



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:33 AM GMT

PDB ID : 3S3A  
Title : Structure of Thermus thermophilus cytochrome ba3 oxidase 120s after Xe de-pressurization  
Authors : Luna, V.M.; Fee, J.A.; Deniz, A.A.; Stout, C.D.  
Deposited on : 2011-05-18  
Resolution : 4.25 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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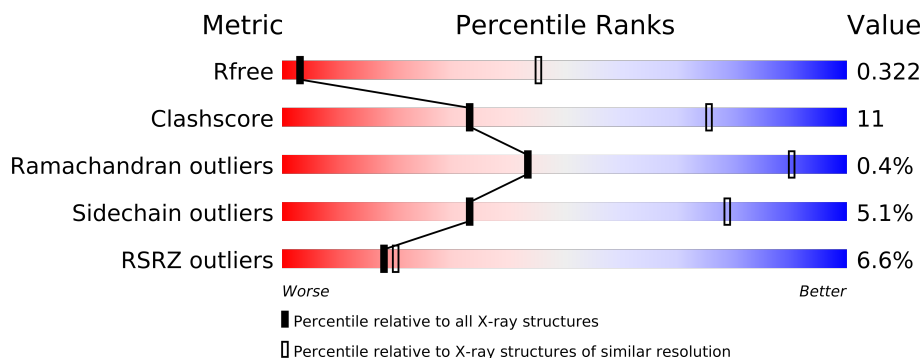
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 4.25 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))
$R_{free}$	66092	1013 (5.02-3.50)
Clashscore	79885	1277 (5.02-3.50)
Ramachandran outliers	78287	1208 (5.02-3.50)
Sidechain outliers	78261	1190 (5.02-3.50)
RSRZ outliers	66119	1013 (5.02-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	568	
2	B	166	
3	C	33	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6056 atoms, of which 0 are hydrogen and 0 are deuterium.

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	554	Total	C	N	O	S	0	0	0
			4384	2971	704	693	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).

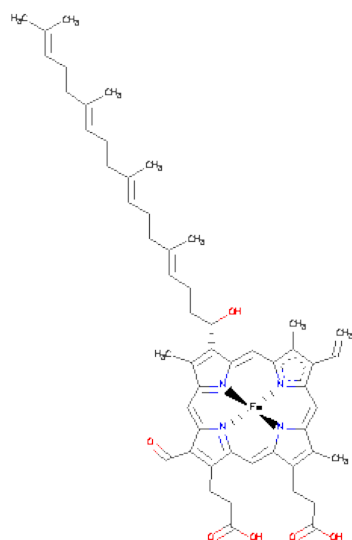
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- 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
			Total	C	Fe	N	O		
5	A	1	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
			Total	C	Fe	N	O		
6	A	1	65	54	1	4	6	0	0

- Molecule 7 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

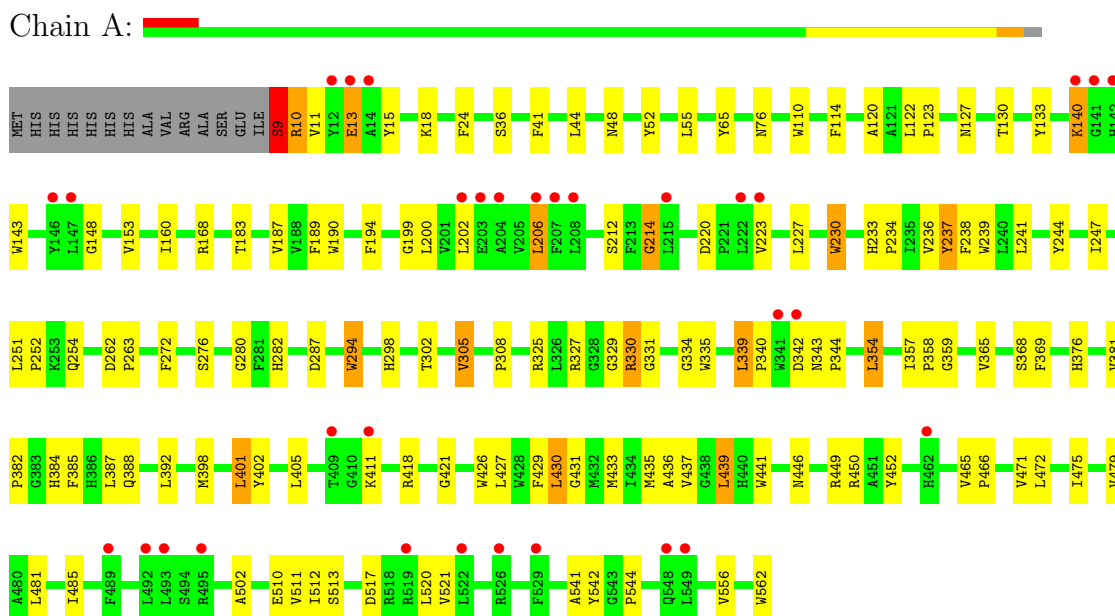
- Molecule 8 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total 4	Xe 4	0	0

