



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:19 am GMT

PDB ID : 4GP5  
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant Y133W from *Thermus thermophilus*  
Authors : Li, Y.; Chen, Y.; Stout, C.D.  
Deposited on : 2012-08-20  
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

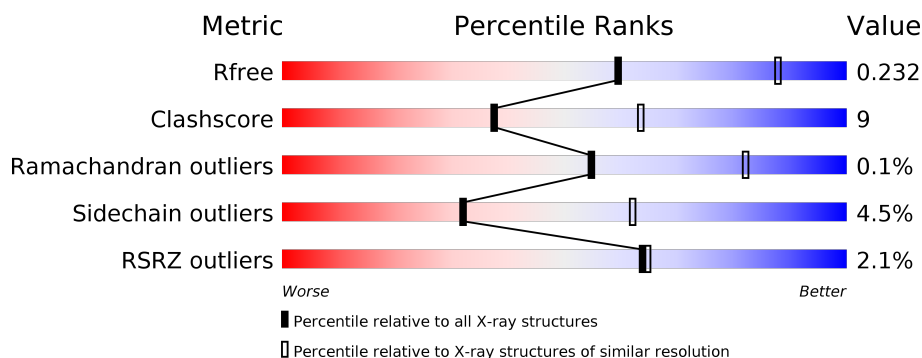
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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>2%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
2	B	168	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>• •</div> </div> </div>
3	C	34	<div> <div></div> <div> <div></div> <div>65%</div> <div>24%</div> <div>• 9%</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
8	OLC	A	605	-	-	-	X
8	OLC	A	606	-	-	-	X
8	OLC	A	607	-	-	-	X
8	OLC	A	608	-	-	-	X
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	B	202	-	-	-	X
8	OLC	B	203	-	-	-	X
8	OLC	B	204	-	-	-	X
8	OLC	B	205	-	-	-	X
8	OLC	C	101	-	-	-	X
8	OLC	C	102	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6429 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	552	Total	C	N	O	S	0	4	0
			4377	2974	698	689	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	TRP	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	1	0
			1288	837	214	233	4			

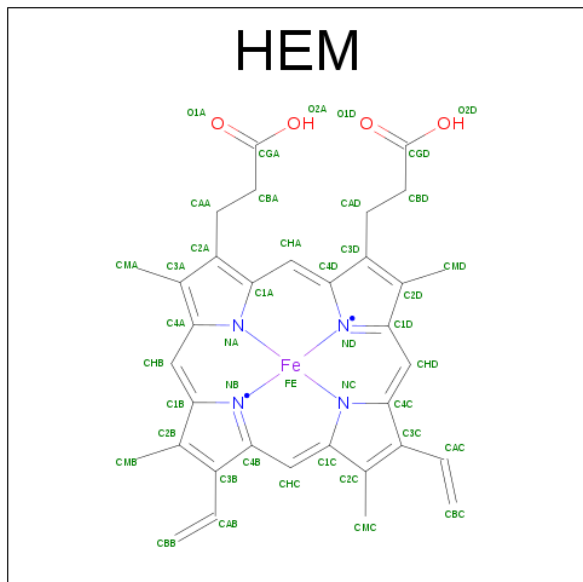
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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).

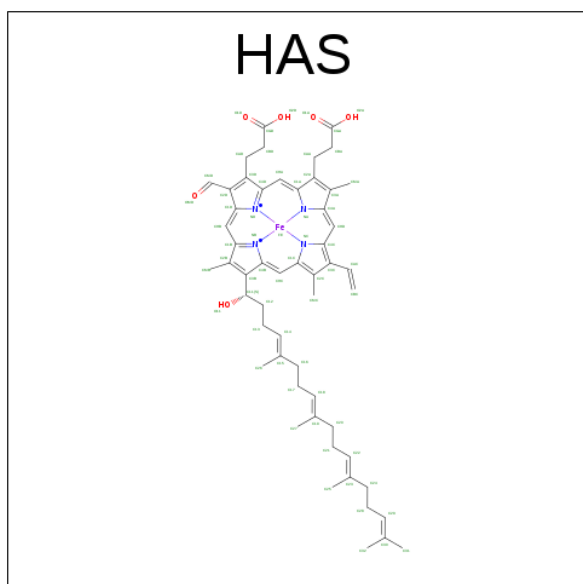
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



