



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 01:26 am GMT

PDB ID : 3S3D  
Title : Structure of Thermus thermophilus cytochrome ba3 oxidase 480s after Xe de-pressurization  
Authors : Luna, V.M.; Fee, J.A.; Deniz, A.A.; Stout, C.D.  
Deposited on : 2011-05-18  
Resolution : 3.75 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

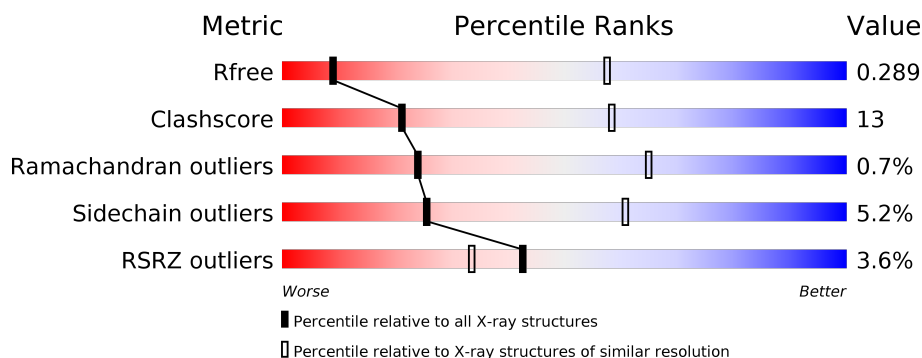
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 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))
$R_{free}$	111664	1140 (4.00-3.52)
Clashscore	122126	1003 (3.98-3.54)
Ramachandran outliers	120053	1172 (4.00-3.52)
Sidechain outliers	120020	1166 (4.00-3.52)
RSRZ outliers	108989	1056 (4.00-3.52)

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  $\geq 3$ , 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	568	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>• •</div> </div> </div>
2	B	166	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>•</div> </div> </div>
3	C	33	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>•</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	XE	A	563	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6063 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	555	Total	C	N	O	S	0	0	0
			4392	2977	705	694	16			

There are 7 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

- 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	216	234	4			

- 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).

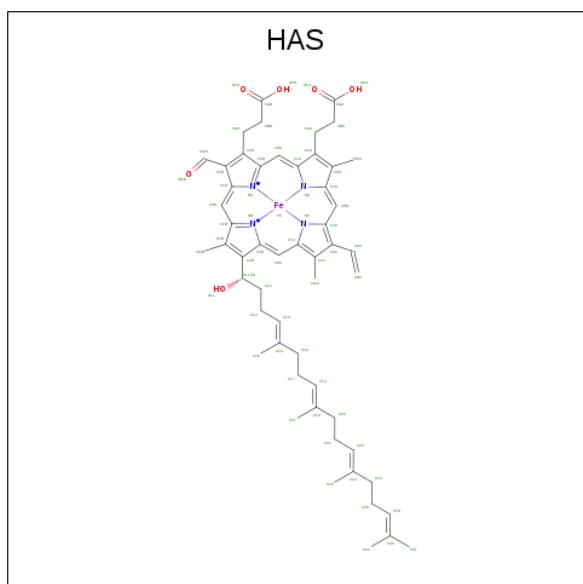
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



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

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

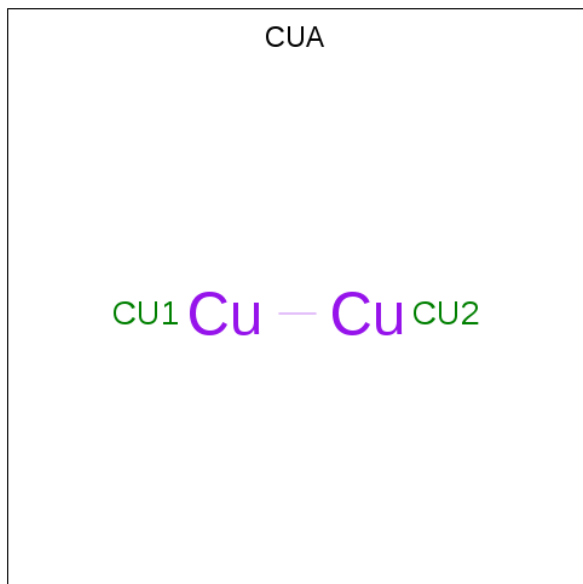


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	
			65	54	1	4	6	

- Molecule 7 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Xe	0	0
			3	3		

- Molecule 8 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).