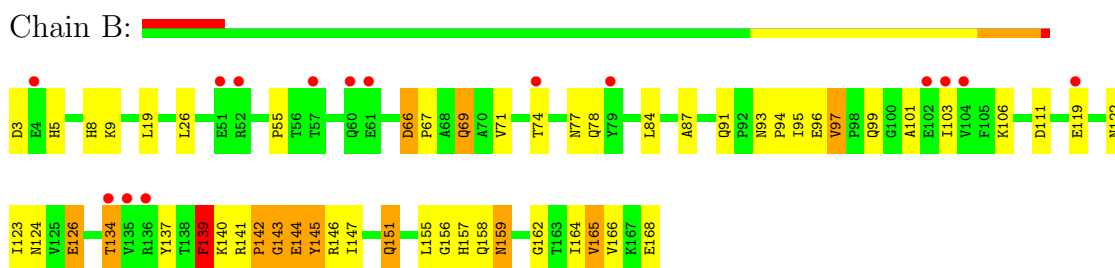
### 3 Residue-property plots

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



#### • 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, $\alpha$ , $\beta$ , $\gamma$	110.29Å 110.29Å 170.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.57 – 4.25 55.15 – 4.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (92.57-4.25) 99.7 (55.15-4.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.79 (at 4.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.279 , 0.330 0.276 , 0.322	Depositor DCC
$R_{free}$ test set	361 reflections (4.82%)	DCC
Wilson B-factor (Å <sup>2</sup> )	146.8	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 38.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 7844 reflections (0.013%)	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	6056	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	1.04	11/4541 (0.2%)	0.71	9/6232 (0.1%)
2	B	1.16	14/1335 (1.0%)	0.80	8/1822 (0.4%)
3	C	0.63	0/265	0.55	0/359
All	All	1.06	25/6141 (0.4%)	0.73	17/8413 (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	2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	GLU	CD-OE1	32.90	1.61	1.25
1	A	510	GLU	CD-OE1	28.14	1.56	1.25
2	B	165	VAL	CB-CG1	16.12	1.86	1.52
1	A	140	LYS	CE-NZ	13.79	1.83	1.49
2	B	168	GLU	CD-OE2	10.60	1.37	1.25
1	A	214	GLY	C-O	9.73	1.39	1.23
1	A	9	SER	C-N	9.72	1.56	1.34
2	B	143	GLY	N-CA	9.43	1.60	1.46
2	B	144	GLU	CD-OE2	9.13	1.35	1.25
2	B	144	GLU	C-O	8.77	1.40	1.23
2	B	145	TYR	CZ-OH	7.79	1.51	1.37
1	A	15	TYR	CZ-OH	6.55	1.49	1.37
2	B	146	ARG	CZ-NH2	6.37	1.41	1.33
1	A	510	GLU	CG-CD	6.29	1.61	1.51
2	B	144	GLU	N-CA	6.12	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	TYR	CE2-CZ	6.08	1.46	1.38
2	B	151	GLN	CD-NE2	-5.83	1.18	1.32
1	A	9	SER	CA-C	5.79	1.68	1.52
1	A	9	SER	CB-OG	5.61	1.49	1.42
2	B	144	GLU	CA-C	5.18	1.66	1.52
2	B	144	GLU	CG-CD	5.18	1.59	1.51
2	B	126	GLU	CD-OE1	5.15	1.31	1.25
2	B	140	LYS	C-O	5.10	1.33	1.23
2	B	3	ASP	CG-OD1	5.08	1.37	1.25
1	A	411	LYS	CE-NZ	5.05	1.61	1.49

