



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:20 am GMT

PDB ID : 4G7S  
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant V236I from *Thermus thermophilus*  
Authors : Li, Y.; Chen, Y.; Stout, C.D.  
Deposited on : 2012-07-20  
Resolution : 2.00 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.

---

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

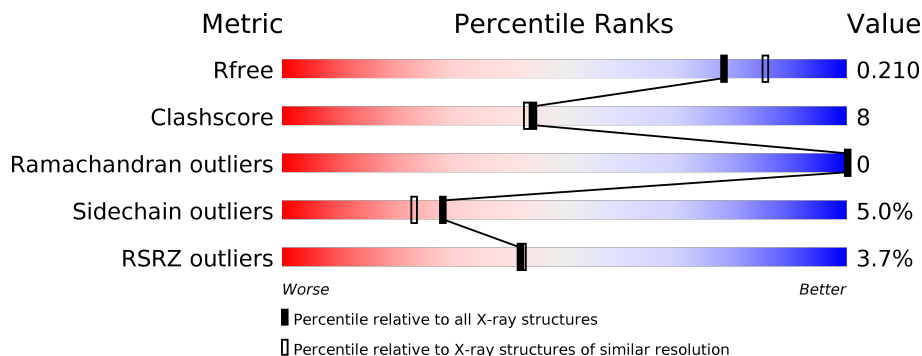
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	569	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>• •</div> </div> </div>
2	B	168	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>• •</div> </div> </div>
3	C	34	<div> <div></div> <div> <div>65%</div> <div>21%</div> <div>6%</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
7	PER	A	604	-	-	-	X
8	OLC	A	605	-	-	-	X
8	OLC	A	607	-	-	-	X
8	OLC	A	609	-	-	-	X
8	OLC	A	610	-	-	-	X
8	OLC	A	611	-	-	-	X
8	OLC	A	613	-	-	-	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 6475 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	554	Total	C	N	O	S	0	3	0
			4368	2966	695	691	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP Q5SJ79
A	-5	HIS	-	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	120	PHE	ALA	engineered mutation	UNP Q5SJ79
A	236	ILE	VAL	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			

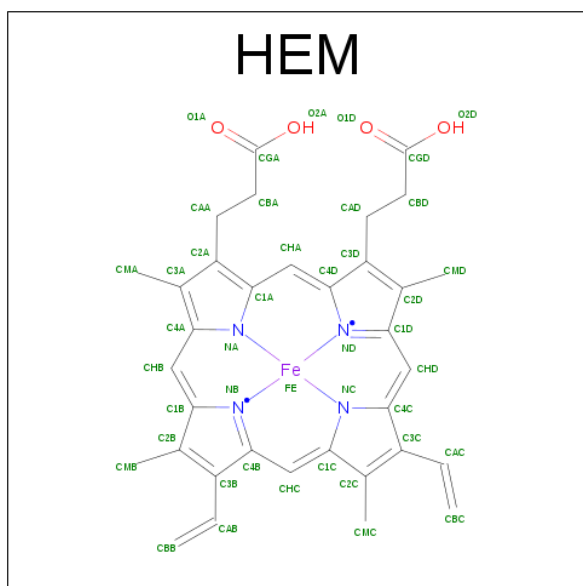
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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).

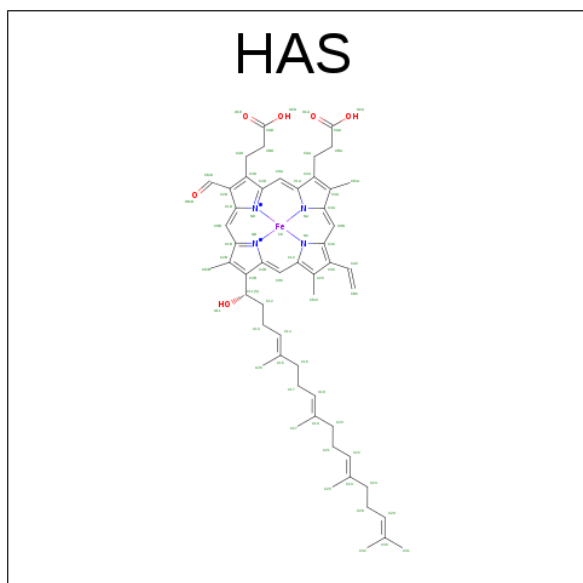
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



