



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:45 PM GMT

PDB ID : 4GP4  
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant Y133F from *Thermus thermophilus*  
Authors : Li, Y.; Chen, Y.; Stout, C.D.  
Deposited on : 2012-08-20  
Resolution : 2.80 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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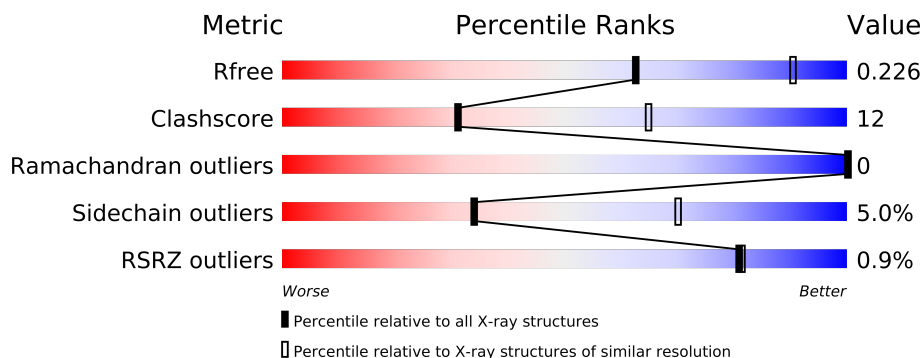
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	168	
3	C	34	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
8	OLC	A	605	-	X
8	OLC	A	606	-	X
8	OLC	A	607	-	X
8	OLC	A	608	-	X
8	OLC	A	609	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
8	OLC	A	610	-	X
8	OLC	A	611	-	X
8	OLC	A	612	-	X
8	OLC	A	613	-	X
8	OLC	A	614	-	X
8	OLC	A	615	-	X
8	OLC	A	616	-	X
8	OLC	A	617	-	X
8	OLC	B	202	-	X
8	OLC	B	203	-	X
8	OLC	B	204	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6458 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	2	0	0
			4361	2960	695	690	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	133	PHE	TYR	engineered mutation	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
			1285	836	213	232	4			

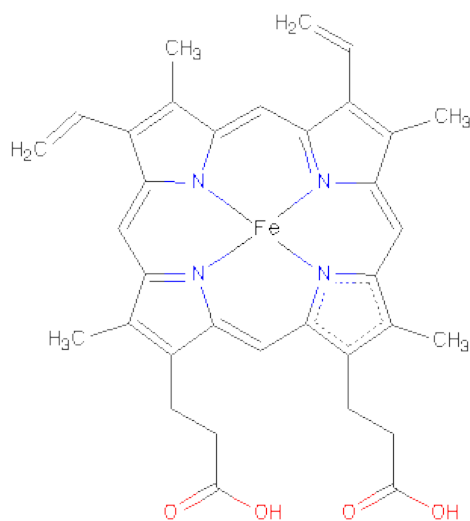
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	0	0	0
			241	169	37	35			

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

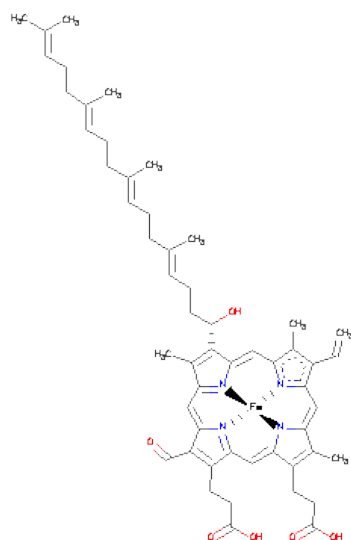
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- 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:  $C_{54}H_{64}FeN_4O_6$ ).



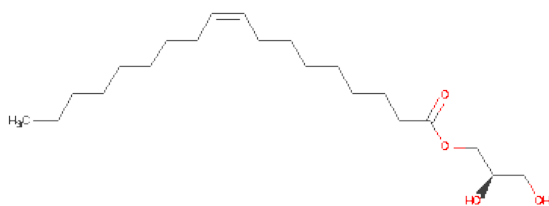
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
6	A	1	65	54	1	4	6	0	0

- Molecule 7 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			2	2		

- Molecule 8 is (2R)-2,3-DIHYDROXYPROPYL(9Z)-OCTADEC-9-ENOATE (three-letter code: OLC) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			25	21	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			23	19	4		
8	A	1	Total	C	O	0	0
			21	19	2		
8	A	1	Total	C	O	0	0
			18	14	4		
8	A	1	Total	C	O	0	0
			17	13	4		
8	A	1	Total	C	O	0	0
			8	4	4		
8	A	1	Total	C	O	0	0
			15	11	4		
8	A	1	Total	C	O	0	0
			20	16	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			21	17	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		

- Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	74	Total O 74 74	0	0
10	B	40	Total O 40 40	0	0
10	C	1	Total O 1 1	0	0

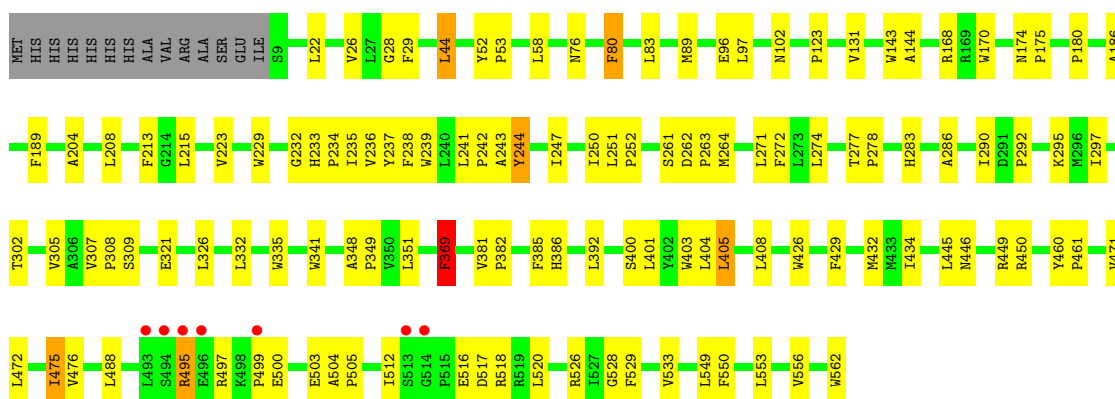


### 3 Residue-property plots

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.

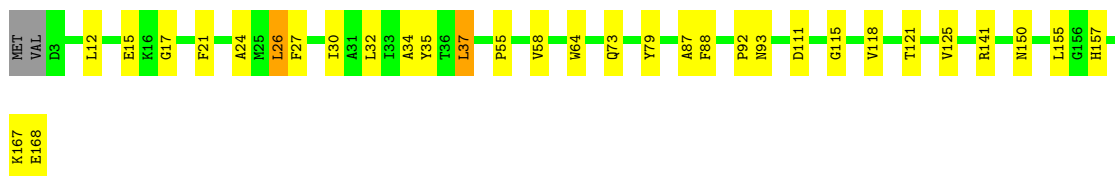
#### • Molecule 1: Cytochrome c oxidase subunit 1

Chain A: 



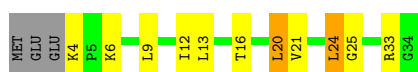
#### • Molecule 2: Cytochrome c oxidase subunit 2

Chain B: 



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

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.14Å 98.58Å 94.80Å 90.00° 127.89° 90.00°	Depositor
Resolution (Å)	74.82 – 2.80 74.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (74.82-2.80) 99.4 (74.50-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.179 , 0.227 0.178 , 0.226	Depositor DCC
$R_{free}$ test set	1312 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 25768 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6458	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OLC, PER, CUA, HEM, HAS, CU

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	0.44	0/4517	0.57	2/6201 (0.0%)
2	B	0.44	0/1321	0.55	0/1805
3	C	0.45	0/247	0.51	0/335
All	All	0.44	0/6085	0.56	2/8341 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	VAL	N-CA-C	-5.79	95.35	111.00
1	A	369	PHE	N-CA-CB	-5.09	101.43	110.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	4361	0	4455	110	0
2	B	1285	0	1260	27	0
3	C	241	0	267	9	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	43	0	30	7	0
6	A	65	0	62	2	0
7	A	2	0	0	0	0
8	A	268	0	393	24	0
8	B	75	0	120	15	0
9	B	2	0	0	0	0
10	A	74	0	0	1	0
10	B	40	0	0	2	1
10	C	1	0	0	0	0
All	All	6458	0	6587	151	1

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 12.

