



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:45 PM GMT

PDB ID : 3S33  
Title : Structure of Thermus thermophilus cytochrome ba3 oxidase 10s after Xe de-pressurization  
Authors : Luna, V.M.; Fee, J.A.; Deniz, A.A.; Stout, C.D.  
Deposited on : 2011-05-17  
Resolution : 4.45 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  
<http://wwpdb.org/validation/2016/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 (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

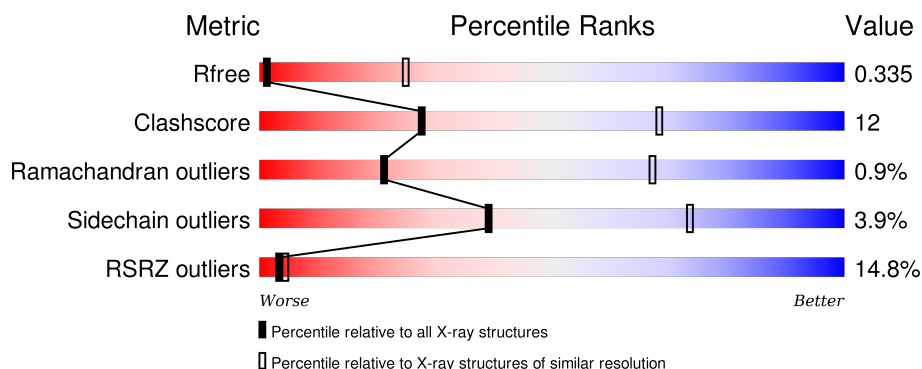
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.45 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	1070 (5.30-3.60)
Clashscore	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1116 (5.30-3.60)
Sidechain outliers	100360	1098 (5.30-3.60)
RSRZ outliers	91569	1074 (5.30-3.60)

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>13%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>
2	B	166	<div> <div>19%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
3	C	33	<div> <div>27%</div> <div>73%</div> <div>27%</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
6	HAS	A	801	-	-	-	X
7	CUA	B	802	-	-	X	-
8	XE	A	564	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6080 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	557	Total	C	N	O	S	0	0	0
			4407	2985	707	699	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).

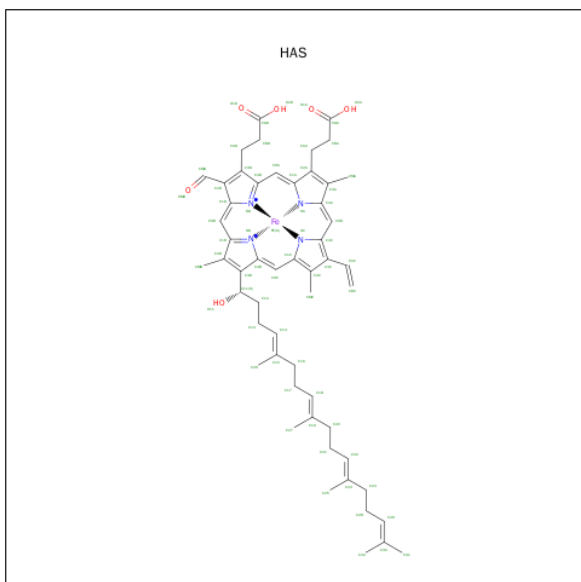
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



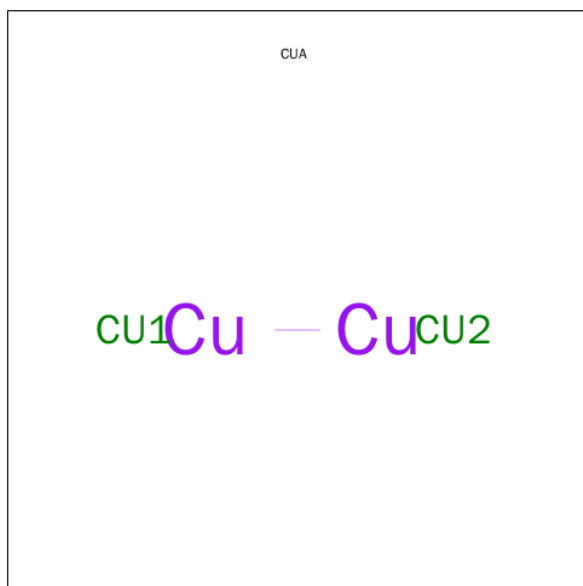
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	0	0
			65	54	1	4	6		