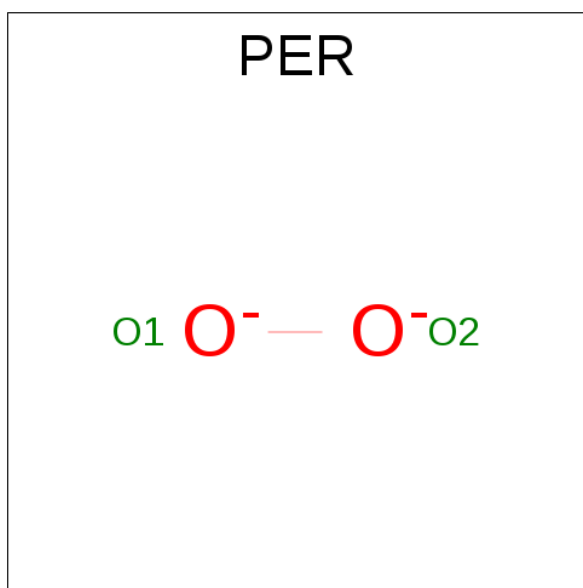
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is HEME-AS (three-letter code: HAS) (formula:  $\text{C}_{54}\text{H}_{64}\text{FeN}_4\text{O}_6$ ).



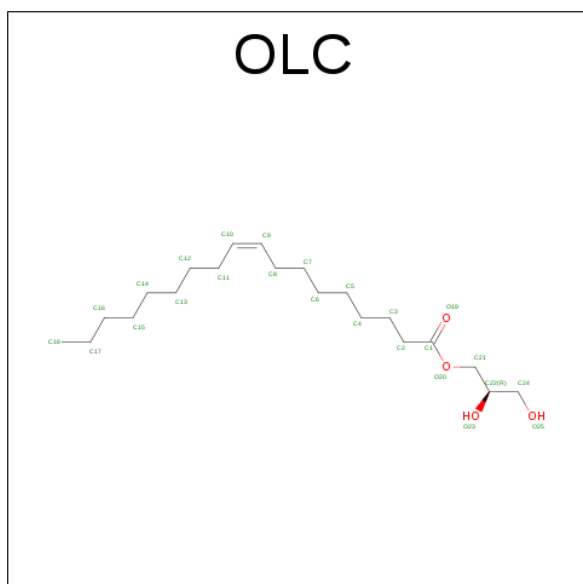
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 65	C 54	Fe 1	N 4	O 6	0	0

- 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>).



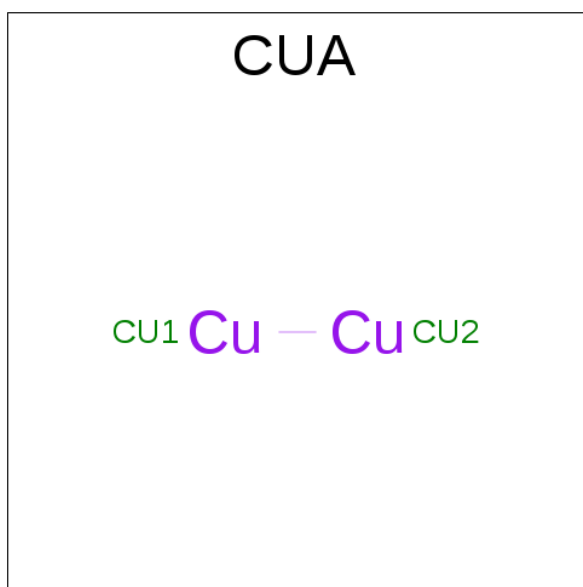
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			25	21	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			23	19	4		
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		
8	B	1	Total	C	O	0	0
			21	19	2		
8	C	1	Total	C	O	0	0
			25	21	4		
8	C	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	0	0
			2	2		

- Molecule 10 is water.

