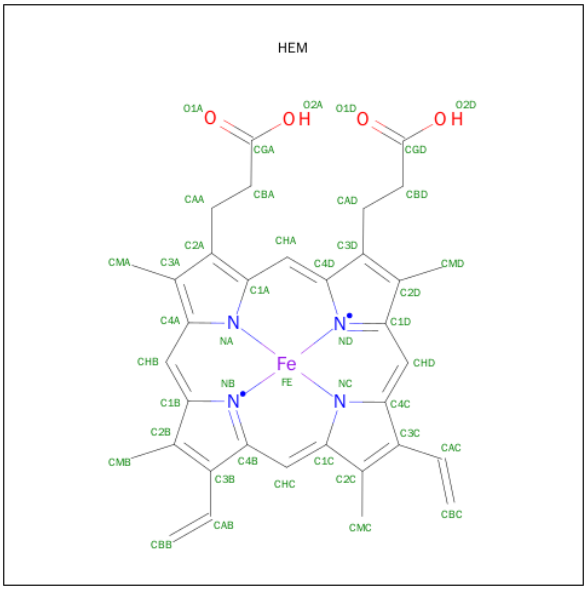
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	33	Total	C	N	O	0	0	0
			259	179	39	41			

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

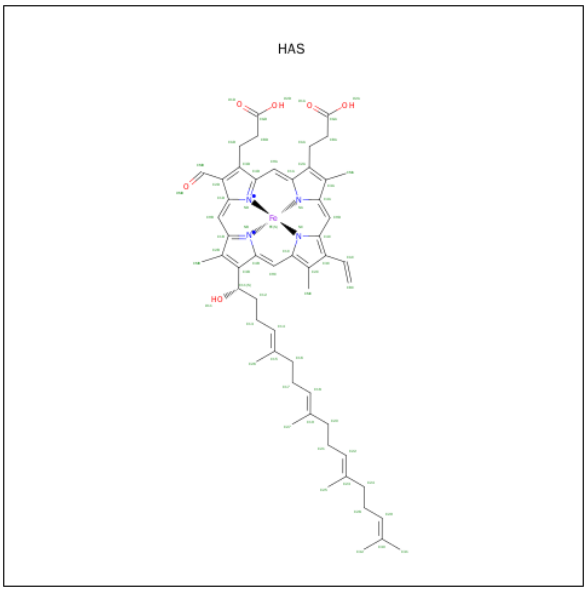
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu 1 1	0	0

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



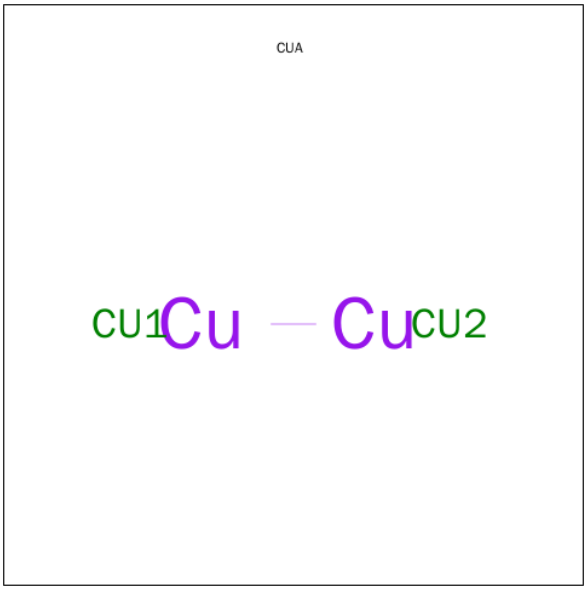
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 6 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 7 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cu	0	0
			2	2		

- Molecule 8 is XENON (three-letter code: XE) (formula: Xe).