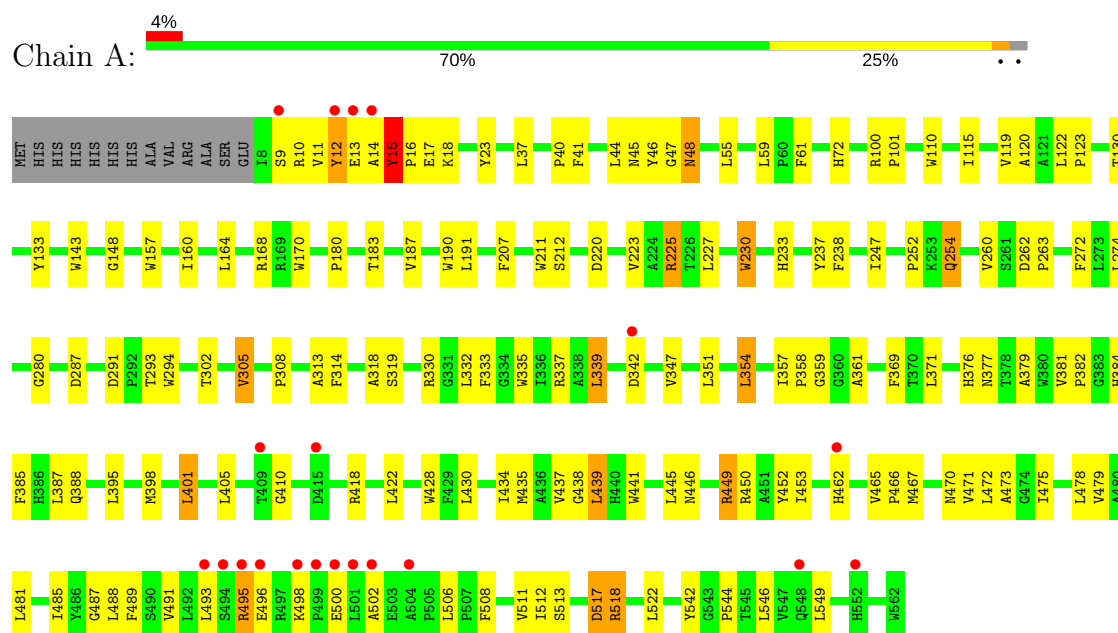


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cu	0	0
			2	2		

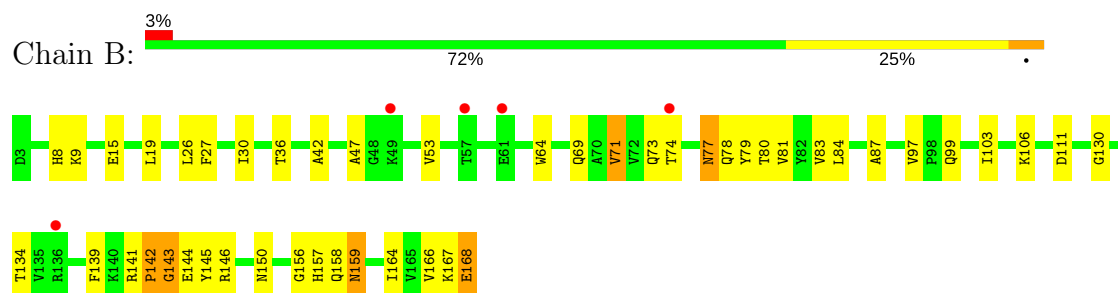
### 3 Residue-property plots [i](#)

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.