- 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	Cu	0	0
			2	2		

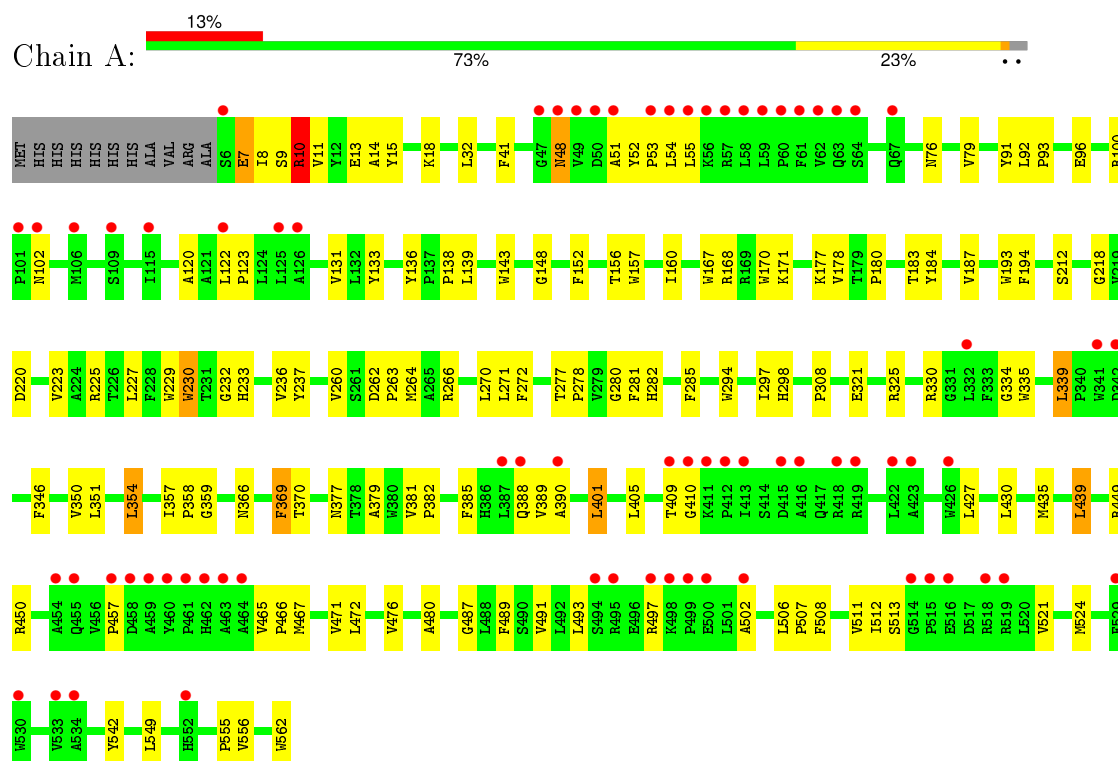
- Molecule 8 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	5	Total	Xe	0	0
			5	5		

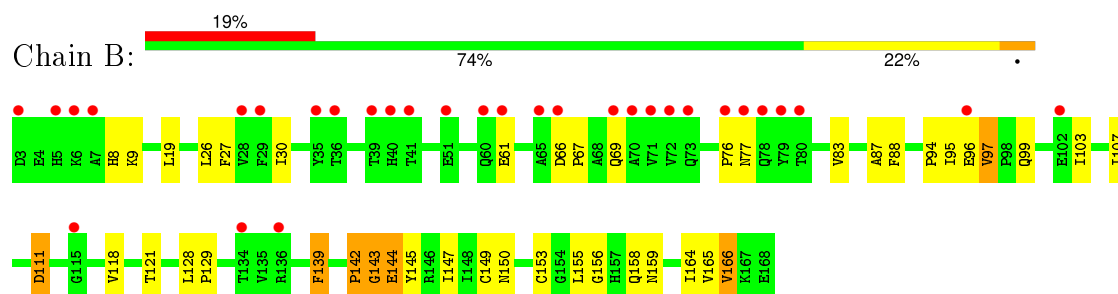
### 3 Residue-property plots [i](#)