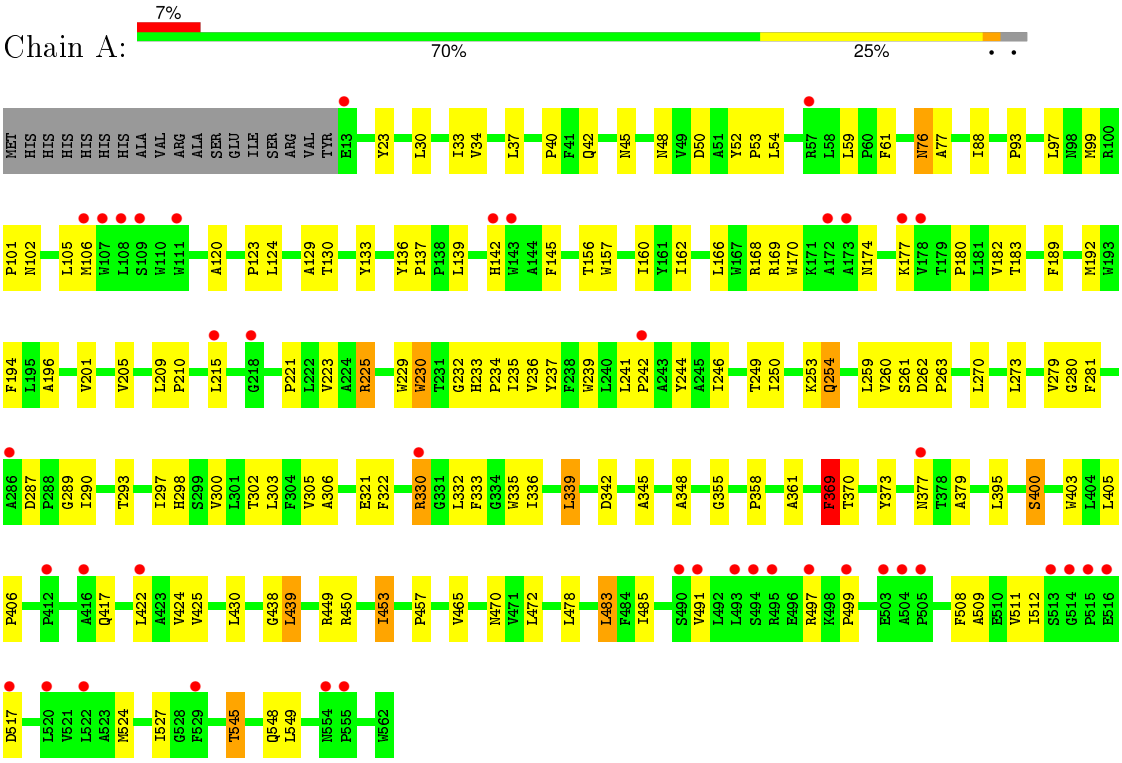
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	7	Total Xe 7 7	0	0

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.

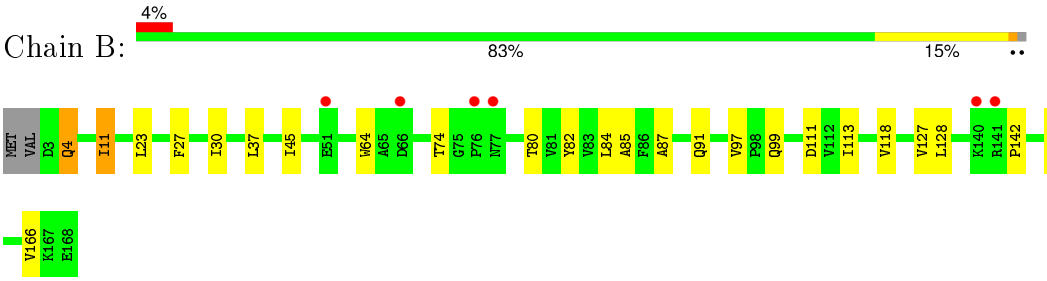
- Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



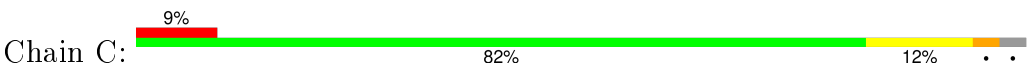
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



- Molecule 3: Cytochrome c oxidase polypeptide 2A

Chain C:




MET
E2
E3
K4
L13
I19
L24
G34

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	119.73Å 119.73Å 153.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.96 – 3.37 26.95 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.8 (26.96-3.37) 99.8 (26.95-3.37)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 3.38Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.292 , 0.336 0.268 , 0.324	Depositor DCC
R_{free} test set	823 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	101.5	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 16295 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6025	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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, HAS, CUA, CU, XE

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	0/4506	0.54	0/6185
2	B	0.39	0/1335	0.54	0/1822
3	C	0.39	0/265	0.55	0/359
All	All	0.41	0/6106	0.54	0/8366

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

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	4350	0	4458	133	0
2	B	1298	0	1282	27	0
3	C	259	0	279	2	0
4	A	1	0	0	0	0
5	A	43	0	30	5	0
6	A	65	0	62	3	0
7	B	2	0	0	0	0
8	A	7	0	0	5	0
All	All	6025	0	6111	142	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 12.