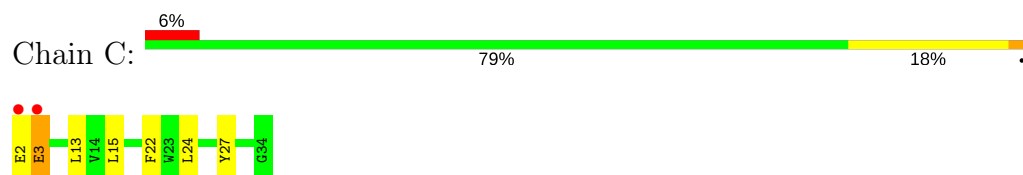
#### • Molecule 1: Cytochrome c oxidase subunit 1



#### • Molecule 2: Cytochrome c oxidase subunit 2



#### • Molecule 3: Cytochrome c oxidase polypeptide 2A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.03Å 110.03Å 170.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.41 – 3.75 50.43 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (92.41-3.75) 99.7 (50.43-3.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.14 (at 3.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.243 , 0.293 0.245 , 0.289	Depositor DCC
$R_{free}$ test set	533 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	91.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 6.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	6063	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 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	0.72	4/4549 (0.1%)	0.65	0/6243
2	B	0.87	4/1335 (0.3%)	0.71	1/1822 (0.1%)
3	C	0.77	0/265	0.60	0/359
All	All	0.75	8/6149 (0.1%)	0.66	1/8424 (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
2	B	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	144	GLU	CB-CG	10.43	1.72	1.52
1	A	15	TYR	CG-CD2	9.07	1.50	1.39
2	B	168	GLU	CD-OE1	8.41	1.34	1.25
1	A	15	TYR	CE2-CZ	7.32	1.48	1.38
2	B	144	GLU	N-CA	6.30	1.58	1.46
1	A	12	TYR	CE2-CZ	5.75	1.46	1.38
1	A	15	TYR	CE1-CZ	5.58	1.45	1.38
2	B	144	GLU	CA-CB	5.26	1.65	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	GLY	C-N-CA	5.41	135.22	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	142	PRO	Peptide

## 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	4392	0	4505	119	17
2	B	1298	0	1280	40	17
3	C	259	0	279	6	0
4	A	1	0	0	0	0
5	A	43	0	30	3	0
6	A	65	0	62	4	0
7	A	3	0	0	2	0
8	B	2	0	0	0	0
All	All	6063	0	6156	159	17

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 13.