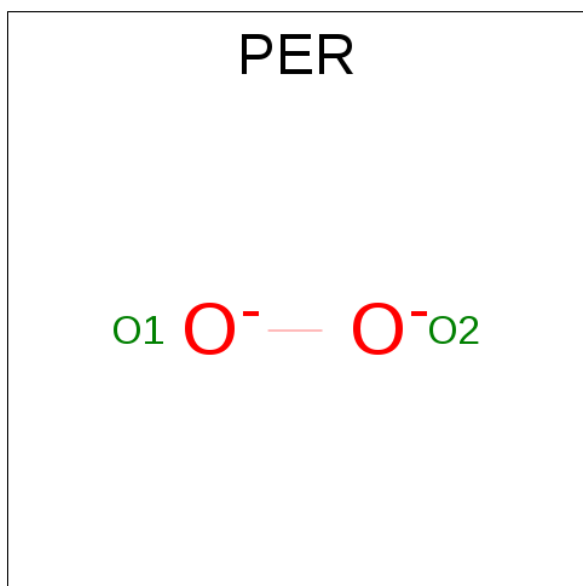
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



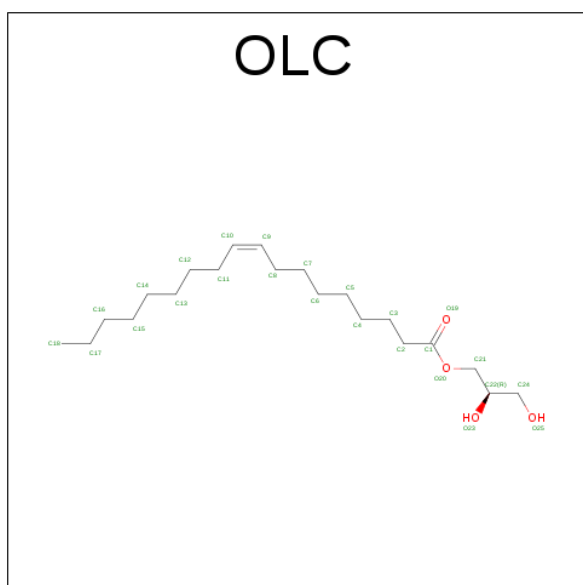
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

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



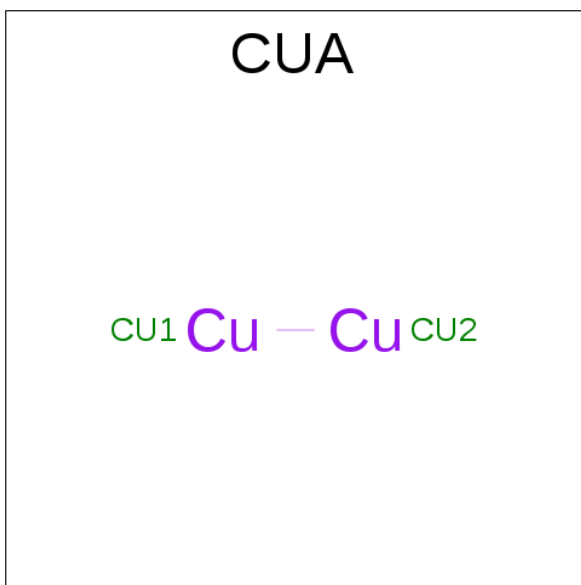
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			2	2		