All (151) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:HIS:NE2	1:A:237:TYR:HE2	1.19	1.37
1:A:233:HIS:NE2	1:A:237:TYR:CE2	2.10	1.19
1:A:263:PRO:HG2	1:A:516:GLU:HG2	1.36	1.07
1:A:263:PRO:HG2	1:A:516:GLU:CG	1.88	1.02
1:A:168:ARG:HH11	8:A:612:OLC:H22	1.24	1.00
1:A:168:ARG:HH22	8:A:613:OLC:H6A	1.27	0.97
1:A:516:GLU:HG3	1:A:517:ASP:H	1.27	0.97
1:A:168:ARG:NH1	8:A:612:OLC:H22	1.91	0.83
1:A:263:PRO:CG	1:A:516:GLU:HG2	2.10	0.81
1:A:168:ARG:NH2	8:A:613:OLC:H6A	1.94	0.80
1:A:476:VAL:HG22	8:A:607:OLC:H16A	1.63	0.79
1:A:341:TRP:CZ2	8:A:617:OLC:H3	2.17	0.79
1:A:233:HIS:O	1:A:236:VAL:HG22	1.85	0.77
2:B:21:PHE:CE2	8:B:204:OLC:H10	2.21	0.74
1:A:516:GLU:CG	1:A:517:ASP:H	2.01	0.74
1:A:341:TRP:CE2	8:A:617:OLC:H3	2.23	0.74
1:A:516:GLU:HG3	1:A:517:ASP:N	2.02	0.70
1:A:495:ARG:HH21	1:A:495:ARG:HA	1.55	0.70
2:B:21:PHE:CZ	8:B:204:OLC:H10	2.26	0.70
1:A:262:ASP:HB3	1:A:263:PRO:HD3	1.76	0.68
1:A:400:SER:HA	1:A:403:TRP:NE1	2.08	0.68
1:A:233:HIS:CD2	1:A:237:TYR:HE2	2.10	0.67
2:B:35:TYR:CE2	8:B:202:OLC:H2A	2.30	0.67
8:B:203:OLC:H6	3:C:33:ARG:HE	1.59	0.66
1:A:297:ILE:HG12	8:A:609:OLC:H14A	1.78	0.66
2:B:32:LEU:HD21	8:B:202:OLC:H7A	1.78	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:381:VAL:HB	1:A:382:PRO:HD3	1.79	0.65
8:A:606:OLC:H6	8:B:203:OLC:H18A	1.78	0.64
8:A:605:OLC:H6	3:C:25:GLY:HA3	1.80	0.64
1:A:305:VAL:O	1:A:308:PRO:HD2	1.98	0.64
2:B:93:ASN:ND2	10:B:320:HOH:O	2.30	0.64
6:A:603:HAS:HBC1	6:A:603:HAS:HMC1	1.81	0.62
2:B:35:TYR:CZ	8:B:202:OLC:H2A	2.35	0.61
1:A:263:PRO:HG2	1:A:516:GLU:HG3	1.83	0.60
1:A:233:HIS:CE1	1:A:237:TYR:HE2	2.09	0.60
1:A:401:LEU:HG	1:A:405:LEU:HD22	1.82	0.60
1:A:168:ARG:HH11	8:A:612:OLC:C22	2.05	0.59
1:A:401:LEU:HD21	1:A:488:LEU:HD13	1.84	0.59
1:A:497:ARG:O	1:A:499:PRO:HD3	2.03	0.59
2:B:17:GLY:HA3	8:B:204:OLC:H3	1.85	0.58
1:A:348:ALA:HB3	1:A:349:PRO:HD3	1.85	0.58
1:A:277:THR:N	1:A:278:PRO:HD2	2.19	0.57
1:A:495:ARG:HA	1:A:495:ARG:NH2	2.20	0.57
1:A:232:GLY:O	1:A:235:ILE:HG22	2.05	0.57
1:A:29:PHE:CE1	1:A:401:LEU:HD11	2.40	0.56
2:B:141:ARG:NH2	8:B:203:OLC:O19	2.39	0.56
8:A:607:OLC:H12	8:A:615:OLC:H14A	1.87	0.56
1:A:401:LEU:O	1:A:405:LEU:HB2	2.05	0.55
1:A:277:THR:N	1:A:278:PRO:CD	2.70	0.55
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.92	0.55