All (159) 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:233:HIS:NE2	1:A:237:TYR:HE2	1.14	1.39
1:A:233:HIS:NE2	1:A:237:TYR:CE2	2.06	1.24
2:B:143:GLY:N	2:B:166:VAL:HG23	1.73	1.02
1:A:15:TYR:HB2	1:A:18:LYS:HD2	1.38	1.02
2:B:143:GLY:H	2:B:166:VAL:HG23	1.23	0.96
3:C:2:GLU:HG3	3:C:3:GLU:H	1.33	0.92
2:B:9:LYS:HE2	2:B:9:LYS:HA	1.49	0.91
5:A:800:HEM:HMC2	5:A:800:HEM:HBC2	1.58	0.85
1:A:233:HIS:CE1	1:A:237:TYR:HE2	1.93	0.84
1:A:335:TRP:O	1:A:339:LEU:HD22	1.79	0.82
2:B:97:VAL:HG23	2:B:166:VAL:HG12	1.63	0.80
1:A:357:ILE:HG23	3:C:15:LEU:HD12	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:PHE:HD1	2:B:15:GLU:OE2	1.65	0.79
1:A:233:HIS:HE2	1:A:237:TYR:HE2	1.03	0.78
1:A:518:ARG:HG2	1:A:518:ARG:HH21	1.49	0.77
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.71	0.76
2:B:156:GLY:HA2	2:B:158:GLN:HE22	1.53	0.74
1:A:449:ARG:HH12	6:A:801:HAS:CGA	2.00	0.73
1:A:435:MET:HG2	1:A:439:LEU:CD2	2.18	0.72
1:A:262:ASP:HB2	1:A:511:VAL:HG11	1.72	0.71
1:A:41:PHE:CE2	1:A:55:LEU:HB2	2.26	0.71
1:A:332:LEU:HD23	1:A:333:PHE:CE2	2.26	0.70
1:A:233:HIS:CD2	1:A:237:TYR:HE2	2.08	0.69
2:B:69:GLN:HA	2:B:69:GLN:NE2	2.08	0.68
1:A:314:PHE:CD1	2:B:15:GLU:OE2	2.46	0.68
1:A:15:TYR:CB	1:A:18:LYS:HD2	2.20	0.67
1:A:467:MET:O	1:A:471:VAL:HG23	1.94	0.67
3:C:2:GLU:HG3	3:C:3:GLU:N	2.10	0.65
1:A:489:PHE:O	1:A:493:LEU:HB2	1.97	0.64
1:A:465:VAL:HG23	1:A:466:PRO:HD3	1.80	0.64
1:A:449:ARG:HD2	1:A:450:ARG:HG3	1.79	0.64
5:A:800:HEM:CMC	5:A:800:HEM:HBC2	2.27	0.63
1:A:410:GLY:CA	1:A:502:ALA:HB2	2.28	0.63
1:A:401:LEU:HG	1:A:405:LEU:HD22	1.82	0.61
2:B:9:LYS:HE2	2:B:9:LYS:CA	2.26	0.60
1:A:272:PHE:CZ	1:A:308:PRO:HB2	2.37	0.60
1:A:10:ARG:O	1:A:13:GLU:N	2.34	0.60
1:A:12:TYR:O	1:A:16:PRO:CA	2.50	0.59
1:A:398:MET:O	1:A:401:LEU:HB2	2.02	0.59
1:A:435:MET:HG2	1:A:439:LEU:HD23	1.84	0.59
1:A:302:THR:O	1:A:305:VAL:HG12	2.02	0.58
1:A:262:ASP:HB3	1:A:263:PRO:HD3	1.86	0.58
2:B:106:LYS:HG2	2:B:134:THR:HG23	1.86	0.58
1:A:359:GLY:HA3	1:A:388:GLN:NE2	2.19	0.58
1:A:481:LEU:O	1:A:485:ILE:HG13	2.04	0.56
1:A:44:LEU:O	1:A:47:GLY:N	2.39	0.56
1:A:401:LEU:HD21	1:A:488:LEU:HD13	1.88	0.56
1:A:14:ALA:HA	1:A:100:ARG:NH1	2.20	0.56
1:A:379:ALA:HB1	1:A:439:LEU:HD12	1.87	0.55
1:A:46:TYR:HA	1:A:453:ILE:HD11	1.86	0.55
2:B:97:VAL:O	2:B:167:LYS:N	2.36	0.55
1:A:59:LEU:HD22	1:A:61:PHE:HE1	1.72	0.55
2:B:145:TYR:HE1	2:B:166:VAL:HG21	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:VAL:O	2:B:166:VAL:HA	2.07	0.55
1:A:260:VAL:HG21	1:A:318:ALA:HB3	1.89	0.54
1:A:357:ILE:HG23	3:C:15:LEU:CD1	2.38	0.54
1:A:518:ARG:HG2	1:A:518:ARG:NH2	2.19	0.54
1:A:358:PRO:HB2	1:A:387:LEU:HD13	1.89	0.53
1:A:133:TYR:CE2	7:A:563:XE:XE	3.39	0.53
1:A:291:ASP:OD2	1:A:293:THR:HB	2.09	0.53
2:B:74:THR:HG21	2:B:80:THR:OG1	2.09	0.53
1:A:12:TYR:O	1:A:16:PRO:HA	2.09	0.52
1:A:230:TRP:C	1:A:230:TRP:CD1	2.82	0.52
1:A:437:VAL:O	1:A:441:TRP:HB2	2.09	0.52
1:A:247:ILE:O	1:A:252:PRO:HD3	2.10	0.52
2:B:71:VAL:HG13	2:B:81:VAL:HG22	1.91	0.51
2:B:74:THR:HG23	2:B:78:GLN:OE1	2.10	0.51
2:B:97:VAL:HG23	2:B:166:VAL:CG1	2.38	0.51
1:A:164:LEU:HD21	1:A:191:LEU:HD21	1.92	0.51
1:A:227:LEU:O	1:A:230:TRP:HB3	2.11	0.51
2:B:143:GLY:N	2:B:166:VAL:CG2	2.60	0.50
1:A:465:VAL:HG23	1:A:466:PRO:CD	2.41	0.50
1:A:122:LEU:HB2	1:A:123:PRO:HD3	1.94	0.50
1:A:475:ILE:O	1:A:479:VAL:HG23	2.10	0.50
1:A:72:HIS:CD2	5:A:800:HEM:ND	2.79	0.50
2:B:47:ALA:HB2	2:B:134:THR:HB	1.94	0.50
2:B:139:PHE:CG	2:B:166:VAL:HG11	2.46	0.49
1:A:487:GLY:O	1:A:491:VAL:HG23	2.14	0.48