All (142) 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:105:LEU:HB2	1:A:162:ILE:HD11	1.32	1.08
1:A:105:LEU:CB	1:A:162:ILE:HD11	1.87	1.03
1:A:361:ALA:HA	3:C:19:ILE:HD13	1.39	1.03
1:A:330:ARG:HH21	1:A:330:ARG:HG3	1.23	1.00
1:A:300:VAL:HG22	2:B:30:ILE:HD12	1.44	0.99
1:A:233:HIS:NE2	1:A:237:TYR:HE2	1.63	0.96
1:A:373:TYR:CE1	2:B:45:ILE:HD13	2.03	0.93
1:A:303:LEU:CD1	2:B:30:ILE:HD11	2.00	0.91
1:A:330:ARG:HH21	1:A:330:ARG:CG	1.85	0.90
1:A:369:PHE:CE2	2:B:45:ILE:HD12	2.09	0.87
1:A:303:LEU:HD12	2:B:30:ILE:HD11	1.58	0.84
1:A:201:VAL:HG22	8:A:808:XE:XE	2.56	0.84
1:A:105:LEU:HB2	1:A:162:ILE:CD1	2.08	0.83
1:A:373:TYR:HE1	2:B:45:ILE:HD13	1.45	0.81
1:A:233:HIS:NE2	1:A:237:TYR:CE2	2.48	0.80
1:A:137:PRO:O	2:B:113:ILE:HD11	1.81	0.79
1:A:76:ASN:HB3	5:A:800:HEM:HAC	1.63	0.79
1:A:293:THR:O	1:A:297:ILE:HD13	1.83	0.77
1:A:88:ILE:CG2	1:A:246:ILE:HD11	2.14	0.77
1:A:221:PRO:HB2	2:B:128:LEU:HD23	1.68	0.76
2:B:142:PRO:HA	2:B:166:VAL:HG23	1.67	0.75
6:A:801:HAS:HBC1	6:A:801:HAS:HMC1	1.67	0.75
1:A:330:ARG:HG3	1:A:330:ARG:NH2	1.98	0.75
1:A:453:ILE:HD13	1:A:453:ILE:H	1.53	0.73
1:A:361:ALA:HA	3:C:19:ILE:CD1	2.19	0.72
1:A:242:PRO:O	1:A:246:ILE:HD13	1.89	0.72
1:A:201:VAL:CG2	8:A:808:XE:XE	3.16	0.71
1:A:322:PHE:HZ	2:B:4:GLN:HG2	1.55	0.71
1:A:45:ASN:ND2	1:A:453:ILE:HD13	2.06	0.70
1:A:40:PRO:HD3	5:A:800:HEM:HBB2	1.74	0.68
1:A:88:ILE:HG23	1:A:246:ILE:HD11	1.73	0.68
1:A:105:LEU:HB3	1:A:162:ILE:HD11	1.73	0.67
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.77	0.66
1:A:373:TYR:HE1	2:B:45:ILE:CD1	2.09	0.66
1:A:261:SER:OG	1:A:263:PRO:HD2	1.96	0.66
1:A:249:THR:OG1	1:A:250:ILE:HD12	1.99	0.62
1:A:76:ASN:HB3	5:A:800:HEM:CAC	2.30	0.62
1:A:373:TYR:CZ	2:B:45:ILE:HD13	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:HB2	1:A:509:ALA:HA	1.82	0.60
1:A:88:ILE:HG21	1:A:246:ILE:HD11	1.82	0.60
1:A:303:LEU:CD1	2:B:30:ILE:CD1	2.78	0.59
1:A:260:VAL:HA	1:A:512:ILE:HD13	1.83	0.59
1:A:355:GLY:O	1:A:358:PRO:HD2	2.03	0.58
1:A:88:ILE:HG21	1:A:246:ILE:CD1	2.35	0.57
1:A:48:ASN:HD21	1:A:457:PRO:HA	1.68	0.57
1:A:233:HIS:CD2	1:A:237:TYR:HE2	2.21	0.56
1:A:300:VAL:HG22	2:B:30:ILE:CD1	2.27	0.55
1:A:137:PRO:O	2:B:113:ILE:CD1	2.53	0.55