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

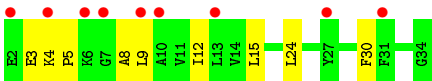


#### • Molecule 2: Cytochrome c oxidase subunit 2



#### • 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, $\alpha$ , $\beta$ , $\gamma$	108.25Å 108.25Å 162.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.06 – 4.45 44.24 – 4.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.06-4.45) 99.7 (44.24-4.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.19	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.17 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.305 , 0.350 0.292 , 0.335	Depositor DCC
$R_{free}$ test set	294 reflections (4.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	155.0	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 6322 reflections (0.016%)	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	6080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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, 0.375 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	0.43	2/4564 (0.0%)	0.55	1/6263 (0.0%)
2	B	0.62	4/1335 (0.3%)	0.58	1/1822 (0.1%)
3	C	0.54	0/265	0.57	0/359
All	All	0.48	6/6164 (0.1%)	0.56	2/8444 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	143	GLY	N-CA	7.83	1.57	1.46
2	B	144	GLU	N-CA	7.16	1.60	1.46
1	A	7	GLU	CB-CG	6.78	1.65	1.52
2	B	144	GLU	CA-C	6.30	1.69	1.52
1	A	7	GLU	CA-C	5.36	1.66	1.52
2	B	144	GLU	CB-CG	5.04	1.61	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ARG	NE-CZ-NH1	-8.42	116.09	120.30
2	B	144	GLU	N-CA-C	6.22	127.78	111.00

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	4407	0	4516	103	35
2	B	1298	0	1280	35	35
3	C	259	0	279	11	0
4	A	1	0	0	0	0
5	A	43	0	30	2	0
6	A	65	0	62	4	0
7	B	2	0	0	2	0
8	A	5	0	0	0	0
All	All	6080	0	6167	144	35