1:A:48:ASN:HB2	1:A:467:MET:SD	2.54	0.48
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.92	0.48
2:B:27:PHE:HA	2:B:30:ILE:HD12	1.96	0.48
1:A:445:LEU:O	1:A:446:ASN:HB2	2.14	0.48
1:A:207:PHE:O	1:A:211:TRP:HB2	2.14	0.47
1:A:120:ALA:HB2	1:A:148:GLY:HA3	1.97	0.47
1:A:157:TRP:HA	1:A:160:ILE:HD12	1.96	0.47
1:A:225:ARG:HD3	1:A:287:ASP:OD1	2.14	0.47
2:B:69:GLN:HA	2:B:69:GLN:HE21	1.77	0.47
1:A:450:ARG:O	2:B:157:HIS:CD2	2.68	0.47
1:A:170:TRP:CH2	1:A:180:PRO:HD3	2.50	0.46
1:A:130:THR:HG22	1:A:130:THR:O	2.16	0.46
2:B:157:HIS:C	2:B:159:ASN:H	2.18	0.46
1:A:377:ASN:HB3	2:B:150:ASN:O	2.15	0.46
2:B:145:TYR:CE1	2:B:166:VAL:HG21	2.50	0.46
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:THR:O	1:A:187:VAL:HG23	2.17	0.45
6:A:801:HAS:HHC	6:A:801:HAS:H122	1.98	0.45
1:A:227:LEU:HD23	1:A:546:LEU:HD21	1.98	0.45
1:A:16:PRO:HD2	1:A:17:GLU:OE1	2.17	0.45
1:A:495:ARG:HD3	1:A:495:ARG:HA	1.70	0.45
1:A:223:VAL:HG12	1:A:549:LEU:HB3	1.99	0.45
1:A:48:ASN:HA	1:A:48:ASN:HD22	1.63	0.44
2:B:145:TYR:HE1	2:B:166:VAL:CG2	2.31	0.44
2:B:77:ASN:HA	2:B:77:ASN:HD22	1.63	0.44
1:A:12:TYR:O	1:A:16:PRO:N	2.51	0.44
1:A:313:ALA:HB2	6:A:801:HAS:H273	2.00	0.44
1:A:381:VAL:HB	1:A:382:PRO:HD3	2.00	0.44
1:A:506:LEU:HB2	1:A:508:PHE:CE1	2.52	0.44
1:A:143:TRP:HB3	1:A:212:SER:O	2.18	0.44
1:A:225:ARG:HH21	1:A:287:ASP:CG	2.21	0.44
1:A:347:VAL:HG21	1:A:422:LEU:HD21	2.00	0.43
1:A:190:TRP:CZ3	1:A:238:PHE:HE2	2.36	0.43
2:B:141:ARG:HA	2:B:142:PRO:HD2	1.56	0.43
2:B:103:ILE:HD13	2:B:139:PHE:HD1	1.83	0.43
1:A:410:GLY:HA3	1:A:502:ALA:HB2	1.97	0.43
1:A:15:TYR:HA	1:A:17:GLU:OE1	2.18	0.43
1:A:337:ARG:HD2	1:A:337:ARG:HA	1.84	0.43
2:B:69:GLN:CA	2:B:69:GLN:NE2	2.80	0.43
1:A:384:HIS:O	1:A:388:GLN:HG2	2.19	0.43
1:A:361:ALA:HB1	3:C:22:PHE:HB2	2.01	0.43
2:B:69:GLN:CA	2:B:69:GLN:HE21	2.31	0.42
1:A:115:ILE:O	1:A:119:VAL:HG23	2.19	0.42
1:A:9:SER:HB3	1:A:12:TYR:CG	2.54	0.42
1:A:220:ASP:HB3	1:A:223:VAL:HG22	1.99	0.42
1:A:441:TRP:HB3	1:A:466:PRO:HB3	2.01	0.42
1:A:44:LEU:O	1:A:45:ASN:C	2.56	0.42
1:A:376:HIS:ND1	6:A:801:HAS:O1D	2.52	0.42
1:A:351:LEU:O	1:A:354:LEU:HB2	2.19	0.42
1:A:518:ARG:CG	1:A:518:ARG:NH2	2.80	0.42
1:A:225:ARG:NH2	1:A:287:ASP:OD2	2.53	0.42
1:A:23:TYR:HB3	1:A:110:TRP:NE1	2.35	0.42
1:A:254:GLN:HE21	1:A:254:GLN:HA	1.84	0.42
1:A:434:ILE:HG22	1:A:473:ALA:HB2	2.02	0.42
1:A:512:ILE:HG22	2:B:8:HIS:ND1	2.34	0.42
2:B:53:VAL:O	2:B:130:GLY:HA2	2.20	0.42
1:A:9:SER:HB3	1:A:12:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:VAL:HG12	2:B:84:LEU:N	2.35	0.42
1:A:280:GLY:HA3	1:A:542:TYR:OH	2.20	0.41
1:A:37:LEU:O	1:A:40:PRO:HD2	2.21	0.41
1:A:517:ASP:O	1:A:518:ARG:C	2.59	0.41
1:A:371:LEU:HD11	3:C:27:TYR:HD1	1.85	0.41
1:A:17:GLU:HB3	1:A:101:PRO:HD2	2.02	0.41
1:A:438:GLY:HA3	1:A:470:ASN:OD1	2.20	0.41
1:A:465:VAL:N	1:A:466:PRO:HD2	2.35	0.41
2:B:64:TRP:HB3	2:B:84:LEU:HD13	2.02	0.41
2:B:145:TYR:HB2	2:B:164:ILE:HB	2.02	0.41
1:A:498:LYS:HB3	1:A:500:GLU:CD	2.41	0.41
1:A:100:ARG:HA	1:A:101:PRO:HD3	1.91	0.41
1:A:342:ASP:O	1:A:418:ARG:NH2	2.54	0.41
1:A:230:TRP:C	1:A:230:TRP:HD1	2.24	0.41
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.56	0.41
1:A:395:LEU:HD21	1:A:428:TRP:CD1	2.56	0.41
2:B:36:THR:O	2:B:42:ALA:HB2	2.21	0.41
2:B:156:GLY:HA2	2:B:158:GLN:NE2	2.27	0.41
1:A:133:TYR:HE2	7:A:563:XE:XE	2.82	0.40
1:A:164:LEU:HA	1:A:164:LEU:HD23	1.96	0.40
1:A:187:VAL:O	1:A:191:LEU:HG	2.21	0.40
1:A:260:VAL:HG13	1:A:319:SER:HA	2.04	0.40
1:A:358:PRO:HB2	1:A:387:LEU:CD1	2.51	0.40
2:B:73:GLN:HB2	2:B:79:TYR:CE1	2.56	0.40