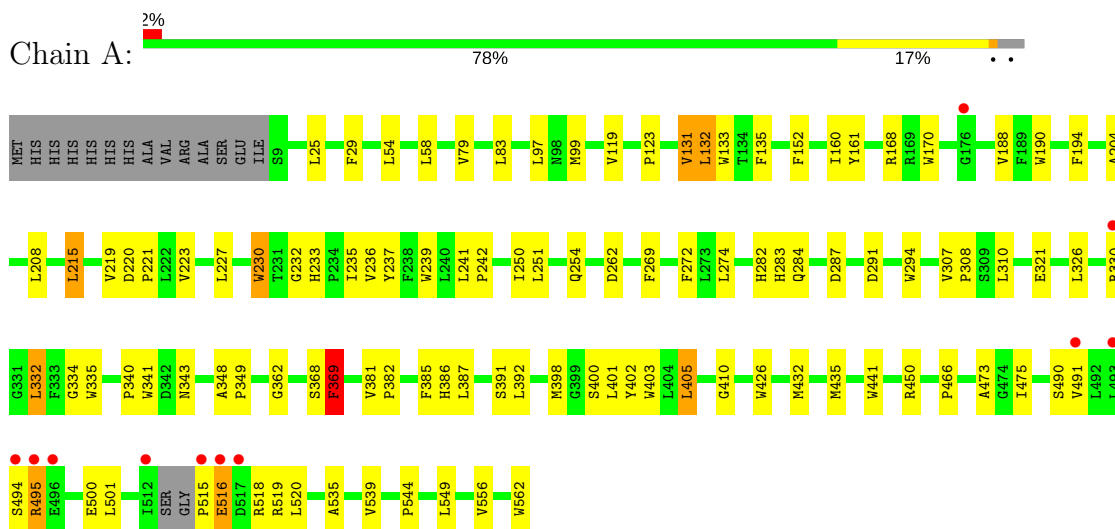
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	47	Total	O	0	0
			47	47		
10	B	17	Total	O	0	0
			17	17		
10	C	3	Total	O	0	0
			3	3		



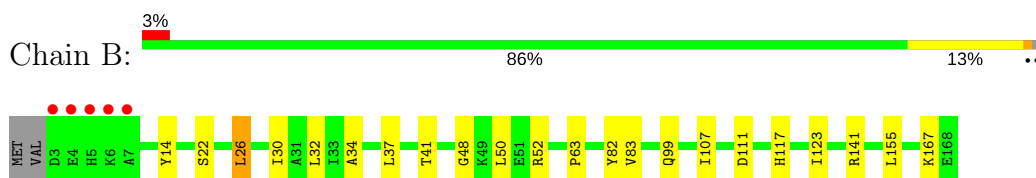
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.09Å 97.96Å 94.65Å 90.00° 127.99° 90.00°	Depositor
Resolution (Å)	74.60 – 2.70 56.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (74.60-2.70) 97.4 (56.78-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.173 , 0.230 0.176 , 0.232	Depositor DCC
$R_{free}$ test set	1401 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6429	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 5.82% 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: 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	0.83	2/4545 (0.0%)	0.80	3/6239 (0.0%)
2	B	0.88	0/1330	0.76	0/1817
3	C	0.88	0/247	0.85	1/335 (0.3%)
All	All	0.84	2/6122 (0.0%)	0.79	4/8391 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	PHE	CD1-CE1	-5.28	1.28	1.39
1	A	368	SER	C-O	-5.23	1.13	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	PHE	N-CA-CB	-8.04	96.12	110.60
1	A	332	LEU	CA-CB-CG	7.57	132.71	115.30
1	A	131	VAL	N-CA-C	-6.27	94.08	111.00
3	C	13	LEU	CA-CB-CG	5.46	127.85	115.30

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	4377	0	4476	87	0
2	B	1288	0	1260	15	0
3	C	241	0	267	5	0
4	A	1	0	0	0	0
5	A	43	0	30	5	0
6	A	65	0	62	1	0
7	A	2	0	0	0	0
8	A	197	0	280	13	0
8	B	96	0	153	9	0
8	C	50	0	80	5	0
9	B	2	0	0	0	0
10	A	47	0	0	13	0
10	B	17	0	0	2	1
10	C	3	0	0	1	0
All	All	6429	0	6608	114	1

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 9.