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 (144) 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)
2:B:99:GLN:OE1	2:B:142:PRO:HG3	1.33	1.26
3:C:3:GLU:CG	3:C:4:LYS:H	1.52	1.20
3:C:3:GLU:HG3	3:C:4:LYS:N	1.71	1.06
3:C:3:GLU:HG3	3:C:4:LYS:H	0.91	1.05
1:A:233:HIS:NE2	1:A:237:TYR:CE2	2.28	1.00
1:A:233:HIS:NE2	1:A:237:TYR:HE2	1.59	0.99
1:A:233:HIS:HE2	1:A:237:TYR:HE2	1.09	0.91
1:A:262:ASP:HB2	1:A:511:VAL:HG11	1.57	0.85
2:B:97:VAL:O	2:B:166:VAL:HA	1.76	0.85
2:B:99:GLN:OE1	2:B:142:PRO:CG	2.24	0.83
1:A:15:TYR:HB2	1:A:18:LYS:HD2	1.65	0.79
2:B:97:VAL:HG23	2:B:166:VAL:HG12	1.65	0.78
1:A:335:TRP:O	1:A:339:LEU:HD22	1.84	0.77
1:A:7:GLU:HB3	1:A:13:GLU:OE2	1.85	0.77
3:C:3:GLU:CG	3:C:4:LYS:N	2.29	0.71
2:B:153:CYS:SG	7:B:802:CUA:CU2	1.79	0.71
1:A:233:HIS:O	1:A:236:VAL:HG22	1.91	0.71
2:B:149:CYS:SG	7:B:802:CUA:CU1	1.81	0.70
2:B:96:GLU:HA	2:B:165:VAL:O	1.93	0.68
1:A:7:GLU:CG	1:A:13:GLU:HG3	2.24	0.67
5:A:800:HEM:HBC2	5:A:800:HEM:HMC1	1.77	0.65
1:A:7:GLU:HG2	1:A:13:GLU:CG	2.27	0.65
3:C:9:LEU:HD23	3:C:12:ILE:HD11	1.79	0.65
1:A:487:GLY:O	1:A:491:VAL:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:HB2	1:A:123:PRO:HD3	1.78	0.64
1:A:379:ALA:HB1	1:A:439:LEU:HD12	1.78	0.64
2:B:145:TYR:CD1	2:B:166:VAL:HG21	2.32	0.63
1:A:7:GLU:HG2	1:A:13:GLU:HG3	1.80	0.63
1:A:449:ARG:HD2	1:A:450:ARG:HG3	1.82	0.62
1:A:233:HIS:CD2	1:A:237:TYR:HE2	2.20	0.60
1:A:357:ILE:HB	1:A:358:PRO:HD3	1.81	0.60
1:A:223:VAL:HG12	1:A:549:LEU:HB3	1.85	0.58
2:B:9:LYS:HE2	2:B:9:LYS:HA	1.85	0.58
1:A:467:MET:O	1:A:471:VAL:HG23	2.03	0.58
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.40	0.57
2:B:145:TYR:CE1	2:B:166:VAL:HG21	2.39	0.57
1:A:230:TRP:C	1:A:230:TRP:CD1	2.77	0.57
2:B:97:VAL:HG23	2:B:166:VAL:CG1	2.32	0.56
1:A:377:ASN:HB3	2:B:150:ASN:HB2	1.88	0.55
1:A:229:TRP:CE3	1:A:232:GLY:HA3	2.42	0.55
1:A:260:VAL:HA	1:A:512:ILE:HD12	1.89	0.54
2:B:94:PRO:HB2	2:B:165:VAL:HG23	1.87	0.54
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.42	0.54
2:B:95:ILE:O	2:B:165:VAL:N	2.30	0.53
2:B:69:GLN:HA	2:B:69:GLN:NE2	2.22	0.53
1:A:7:GLU:CG	1:A:13:GLU:CG	2.85	0.52
2:B:147:ILE:HD11	2:B:164:ILE:HG13	1.91	0.52
1:A:52:TYR:N	1:A:53:PRO:HD2	2.25	0.52
1:A:272:PHE:CZ	1:A:308:PRO:HB2	2.45	0.51
5:A:800:HEM:HBC2	5:A:800:HEM:CMC	2.40	0.51
1:A:271:LEU:HB2	1:A:308:PRO:HG3	1.93	0.51
3:C:3:GLU:CD	3:C:4:LYS:H	2.12	0.50
1:A:366:ASN:CB	6:A:801:HAS:HMD	2.42	0.50
1:A:427:LEU:HB3	1:A:480:ALA:HB2	1.93	0.50
1:A:506:LEU:O	1:A:508:PHE:N	2.41	0.49
1:A:346:PHE:CZ	1:A:350:VAL:HG21	2.47	0.49
1:A:262:ASP:HB2	1:A:511:VAL:CG1	2.34	0.49
1:A:7:GLU:HG2	1:A:13:GLU:HG2	1.94	0.49
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.98	0.49
1:A:7:GLU:HG3	1:A:13:GLU:HG3	1.95	0.48
1:A:220:ASP:HB3	1:A:223:VAL:HG22	1.96	0.48
1:A:41:PHE:CE1	1:A:55:LEU:HD13	2.48	0.48
1:A:357:ILE:HG23	3:C:15:LEU:HD12	1.95	0.48
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.94	0.48
1:A:15:TYR:O	1:A:18:LYS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ALA:HA	1:A:100:ARG:NH1	2.28	0.48
1:A:18:LYS:HE2	1:A:502:ALA:O	2.14	0.47
1:A:230:TRP:C	1:A:230:TRP:HD1	2.17	0.47
1:A:410:GLY:CA	1:A:502:ALA:HB2	2.45	0.47
2:B:27:PHE:HA	2:B:30:ILE:HD12	1.96	0.47