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.42	0.54
1:A:475:ILE:HD11	8:A:607:OLC:H13A	1.90	0.53
1:A:204:ALA:HA	1:A:208:LEU:HB2	1.89	0.53
1:A:369:PHE:CD2	1:A:369:PHE:C	2.81	0.53
1:A:529:PHE:O	1:A:533:VAL:HG23	2.10	0.51
1:A:241:LEU:N	1:A:242:PRO:CD	2.74	0.51
2:B:26:LEU:O	2:B:30:ILE:HG13	2.11	0.51
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.46	0.50
1:A:52:TYR:N	1:A:53:PRO:CD	2.75	0.50
1:A:123:PRO:HG3	1:A:144:ALA:HB3	1.93	0.50
3:C:4:LYS:HE3	3:C:6:LYS:HG2	1.94	0.50
1:A:550:PHE:HA	1:A:553:LEU:HD21	1.93	0.50
2:B:34:ALA:O	2:B:37:LEU:HB2	2.12	0.50
1:A:250:ILE:HD13	1:A:403:TRP:CH2	2.47	0.50
1:A:400:SER:HA	1:A:403:TRP:CD1	2.45	0.49
1:A:277:THR:H	1:A:278:PRO:HD2	1.76	0.49
1:A:277:THR:H	1:A:278:PRO:CD	2.26	0.49
1:A:168:ARG:NH1	8:A:612:OLC:C22	2.71	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:404:LEU:O	1:A:408:LEU:HG	2.13	0.49
2:B:21:PHE:CD2	8:B:204:OLC:H9	2.47	0.49
2:B:141:ARG:HH12	8:B:203:OLC:H24A	1.77	0.48
1:A:89:MET:HG3	1:A:189:PHE:CE2	2.48	0.48
1:A:369:PHE:C	1:A:369:PHE:HD2	2.17	0.48
1:A:28:GLY:HA2	1:A:83:LEU:HD12	1.96	0.48
1:A:229:TRP:CE3	1:A:283:HIS:CD2	3.01	0.48
1:A:236:VAL:HB	6:A:603:HAS:C3C	2.45	0.47
1:A:271:LEU:HB3	1:A:308:PRO:HG3	1.96	0.47
1:A:272:PHE:CZ	1:A:308:PRO:HB2	2.50	0.47
1:A:386:HIS:CE1	5:A:602:HEM:C1A	3.02	0.47
1:A:233:HIS:N	1:A:234:PRO:HD2	2.30	0.47
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.50	0.47
2:B:118:VAL:HB	2:B:121:THR:OG1	2.14	0.47
1:A:143:TRP:HB2	1:A:213:PHE:CE2	2.50	0.47
1:A:434:ILE:HG21	1:A:472:LEU:HD23	1.97	0.47
1:A:286:ALA:HB1	2:B:125:VAL:HA	1.96	0.47
1:A:235:ILE:O	1:A:238:PHE:HB3	2.15	0.46
1:A:392:LEU:O	1:A:392:LEU:HD22	2.14	0.46
2:B:35:TYR:OH	8:B:202:OLC:H24A	2.15	0.46
1:A:243:ALA:O	1:A:247:ILE:HD12	2.15	0.46
1:A:76:ASN:HB3	5:A:602:HEM:CAC	2.45	0.46
1:A:251:LEU:HD13	1:A:349:PRO:HG2	1.98	0.46
1:A:449:ARG:HG3	1:A:450:ARG:HG3	1.96	0.46
8:A:606:OLC:H9	3:C:21:VAL:HG11	1.97	0.46
1:A:52:TYR:N	1:A:53:PRO:HD2	2.30	0.46
1:A:28:GLY:O	1:A:80:PHE:HB2	2.16	0.45
8:A:617:OLC:H13	8:A:617:OLC:H10	1.32	0.45
5:A:602:HEM:HBC2	5:A:602:HEM:CMC	2.47	0.45
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.52	0.45
1:A:562:TRP:HA	2:B:155:LEU:HG	1.97	0.45
8:B:203:OLC:H6	3:C:33:ARG:HH11	1.81	0.45
8:A:605:OLC:O25	8:B:203:OLC:H7	2.16	0.44
1:A:445:LEU:O	1:A:446:ASN:HB2	2.17	0.44