2:B:97:VAL:HG23	2:B:166:VAL:HG12	1.87	0.55
1:A:45:ASN:HD21	1:A:453:ILE:HD13	1.69	0.55
1:A:156:THR:O	1:A:160:ILE:HG13	2.06	0.54
1:A:395:LEU:HD22	1:A:425:VAL:HG13	1.90	0.54
1:A:300:VAL:CG2	2:B:30:ILE:HD12	2.27	0.54
1:A:438:GLY:HA3	1:A:470:ASN:OD1	2.08	0.53
1:A:205:VAL:HA	1:A:209:LEU:HD12	1.91	0.53
1:A:229:TRP:CE3	1:A:232:GLY:HA3	2.45	0.52
1:A:157:TRP:HA	1:A:160:ILE:HD12	1.92	0.52
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.46	0.51
1:A:270:LEU:HD22	1:A:524:MET:HG2	1.91	0.51
1:A:379:ALA:HB1	1:A:439:LEU:HD12	1.93	0.51
1:A:33:ILE:O	1:A:37:LEU:HG	2.11	0.51
1:A:449:ARG:HH12	6:A:801:HAS:CGA	2.23	0.51
1:A:289:GLY:O	1:A:290:ILE:HD13	2.12	0.50
1:A:373:TYR:OH	2:B:45:ILE:HD13	2.12	0.50
1:A:225:ARG:HD3	1:A:287:ASP:OD1	2.12	0.50
1:A:124:LEU:HD23	1:A:129:ALA:HB3	1.93	0.50
1:A:101:PRO:HA	1:A:166:LEU:HD21	1.94	0.49
1:A:99:MET:HE2	1:A:169:ARG:HE	1.77	0.49
1:A:174:ASN:HB3	1:A:177:LYS:HD3	1.93	0.49
1:A:322:PHE:CZ	2:B:4:GLN:HG2	2.41	0.49
1:A:262:ASP:N	1:A:263:PRO:CD	2.76	0.49
1:A:302:THR:HG22	6:A:801:HAS:HMB2	1.94	0.49
1:A:512:ILE:HD12	1:A:512:ILE:N	2.28	0.49
1:A:241:LEU:HA	1:A:244:TYR:HB2	1.93	0.49
1:A:233:HIS:O	1:A:236:VAL:HG22	2.12	0.48
2:B:84:LEU:HB3	2:B:91:GLN:HB3	1.94	0.48
1:A:259:LEU:O	1:A:512:ILE:CD1	2.61	0.48
1:A:333:PHE:HA	1:A:336:ILE:HD13	1.95	0.48
1:A:30:LEU:O	1:A:34:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:TYR:O	1:A:139:LEU:HB2	2.14	0.48
1:A:52:TYR:N	1:A:53:PRO:HD2	2.29	0.48
1:A:449:ARG:HD2	1:A:450:ARG:HG3	1.96	0.47
1:A:223:VAL:HG12	1:A:549:LEU:HB3	1.95	0.47
1:A:201:VAL:HG23	8:A:808:XE:XE	2.92	0.47
1:A:332:LEU:HD23	1:A:333:PHE:CE1	2.50	0.47
1:A:417:GLN:NE2	1:A:491:VAL:HG22	2.30	0.47
1:A:281:PHE:HB2	1:A:298:HIS:CG	2.50	0.47
1:A:233:HIS:CE1	1:A:237:TYR:HE2	2.29	0.46
1:A:201:VAL:HA	8:A:808:XE:XE	2.94	0.46
1:A:345:ALA:HB1	1:A:403:TRP:HD1	1.80	0.46
1:A:232:GLY:HA2	8:A:810:XE:XE	2.94	0.46
1:A:230:TRP:C	1:A:230:TRP:CD1	2.90	0.45
1:A:77:ALA:HB2	5:A:800:HEM:CMD	2.46	0.45
1:A:77:ALA:HB2	5:A:800:HEM:HMD3	1.99	0.45
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.98	0.45
1:A:246:ILE:HD12	1:A:246:ILE:N	2.31	0.45
2:B:118:VAL:HG22	2:B:147:ILE:HG12	1.98	0.45
1:A:259:LEU:O	1:A:512:ILE:HD12	2.18	0.44