1:A:435:MET:HG2	1:A:439:LEU:CD2	2.44	0.47
1:A:136:TYR:O	1:A:139:LEU:HB2	2.15	0.47
1:A:401:LEU:O	1:A:405:LEU:HB2	2.15	0.47
1:A:218:GLY:HA3	1:A:555:PRO:HB2	1.97	0.47
1:A:41:PHE:CE2	1:A:55:LEU:HB2	2.49	0.47
1:A:10:ARG:HE	1:A:10:ARG:HB2	1.30	0.47
3:C:3:GLU:OE2	3:C:4:LYS:N	2.48	0.46
1:A:170:TRP:CH2	1:A:180:PRO:HD3	2.50	0.46
1:A:465:VAL:HG23	1:A:466:PRO:HD3	1.97	0.46
1:A:282:HIS:HA	1:A:285:PHE:CZ	2.50	0.46
1:A:351:LEU:HA	1:A:354:LEU:HD22	1.97	0.46
1:A:120:ALA:HB2	1:A:148:GLY:HA3	1.98	0.46
1:A:79:VAL:HA	1:A:152:PHE:CZ	2.51	0.46
1:A:264:MET:CE	1:A:264:MET:HA	2.46	0.46
3:C:4:LYS:HD2	3:C:9:LEU:CD1	2.45	0.45
1:A:280:GLY:HA3	1:A:542:TYR:OH	2.17	0.45
3:C:5:PRO:HB2	3:C:8:ALA:HB3	1.99	0.45
1:A:270:LEU:HD22	1:A:524:MET:HG2	1.98	0.45
1:A:389:VAL:HG13	1:A:390:ALA:N	2.32	0.45
2:B:145:TYR:HD1	2:B:166:VAL:HG21	1.78	0.45
1:A:157:TRP:HA	1:A:160:ILE:HD12	2.00	0.45
1:A:227:LEU:O	1:A:230:TRP:HB3	2.18	0.44
2:B:69:GLN:HA	2:B:69:GLN:HE21	1.80	0.44
1:A:138:PRO:HG2	2:B:111:ASP:O	2.16	0.44
2:B:96:GLU:HG2	2:B:165:VAL:HB	1.99	0.44
2:B:8:HIS:HD2	2:B:9:LYS:HE3	1.83	0.44
2:B:69:GLN:CA	2:B:69:GLN:HE21	2.29	0.44
1:A:167:TRP:CZ2	1:A:171:LYS:HE3	2.53	0.44
1:A:281:PHE:H	1:A:298:HIS:CD2	2.36	0.44
1:A:330:ARG:HB2	1:A:334:GLY:HA3	1.99	0.44
2:B:156:GLY:HA2	2:B:158:GLN:HE22	1.83	0.44
1:A:277:THR:N	1:A:278:PRO:CD	2.81	0.44
1:A:51:ALA:O	1:A:54:LEU:HB3	2.17	0.44
1:A:321:GLU:O	1:A:325:ARG:HG2	2.18	0.43
1:A:92:LEU:N	1:A:93:PRO:HD2	2.34	0.43
2:B:164:ILE:CG2	2:B:166:VAL:HG13	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:VAL:HG11	1:A:521:VAL:HG12	2.00	0.43
2:B:145:TYR:HD1	2:B:166:VAL:CG2	2.32	0.43
1:A:281:PHE:H	1:A:298:HIS:HD2	1.65	0.43
2:B:118:VAL:HB	2:B:121:THR:OG1	2.19	0.43
2:B:66:ASP:HA	2:B:67:PRO:HD3	1.88	0.43
1:A:562:TRP:HA	2:B:155:LEU:HG	2.01	0.43
1:A:271:LEU:CB	1:A:308:PRO:HG3	2.48	0.42
6:A:801:HAS:HHA	6:A:801:HAS:HAA2	1.84	0.42
1:A:427:LEU:HD22	1:A:476:VAL:HG13	2.00	0.42
1:A:556:VAL:HG21	2:B:129:PRO:HB2	2.01	0.42
1:A:409:THR:O	1:A:497:ARG:NE	2.53	0.42
1:A:381:VAL:HB	1:A:382:PRO:HD3	2.00	0.42
1:A:359:GLY:HA3	1:A:388:GLN:NE2	2.35	0.42
1:A:225:ARG:HD2	2:B:128:LEU:HD21	2.02	0.42
1:A:156:THR:CB	1:A:193:TRP:HE1	2.33	0.42
1:A:48:ASN:HD21	1:A:457:PRO:HA	1.85	0.42
1:A:262:ASP:N	1:A:263:PRO:CD	2.83	0.41
2:B:97:VAL:N	2:B:165:VAL:O	2.43	0.41
1:A:131:VAL:HG12	1:A:139:LEU:HB3	2.02	0.41
1:A:184:TYR:CD2	1:A:266:ARG:HG2	2.55	0.41
1:A:236:VAL:HB	6:A:801:HAS:C3C	2.50	0.41
1:A:435:MET:HG2	1:A:439:LEU:HD23	2.01	0.41
1:A:91:TYR:CE2	1:A:506:LEU:HD11	2.56	0.41
1:A:370:THR:HB	3:C:30:PHE:CZ	2.56	0.41
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.55	0.41
1:A:178:VAL:HG11	1:A:521:VAL:CG1	2.51	0.41
1:A:465:VAL:N	1:A:466:PRO:HD2	2.37	0.41
1:A:377:ASN:HB3	2:B:150:ASN:O	2.21	0.40
1:A:96:GLU:OE2	1:A:180:PRO:HB2	2.21	0.40
2:B:103:ILE:HD13	2:B:139:PHE:CD1	2.56	0.40
2:B:83:VAL:HB	2:B:107:ILE:HG12	2.03	0.40
1:A:143:TRP:HA	1:A:212:SER:HB2	2.03	0.40
1:A:294:TRP:HA	1:A:297:ILE:HD12	2.04	0.40
1:A:388:GLN:HB2	6:A:801:HAS:HAC	2.02	0.40
1:A:9:SER:OG	1:A:497:ARG:NH2	2.55	0.40
1:A:32:LEU:HA	1:A:76:ASN:ND2	2.37	0.40
1:A:183:THR:O	1:A:187:VAL:HG23	2.21	0.40
1:A:489:PHE:O	1:A:493:LEU:HB2	2.22	0.40