- 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 19 17 2	0	0
8	A	1	Total C O 23 19 4	0	0
8	A	1	Total C O 14 12 2	0	0
8	A	1	Total C O 12 10 2	0	0
8	A	1	Total C O 15 11 4	0	0
8	A	1	Total C O 20 16 4	0	0
8	A	1	Total C O 25 21 4	0	0
8	A	1	Total C O 21 17 4	0	0
8	A	1	Total C O 25 21 4	0	0
8	B	1	Total C O 20 18 2	0	0
8	B	1	Total C O 24 20 4	0	0
8	B	1	Total C O 16 12 4	0	0
8	B	1	Total C O 20 18 2	0	0
8	C	1	Total C O 23 19 4	0	0
8	C	1	Total C 9 9	0	0

- 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 2	Cu 2	0	0

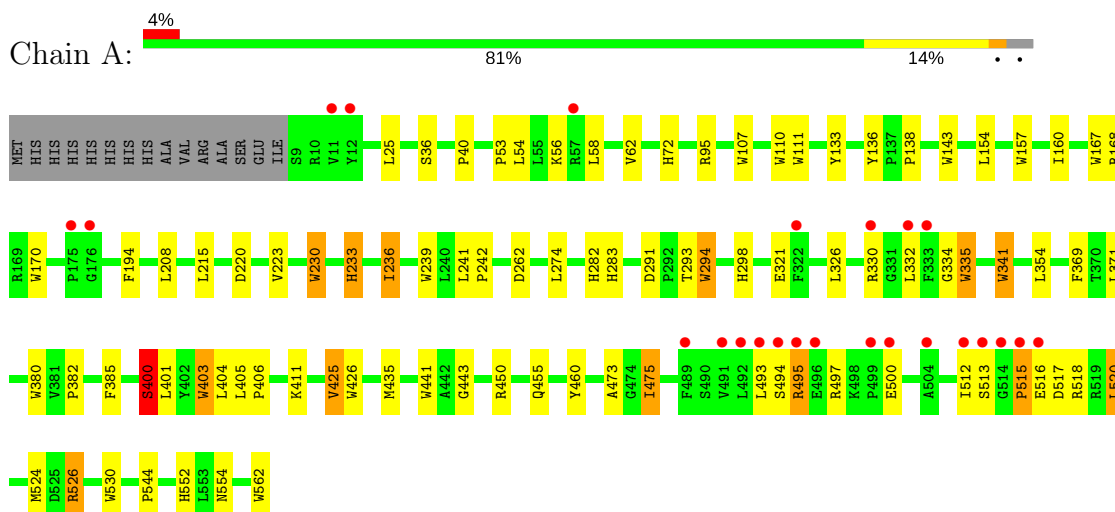
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	106	Total 106	O 106	0	0
10	B	67	Total 67	O 67	0	0
10	C	6	Total 6	O 6	0	0

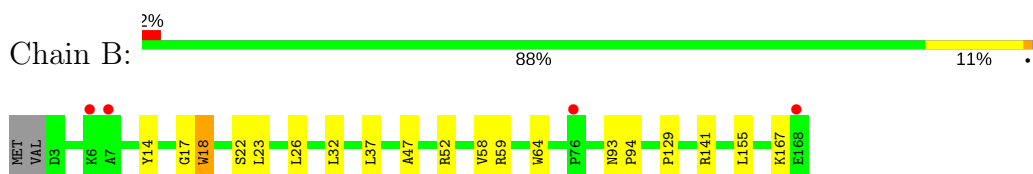
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

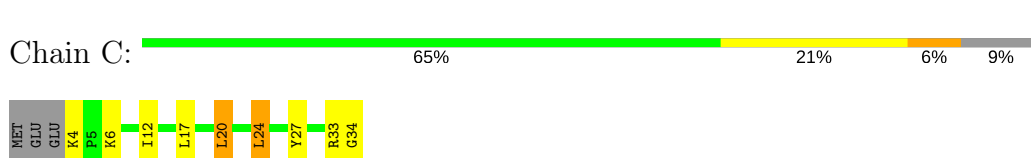
#### • Molecule 1: Cytochrome c oxidase subunit 1