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	ARG	NE-CZ-NH1	-14.15	113.22	120.30
1	A	206	LEU	CB-CG-CD2	8.95	126.22	111.00
1	A	9	SER	O-C-N	-8.74	108.71	122.70
1	A	10	ARG	NE-CZ-NH2	7.85	124.22	120.30
1	A	327	ARG	NH1-CZ-NH2	6.86	126.95	119.40
1	A	9	SER	C-N-CA	6.82	138.76	121.70
1	A	294	TRP	CD1-NE1-CE2	6.57	114.91	109.00
2	B	144	GLU	N-CA-C	6.35	128.14	111.00
2	B	143	GLY	N-CA-C	6.14	128.46	113.10
2	B	3	ASP	CB-CG-OD1	-6.09	112.82	118.30
2	B	165	VAL	CA-CB-CG1	6.00	119.90	110.90
2	B	146	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	13	GLU	OE1-CD-OE2	-5.53	116.67	123.30
2	B	139	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	A	114	PHE	CG-CD2-CE2	-5.40	114.86	120.80
2	B	165	VAL	CA-CB-CG2	-5.31	102.93	110.90
2	B	66	ASP	CB-CG-OD1	5.27	123.05	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	GLY	Mainchain
1	A	9	SER	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4384	0	4494	95	24
2	B	1298	0	1280	37	24
3	C	259	0	279	13	0
4	A	1	0	0	0	0
5	A	43	0	30	2	0
6	A	65	0	62	8	0
7	B	2	0	0	0	0
8	A	4	0	0	0	0
All	All	6056	0	6145	135	24