All (35) 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:9:SER:O	2:B:143:GLY:CA[3_444]	1.03	1.17
1:A:7:GLU:C	2:B:144:GLU:CA[3_444]	1.17	1.03
1:A:9:SER:C	2:B:143:GLY:N[3_444]	1.17	1.03
1:A:9:SER:O	2:B:143:GLY:N[3_444]	1.19	1.01
1:A:8:ILE:N	2:B:144:GLU:CA[3_444]	1.30	0.90
1:A:8:ILE:N	2:B:144:GLU:C[3_444]	1.32	0.88
1:A:10:ARG:N	2:B:143:GLY:N[3_444]	1.36	0.84
1:A:7:GLU:C	2:B:144:GLU:C[3_444]	1.45	0.75
1:A:7:GLU:CA	2:B:144:GLU:CA[3_444]	1.49	0.71
1:A:10:ARG:NH1	2:B:139:PHE:CB[3_444]	1.51	0.69
1:A:9:SER:C	2:B:142:PRO:C[3_444]	1.58	0.62
1:A:9:SER:C	2:B:143:GLY:CA[3_444]	1.64	0.56
1:A:11:VAL:N	2:B:142:PRO:C[3_444]	1.67	0.53
1:A:7:GLU:O	2:B:145:TYR:N[3_444]	1.75	0.45
1:A:10:ARG:CA	2:B:143:GLY:N[3_444]	1.76	0.44
1:A:10:ARG:N	2:B:142:PRO:C[3_444]	1.78	0.42
1:A:7:GLU:C	2:B:145:TYR:N[3_444]	1.78	0.42
1:A:11:VAL:N	2:B:142:PRO:CB[3_444]	1.85	0.35
1:A:9:SER:O	2:B:142:PRO:C[3_444]	1.86	0.34
1:A:8:ILE:N	2:B:144:GLU:N[3_444]	1.92	0.28
1:A:13:GLU:OE1	2:B:166:VAL:N[3_444]	1.96	0.24
1:A:11:VAL:N	2:B:142:PRO:CA[3_444]	1.96	0.24
1:A:7:GLU:C	2:B:144:GLU:N[3_444]	1.98	0.22
1:A:10:ARG:NH1	2:B:139:PHE:CG[3_444]	2.01	0.19
1:A:8:ILE:N	2:B:145:TYR:N[3_444]	2.01	0.19
1:A:10:ARG:C	2:B:143:GLY:N[3_444]	2.02	0.18
1:A:9:SER:C	2:B:142:PRO:O[3_444]	2.08	0.12
1:A:7:GLU:O	2:B:143:GLY:O[3_444]	2.09	0.11
1:A:7:GLU:CA	2:B:144:GLU:CB[3_444]	2.11	0.09
1:A:13:GLU:OE2	2:B:143:GLY:O[3_444]	2.13	0.07
1:A:10:ARG:CA	2:B:142:PRO:CA[3_444]	2.13	0.07
1:A:9:SER:O	2:B:142:PRO:O[3_444]	2.13	0.07
1:A:10:ARG:CB	2:B:142:PRO:CA[3_444]	2.17	0.03
1:A:7:GLU:CD	2:B:144:GLU:CG[3_444]	2.17	0.03
1:A:10:ARG:C	2:B:142:PRO:C[3_444]	2.18	0.02