All (17) 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)
1:A:13:GLU:OE1	2:B:166:VAL:O[3_454]	1.49	0.71
1:A:10:ARG:N	2:B:142:PRO:C[3_454]	1.53	0.67
1:A:10:ARG:CA	2:B:142:PRO:CB[3_454]	1.61	0.59
1:A:10:ARG:N	2:B:142:PRO:CB[3_454]	1.62	0.58
1:A:10:ARG:N	2:B:142:PRO:CA[3_454]	1.70	0.50
1:A:13:GLU:OE1	2:B:166:VAL:C[3_454]	1.80	0.40
1:A:10:ARG:CB	2:B:142:PRO:CB[3_454]	1.85	0.35
1:A:11:VAL:N	2:B:142:PRO:CB[3_454]	1.95	0.25
1:A:10:ARG:NH1	2:B:139:PHE:CB[3_454]	1.96	0.24
1:A:11:VAL:O	2:B:168:GLU:OE1[3_454]	1.96	0.24
1:A:10:ARG:CB	2:B:142:PRO:CA[3_454]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:CD	2:B:99:GLN:CB[3_454]	2.02	0.18
1:A:10:ARG:C	2:B:142:PRO:CB[3_454]	2.05	0.15
1:A:15:TYR:CD2	2:B:168:GLU:OE2[3_454]	2.07	0.13
1:A:10:ARG:N	2:B:143:GLY:N[3_454]	2.09	0.11
1:A:10:ARG:CA	2:B:142:PRO:CA[3_454]	2.13	0.07
1:A:10:ARG:NH2	2:B:139:PHE:CB[3_454]	2.17	0.03