1:A:123:PRO:HB3	1:A:142:HIS:HB3	1.98	0.44
1:A:182:VAL:HG21	1:A:508:PHE:HE2	1.82	0.44
1:A:342:ASP:HA	1:A:422:LEU:HD11	1.99	0.44
1:A:303:LEU:O	1:A:306:ALA:HB3	2.18	0.44
1:A:196:ALA:HB1	1:A:234:PRO:CG	2.48	0.44
1:A:42:GLN:O	1:A:45:ASN:HB3	2.17	0.44
1:A:120:ALA:HA	1:A:145:PHE:HA	1.99	0.43
1:A:254:GLN:HE21	1:A:254:GLN:HB3	1.56	0.43
1:A:209:LEU:N	1:A:210:PRO:HD2	2.33	0.43
1:A:205:VAL:O	1:A:210:PRO:HD3	2.18	0.43
1:A:50:ASP:O	1:A:53:PRO:HD2	2.18	0.43
1:A:192:MET:HB2	1:A:273:LEU:HA	2.00	0.43
2:B:64:TRP:CZ2	2:B:82:TYR:HD2	2.37	0.43
1:A:333:PHE:HA	1:A:336:ILE:CD1	2.49	0.43
1:A:233:HIS:CD2	1:A:237:TYR:CE2	3.03	0.43
1:A:330:ARG:CG	1:A:330:ARG:NH2	2.57	0.42
2:B:74:THR:HG21	2:B:80:THR:OG1	2.18	0.42
2:B:97:VAL:O	2:B:166:VAL:HA	2.18	0.42
1:A:261:SER:HG	1:A:263:PRO:HD2	1.84	0.42
1:A:262:ASP:HB2	1:A:511:VAL:HG11	2.00	0.42
1:A:33:ILE:HD13	1:A:485:ILE:HG23	2.01	0.42
1:A:189:PHE:CE1	1:A:242:PRO:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:ALA:HB3	2:B:127:VAL:HG11	2.02	0.42
1:A:290:ILE:HD12	1:A:545:THR:HG21	2.02	0.42
1:A:336:ILE:HA	1:A:339:LEU:HD22	2.02	0.42
1:A:453:ILE:CD1	1:A:453:ILE:H	2.26	0.41
1:A:290:ILE:HD12	1:A:545:THR:CG2	2.50	0.41
1:A:336:ILE:HD12	1:A:336:ILE:H	1.85	0.41
1:A:233:HIS:H	1:A:234:PRO:HD2	1.86	0.41
1:A:348:ALA:HA	1:A:425:VAL:HG11	2.02	0.41
1:A:93:PRO:O	1:A:97:LEU:HG	2.21	0.41
1:A:235:ILE:HG12	1:A:239:TRP:NE1	2.36	0.41
1:A:45:ASN:ND2	1:A:453:ILE:CD1	2.78	0.41
1:A:424:VAL:HG22	1:A:483:LEU:HB3	2.02	0.41
1:A:93:PRO:HB3	1:A:183:THR:HA	2.03	0.41
1:A:59:LEU:HB3	1:A:61:PHE:CE1	2.55	0.41
1:A:225:ARG:NH2	1:A:287:ASP:OD2	2.54	0.40
1:A:279:VAL:O	1:A:281:PHE:N	2.55	0.40
1:A:377:ASN:HB3	2:B:150:ASN:HB2	2.02	0.40
1:A:400:SER:HA	1:A:403:TRP:NE1	2.36	0.40
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.56	0.40
1:A:497:ARG:HG2	1:A:499:PRO:HG3	2.03	0.40
1:A:170:TRP:CH2	1:A:180:PRO:HD3	2.55	0.40
1:A:260:VAL:HB	2:B:11:ILE:HD13	2.03	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	548/568 (96%)	496 (90%)	47 (9%)	5 (1%)	21 63
2	B	164/168 (98%)	145 (88%)	17 (10%)	2 (1%)	16 56
3	C	31/34 (91%)	29 (94%)	1 (3%)	1 (3%)	5 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	743/770 (96%)	670 (90%)	65 (9%)	8 (1%)	17 58