All (114) 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	0.87	1.36
1:A:233:HIS:NE2	1:A:237:TYR:CE2	1.78	1.32
8:A:607:OLC:H2	10:A:713:HOH:O	1.35	1.24
10:A:744:HOH:O	8:B:203:OLC:H17	1.45	1.16
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:HG2	0.94	1.07
1:A:330[B]:ARG:NH1	1:A:330[B]:ARG:HG2	1.64	1.03
1:A:168:ARG:HH22	8:A:610:OLC:H6A	1.24	1.03
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:CG	1.70	1.01
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.81	0.98
1:A:515:PRO:HA	1:A:516:GLU:HB2	1.44	0.95
8:B:204:OLC:H3	10:B:313:HOH:O	1.71	0.90
10:A:744:HOH:O	8:C:101:OLC:H11	1.86	0.76
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.63	0.76
3:C:4:LYS:HG3	3:C:6:LYS:HG2	1.70	0.72
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.76	0.71
1:A:133:TRP:CD1	10:A:709:HOH:O	2.46	0.67
1:A:168:ARG:NH2	8:A:610:OLC:H6A	2.06	0.66
1:A:381:VAL:HB	1:A:382:PRO:HD3	1.78	0.66
5:A:602:HEM:HBC2	5:A:602:HEM:HMC1	1.78	0.65
1:A:341:TRP:O	8:A:606:OLC:H24A	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ARG:HH12	8:B:203:OLC:H22	1.63	0.63
1:A:161:TYR:CE2	8:A:609:OLC:H21	2.34	0.62
1:A:233:HIS:O	1:A:236:VAL:HG22	2.01	0.60
1:A:160:ILE:HG12	1:A:190:TRP:HB3	1.85	0.59
3:C:18:THR:HG23	8:C:102:OLC:H12	1.85	0.59
1:A:133:TRP:HD1	10:A:709:HOH:O	1.85	0.58
1:A:362:GLY:HA3	10:A:721:HOH:O	2.02	0.58
1:A:450:ARG:NH1	10:A:709:HOH:O	2.37	0.57
2:B:14:TYR:CD2	3:C:9:LEU:HD11	2.40	0.56
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.40	0.56
1:A:204:ALA:HA	1:A:208:LEU:HB2	1.89	0.55
8:A:606:OLC:H15	8:A:611:OLC:H12	1.89	0.55
1:A:562:TRP:HA	2:B:155:LEU:HG	1.88	0.54
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.43	0.54
8:B:204:OLC:H7	10:B:312:HOH:O	2.07	0.54
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.91	0.53
8:B:204:OLC:C10	10:C:201:HOH:O	2.57	0.53
10:A:744:HOH:O	8:C:101:OLC:C11	2.52	0.53
2:B:26:LEU:O	2:B:30:ILE:HG13	2.09	0.52
1:A:219:VAL:O	1:A:221:PRO:HD3	2.10	0.52
1:A:232:GLY:O	1:A:235:ILE:HG22	2.10	0.52
1:A:450:ARG:HB2	10:A:726:HOH:O	2.10	0.51
1:A:535:ALA:O	1:A:539:VAL:HG23	2.09	0.51
1:A:168:ARG:HH11	8:A:609:OLC:H22	1.75	0.51
1:A:400:SER:HA	1:A:403:TRP:NE1	2.26	0.51
1:A:307:VAL:N	1:A:308:PRO:HD2	2.25	0.51
1:A:168:ARG:NH2	8:A:610:OLC:H3A	2.26	0.51
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.94	0.50
1:A:385:PHE:CG	6:A:603:HAS:HMA2	2.46	0.50
1:A:348:ALA:HB3	1:A:349:PRO:CD	2.42	0.50
2:B:141:ARG:NH2	8:B:203:OLC:O19	2.44	0.50
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.99	0.50
1:A:432:MET:HE2	5:A:602:HEM:HAB	1.94	0.50
1:A:387:LEU:O	1:A:391:SER:HB3	2.12	0.49