## 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	555/568 (98%)	522 (94%)	29 (5%)	4 (1%)	26	71
2	B	164/166 (99%)	153 (93%)	8 (5%)	3 (2%)	11	55
3	C	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
All	All	750/767 (98%)	705 (94%)	38 (5%)	7 (1%)	21	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
2	B	87	ALA
1	A	102	ASN
1	A	369	PHE
2	B	88	PHE
2	B	76	PRO
1	A	507	PRO

### 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	453/462 (98%)	440 (97%)	13 (3%)	50	79
2	B	136/136 (100%)	126 (93%)	10 (7%)	17	56
3	C	26/26 (100%)	25 (96%)	1 (4%)	40	74
All	All	615/624 (99%)	591 (96%)	24 (4%)	39	73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	133	TYR

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Mol	Chain	Res	Type
1	A	168	ARG
1	A	177	LYS
1	A	230	TRP
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	472	LEU
1	A	513	SER
2	B	19	LEU
2	B	26	LEU
2	B	61	GLU
2	B	77	ASN
2	B	97	VAL
2	B	111	ASP
2	B	139	PHE
2	B	142	PRO
2	B	159	ASN
2	B	166	VAL
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	48	ASN
1	A	76	ASN
1	A	254	GLN
1	A	298	HIS
2	B	8	HIS
2	B	69	GLN
2	B	77	ASN
2	B	117	HIS
2	B	122	ASN
2	B	158	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 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	2.18	5 (16%)	24,82,82	2.25	7 (29%)
6	HAS	A	801	1	45,72,72	2.05	12 (26%)	47,109,109	3.37	21 (44%)
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	1	-	0/30/82/82	0/0/8/8
7	CUA	B	802	2	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C3B-C4B	-7.61	1.45	1.51
6	A	801	HAS	C4C-NC	-5.47	1.29	1.36
5	A	800	HEM	C3D-C4D	-5.44	1.44	1.51
5	A	800	HEM	C2C-C1C	-4.08	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	C4B-NB	-2.29	1.33	1.36
5	A	800	HEM	C2D-C1D	-2.21	1.44	1.51
6	A	801	HAS	C3C-CAC	2.08	1.52	1.47
5	A	800	HEM	CAA-C2A	2.12	1.55	1.52
6	A	801	HAS	CMC-C2C	2.27	1.56	1.51
6	A	801	HAS	CAA-C2A	2.38	1.56	1.52
6	A	801	HAS	C4A-CHD	3.09	1.48	1.39
6	A	801	HAS	C1D-CHB	3.12	1.48	1.39
6	A	801	HAS	C1C-CHC	3.37	1.49	1.39
6	A	801	HAS	C2D-C3D	3.74	1.45	1.40
6	A	801	HAS	C1A-CHA	3.84	1.50	1.39
6	A	801	HAS	C2A-C3A	4.54	1.51	1.37
6	A	801	HAS	C3C-C2C	6.94	1.49	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	CMC-C2C-C1C	-9.15	113.22	128.36
6	A	801	HAS	CAA-C2A-C1A	-8.42	117.86	127.01
6	A	801	HAS	CMA-C3A-C4A	-8.16	114.86	128.36
6	A	801	HAS	CMC-C2C-C3C	-7.37	110.68	125.09
6	A	801	HAS	CMA-C3A-C2A	-5.67	113.38	125.24
6	A	801	HAS	C4D-C3D-C2D	-5.15	101.92	107.07
6	A	801	HAS	CAD-CBD-CGD	-5.11	103.38	112.75
6	A	801	HAS	CAA-C2A-C3A	-3.87	117.94	129.00
6	A	801	HAS	C13-C12-C11	-3.60	109.73	114.51
5	A	800	HEM	C3B-CAB-CBB	-3.54	119.03	124.46
6	A	801	HAS	C3C-CAC-CBC	-3.23	119.71	126.32
6	A	801	HAS	C13-C14-C15	-2.25	122.86	127.76
6	A	801	HAS	CAA-CBA-CGA	-2.25	108.62	112.75
6	A	801	HAS	C20-C21-C22	-2.06	106.29	111.69
6	A	801	HAS	OMD-CMD-C2D	-2.02	121.03	125.11
5	A	800	HEM	C2D-C3D-C4D	2.07	105.01	101.50
6	A	801	HAS	C27-C19-C20	2.25	118.85	115.41
6	A	801	HAS	C26-C15-C16	2.65	119.46	115.41
5	A	800	HEM	CMD-C2D-C3D	2.72	126.39	114.35
6	A	801	HAS	CBD-CAD-C3D	2.75	117.46	112.53
6	A	801	HAS	C3C-C4C-NC	3.21	117.00	110.94
6	A	801	HAS	CBA-CAA-C2A	3.67	119.10	112.53
6	A	801	HAS	C25-C23-C24	3.68	121.03	115.41