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	GLY
2	B	87	ALA
1	A	102	ASN
1	A	130	THR
1	A	369	PHE
2	B	4	GLN
3	C	4	LYS
1	A	400	SER

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	446/462 (96%)	420 (94%)	26 (6%)	25 64
2	B	136/138 (99%)	129 (95%)	7 (5%)	29 67
3	C	26/27 (96%)	22 (85%)	4 (15%)	3 16
All	All	608/627 (97%)	571 (94%)	37 (6%)	23 62

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	TYR
1	A	54	LEU
1	A	76	ASN
1	A	106	MET
1	A	133	TYR
1	A	168	ARG
1	A	215	LEU
1	A	225	ARG

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Mol	Chain	Res	Type
1	A	230	TRP
1	A	254	GLN
1	A	305	VAL
1	A	330	ARG
1	A	339	LEU
1	A	369	PHE
1	A	370	THR
1	A	430	LEU
1	A	439	LEU
1	A	453	ILE
1	A	465	VAL
1	A	472	LEU
1	A	478	LEU
1	A	483	LEU
1	A	517	ASP
1	A	527	ILE
1	A	545	THR
1	A	548	GLN
2	B	11	ILE
2	B	23	LEU
2	B	27	PHE
2	B	37	LEU
2	B	99	GLN
2	B	111	ASP
2	B	146	ARG
3	C	2	GLU
3	C	4	LYS
3	C	13	LEU
3	C	24	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	76	ASN
1	A	254	GLN
1	A	298	HIS
2	B	99	GLN
2	B	122	ASN