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.46	0.49
10:A:744:HOH:O	8:C:101:OLC:C12	2.60	0.49
1:A:343:ASN:OD1	1:A:402[B]:TYR:CE2	2.66	0.49
1:A:426:TRP:CB	8:A:606:OLC:H3A	2.42	0.48
1:A:132:LEU:HB2	10:A:709:HOH:O	2.13	0.48
1:A:241:LEU:N	1:A:242:PRO:CD	2.76	0.48
1:A:79:VAL:HA	1:A:152:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.49	0.47
8:A:613:OLC:H11	8:A:613:OLC:H8	1.70	0.47
1:A:401:LEU:HG	1:A:405:LEU:HD22	1.96	0.47
1:A:168:ARG:HH11	8:A:609:OLC:C22	2.27	0.47
1:A:435:MET:HB2	1:A:473:ALA:HB1	1.97	0.47
1:A:119:VAL:O	1:A:123:PRO:HD2	2.15	0.46
1:A:251:LEU:HA	1:A:254:GLN:HG3	1.97	0.46
1:A:221:PRO:HD3	1:A:556:VAL:HG22	1.98	0.46
1:A:220:ASP:O	1:A:223:VAL:HG12	2.15	0.46
1:A:495:ARG:HH21	1:A:495:ARG:HA	1.81	0.46
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.85	0.45
1:A:432:MET:CE	5:A:602:HEM:HAB	2.47	0.45
10:A:744:HOH:O	8:C:101:OLC:H12A	2.17	0.45
1:A:310:LEU:HD13	2:B:22:SER:HB2	1.99	0.45
2:B:32:LEU:HD21	8:B:202:OLC:H7A	1.99	0.45
1:A:227:LEU:O	1:A:230:TRP:HB3	2.17	0.44
1:A:188:VAL:HG21	1:A:269:PHE:HB3	2.00	0.44
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.52	0.44
1:A:291:ASP:HA	2:B:48:GLY:HA3	2.00	0.44
1:A:168:ARG:NH1	8:A:609:OLC:H22	2.32	0.44
1:A:369:PHE:CD2	1:A:369:PHE:C	2.90	0.44
1:A:405:LEU:HD23	1:A:491:VAL:HG11	2.00	0.44
1:A:386:HIS:CE1	5:A:602:HEM:C1A	3.06	0.44
2:B:63:PRO:HB2	2:B:82:TYR:CG	2.53	0.44
1:A:386:HIS:CE1	5:A:602:HEM:NA	2.86	0.43
1:A:410:GLY:HA2	1:A:501:LEU:HB2	2.00	0.43
1:A:233:HIS:NE2	1:A:237:TYR:CZ	2.66	0.43
1:A:519:ARG:HB2	1:A:519:ARG:HE	1.63	0.43
1:A:29:PHE:CE1	1:A:401:LEU:CD1	3.02	0.42
2:B:83:VAL:HB	2:B:107:ILE:HG23	2.01	0.42
2:B:117:HIS:HD2	2:B:123:ILE:O	2.02	0.42
1:A:215:LEU:HD12	1:A:215:LEU:HA	1.86	0.42
1:A:330[B]:ARG:NH1	1:A:330[B]:ARG:CG	2.42	0.42
8:A:607:OLC:H4A	10:A:706:HOH:O	2.18	0.42
1:A:284:GLN:HG2	1:A:287:ASP:OD1	2.19	0.42
8:B:203:OLC:H6	3:C:33:ARG:HH11	1.84	0.42
2:B:34:ALA:O	2:B:37:LEU:HB2	2.20	0.42
1:A:398:MET:O	1:A:401:LEU:HB2	2.20	0.42
1:A:272:PHE:CE1	1:A:308:PRO:HB2	2.55	0.41
1:A:97:LEU:O	1:A:99:MET:HG3	2.19	0.41
2:B:41:THR:HG21	3:C:31:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:HD23	2:B:50:LEU:HD11	2.03	0.41
2:B:141:ARG:NH1	8:B:203:OLC:H22	2.33	0.41
1:A:25:LEU:HA	1:A:25:LEU:HD23	1.90	0.41
1:A:441:TRP:CG	1:A:466:PRO:HG3	2.56	0.41
1:A:254:GLN:O	1:A:340:PRO:HG2	2.21	0.40
1:A:230:TRP:CD1	1:A:230:TRP:C	2.95	0.40
1:A:250:ILE:HG22	1:A:254:GLN:HE21	1.86	0.40
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.56	0.40
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.97	0.40