1:A:556:VAL:HG12	2:B:55:PRO:HG3	1.99	0.44
1:A:264:MET:HG3	2:B:15:GLU:OE2	2.18	0.44
1:A:292:PRO:HB2	8:A:609:OLC:H3A	2.00	0.44
1:A:44:LEU:HD12	1:A:471:VAL:HA	2.00	0.44
2:B:32:LEU:HD21	8:B:202:OLC:C7	2.45	0.44
1:A:22:LEU:O	1:A:26:VAL:HG23	2.17	0.44
3:C:4:LYS:HG3	3:C:6:LYS:HG2	2.00	0.44
1:A:386:HIS:CE1	5:A:602:HEM:NA	2.86	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:87:ALA:HA	2:B:88:PHE:HA	1.68	0.43
2:B:73:GLN:HB2	2:B:79:TYR:CE1	2.54	0.43
8:A:607:OLC:H12	8:A:615:OLC:C14	2.48	0.43
1:A:186:ALA:O	1:A:189:PHE:HB3	2.19	0.43
1:A:450:ARG:O	2:B:157:HIS:CD2	2.71	0.43
1:A:445:LEU:HD23	1:A:445:LEU:HA	1.79	0.43
1:A:504:ALA:HA	1:A:505:PRO:HD3	1.88	0.43
1:A:405:LEU:HA	1:A:405:LEU:HD12	1.84	0.42
1:A:302:THR:O	1:A:305:VAL:HG12	2.18	0.42
1:A:386:HIS:HE1	5:A:602:HEM:C1A	2.38	0.42
1:A:241:LEU:HA	1:A:244:TYR:HB2	2.02	0.42
1:A:168:ARG:HH22	8:A:613:OLC:C6	2.14	0.42
8:A:607:OLC:H2	8:A:607:OLC:H5A	1.88	0.42
1:A:400:SER:HB3	10:A:704:HOH:O	2.20	0.42
1:A:290:ILE:HB	1:A:295:LYS:HE3	2.01	0.42
3:C:16:THR:HG22	3:C:20:LEU:HD22	2.00	0.42
1:A:432:MET:CE	5:A:602:HEM:HAB	2.50	0.42
5:A:602:HEM:HBC2	5:A:602:HEM:HMC2	2.02	0.42
1:A:516:GLU:CG	1:A:517:ASP:N	2.67	0.42
1:A:174:ASN:N	1:A:175:PRO:CD	2.82	0.42
1:A:307:VAL:N	1:A:308:PRO:CD	2.82	0.42
2:B:21:PHE:O	2:B:24:ALA:HB3	2.19	0.41
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.55	0.41
1:A:475:ILE:HG13	1:A:476:VAL:N	2.35	0.41
3:C:24:LEU:HD12	3:C:24:LEU:HA	1.84	0.41
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.94	0.41
2:B:92:PRO:HG3	10:B:339:HOH:O	2.21	0.41
2:B:115:GLY:HA3	2:B:150:ASN:H	1.85	0.41
2:B:58:VAL:HG22	2:B:64:TRP:HB2	2.03	0.41
1:A:460:TYR:N	1:A:461:PRO:CD	2.83	0.41
1:A:528:GLY:HA2	8:A:613:OLC:H2	2.02	0.41
8:A:608:OLC:H11	8:A:615:OLC:H14	2.03	0.41
1:A:351:LEU:HB3	1:A:429:PHE:CD2	2.56	0.41
1:A:426:TRP:NE1	8:A:608:OLC:H21	2.36	0.40
1:A:261:SER:HB3	1:A:264:MET:HB2	2.04	0.40
3:C:9:LEU:O	3:C:12:ILE:HG13	2.21	0.40
1:A:102:ASN:OD1	1:A:102:ASN:C	2.60	0.40
1:A:96:GLU:OE2	1:A:180:PRO:HB2	2.20	0.40
2:B:27:PHE:HD1	2:B:27:PHE:HA	1.79	0.40
1:A:247:ILE:O	1:A:252:PRO:HD3	2.22	0.40
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.89	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:B:308:HOH:O	10:B:324:HOH:O[2_556]	1.72	0.48