5	A	800	HEM	CMB-C2B-C3B	3.81	126.03	116.53
5	A	800	HEM	CAD-C3D-C4D	4.32	127.71	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	HEM	CMC-C2C-C3C	4.55	127.88	116.53
5	A	800	HEM	CAD-C3D-C2D	4.89	127.27	113.22
6	A	801	HAS	CAD-C3D-C4D	5.24	132.69	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	HEM	2	0
6	A	801	HAS	4	0
7	B	802	CUA	2	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	557/568 (98%)	0.45	72 (12%) 5 6	131, 131, 131, 131	0
2	B	166/166 (100%)	0.82	31 (18%) 2 3	131, 131, 131, 131	0
3	C	33/33 (100%)	1.09	9 (27%) 1 2	131, 131, 131, 131	0
All	All	756/767 (98%)	0.56	112 (14%) 3 4	131, 131, 131, 131	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	GLN	6.9
1	A	419	ARG	6.8
1	A	48	ASN	5.8
1	A	498	LYS	5.2
1	A	62	VAL	5.0
1	A	458	ASP	4.9
1	A	519	ARG	4.8
2	B	102	GLU	4.7
2	B	79	TYR	4.6
1	A	61	PHE	4.5
1	A	497	ARG	4.5
3	C	10	ALA	4.4
1	A	6	SER	4.3
2	B	78	GLN	4.3
2	B	69	GLN	4.3
1	A	415	ASP	4.2
2	B	77	ASN	4.1
1	A	515	PRO	4.1
1	A	533	VAL	3.9
1	A	410	GLY	3.9
1	A	464	ALA	3.9
1	A	411	LYS	3.9
1	A	463	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	7	ALA	3.8
2	B	66	ASP	3.8
1	A	499	PRO	3.7
1	A	412	PRO	3.7
1	A	457	PRO	3.7
1	A	342	ASP	3.6
1	A	54	LEU	3.6
3	C	6	LYS	3.6
2	B	136	ARG	3.5
1	A	518	ARG	3.5
1	A	57	ARG	3.5
1	A	332	LEU	3.5
1	A	50	ASP	3.4
1	A	462	HIS	3.4
1	A	49	VAL	3.4
1	A	56	LYS	3.4
2	B	80	THR	3.3
2	B	71	VAL	3.3
2	B	96	GLU	3.3
2	B	5	HIS	3.2
3	C	2	GLU	3.2
1	A	409	THR	3.1
1	A	59	LEU	3.1
1	A	502	ALA	3.1
1	A	388	GLN	3.0
1	A	454	ALA	3.0
1	A	514	GLY	3.0
1	A	552	HIS	3.0
3	C	9	LEU	3.0
1	A	53	PRO	3.0
2	B	39	THR	2.9
1	A	102	ASN	2.9
1	A	58	LEU	2.9
1	A	530	TRP	2.9
1	A	460	TYR	2.9
1	A	495	ARG	2.9
1	A	60	PRO	2.8
2	B	36	THR	2.8
2	B	76	PRO	2.8
3	C	7	GLY	2.8
1	A	418	ARG	2.8
1	A	422	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	73	GLN	2.7
3	C	31	PHE	2.7
1	A	125	LEU	2.7
1	A	455	GLN	2.7
1	A	106	MET	2.7
2	B	35	TYR	2.7
1	A	55	LEU	2.7
2	B	41	THR	2.7
2	B	3	ASP	2.6
1	A	101	PRO	2.6
1	A	416	ALA	2.6
1	A	461	PRO	2.6
3	C	27	TYR	2.6
1	A	67	GLN	2.5
3	C	4	LYS	2.5
1	A	51	ALA	2.5
2	B	115	GLY	2.5
1	A	47	GLY	2.5
2	B	51	GLU	2.5
1	A	390	ALA	2.5
1	A	534	ALA	2.4
1	A	122	LEU	2.4
1	A	459	ALA	2.4
2	B	70	ALA	2.4
1	A	109	SER	2.4
2	B	6	LYS	2.3
1	A	426	TRP	2.3
1	A	529	PHE	2.3
1	A	64	SER	2.3
1	A	516	GLU	2.3
2	B	40	HIS	2.3
1	A	494	SER	2.2
2	B	72	VAL	2.2
1	A	500	GLU	2.2
2	B	65	ALA	2.2
1	A	115	ILE	2.2
3	C	13	LEU	2.2
2	B	61	GLU	2.2
1	A	341	TRP	2.1
2	B	60	GLN	2.1
2	B	28	VAL	2.1
2	B	29	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	413	ILE	2.1
1	A	126	ALA	2.0
1	A	423	ALA	2.0
1	A	387	LEU	2.0
2	B	134	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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	XE	A	564	1/1	0.89	0.65	2.01	130,130,130,130	1
8	XE	A	565	1/1	0.81	0.40	1.56	130,130,130,130	1
6	HAS	A	801	65/65	0.77	0.46	0.51	130,130,130,130	0
8	XE	A	566	1/1	0.87	0.18	0.08	130,130,130,130	1
5	HEM	A	800	43/43	0.92	0.35	-0.09	130,130,130,130	0
8	XE	A	567	1/1	0.72	0.36	-0.35	130,130,130,130	1
7	CUA	B	802	2/2	0.98	0.18	-1.31	130,130,130,130	0
8	XE	A	563	1/1	0.96	0.19	-2.75	130,130,130,130	1
4	CU	A	803	1/1	0.93	0.47	-	130,130,130,130	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.