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (135) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:357:ILE:CG1	1:A:357:ILE:CD1	1.75	1.63
6:A:801:HAS:C12	6:A:801:HAS:C13	1.75	1.60
2:B:165:VAL:CB	2:B:165:VAL:CG1	1.86	1.54
1:A:140:LYS:CE	1:A:140:LYS:NZ	1.83	1.41
1:A:262:ASP:HB2	1:A:511:VAL:HG11	1.43	1.00
1:A:562:TRP:HA	2:B:155:LEU:HG	1.55	0.87
6:A:801:HAS:C12	6:A:801:HAS:C14	2.55	0.84
3:C:2:GLU:HG3	3:C:3:GLU:H	1.45	0.81
1:A:233:HIS:NE2	1:A:237:TYR:HE2	1.80	0.80
1:A:233:HIS:NE2	1:A:237:TYR:CE2	2.51	0.77
1:A:357:ILE:HG23	3:C:15:LEU:HD12	1.70	0.73
1:A:233:HIS:HE2	1:A:237:TYR:HE2	1.38	0.72
6:A:801:HAS:C11	6:A:801:HAS:C13	2.67	0.70
1:A:376:HIS:HB3	2:B:124:ASN:ND2	2.06	0.70
1:A:449:ARG:HH12	6:A:801:HAS:CGA	2.04	0.70
1:A:18:LYS:HE2	1:A:502:ALA:O	1.91	0.69
2:B:97:VAL:HG23	2:B:166:VAL:HG12	1.73	0.69
1:A:357:ILE:CB	1:A:357:ILE:CD1	2.71	0.68
1:A:263:PRO:HB3	1:A:520:LEU:HD23	1.77	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:165:VAL:CG2	2:B:165:VAL:CG1	2.70	0.66
1:A:365:VAL:HG11	3:C:26:VAL:HG21	1.77	0.66
1:A:52:TYR:CZ	1:A:65:TYR:HD1	2.13	0.66
2:B:69:GLN:HA	2:B:69:GLN:HE21	1.61	0.65
1:A:446:ASN:OD1	2:B:119:GLU:HG3	1.97	0.64
2:B:106:LYS:HG2	2:B:134:THR:HG23	1.80	0.64
1:A:354:LEU:HA	1:A:357:ILE:HD12	1.80	0.63
2:B:69:GLN:HA	2:B:69:GLN:NE2	2.14	0.63
1:A:160:ILE:HG12	1:A:190:TRP:HB3	1.81	0.61
1:A:241:LEU:HA	1:A:244:TYR:HB2	1.83	0.60
1:A:302:THR:O	1:A:305:VAL:HG12	2.02	0.60
1:A:220:ASP:HB3	1:A:223:VAL:HG22	1.84	0.60
1:A:227:LEU:O	1:A:230:TRP:HB3	2.03	0.59
2:B:69:GLN:CA	2:B:69:GLN:HE21	2.15	0.58
1:A:325:ARG:HA	1:A:329:GLY:H	1.67	0.58
1:A:359:GLY:HA3	1:A:388:GLN:NE2	2.19	0.57
2:B:122:ASN:HD21	3:C:33:ARG:HB2	1.69	0.57
1:A:122:LEU:HB2	1:A:123:PRO:HD3	1.87	0.57
2:B:9:LYS:HE2	2:B:9:LYS:HA	1.86	0.57
2:B:147:ILE:HD11	2:B:164:ILE:HG13	1.86	0.57
1:A:233:HIS:O	1:A:236:VAL:HG22	2.06	0.55
3:C:2:GLU:HG3	3:C:3:GLU:N	2.20	0.55
1:A:294:TRP:CZ2	1:A:544:PRO:HB2	2.42	0.55
1:A:357:ILE:HG23	3:C:15:LEU:CD1	2.37	0.54
5:A:800:HEM:HBC2	5:A:800:HEM:HMC2	1.89	0.54
1:A:398:MET:O	1:A:401:LEU:HB2	2.08	0.54
1:A:52:TYR:CZ	1:A:65:TYR:CD1	2.96	0.53
1:A:272:PHE:CZ	1:A:308:PRO:HB2	2.43	0.53
1:A:127:ASN:HD21	1:A:562:TRP:HD1	1.56	0.53
2:B:123:ILE:HD11	2:B:137:TYR:CD1	2.44	0.53
1:A:230:TRP:C	1:A:230:TRP:CD1	2.83	0.53
1:A:272:PHE:O	1:A:276:SER:OG	2.19	0.52
3:C:4:LYS:HE3	3:C:6:LYS:HG2	1.91	0.52
1:A:44:LEU:HD23	1:A:471:VAL:HA	1.92	0.52
1:A:365:VAL:HG22	3:C:23:TRP:HA	1.91	0.52
1:A:450:ARG:NH2	2:B:151:GLN:OE1	2.41	0.52
1:A:140:LYS:HE3	1:A:212:SER:HA	1.92	0.51
1:A:335:TRP:O	1:A:339:LEU:HD22	2.10	0.51
1:A:298:HIS:CE1	1:A:541:ALA:HB1	2.46	0.51
1:A:127:ASN:ND2	1:A:562:TRP:HD1	2.09	0.51
1:A:381:VAL:HB	1:A:382:PRO:HD3	1.93	0.50
1:A:236:VAL:HG11	6:A:801:HAS:HHD	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:282:HIS:CD2	6:A:801:HAS:CMD	2.95	0.50
1:A:189:PHE:CZ	1:A:238:PHE:CD2	3.00	0.50
1:A:153:VAL:HG11	1:A:200:LEU:HD23	1.93	0.50
1:A:450:ARG:O	2:B:157:HIS:CD2	2.64	0.49
3:C:20:LEU:O	3:C:24:LEU:HB2	2.13	0.49
5:A:800:HEM:HBC2	5:A:800:HEM:CMC	2.43	0.49
1:A:24:PHE:CE1	1:A:110:TRP:HB2	2.47	0.49
1:A:280:GLY:HA3	1:A:542:TYR:OH	2.12	0.49
1:A:354:LEU:HA	1:A:357:ILE:CD1	2.43	0.48
1:A:441:TRP:HB3	1:A:466:PRO:HB3	1.95	0.48
1:A:465:VAL:HG23	1:A:466:PRO:HD3	1.95	0.48
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.95	0.48
1:A:247:ILE:HD11	1:A:392:LEU:HD11	1.96	0.48
1:A:387:LEU:HD21	1:A:436:ALA:HB2	1.96	0.48
2:B:74:THR:HG23	2:B:78:GLN:OE1	2.13	0.47
2:B:84:LEU:HB3	2:B:91:GLN:HB3	1.97	0.47
2:B:157:HIS:C	2:B:159:ASN:H	2.18	0.47
3:C:2:GLU:CG	3:C:3:GLU:H	2.20	0.47
2:B:139:PHE:CD2	2:B:145:TYR:CE1	3.03	0.46
1:A:183:THR:O	1:A:187:VAL:HG23	2.15	0.46
1:A:202:LEU:O	1:A:206:LEU:HB2	2.14	0.46
2:B:122:ASN:ND2	3:C:33:ARG:HB2	2.30	0.46
1:A:120:ALA:HB2	1:A:148:GLY:HA3	1.98	0.46
1:A:330:ARG:HB2	1:A:334:GLY:HA3	1.98	0.46
1:A:384:HIS:O	1:A:388:GLN:HG2	2.16	0.45
2:B:141:ARG:HG3	2:B:142:PRO:HD2	1.98	0.45
1:A:130:THR:HB	1:A:562:TRP:CG	2.51	0.45
1:A:294:TRP:HZ2	1:A:544:PRO:HB2	1.80	0.45
1:A:251:LEU:N	1:A:252:PRO:CD	2.80	0.45
3:C:9:LEU:HD23	3:C:12:ILE:HD11	1.99	0.45
1:A:254:GLN:NE2	1:A:343:ASN:HD21	2.14	0.44
1:A:325:ARG:HA	1:A:329:GLY:N	2.31	0.44
1:A:357:ILE:HB	1:A:358:PRO:HD3	1.98	0.44
1:A:199:GLY:HA3	1:A:230:TRP:CG	2.53	0.44
1:A:429:PHE:O	1:A:433:MET:HG2	2.17	0.44
2:B:66:ASP:HA	2:B:67:PRO:HD3	1.77	0.44
2:B:147:ILE:HB	2:B:162:GLY:HA3	2.00	0.44
1:A:287:ASP:OD2	2:B:126:GLU:HG3	2.18	0.44
1:A:437:VAL:O	1:A:441:TRP:HB2	2.18	0.43
1:A:233:HIS:H	1:A:234:PRO:HD2	1.82	0.43
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.53	0.43
2:B:93:ASN:HA	2:B:94:PRO:HA	1.75	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:401:LEU:HG	1:A:405:LEU:HD22	2.00	0.43
1:A:41:PHE:CZ	1:A:55:LEU:HD13	2.53	0.43
1:A:143:TRP:HA	1:A:212:SER:HB2	2.01	0.43
2:B:139:PHE:HD2	2:B:145:TYR:CE1	2.37	0.43
1:A:402:TYR:OH	1:A:421:GLY:HA3	2.18	0.43
1:A:426:TRP:O	1:A:430:LEU:HB2	2.19	0.43
1:A:343:ASN:HA	1:A:344:PRO:HD2	1.94	0.42
2:B:96:GLU:HA	2:B:165:VAL:O	2.19	0.42
1:A:435:MET:HG2	1:A:439:LEU:CD2	2.50	0.42
1:A:262:ASP:HB2	1:A:511:VAL:CG1	2.32	0.42
2:B:69:GLN:CA	2:B:69:GLN:NE2	2.78	0.42
2:B:156:GLY:HA2	2:B:158:GLN:HE22	1.84	0.42
1:A:384:HIS:CE1	6:A:801:HAS:CHC	3.03	0.42
2:B:97:VAL:O	2:B:166:VAL:HA	2.20	0.42
1:A:339:LEU:HB3	1:A:340:PRO:CD	2.49	0.42
1:A:254:GLN:NE2	1:A:343:ASN:ND2	2.68	0.41
1:A:41:PHE:CE1	1:A:55:LEU:HD13	2.55	0.41
1:A:517:ASP:O	1:A:521:VAL:HG23	2.20	0.41
2:B:165:VAL:CG1	2:B:165:VAL:HB	2.26	0.41
1:A:385:PHE:CE2	6:A:801:HAS:HAA1	2.56	0.41
2:B:95:ILE:O	2:B:165:VAL:N	2.39	0.41
1:A:368:SER:OG	3:C:23:TRP:NE1	2.48	0.41
1:A:512:ILE:CG2	2:B:8:HIS:HB2	2.50	0.41
1:A:427:LEU:O	1:A:431:GLY:N	2.43	0.41
1:A:481:LEU:O	1:A:485:ILE:HG13	2.20	0.41
1:A:236:VAL:HA	1:A:239:TRP:CE3	2.57	0.40
1:A:325:ARG:HA	1:A:329:GLY:HA3	2.03	0.40
1:A:342:ASP:O	1:A:418:ARG:NH2	2.52	0.40
1:A:475:ILE:O	1:A:479:VAL:HG23	2.21	0.40
2:B:99:GLN:C	2:B:101:ALA:H	2.23	0.40
2:B:97:VAL:HG11	2:B:103:ILE:HG12	2.03	0.40
1:A:556:VAL:CG1	2:B:55:PRO:HG3	2.52	0.40