## 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%)	520 (94%)	32 (6%)	0	100	100
2	B	164/168 (98%)	160 (98%)	4 (2%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	745/770 (97%)	709 (95%)	36 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	445/462 (96%)	424 (95%)	21 (5%)	36	73
2	B	133/138 (96%)	127 (96%)	6 (4%)	38	74
3	C	24/27 (89%)	21 (88%)	3 (12%)	7	19
All	All	602/627 (96%)	572 (95%)	30 (5%)	34	70

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	58	LEU

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Mol	Chain	Res	Type
1	A	80	PHE
1	A	215	LEU
1	A	223	VAL
1	A	244	TYR
1	A	274	LEU
1	A	309	SER
1	A	326	LEU
1	A	332	LEU
1	A	369	PHE
1	A	405	LEU
1	A	475	ILE
1	A	495	ARG
1	A	500	GLU
1	A	503	GLU
1	A	512	ILE
1	A	518	ARG
1	A	520	LEU
1	A	526	ARG
1	A	549	LEU
2	B	12	LEU
2	B	26	LEU
2	B	37	LEU
2	B	111	ASP
2	B	167	LYS
2	B	168	GLU
3	C	13	LEU
3	C	20	LEU
3	C	24	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	602	1	49,50,50	8.31	26 (53%)	46,82,82	2.88	16 (34%)
6	HAS	A	603	1,7	72,72,72	2.76	26 (36%)	86,109,109	2.17	20 (23%)
7	PER	A	604	4,6	1,1,1	1.56	0	0,0,0	0.00	-
8	OLC	A	605	-	24,24,24	0.49	0	25,25,25	0.71	0
8	OLC	A	606	-	24,24,24	0.42	0	25,25,25	0.61	0
8	OLC	A	607	-	24,24,24	0.51	0	25,25,25	0.69	0
8	OLC	A	608	-	22,22,24	1.35	1 (4%)	23,23,25	0.58	0
8	OLC	A	609	-	19,20,24	0.38	0	19,20,25	0.53	0
8	OLC	A	610	-	16,17,24	0.53	0	17,18,25	0.54	0
8	OLC	A	611	-	15,16,24	0.48	0	16,17,25	0.67	0
8	OLC	A	612	-	6,7,24	0.23	0	5,7,25	0.27	0
8	OLC	A	613	-	14,14,24	1.52	1 (7%)	15,15,25	0.73	0
8	OLC	A	614	-	19,19,24	1.47	1 (5%)	20,20,25	1.66	1 (5%)
8	OLC	A	615	-	24,24,24	0.41	0	25,25,25	0.79	0
8	OLC	A	616	-	20,20,24	1.34	1 (5%)	21,21,25	0.88	0
8	OLC	A	617	-	24,24,24	0.42	0	25,25,25	0.83	1 (4%)
9	CUA	B	201	2	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	B	202	-	24,24,24	0.48	0	25,25,25	0.65	0
8	OLC	B	203	-	24,24,24	0.54	0	25,25,25	0.71	0
8	OLC	B	204	-	24,24,24	0.45	0	25,25,25	0.53	0

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	602	1	-	0/14/114/114	0/0/8/8
6	HAS	A	603	1,7	-	0/36/82/82	0/0/8/8
7	PER	A	604	4,6	-	0/0/0/0	0/0/0/0
8	OLC	A	605	-	-	0/24/24/24	0/0/0/0
8	OLC	A	606	-	-	0/24/24/24	0/0/0/0
8	OLC	A	607	-	-	0/24/24/24	0/0/0/0
8	OLC	A	608	-	-	0/22/22/24	0/0/0/0
8	OLC	A	609	-	-	0/19/19/24	0/0/0/0
8	OLC	A	610	-	-	0/17/17/24	0/0/0/0
8	OLC	A	611	-	-	0/16/16/24	0/0/0/0
8	OLC	A	612	-	-	0/5/6/24	0/0/0/0
8	OLC	A	613	-	-	0/14/14/24	0/0/0/0
8	OLC	A	614	-	-	0/19/19/24	0/0/0/0
8	OLC	A	615	-	-	0/24/24/24	0/0/0/0
8	OLC	A	616	-	-	0/20/20/24	0/0/0/0
8	OLC	A	617	-	-	0/24/24/24	0/0/0/0
9	CUA	B	201	2	-	0/0/0/0	0/0/0/0
8	OLC	B	202	-	-	0/24/24/24	0/0/0/0
8	OLC	B	203	-	-	0/24/24/24	0/0/0/0
8	OLC	B	204	-	-	0/24/24/24	0/0/0/0