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.57Å 98.39Å 94.58Å 90.00° 127.64° 90.00°	Depositor
Resolution (Å)	74.89 – 2.00 56.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (74.89-2.00) 93.5 (56.84-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.182 , 0.207 0.183 , 0.210	Depositor DCC
$R_{free}$ test set	3314 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.6	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 70.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6475	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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	1.33	25/4535 (0.6%)	1.05	11/6227 (0.2%)
2	B	1.27	2/1330 (0.2%)	1.03	3/1817 (0.2%)
3	C	1.19	0/247	1.17	2/335 (0.6%)
All	All	1.31	27/6112 (0.4%)	1.05	16/8379 (0.2%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	TRP	CD2-CE2	7.41	1.50	1.41
1	A	400	SER	CB-OG	7.18	1.51	1.42
1	A	341	TRP	CD2-CE2	6.46	1.49	1.41
1	A	460	TYR	CB-CG	6.28	1.61	1.51
1	A	298	HIS	CG-CD2	6.27	1.46	1.35
1	A	107	TRP	CD2-CE2	6.23	1.48	1.41
1	A	443	GLY	N-CA	6.13	1.55	1.46
1	A	403	TRP	CD2-CE2	5.93	1.48	1.41
1	A	294	TRP	CD2-CE2	5.87	1.48	1.41
2	B	18	TRP	CD2-CE2	5.79	1.48	1.41
1	A	170	TRP	CD2-CE2	5.76	1.48	1.41
1	A	426	TRP	CD2-CE2	5.75	1.48	1.41
1	A	157	TRP	CD2-CE2	5.72	1.48	1.41
1	A	335	TRP	CD2-CE2	5.71	1.48	1.41
1	A	111	TRP	CD2-CE2	5.70	1.48	1.41
1	A	167	TRP	CD2-CE2	5.61	1.48	1.41
1	A	72	HIS	CG-CD2	5.57	1.45	1.35
1	A	239	TRP	CG-CD1	5.42	1.44	1.36
1	A	400	SER	CA-CB	5.34	1.60	1.52
2	B	64	TRP	CD2-CE2	5.31	1.47	1.41
1	A	380	TRP	CD2-CE3	5.20	1.48	1.40
1	A	53	PRO	N-CA	5.15	1.56	1.47
1	A	530	TRP	CD2-CE2	5.05	1.47	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	TRP	CD2-CE2	5.04	1.47	1.41
1	A	230	TRP	CD2-CE2	5.03	1.47	1.41
1	A	143	TRP	CD2-CE2	5.03	1.47	1.41
1	A	136	TYR	CE2-CZ	5.00	1.45	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ARG	NE-CZ-NH1	-12.15	114.22	120.30
2	B	59	ARG	NE-CZ-NH2	9.41	125.01	120.30
3	C	24	LEU	CB-CG-CD1	8.53	125.50	111.00
1	A	450	ARG	NE-CZ-NH1	-7.78	116.41	120.30
1	A	95	ARG	NE-CZ-NH2	7.75	124.17	120.30
1	A	208	LEU	CB-CG-CD1	-7.26	98.66	111.00
1	A	25	LEU	CB-CG-CD1	-6.54	99.89	111.00
3	C	20	LEU	CB-CG-CD1	6.30	121.72	111.00
1	A	332	LEU	CA-CB-CG	5.99	129.07	115.30
1	A	475	ILE	CB-CG1-CD1	-5.55	98.36	113.90
1	A	404	LEU	CB-CG-CD1	5.49	120.34	111.00
2	B	23	LEU	CB-CG-CD2	-5.46	101.71	111.00
1	A	515	PRO	C-N-CA	5.41	135.21	121.70
1	A	233	HIS	N-CA-CB	5.26	120.07	110.60
2	B	22	SER	CB-CA-C	5.22	120.02	110.10
1	A	425	VAL	CA-CB-CG1	5.12	118.58	110.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	4368	0	4462	64	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	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	65	0	62	5	0
7	A	2	0	0	0	0
8	A	174	0	247	31	0
8	B	80	0	112	12	0
8	C	32	0	50	2	0
9	B	2	0	0	0	0
10	A	106	0	0	3	0
10	B	67	0	0	1	0
10	C	6	0	0	1	0
All	All	6475	0	6490	96	0

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 8.