All (1) 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)
10:B:303:HOH:O	10:B:303:HOH:O[2_554]	1.73	0.47

## 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	551/568 (97%)	525 (95%)	25 (4%)	1 (0%)	51	79
2	B	165/168 (98%)	161 (98%)	4 (2%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	745/770 (97%)	715 (96%)	29 (4%)	1 (0%)	55	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	VAL

### 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	448/462 (97%)	429 (96%)	19 (4%)	34	65
2	B	134/138 (97%)	129 (96%)	5 (4%)	39	70
3	C	24/27 (89%)	21 (88%)	3 (12%)	5	12
All	All	606/627 (97%)	579 (96%)	27 (4%)	32	62

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	58	LEU
1	A	132	LEU
1	A	215	LEU
1	A	230	TRP
1	A	262	ASP
1	A	274	LEU
1	A	326	LEU
1	A	332	LEU
1	A	369	PHE
1	A	405	LEU
1	A	475	ILE
1	A	490	SER
1	A	494	SER
1	A	495	ARG
1	A	500	GLU
1	A	516	GLU
1	A	518	ARG
1	A	520	LEU
2	B	26	LEU
2	B	52	ARG
2	B	99	GLN
2	B	111	ASP
2	B	167	LYS
3	C	13	LEU
3	C	20	LEU

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Mol	Chain	Res	Type
3	C	24	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	69	GLN
2	B	99	GLN
2	B	117	HIS

### 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 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	28,50,50	2.72	11 (39%)	17,82,82	2.13	7 (41%)
6	HAS	A	603	1,7	55,72,72	4.44	17 (30%)	48,109,109	2.36	11 (22%)
7	PER	A	604	4,6	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	A	605	-	24,24,24	0.54	0	25,25,25	0.81	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	OLC	A	606	-	22,22,24	0.49	0	23,23,25	0.61	1 (4%)
8	OLC	A	607	-	17,17,24	0.68	0	18,18,25	0.57	0
8	OLC	A	608	-	16,16,24	0.93	1 (6%)	17,17,25	0.79	1 (5%)
8	OLC	A	609	-	7,7,24	0.64	0	6,7,25	0.69	0
8	OLC	A	610	-	14,14,24	0.57	0	15,15,25	0.60	0
8	OLC	A	611	-	19,19,24	0.46	0	20,20,25	0.75	1 (5%)
8	OLC	A	612	-	24,24,24	0.62	1 (4%)	25,25,25	1.00	3 (12%)
8	OLC	A	613	-	20,20,24	0.55	0	21,21,25	0.68	0
8	OLC	A	614	-	24,24,24	0.54	0	25,25,25	0.70	0
9	CUA	B	201	2	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	B	202	-	24,24,24	0.54	0	25,25,25	0.49	0
8	OLC	B	203	-	24,24,24	0.68	1 (4%)	25,25,25	1.11	3 (12%)
8	OLC	B	204	-	24,24,24	0.54	0	25,25,25	0.42	0
8	OLC	B	205	-	20,20,24	0.56	0	20,20,25	0.52	0
8	OLC	C	101	-	24,24,24	0.55	0	25,25,25	0.95	1 (4%)
8	OLC	C	102	-	24,24,24	0.45	0	25,25,25	0.54	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	-	0/6/54/54	0/0/8/8
6	HAS	A	603	1,7	-	0/35/122/122	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	-	-	0/22/22/24	0/0/0/0
8	OLC	A	607	-	-	0/17/17/24	0/0/0/0
8	OLC	A	608	-	-	0/16/16/24	0/0/0/0
8	OLC	A	609	-	-	0/6/6/24	0/0/0/0
8	OLC	A	610	-	-	0/14/14/24	0/0/0/0
8	OLC	A	611	-	-	0/19/19/24	0/0/0/0
8	OLC	A	612	-	-	0/24/24/24	0/0/0/0
8	OLC	A	613	-	-	0/20/20/24	0/0/0/0
8	OLC	A	614	-	-	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
8	OLC	B	205	-	-	0/19/19/24	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	C	101	-	-	0/24/24/24	0/0/0/0
8	OLC	C	102	-	-	0/24/24/24	0/0/0/0