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	C2B-C1B	-42.48	1.33	1.44
5	A	602	HEM	C2D-C1D	24.57	1.50	1.44
5	A	602	HEM	C3D-C4D	20.86	1.49	1.44
5	A	602	HEM	CHB-C1B	10.55	1.50	1.35
5	A	602	HEM	C4A-C3A	8.19	1.50	1.40
6	A	603	HAS	C4D-ND	7.66	1.48	1.37
6	A	603	HAS	C3C-CAC	-7.60	1.33	1.48
6	A	603	HAS	C2D-C1D	7.34	1.52	1.40
6	A	603	HAS	C4A-C3A	7.03	1.48	1.40
5	A	602	HEM	CHD-C4C	6.79	1.49	1.36
5	A	602	HEM	CHC-C1C	6.45	1.48	1.36
5	A	602	HEM	FE-NB	6.10	2.20	1.97
8	A	614	OLC	C13-C12	-6.08	1.52	1.55
8	A	608	OLC	C16-C15	-5.95	1.52	1.55
6	A	603	HAS	C4C-C3C	5.89	1.49	1.41
5	A	602	HEM	C3D-C2D	-5.80	1.33	1.43
6	A	603	HAS	C1D-ND	5.71	1.47	1.36
8	A	616	OLC	C14-C13	-5.63	1.52	1.55
6	A	603	HAS	C3C-C2C	5.49	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	613	OLC	C8-C7	-5.42	1.53	1.55
5	A	602	HEM	C1A-NA	4.96	1.46	1.36
6	A	603	HAS	C4C-NC	4.70	1.43	1.37
6	A	603	HAS	C1C-C2C	-4.28	1.34	1.40
6	A	603	HAS	C4D-CHA	4.17	1.51	1.38
5	A	602	HEM	C1A-CHA	4.13	1.51	1.39
6	A	603	HAS	C1A-C2A	4.03	1.50	1.43
5	A	602	HEM	C1A-C2A	4.02	1.50	1.43
5	A	602	HEM	C3B-C4B	3.96	1.49	1.44
6	A	603	HAS	C1C-CHC	3.87	1.50	1.39
6	A	603	HAS	C1D-CHB	3.84	1.50	1.39
5	A	602	HEM	CBB-CAB	3.82	1.51	1.28
6	A	603	HAS	C2D-C3D	-3.72	1.34	1.41
6	A	603	HAS	C4C-CHD	3.63	1.49	1.38
5	A	602	HEM	C3B-C2B	3.52	1.49	1.43
5	A	602	HEM	C2C-C1C	-3.33	1.33	1.43
6	A	603	HAS	FE-NC	3.15	2.05	1.92
5	A	602	HEM	CHC-C4B	-2.97	1.32	1.39
6	A	603	HAS	O1D-CGD	2.96	1.32	1.22
6	A	603	HAS	CBC-CAC	2.93	1.51	1.28
5	A	602	HEM	CHD-C1D	-2.86	1.32	1.39
6	A	603	HAS	FE-NB	2.85	2.04	1.92
5	A	602	HEM	C3C-CAC	2.83	1.49	1.40
6	A	603	HAS	C4A-CHD	-2.76	1.32	1.39
6	A	603	HAS	FE-NA	2.73	2.04	1.92
5	A	602	HEM	FE-NA	2.60	2.03	1.92
6	A	603	HAS	C4D-C3D	2.59	1.52	1.43
5	A	602	HEM	C3C-C2C	2.58	1.48	1.43
5	A	602	HEM	C1C-NC	-2.49	1.34	1.38
6	A	603	HAS	O2D-CGD	-2.44	1.21	1.30
5	A	602	HEM	C4A-CHB	-2.41	1.33	1.39
5	A	602	HEM	CHA-C4D	-2.40	1.32	1.35
6	A	603	HAS	C4B-C3B	2.34	1.51	1.43
5	A	602	HEM	C3B-CAB	-2.20	1.33	1.40
6	A	603	HAS	C1A-CHA	-2.09	1.34	1.39
5	A	602	HEM	C4D-ND	-2.07	1.35	1.39
6	A	603	HAS	C3B-C2B	-2.06	1.33	1.40