All (24) 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	Distance(Å)	Clash(Å)
1:A:9:SER:C	2:B:143:GLY:N[4_445]	1.17	1.03
1:A:9:SER:O	2:B:143:GLY:CA[4_445]	1.44	0.76
1:A:9:SER:C	2:B:143:GLY:CA[4_445]	1.45	0.75
1:A:10:ARG:N	2:B:143:GLY:N[4_445]	1.57	0.63
1:A:9:SER:CA	2:B:143:GLY:CA[4_445]	1.59	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:13:GLU:OE2	2:B:165:VAL:CG1[4_445]	1.65	0.55
1:A:9:SER:O	2:B:143:GLY:C[4_445]	1.78	0.42
1:A:9:SER:CB	2:B:143:GLY:CA[4_445]	1.79	0.41
1:A:11:VAL:N	2:B:142:PRO:CB[4_445]	1.83	0.37
1:A:9:SER:CA	2:B:143:GLY:N[4_445]	1.85	0.35
1:A:9:SER:O	2:B:143:GLY:O[4_445]	1.85	0.35
1:A:9:SER:O	2:B:143:GLY:N[4_445]	1.89	0.31
1:A:10:ARG:NH1	2:B:139:PHE:CB[4_445]	2.02	0.18
1:A:13:GLU:CD	2:B:165:VAL:CG1[4_445]	2.02	0.18
1:A:9:SER:C	2:B:143:GLY:C[4_445]	2.03	0.17
1:A:9:SER:OG	2:B:142:PRO:O[4_445]	2.03	0.17
1:A:10:ARG:N	2:B:142:PRO:C[4_445]	2.04	0.16
1:A:13:GLU:OE2	2:B:165:VAL:CB[4_445]	2.08	0.12
1:A:9:SER:N	2:B:144:GLU:N[4_445]	2.11	0.09
1:A:9:SER:N	2:B:143:GLY:C[4_445]	2.13	0.07
1:A:13:GLU:OE2	2:B:165:VAL:CA[4_445]	2.15	0.05
1:A:9:SER:CA	2:B:142:PRO:C[4_445]	2.17	0.03
1:A:9:SER:CA	2:B:142:PRO:O[4_445]	2.18	0.02
1:A:13:GLU:OE2	2:B:165:VAL:C[4_445]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	552/568 (97%)	516 (94%)	34 (6%)	2 (0%)	43	90
2	B	164/166 (99%)	152 (93%)	11 (7%)	1 (1%)	33	86
3	C	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
All	All	747/767 (97%)	698 (93%)	46 (6%)	3 (0%)	43	90