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	CHD-C4A	-17.67	1.34	1.51
6	A	603	HAS	C1B-NB	-12.15	1.33	1.49
6	A	603	HAS	CHC-C4B	-10.88	1.32	1.53
6	A	603	HAS	C4B-NB	-10.38	1.35	1.49
5	A	602	HEM	C3B-CAB	-7.73	1.32	1.47
6	A	603	HAS	CHA-C1A	-7.72	1.33	1.51
6	A	603	HAS	C3C-CAC	-7.29	1.33	1.47
6	A	603	HAS	CHB-C1B	-5.37	1.31	1.53
6	A	603	HAS	C4D-ND	-3.36	1.45	1.49
5	A	602	HEM	C4B-CHC	-3.03	1.32	1.40
5	A	602	HEM	C4D-ND	-3.01	1.33	1.36
6	A	603	HAS	C1D-ND	-2.82	1.45	1.49
5	A	602	HEM	C1D-CHD	-2.79	1.32	1.40
6	A	603	HAS	C1C-C2C	-2.49	1.34	1.38
5	A	602	HEM	C4A-CHB	-2.34	1.33	1.40
5	A	602	HEM	C1C-NC	-2.31	1.34	1.36
6	A	603	HAS	CHD-C4C	-2.09	1.49	1.51
6	A	603	HAS	CMB-C2B	2.05	1.54	1.50
8	A	608	OLC	O20-C1	2.20	1.39	1.33
8	A	612	OLC	O20-C1	2.30	1.40	1.33
8	B	203	OLC	O20-C1	2.59	1.40	1.33
5	A	602	HEM	CBB-CAB	3.11	1.50	1.28
6	A	603	HAS	CBC-CAC	3.25	1.51	1.28
6	A	603	HAS	CMD-C2D	3.35	1.51	1.45
5	A	602	HEM	C1A-CHA	3.38	1.49	1.40
5	A	602	HEM	C1A-NA	3.98	1.44	1.36
5	A	602	HEM	C3C-C2C	4.36	1.46	1.40
6	A	603	HAS	C3C-C2C	6.69	1.49	1.40
5	A	602	HEM	C3B-C2B	6.78	1.49	1.40
6	A	603	HAS	C1A-C2A	7.49	1.48	1.38
6	A	603	HAS	C4A-C3A	8.83	1.50	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	CAA-C2A-C1A	-5.80	123.22	127.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	CHD-C4A-C3A	-5.15	120.92	129.53
6	A	603	HAS	CHC-C1C-C2C	-4.38	121.87	129.45
5	A	602	HEM	C3B-C4B-NB	-4.37	103.56	109.21
5	A	602	HEM	CMA-C3A-C4A	-3.57	122.98	128.46
6	A	603	HAS	CAD-CBD-CGD	-3.35	106.94	112.66
5	A	602	HEM	C4C-C3C-C2C	-2.55	105.12	106.90
5	A	602	HEM	C1D-C2D-C3D	-2.49	105.26	107.00
5	A	602	HEM	CMD-C2D-C1D	-2.43	124.73	128.46
6	A	603	HAS	CMB-C2B-C3B	-2.32	123.76	129.77
6	A	603	HAS	C4C-C3C-C2C	-2.30	100.70	104.13
5	A	602	HEM	CBD-CAD-C3D	-2.18	108.31	112.47
8	A	608	OLC	C21-O20-C1	2.03	123.23	117.13
8	A	612	OLC	O20-C1-O19	2.04	128.61	123.55
8	B	203	OLC	O20-C1-O19	2.15	128.89	123.55
8	A	605	OLC	O20-C21-C22	2.23	116.65	105.72
8	A	611	OLC	O20-C21-C22	2.27	116.83	105.72
8	A	612	OLC	O20-C21-C22	2.32	117.09	105.72
6	A	603	HAS	OMD-CMD-C2D	2.35	127.28	124.29
8	A	606	OLC	C21-O20-C1	2.36	124.23	117.13
8	A	612	OLC	C21-O20-C1	2.45	124.49	117.13
8	C	101	OLC	C21-O20-C1	2.48	124.60	117.13
8	B	203	OLC	O20-C21-C22	2.51	118.05	105.72
6	A	603	HAS	C1B-CHB-C1D	2.62	124.16	116.30
8	B	203	OLC	C21-O20-C1	3.37	127.26	117.13
5	A	602	HEM	C4A-C3A-C2A	3.85	109.68	107.00
6	A	603	HAS	CHA-C4D-ND	5.64	121.39	110.75
6	A	603	HAS	C4A-CHD-C4C	5.65	125.46	112.83
6	A	603	HAS	CHC-C4B-NB	7.69	125.25	110.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	HEM	5	0
6	A	603	HAS	1	0
8	A	606	OLC	3	0
8	A	607	OLC	2	0
8	A	609	OLC	4	0
8	A	610	OLC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	611	OLC	1	0
8	A	613	OLC	1	0
8	B	202	OLC	1	0
8	B	203	OLC	5	0
8	B	204	OLC	3	0
8	C	101	OLC	4	0
8	C	102	OLC	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	552/568 (97%)	-0.45	11 (1%) 65 66	12, 24, 47, 74	0
2	B	166/168 (98%)	-0.42	5 (3%) 51 50	14, 25, 41, 68	0
3	C	31/34 (91%)	-0.81	0 100 100	19, 23, 40, 45	0
All	All	749/770 (97%)	-0.46	16 (2%) 64 65	12, 24, 45, 74	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	ARG	4.6
2	B	4	GLU	4.0
2	B	6	LYS	3.8
1	A	496	GLU	3.7
1	A	176	GLY	3.2
1	A	330[A]	ARG	3.1
2	B	5	HIS	3.0
1	A	494	SER	2.8
2	B	3	ASP	2.7
1	A	515	PRO	2.4
1	A	516	GLU	2.4
1	A	491	VAL	2.3
1	A	493	LEU	2.2
1	A	512	ILE	2.1
2	B	7	ALA	2.1
1	A	517	ASP	2.1