## 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	553/568 (97%)	514 (93%)	35 (6%)	4 (1%)	24	65
2	B	164/166 (99%)	151 (92%)	12 (7%)	1 (1%)	27	67
3	C	31/33 (94%)	29 (94%)	2 (6%)	0	100	100
All	All	748/767 (98%)	694 (93%)	49 (7%)	5 (1%)	24	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	ARG
1	A	496	GLU
1	A	518	ARG
2	B	87	ALA
1	A	517	ASP

### 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	451/462 (98%)	429 (95%)	22 (5%)	27	62
2	B	136/136 (100%)	129 (95%)	7 (5%)	26	61
3	C	26/26 (100%)	23 (88%)	3 (12%)	6	31
All	All	613/624 (98%)	581 (95%)	32 (5%)	25	61

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	TYR
1	A	48	ASN
1	A	168	ARG
1	A	225	ARG
1	A	230	TRP
1	A	254	GLN
1	A	274	LEU
1	A	305	VAL
1	A	339	LEU
1	A	354	LEU
1	A	369	PHE
1	A	401	LEU
1	A	430	LEU
1	A	439	LEU
1	A	449	ARG
1	A	452	TYR
1	A	462	HIS
1	A	472	LEU
1	A	478	LEU
1	A	495	ARG
1	A	513	SER
1	A	522	LEU
2	B	19	LEU
2	B	26	LEU
2	B	71	VAL
2	B	77	ASN
2	B	111	ASP
2	B	146	ARG
2	B	159	ASN
3	C	3	GLU
3	C	13	LEU
3	C	24	LEU