All (96) 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:168:ARG:HH22	8:A:609:OLC:C2	1.62	1.11
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:CG	1.67	1.07
1:A:168:ARG:NH1	8:A:609:OLC:H7A	1.77	0.99
1:A:168:ARG:HH12	8:A:609:OLC:H5	1.26	0.99
1:A:330[B]:ARG:NH1	1:A:330[B]:ARG:HG2	1.54	0.94
1:A:168:ARG:HH12	8:A:609:OLC:C5	1.80	0.93
3:C:34:GLY:OXT	10:C:204:HOH:O	1.89	0.90
1:A:168:ARG:HH22	8:A:609:OLC:H2A	1.43	0.83
1:A:495:ARG:HH21	1:A:495:ARG:HA	1.42	0.83
8:A:606:OLC:H13A	8:A:611:OLC:H12	1.61	0.82
1:A:168:ARG:NH2	8:A:609:OLC:O23	2.12	0.81
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:HG2	0.74	0.81
1:A:516:GLU:CG	1:A:516:GLU:O	2.30	0.79
2:B:141:ARG:HH12	8:B:203:OLC:H24A	1.49	0.77
1:A:168:ARG:HH22	8:A:609:OLC:H2	1.45	0.77
2:B:141:ARG:NH1	8:B:203:OLC:H24A	2.00	0.76
1:A:168:ARG:NH2	8:A:609:OLC:C2	2.46	0.75
8:B:203:OLC:H7A	8:C:101:OLC:O25	1.88	0.74
1:A:330[B]:ARG:NH1	1:A:330[B]:ARG:CG	2.35	0.74
8:A:605:OLC:H12	8:A:611:OLC:H14A	1.70	0.73
1:A:168:ARG:HH12	8:A:609:OLC:H7A	1.53	0.72
1:A:236:ILE:HD13	6:A:603:HAS:C3C	2.21	0.70
8:A:605:OLC:C12	8:A:611:OLC:H14A	2.23	0.69
1:A:516:GLU:HG3	1:A:516:GLU:O	1.92	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ILE:HD13	6:A:603:HAS:C2C	2.25	0.67
1:A:168:ARG:NH1	8:A:609:OLC:C7	2.60	0.62
1:A:168:ARG:NH1	8:A:609:OLC:C5	2.59	0.62
1:A:168:ARG:NH2	8:A:609:OLC:H2A	2.11	0.61
1:A:168:ARG:HH11	8:A:609:OLC:H7A	1.65	0.60
8:A:606:OLC:H13A	8:A:611:OLC:C12	2.30	0.59
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.91	0.58
2:B:18:TRP:CE3	3:C:12:ILE:HD13	2.40	0.56
2:B:14:TYR:OH	8:B:204:OLC:H24A	2.06	0.55
1:A:168:ARG:HH22	8:A:609:OLC:C1	2.19	0.55
8:B:203:OLC:H6	3:C:33:ARG:HE	1.72	0.54
8:A:611:OLC:H13A	8:A:611:OLC:C8	2.37	0.54
1:A:236:ILE:HD12	1:A:236:ILE:C	2.28	0.54
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.90	0.54
1:A:354:LEU:HD21	6:A:603:HAS:H323	1.88	0.54
8:A:610:OLC:O19	8:A:611:OLC:O23	2.25	0.53
1:A:526:ARG:NH2	10:A:781:HOH:O	2.29	0.53
1:A:168:ARG:NH2	8:A:609:OLC:H2	2.19	0.52
2:B:141:ARG:NH1	8:B:203:OLC:O19	2.41	0.52
1:A:526:ARG:HB3	1:A:526:ARG:CZ	2.40	0.52
2:B:14:TYR:CZ	8:B:204:OLC:H24A	2.45	0.51
1:A:241:LEU:N	1:A:242:PRO:CD	2.74	0.51
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.46	0.51
5:A:602:HEM:CMC	5:A:602:HEM:HBC2	2.41	0.51
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.94	0.50
1:A:516:GLU:HG2	1:A:516:GLU:O	2.10	0.50
2:B:32:LEU:HD21	8:B:202:OLC:H7A	1.92	0.50