### 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	OLC	A	608	17/25	0.61	0.35	17.30	57,64,77,77	0
8	OLC	C	102	25/25	0.74	0.28	17.17	81,85,91,93	0
8	OLC	B	204	25/25	0.71	0.42	10.77	76,87,96,97	0
8	OLC	A	607	18/25	0.84	0.25	9.84	48,54,64,65	0
8	OLC	A	605	25/25	0.73	0.34	8.70	72,80,92,92	0
8	OLC	A	611	20/25	0.81	0.27	7.02	55,59,69,69	0
8	OLC	A	614	25/25	0.83	0.29	6.04	55,63,70,73	0
8	OLC	A	610	15/25	0.78	0.54	5.78	68,80,86,86	0
8	OLC	C	101	25/25	0.84	0.24	5.53	41,55,75,75	0
8	OLC	A	613	21/25	0.81	0.27	4.58	49,64,82,84	0
8	OLC	B	205	21/25	0.82	0.28	3.93	56,61,71,72	0
8	OLC	B	203	25/25	0.80	0.26	3.88	52,68,79,80	0
8	OLC	B	202	25/25	0.80	0.27	3.79	56,61,70,71	0
8	OLC	A	606	23/25	0.87	0.22	2.87	39,43,52,52	0
8	OLC	A	612	25/25	0.90	0.19	2.18	40,44,50,51	0
6	HAS	A	603	65/65	0.98	0.13	0.19	10,16,26,27	0
7	PER	A	604	2/2	1.00	0.11	-0.33	20,20,20,22	0
5	HEM	A	602	43/43	0.98	0.11	-0.43	10,15,19,26	0
9	CUA	B	201	2/2	1.00	0.08	-3.05	18,18,18,20	0
4	CU	A	601	1/1	1.00	0.09	-	19,19,19,19	0
8	OLC	A	609	8/25	0.91	0.34	-	55,56,57,57	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.