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	GLY
1	A	330	ARG

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Mol	Chain	Res	Type
2	B	87	ALA

### 5.3.2 Protein sidechains ⓘ

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	450/462 (97%)	433 (96%)	17 (4%)	44	85
2	B	136/136 (100%)	124 (91%)	12 (9%)	14	58
3	C	26/26 (100%)	24 (92%)	2 (8%)	18	64
All	All	612/624 (98%)	581 (95%)	31 (5%)	33	79

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	36	SER
1	A	48	ASN
1	A	76	ASN
1	A	133	TYR
1	A	168	ARG
1	A	230	TRP
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	452	TYR
1	A	472	LEU
1	A	513	SER
2	B	5	HIS
2	B	19	LEU
2	B	26	LEU
2	B	69	GLN
2	B	71	VAL

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Mol	Chain	Res	Type
2	B	77	ASN
2	B	97	VAL
2	B	111	ASP
2	B	134	THR
2	B	139	PHE
2	B	142	PRO
2	B	159	ASN
3	C	3	GLU
3	C	13	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) 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	554	ASN
2	B	69	GLN
2	B	77	ASN
2	B	122	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 8 ligands modelled in this entry, 5 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	49,50,50	2.49	14 (28%)	46,82,82	1.91	5 (10%)
6	HAS	A	801	1	72,72,72	3.68	29 (40%)	86,109,109	5.12	42 (48%)
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	-	0/14/114/114	0/0/8/8
6	HAS	A	801	1	-	0/36/82/82	0/0/8/8
7	CUA	B	802	2	-	0/0/0/0	0/0/0/0