1:A:401:LEU:O	1:A:405:LEU:HB2	2.11	0.50
6:A:603:HAS:HBC1	6:A:603:HAS:HMC1	1.93	0.49
1:A:435:MET:HB2	1:A:473:ALA:HB1	1.94	0.49
8:A:611:OLC:H21A	10:A:711:HOH:O	2.12	0.49
1:A:400:SER:HA	1:A:403:TRP:NE1	2.28	0.49
1:A:56:LYS:HG2	1:A:62:VAL:O	2.13	0.49
3:C:4:LYS:HG3	3:C:6:LYS:HG2	1.95	0.49
1:A:138:PRO:HG2	2:B:129:PRO:HG2	1.95	0.48
1:A:168:ARG:HH12	8:A:609:OLC:H5A	1.74	0.47
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.50	0.47
1:A:168:ARG:HH12	8:A:609:OLC:H2	1.80	0.47
8:B:203:OLC:H7A	8:C:101:OLC:C24	2.44	0.47
1:A:168:ARG:NH1	8:A:609:OLC:H5A	2.31	0.46
1:A:495:ARG:HA	1:A:495:ARG:NH2	2.23	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:605:OLC:H12A	8:A:611:OLC:H14A	1.97	0.46
1:A:411:LYS:HE3	1:A:497:ARG:NH2	2.30	0.46
1:A:405:LEU:CB	1:A:406:PRO:HD3	2.47	0.45
8:A:609:OLC:H2	8:A:609:OLC:H5	1.29	0.45
1:A:341:TRP:HB3	8:A:606:OLC:H24A	1.99	0.45
8:A:612:OLC:H8	8:A:612:OLC:H11	1.81	0.44
1:A:154:LEU:HA	1:A:154:LEU:HD23	1.82	0.44
1:A:562:TRP:HA	2:B:155:LEU:HG	1.99	0.44
1:A:291:ASP:OD2	1:A:293:THR:HB	2.18	0.44
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.99	0.43
1:A:293:THR:HG23	8:B:205:OLC:H8	1.99	0.43
5:A:602:HEM:HBC2	5:A:602:HEM:HMC2	2.00	0.43
1:A:371:LEU:HD21	3:C:27:TYR:HD1	1.83	0.43
2:B:47:ALA:HA	10:B:351:HOH:O	2.17	0.43
1:A:552:HIS:HB3	2:B:52:ARG:NH1	2.33	0.43
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.90	0.43
8:A:613:OLC:H13	8:A:613:OLC:H10	1.04	0.42
1:A:515:PRO:HA	1:A:516:GLU:HB3	2.01	0.42
2:B:17:GLY:HA3	8:B:204:OLC:H3	2.01	0.42
1:A:520:LEU:HD22	1:A:524:MET:HG3	2.02	0.42
6:A:603:HAS:HHA	6:A:603:HAS:HAA2	1.83	0.42
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.55	0.41
1:A:554:ASN:HB2	2:B:52:ARG:HD2	2.02	0.41
1:A:233:HIS:O	1:A:236:ILE:HG13	2.21	0.41
1:A:36:SER:O	1:A:40:PRO:HD3	2.20	0.41
8:A:611:OLC:H8A	8:A:611:OLC:H13A	2.02	0.41
1:A:517:ASP:OD2	1:A:520:LEU:HB2	2.22	0.40
2:B:141:ARG:NH2	8:B:203:OLC:O19	2.54	0.40
2:B:93:ASN:HA	2:B:94:PRO:HA	1.90	0.40
1:A:382:PRO:HG2	10:A:742:HOH:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	554/569 (97%)	539 (97%)	15 (3%)	0	100	100
2	B	165/168 (98%)	163 (99%)	2 (1%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	748/771 (97%)	731 (98%)	17 (2%)	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	447/464 (96%)	424 (95%)	23 (5%)	28	22
2	B	134/138 (97%)	130 (97%)	4 (3%)	46	46
3	C	24/27 (89%)	21 (88%)	3 (12%)	5	3
All	All	605/629 (96%)	575 (95%)	30 (5%)	28	23