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 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
5	HEM	A	800	1	30,50,50	2.13	8 (26%)	24,82,82	2.26	9 (37%)
6	HAS	A	801	-	45,72,72	1.64	7 (15%)	47,109,109	1.87	13 (27%)
7	CUA	B	802	2	0,1,1	0.00	-	0,0,0	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	A	800	1	-	0/10/54/54	0/0/8/8
6	HAS	A	801	-	-	0/30/82/82	0/0/8/8
7	CUA	B	802	2	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C3B-C4B	-6.86	1.45	1.51
5	A	800	HEM	C3D-C4D	-5.08	1.45	1.51
5	A	800	HEM	C2C-C1C	-3.75	1.45	1.52
5	A	800	HEM	C2D-C1D	-2.08	1.45	1.51
5	A	800	HEM	C3C-CAC	2.09	1.55	1.51
5	A	800	HEM	C1C-NC	2.24	1.38	1.36
5	A	800	HEM	FE-NC	2.32	2.05	1.95
5	A	800	HEM	C4C-NC	2.36	1.38	1.36
6	A	801	HAS	C1A-CHA	2.77	1.47	1.39
6	A	801	HAS	C4A-CHD	2.80	1.47	1.39
6	A	801	HAS	C1D-CHB	3.05	1.48	1.39
6	A	801	HAS	C1C-CHC	3.06	1.48	1.39
6	A	801	HAS	C2A-C3A	3.43	1.47	1.37
6	A	801	HAS	C2D-C3D	5.12	1.47	1.40
6	A	801	HAS	C3C-C2C	5.79	1.47	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	801	HAS	C4D-C3D-C2D	-5.62	101.45	107.07
6	A	801	HAS	CAD-CBD-CGD	-4.22	105.02	112.75
5	A	800	HEM	C3B-CAB-CBB	-3.53	119.04	124.46
6	A	801	HAS	C13-C12-C11	-2.98	110.55	114.51
6	A	801	HAS	OMD-CMD-C2D	-2.70	119.66	125.11
6	A	801	HAS	C17-C18-C19	-2.07	123.26	127.76
6	A	801	HAS	C24-C28-C29	-2.07	106.28	111.69
5	A	800	HEM	CBA-CAA-C2A	-2.04	108.86	112.53
5	A	800	HEM	C3B-C4B-CHC	2.19	126.25	123.16
5	A	800	HEM	C2D-C3D-C4D	2.24	105.30	101.50
6	A	801	HAS	C2D-C1D-ND	2.39	112.31	109.21
6	A	801	HAS	CMC-C2C-C3C	2.44	129.87	125.09
6	A	801	HAS	C27-C19-C20	2.48	119.20	115.41
6	A	801	HAS	C26-C15-C16	2.54	119.29	115.41
5	A	800	HEM	CMD-C2D-C3D	2.56	125.68	114.35
6	A	801	HAS	C4B-C3B-C11	2.74	129.98	127.01
6	A	801	HAS	C25-C23-C24	2.75	119.61	115.41
6	A	801	HAS	CAD-C3D-C4D	2.88	130.14	127.01
5	A	800	HEM	CMB-C2B-C3B	3.79	125.98	116.53
5	A	800	HEM	CMC-C2C-C3C	4.07	126.70	116.53
5	A	800	HEM	CAD-C3D-C4D	4.50	128.34	112.47
5	A	800	HEM	CAD-C3D-C2D	4.57	126.36	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	HEM	5	0
6	A	801	HAS	3	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	550/568 (96%)	0.29	42 (7%) 17 18	85, 85, 85, 85	0
2	B	166/168 (98%)	0.17	6 (3%) 46 47	85, 85, 85, 85	0
3	C	33/34 (97%)	0.02	3 (9%) 11 12	85, 85, 85, 85	0
All	All	749/770 (97%)	0.25	51 (6%) 20 22	85, 85, 85, 85	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	SER	5.7
1	A	493	LEU	5.6
1	A	514	GLY	4.8
1	A	515	PRO	4.6
1	A	142	HIS	4.1
1	A	513	SER	3.9
1	A	499	PRO	3.7
1	A	495	ARG	3.6
1	A	497	ARG	3.5
1	A	111	TRP	3.1
1	A	107	TRP	3.1
1	A	177	LYS	3.0
1	A	516	GLU	3.0
1	A	109	SER	3.0
3	C	2	GLU	3.0
2	B	76	PRO	3.0
1	A	555	PRO	3.0
1	A	215	LEU	2.9
1	A	517	ASP	2.8
1	A	503	GLU	2.8
1	A	143	TRP	2.7
1	A	57	ARG	2.7
1	A	218	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	108	LEU	2.6
1	A	422	LEU	2.5
1	A	490	SER	2.5
1	A	330	ARG	2.4
2	B	140	LYS	2.4
1	A	505	PRO	2.4
2	B	141	ARG	2.4
2	B	66	ASP	2.4
3	C	4	LYS	2.4
1	A	178	VAL	2.4
1	A	172	ALA	2.3
1	A	504	ALA	2.3
1	A	173	ALA	2.3
1	A	554	ASN	2.2
1	A	13	GLU	2.2
1	A	412	PRO	2.2
1	A	242	PRO	2.2
1	A	522	LEU	2.2
1	A	106	MET	2.1
1	A	491	VAL	2.1
2	B	77	ASN	2.1
1	A	520	LEU	2.1
1	A	377	ASN	2.1
1	A	529	PHE	2.1
3	C	34	GLY	2.1
1	A	286	ALA	2.1
1	A	416	ALA	2.0
2	B	51	GLU	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, 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
8	XE	A	811	1/1	0.83	0.38	1.14	85,85,85,85	1
5	HEM	A	800	43/43	0.97	0.25	0.31	85,85,85,85	0
8	XE	A	808	1/1	0.86	0.18	-0.07	85,85,85,85	1
6	HAS	A	801	65/65	0.95	0.23	-0.19	85,85,85,85	0
8	XE	A	807	1/1	0.90	0.18	-0.74	85,85,85,85	1
8	XE	A	809	1/1	0.83	0.18	-1.40	85,85,85,85	1
7	CUA	B	802	2/2	0.99	0.11	-1.84	85,85,85,85	0
8	XE	A	805	1/1	0.81	0.11	-2.38	85,85,85,85	0
8	XE	A	806	1/1	0.89	0.12	-2.62	85,85,85,85	1
8	XE	A	810	1/1	0.96	0.19	-	85,85,85,85	1
4	CU	A	803	1/1	0.95	0.10	-	85,85,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.