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	48	ASN
1	A	76	ASN
1	A	254	GLN
1	A	298	HIS
1	A	388	GLN
1	A	554	ASN
2	B	69	GLN
2	B	77	ASN
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 7 ligands modelled in this entry, 4 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	27,50,50	2.21	6 (22%)	17,82,82	1.75	3 (17%)
6	HAS	A	801	1	56,72,72	4.03	17 (30%)	49,109,109	2.75	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	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	-	0/6/54/54	0/0/8/8
6	HAS	A	801	1	-	0/35/122/122	0/0/8/8
8	CUA	B	802	2	-	0/0/0/0	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	C1B-NB	-10.80	1.34	1.49
6	A	801	HAS	C4B-NB	-10.47	1.34	1.49
6	A	801	HAS	C1D-ND	-9.87	1.35	1.49
6	A	801	HAS	C4D-ND	-9.72	1.35	1.49
6	A	801	HAS	C1D-C2D	-8.21	1.38	1.51
5	A	800	HEM	C3C-C2C	-5.18	1.33	1.40
5	A	800	HEM	C3B-C2B	-5.04	1.33	1.40
6	A	801	HAS	CHD-C4A	-4.37	1.46	1.51
6	A	801	HAS	CHD-C4C	-3.61	1.47	1.51
6	A	801	HAS	CHA-C4D	-3.04	1.47	1.53
6	A	801	HAS	CHC-C4B	-2.56	1.48	1.53
6	A	801	HAS	FE-NA	2.04	2.10	1.95
5	A	800	HEM	CAA-C2A	2.34	1.55	1.52
6	A	801	HAS	C2A-C3A	2.84	1.46	1.37
5	A	800	HEM	C3C-CAC	3.54	1.54	1.47
5	A	800	HEM	C3B-CAB	3.56	1.55	1.47
6	A	801	HAS	C3C-C2C	4.84	1.47	1.40
5	A	800	HEM	C3D-C2D	4.97	1.52	1.37
6	A	801	HAS	C2B-C3B	5.49	1.39	1.34
6	A	801	HAS	C4A-C3A	7.47	1.48	1.38
6	A	801	HAS	C1C-C2C	8.45	1.49	1.38
6	A	801	HAS	C1A-C2A	8.49	1.49	1.38
6	A	801	HAS	C3D-C2D	9.28	1.45	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	CHD-C4A-C3A	-5.37	120.55	129.53
6	A	801	HAS	CHD-C4C-C3C	-5.06	122.97	129.61
6	A	801	HAS	OMD-CMD-C2D	-4.95	118.24	124.28
5	A	800	HEM	CAD-CBD-CGD	-4.08	105.69	112.66
6	A	801	HAS	CHC-C1C-C2C	-4.02	122.48	129.45
6	A	801	HAS	CAA-CBA-CGA	-3.38	106.89	112.66
5	A	800	HEM	C1D-C2D-C3D	-3.31	104.69	107.00
6	A	801	HAS	CAD-CBD-CGD	-3.11	107.35	112.66
6	A	801	HAS	C4A-C3A-C2A	-2.86	102.54	105.81
6	A	801	HAS	C13-C12-C11	-2.78	110.25	114.46
5	A	800	HEM	CBD-CAD-C3D	-2.45	107.80	112.47
6	A	801	HAS	C1A-C2A-C3A	-2.29	102.52	105.93
6	A	801	HAS	C24-C28-C29	-2.19	104.55	111.87
6	A	801	HAS	CMB-C2B-C1B	2.64	127.94	120.24
6	A	801	HAS	C26-C15-C16	2.65	119.86	115.29
6	A	801	HAS	CMC-C2C-C3C	2.70	129.80	124.88
6	A	801	HAS	C25-C23-C24	2.75	120.03	115.29
6	A	801	HAS	CHB-C1B-C2B	3.19	124.64	114.70
6	A	801	HAS	C1B-CHB-C1D	3.91	128.04	116.30
6	A	801	HAS	CAD-C3D-C4D	4.48	131.44	122.48
6	A	801	HAS	CAA-C2A-C1A	4.51	130.46	127.30
6	A	801	HAS	CHA-C4D-ND	5.28	120.71	110.75
6	A	801	HAS	CHC-C4B-NB	5.55	121.21	110.75
6	A	801	HAS	C4A-CHD-C4C	6.15	127.06	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	HEM	3	0
6	A	801	HAS	4	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	555/568 (97%)	-0.17	20 (3%) 42 33	61, 61, 61, 61	0
2	B	166/166 (100%)	0.03	5 (3%) 50 38	61, 61, 61, 61	0
3	C	33/33 (100%)	-0.50	2 (6%) 21 15	61, 61, 61, 61	0
All	All	754/767 (98%)	-0.14	27 (3%) 42 33	61, 61, 61, 61	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	502	ALA	5.2
1	A	498	LYS	4.4
1	A	501	LEU	3.8
1	A	9	SER	3.8
3	C	2	GLU	3.7
1	A	499	PRO	3.3
1	A	500	GLU	3.1
2	B	61	GLU	3.1
1	A	14	ALA	3.1
1	A	342	ASP	3.0
1	A	548	GLN	3.0
2	B	136	ARG	2.9
1	A	494	SER	2.8
3	C	3	GLU	2.7
2	B	57	THR	2.5
1	A	552	HIS	2.5
1	A	415	ASP	2.4
1	A	409	THR	2.4
1	A	12	TYR	2.4
1	A	462	HIS	2.3
1	A	495	ARG	2.3
1	A	493	LEU	2.2
1	A	13	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	504	ALA	2.2
2	B	49	LYS	2.2
1	A	496	GLU	2.1
2	B	74	THR	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
7	XE	A	565	1/1	0.88	0.62	61,61,61,61	1
4	CU	A	803	1/1	0.93	0.20	61,61,61,61	0
6	HAS	A	801	65/65	0.94	0.28	61,61,61,61	0
5	HEM	A	800	43/43	0.96	0.23	61,61,61,61	0
7	XE	A	563	1/1	0.96	0.58	61,61,61,61	1
7	XE	A	564	1/1	0.97	0.23	61,61,61,61	1
8	CUA	B	802	2/2	0.99	0.09	61,61,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.