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

Mol	Chain	Res	Type
1	A	54	LEU
1	A	58	LEU
1	A	133	TYR
1	A	215	LEU
1	A	230	TRP
1	A	236	ILE
1	A	262	ASP
1	A	274	LEU
1	A	326	LEU
1	A	369	PHE
1	A	400	SER
1	A	425	VAL
1	A	455	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	475	ILE
1	A	493	LEU
1	A	494	SER
1	A	495	ARG
1	A	500	GLU
1	A	512	ILE
1	A	513	SER
1	A	518	ARG
1	A	520	LEU
1	A	526	ARG
2	B	26	LEU
2	B	37	LEU
2	B	58	VAL
2	B	167	LYS
3	C	17	LEU
3	C	20	LEU
3	C	24	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	8	HIS

### 5.3.3 RNA [i](#)

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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	2.17	9 (32%)	17,82,82	2.85	7 (41%)
6	HAS	A	603	1,7	55,72,72	4.06	17 (30%)	48,109,109	2.67	15 (31%)
7	PER	A	604	4,6	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	A	605	-	15,18,24	0.23	0	14,18,25	1.12	1 (7%)
8	OLC	A	606	-	22,22,24	0.69	0	23,23,25	1.13	2 (8%)
8	OLC	A	607	-	13,13,24	0.65	0	13,13,25	0.84	0
8	OLC	A	608	-	8,11,24	0.47	0	7,11,25	0.94	1 (14%)
8	OLC	A	609	-	14,14,24	1.19	1 (7%)	15,15,25	1.67	2 (13%)
8	OLC	A	610	-	19,19,24	0.39	0	20,20,25	0.87	0
8	OLC	A	611	-	24,24,24	0.66	1 (4%)	25,25,25	1.15	3 (12%)
8	OLC	A	612	-	20,20,24	0.50	0	21,21,25	0.84	0
8	OLC	A	613	-	24,24,24	0.35	0	25,25,25	1.19	3 (12%)
9	CUA	B	201	2	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	B	202	-	19,19,24	0.64	1 (5%)	19,19,25	0.77	0
8	OLC	B	203	-	23,23,24	0.98	1 (4%)	24,24,25	1.76	5 (20%)
8	OLC	B	204	-	15,15,24	0.50	0	16,16,25	0.75	0
8	OLC	B	205	-	19,19,24	0.53	0	19,19,25	0.59	0
8	OLC	C	101	-	22,22,24	0.58	0	23,23,25	1.10	1 (4%)
8	OLC	C	102	-	8,8,24	0.11	0	7,7,25	0.38	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	-	-	0/14/16/24	0/0/0/0
8	OLC	A	606	-	-	0/22/22/24	0/0/0/0
8	OLC	A	607	-	-	0/12/12/24	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	A	608	-	-	0/7/9/24	0/0/0/0
8	OLC	A	609	-	-	0/14/14/24	0/0/0/0
8	OLC	A	610	-	-	0/19/19/24	0/0/0/0
8	OLC	A	611	-	-	0/24/24/24	0/0/0/0
8	OLC	A	612	-	-	0/20/20/24	0/0/0/0
8	OLC	A	613	-	-	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	-	-	0/18/18/24	0/0/0/0
8	OLC	B	203	-	-	0/23/23/24	0/0/0/0
8	OLC	B	204	-	-	0/15/15/24	0/0/0/0