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEM	C3B-C4B-NB	-11.90	105.48	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C4C-C3C-C2C	-10.47	99.55	106.87
5	A	602	HEM	CHC-C4B-NB	7.40	130.74	124.58
6	A	603	HAS	C2C-C1C-NC	7.03	114.72	109.41
8	A	614	OLC	C13-C12-C11	-6.89	110.79	117.97
5	A	602	HEM	C1B-NB-C4B	5.93	111.23	105.16
6	A	603	HAS	C3A-C4A-NA	4.69	112.95	109.41
6	A	603	HAS	C4D-ND-C1D	-4.46	100.89	106.76
5	A	602	HEM	CHD-C4C-NC	4.17	128.36	124.73
6	A	603	HAS	C4B-C3B-C11	4.12	132.10	124.67
6	A	603	HAS	C2B-C1B-NB	3.87	112.33	109.41
5	A	602	HEM	C1A-CHA-C4D	-3.67	122.64	127.47
5	A	602	HEM	C4A-CHB-C1B	-3.57	122.78	127.47
5	A	602	HEM	C2D-C1D-ND	-3.51	108.79	112.93
5	A	602	HEM	C4D-ND-C1D	3.45	108.69	105.16
6	A	603	HAS	C4A-C3A-C2A	-3.37	104.65	107.00
5	A	602	HEM	C4C-NC-C1C	3.36	109.03	105.53
6	A	603	HAS	CMC-C2C-C1C	-3.27	123.59	128.62
6	A	603	HAS	C4B-C3B-C2B	-3.26	104.59	106.87
6	A	603	HAS	C2A-C1A-CHA	-3.00	120.31	126.00
6	A	603	HAS	C3C-C2C-C1C	2.85	108.67	107.00
6	A	603	HAS	C1B-CHB-C1D	-2.81	123.77	127.47
5	A	602	HEM	CHA-C1A-NA	2.72	129.11	124.58
6	A	603	HAS	C3A-C4A-CHD	-2.67	120.94	126.00
5	A	602	HEM	C4A-C3A-C2A	2.64	108.83	107.00
6	A	603	HAS	CAA-CBA-CGA	-2.58	105.16	113.47
6	A	603	HAS	C4D-CHA-C1A	-2.42	124.28	127.47
6	A	603	HAS	C3B-C4B-NB	2.41	112.24	109.90
6	A	603	HAS	C2D-C1D-ND	2.37	110.94	108.64
5	A	602	HEM	CHD-C1D-ND	2.36	126.55	124.58
5	A	602	HEM	CMA-C3A-C4A	-2.35	125.00	128.62
5	A	602	HEM	CHA-C4D-ND	2.33	127.51	124.31
5	A	602	HEM	C2A-C1A-NA	-2.31	106.52	109.73
6	A	603	HAS	CHB-C1D-ND	-2.30	120.74	124.58
8	A	617	OLC	C3-C2-C1	-2.29	104.55	113.51
5	A	602	HEM	CBD-CAD-C3D	-2.16	109.66	114.37
6	A	603	HAS	CMA-C3A-C4A	-2.16	125.30	128.62
6	A	603	HAS	O1A-CGA-CBA	-2.12	115.75	123.03

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%)	-0.59	7 (1%) 74 75	15, 25, 45, 87	3 (0%)
2	B	166/168 (98%)	-0.69	0 100 100	17, 25, 43, 61	1 (0%)
3	C	31/34 (91%)	-0.80	0 100 100	17, 24, 37, 48	0
All	All	751/770 (97%)	-0.62	7 (0%) 81 81	15, 25, 45, 87	4 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	SER	6.5
1	A	495	ARG	4.2
1	A	494	SER	3.5
1	A	514	GLY	3.4
1	A	496	GLU	2.6
1	A	499	PRO	2.5
1	A	493	LEU	2.3

### 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(Å <sup>2</sup> )	Q<0.9
8	OLC	A	606	25/25	0.27	8.94	35,58,90,105	0
8	OLC	A	605	25/25	0.30	6.79	26,45,69,79	0
8	OLC	A	617	25/25	0.24	5.81	35,47,62,70	0
8	OLC	A	616	21/25	0.30	5.55	35,45,61,72	0
8	OLC	A	611	17/25	0.26	5.29	35,47,97,98	0
8	OLC	A	614	20/25	0.24	5.23	32,50,64,65	0
8	OLC	A	613	15/25	0.42	4.95	41,48,71,73	0
8	OLC	B	204	25/25	0.33	4.45	38,50,66,77	0
8	OLC	B	202	25/25	0.24	4.32	32,44,52,55	0
8	OLC	A	609	21/25	0.23	4.23	37,43,63,71	0
8	OLC	A	607	25/25	0.21	3.55	40,44,65,79	0
8	OLC	B	203	25/25	0.21	2.69	36,53,75,82	0
8	OLC	A	615	25/25	0.18	2.43	31,44,58,69	0
8	OLC	A	610	18/25	0.17	2.40	32,43,62,65	0
8	OLC	A	608	23/25	0.19	2.34	27,39,49,55	0
8	OLC	A	612	8/25	0.25	2.26	39,44,48,49	0
6	HAS	A	603	65/65	0.16	1.33	14,19,24,27	0
9	CUA	B	201	2/2	0.13	0.07	17,17,17,17	0
5	HEM	A	602	43/43	0.12	-0.24	13,17,20,21	0
7	PER	A	604	2/2	0.11	-0.33	23,23,23,24	0
4	CU	A	601	1/1	0.08	-5.96	17,17,17,17	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.