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	C1C-C2C	12.09	1.55	1.40
6	A	801	HAS	CMC-C2C	10.30	1.73	1.51
6	A	801	HAS	C4C-C3C	9.49	1.53	1.41
6	A	801	HAS	C3C-C2C	7.91	1.55	1.41
6	A	801	HAS	C4D-CHA	7.73	1.62	1.38
6	A	801	HAS	C2D-C3D	6.97	1.53	1.41
6	A	801	HAS	C4A-C3A	6.91	1.48	1.40
6	A	801	HAS	C12-C13	6.34	1.75	1.53
6	A	801	HAS	C2A-C3A	5.97	1.55	1.37
6	A	801	HAS	C1D-CHB	5.94	1.56	1.39
5	A	800	HEM	C3D-C4D	5.92	1.46	1.44
6	A	801	HAS	O1A-CGA	5.57	1.42	1.22
6	A	801	HAS	C1A-C2A	5.45	1.52	1.43
6	A	801	HAS	C3B-C11	5.45	1.57	1.52
5	A	800	HEM	C3D-C2D	5.45	1.53	1.43
5	A	800	HEM	C3B-C2B	-5.42	1.34	1.43
5	A	800	HEM	C3C-C2C	-5.34	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C2D-C1D	5.02	1.45	1.44
6	A	801	HAS	C1B-CHB	4.83	1.53	1.38
6	A	801	HAS	C2D-C1D	4.83	1.48	1.40
5	A	800	HEM	C3C-CAC	4.81	1.55	1.40
5	A	800	HEM	C3B-CAB	4.58	1.54	1.40
6	A	801	HAS	FE-NA	4.47	2.11	1.92
5	A	800	HEM	C4A-C3A	4.40	1.45	1.40
6	A	801	HAS	FE-NB	4.34	2.11	1.92
5	A	800	HEM	C2B-C1B	3.77	1.45	1.44
6	A	801	HAS	O11-C11	3.71	1.51	1.42
6	A	801	HAS	FE-ND	3.60	2.07	1.92
6	A	801	HAS	C3B-C2B	3.38	1.53	1.40
5	A	800	HEM	FE-NA	3.32	2.06	1.92
6	A	801	HAS	C4B-CHC	-3.00	1.29	1.38
6	A	801	HAS	C3C-CAC	2.94	1.53	1.48
5	A	800	HEM	CMC-C2C	2.73	1.55	1.47
5	A	800	HEM	FE-ND	2.71	2.07	1.97
6	A	801	HAS	C14-C15	2.62	1.38	1.32
5	A	800	HEM	CMD-C2D	2.62	1.55	1.47
5	A	800	HEM	CMB-C2B	2.54	1.55	1.47
6	A	801	HAS	C4B-NB	-2.27	1.33	1.37
6	A	801	HAS	C1A-CHA	2.23	1.46	1.39
6	A	801	HAS	O1D-CGD	2.22	1.30	1.22
6	A	801	HAS	C4C-NC	-2.16	1.34	1.37
6	A	801	HAS	C1B-C2B	2.16	1.50	1.43
6	A	801	HAS	C2D-CMD	2.05	1.51	1.46

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	C4B-C3B-C2B	-23.71	90.30	106.87
6	A	801	HAS	C3B-C4B-NB	15.75	125.17	109.90
6	A	801	HAS	C4B-CHC-C1C	13.67	145.46	127.47
6	A	801	HAS	C3A-C4A-NA	11.92	118.41	109.41
6	A	801	HAS	C4A-C3A-C2A	-11.91	98.71	107.00
6	A	801	HAS	C1B-C2B-C3B	10.74	113.29	107.00
6	A	801	HAS	C3C-C2C-C1C	-10.72	100.73	107.00
6	A	801	HAS	C4C-CHD-C4A	9.47	139.94	127.47
6	A	801	HAS	CHD-C4A-NA	-9.25	109.12	124.58
5	A	800	HEM	C3B-C4B-NB	-8.58	107.86	114.00
6	A	801	HAS	C1B-CHB-C1D	-6.79	118.54	127.47
6	A	801	HAS	C4C-C3C-C2C	-6.42	102.38	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	CHC-C1C-NC	-6.30	114.05	124.58
6	A	801	HAS	C2C-C1C-NC	5.57	113.62	109.41
5	A	800	HEM	C4D-ND-C1D	5.48	110.77	105.16
6	A	801	HAS	C2C-C3C-CAC	-5.16	116.76	127.33
6	A	801	HAS	C3C-CAC-CBC	-5.05	115.50	125.95
6	A	801	HAS	CMC-C2C-C3C	-4.96	117.15	124.97
6	A	801	HAS	C4D-CHA-C1A	-4.71	121.27	127.47
6	A	801	HAS	C2B-C3B-C11	-4.49	116.54	126.14
6	A	801	HAS	C2B-C1B-NB	-4.17	106.26	109.41
6	A	801	HAS	CBD-CAD-C3D	4.16	120.13	112.35
6	A	801	HAS	C12-C13-C14	-4.00	101.22	112.46
6	A	801	HAS	CBA-CAA-C2A	-3.98	105.68	112.69
6	A	801	HAS	C25-C23-C24	3.79	121.14	115.39
6	A	801	HAS	CMB-C2B-C3B	-3.54	118.28	124.94
6	A	801	HAS	C3D-C4D-ND	3.53	112.28	109.64
6	A	801	HAS	C13-C12-C11	-3.44	108.53	114.06
6	A	801	HAS	CMA-C3A-C2A	3.38	131.32	124.94
6	A	801	HAS	C4B-C3B-C11	-3.31	118.70	124.67
6	A	801	HAS	C3A-C4A-CHD	3.25	132.16	126.00
6	A	801	HAS	C1D-C2D-C3D	-3.06	105.17	107.90
6	A	801	HAS	C4D-C3D-C2D	-2.97	104.33	106.80
5	A	800	HEM	C2D-C1D-ND	-2.87	109.54	112.93
6	A	801	HAS	CMC-C2C-C1C	-2.82	124.29	128.62
6	A	801	HAS	C2C-C1C-CHC	2.79	131.30	126.00
6	A	801	HAS	C27-C19-C20	2.61	119.36	115.39
5	A	800	HEM	C1B-NB-C4B	2.56	107.78	105.16
6	A	801	HAS	C4D-ND-C1D	2.53	110.10	106.76
6	A	801	HAS	OMD-CMD-C2D	-2.47	119.99	125.32
6	A	801	HAS	C12-C11-C3B	-2.40	106.19	112.64
6	A	801	HAS	CAD-CBD-CGD	-2.31	106.03	113.47
6	A	801	HAS	C16-C17-C18	-2.24	105.22	111.62
6	A	801	HAS	C20-C21-C22	-2.19	105.35	111.62
6	A	801	HAS	CAD-C3D-C4D	2.12	128.50	124.67
6	A	801	HAS	O11-C11-C3B	2.11	118.86	111.89
5	A	800	HEM	CAD-C3D-C4D	2.09	128.29	124.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	554/568 (97%)	0.47	32 (5%)	22 22	123, 123, 123, 123	0
2	B	166/166 (100%)	0.55	15 (9%)	10 14	123, 123, 123, 123	0
3	C	33/33 (100%)	0.03	2 (6%)	21 21	123, 123, 123, 123	0
All	All	753/767 (98%)	0.47	49 (6%)	18 20	123, 123, 123, 123	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	136	ARG	4.5
2	B	61	GLU	4.5
1	A	203	GLU	4.0
1	A	14	ALA	3.6
1	A	342	ASP	3.6
1	A	493	LEU	3.4
1	A	548	GLN	3.3
1	A	206	LEU	3.3
3	C	2	GLU	3.2
1	A	146	TYR	3.2
3	C	3	GLU	3.2
2	B	51	GLU	3.1
2	B	52	ARG	3.0
1	A	142	HIS	3.0
2	B	60	GLN	2.9
1	A	12	TYR	2.8
1	A	549	LEU	2.7
2	B	104	VAL	2.7
1	A	207	PHE	2.7
1	A	208	LEU	2.7
1	A	202	LEU	2.6
2	B	74	THR	2.6
2	B	79	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	57	THR	2.5
1	A	141	GLY	2.4
1	A	222	LEU	2.4
1	A	522	LEU	2.4
2	B	103	ILE	2.4
1	A	519	ARG	2.4
1	A	462	HIS	2.4
1	A	147	LEU	2.4
1	A	215	LEU	2.3
1	A	489	PHE	2.3
1	A	204	ALA	2.3
2	B	119	GLU	2.3
1	A	529	PHE	2.2
2	B	135	VAL	2.2
1	A	140	LYS	2.2
2	B	102	GLU	2.2
1	A	411	LYS	2.2
1	A	409	THR	2.2
1	A	495	ARG	2.2
1	A	223	VAL	2.1
1	A	492	LEU	2.1
1	A	341	TRP	2.1
2	B	4	GLU	2.1
1	A	526	ARG	2.1
2	B	134	THR	2.1
1	A	13	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

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<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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	HAS	A	801	65/65	0.36	0.72	123,123,123,123	0
8	XE	A	565	1/1	1.33	-	123,123,123,123	1
8	XE	A	563	1/1	0.64	-	123,123,123,123	1
8	XE	A	566	1/1	0.84	-	123,123,123,123	1
5	HEM	A	800	43/43	0.28	-	123,123,123,123	0
4	CU	A	803	1/1	0.22	-	123,123,123,123	0
7	CUA	B	802	2/2	0.12	-	123,123,123,123	0
8	XE	A	564	1/1	0.35	-	123,123,123,123	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.