8	OLC	B	205	-	-	0/18/18/24	0/0/0/0
8	OLC	C	101	-	-	0/22/22/24	0/0/0/0
8	OLC	C	102	-	-	0/6/6/24	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	CHD-C4A	-14.75	1.36	1.51
6	A	603	HAS	C1B-NB	-10.45	1.35	1.49
6	A	603	HAS	CHC-C4B	-10.11	1.34	1.53
6	A	603	HAS	C4B-NB	-8.79	1.37	1.49
6	A	603	HAS	CHA-C1A	-8.10	1.32	1.51
6	A	603	HAS	C3C-CAC	-6.92	1.34	1.47
5	A	602	HEM	C3B-CAB	-6.10	1.35	1.47
6	A	603	HAS	CHB-C1B	-4.85	1.33	1.53
6	A	603	HAS	CHD-C4C	-3.48	1.47	1.51
6	A	603	HAS	C4D-ND	-2.71	1.46	1.49
6	A	603	HAS	CHA-C4D	-2.41	1.48	1.53
5	A	602	HEM	C1D-CHD	-2.38	1.33	1.40
6	A	603	HAS	C1D-C2D	-2.34	1.47	1.51
5	A	602	HEM	CMB-C2B	2.26	1.56	1.51
8	B	202	OLC	O20-C1	2.27	1.40	1.32
5	A	602	HEM	CMA-C3A	2.29	1.56	1.51
6	A	603	HAS	CMB-C2B	2.48	1.54	1.50
6	A	603	HAS	CMD-C2D	2.50	1.49	1.45
8	A	611	OLC	O20-C1	2.52	1.40	1.33
6	A	603	HAS	CBC-CAC	2.58	1.47	1.28
5	A	602	HEM	C1A-CHA	2.60	1.47	1.40
5	A	602	HEM	CBB-CAB	3.01	1.50	1.28
5	A	602	HEM	C4C-NC	3.05	1.40	1.36
8	B	203	OLC	O20-C1	3.47	1.43	1.33
8	A	609	OLC	O20-C1	3.71	1.44	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	C3C-C2C	3.89	1.45	1.40
5	A	602	HEM	C1A-NA	5.28	1.47	1.36
6	A	603	HAS	C1A-C2A	6.40	1.47	1.38
6	A	603	HAS	C3C-C2C	8.24	1.51	1.40
6	A	603	HAS	C4A-C3A	8.49	1.49	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEM	CMD-C2D-C1D	-6.59	118.33	128.46
6	A	603	HAS	CAA-C2A-C1A	-6.55	122.69	127.30
6	A	603	HAS	CHD-C4A-C3A	-5.58	120.19	129.53
5	A	602	HEM	C4C-C3C-C2C	-5.51	103.05	106.90
6	A	603	HAS	CHD-C4C-C3C	-5.34	122.61	129.61
6	A	603	HAS	CAA-CBA-CGA	-4.52	104.94	112.66
5	A	602	HEM	CMA-C3A-C4A	-3.74	122.71	128.46
6	A	603	HAS	C4C-C3C-C2C	-3.40	99.05	104.13
5	A	602	HEM	CBD-CAD-C3D	-3.35	106.08	112.47
5	A	602	HEM	CAD-CBD-CGD	-3.32	107.00	112.66
8	A	613	OLC	C3-C2-C1	-3.07	102.39	113.58
8	A	606	OLC	O20-C21-C22	-3.05	90.77	105.72
6	A	603	HAS	CHC-C1C-C2C	-2.95	124.35	129.45
8	A	613	OLC	C13-C12-C11	-2.90	102.59	113.74
5	A	602	HEM	CBA-CAA-C2A	-2.78	107.16	112.48
6	A	603	HAS	C20-C19-C18	-2.68	115.61	121.10
8	A	605	OLC	C13-C14-C15	-2.29	102.63	114.45
8	B	203	OLC	O23-C22-C24	-2.26	98.15	108.84
8	A	613	OLC	C3-C4-C5	-2.17	103.30	114.45
6	A	603	HAS	CMB-C2B-C3B	-2.13	124.26	129.77
8	A	608	OLC	C3-C4-C5	-2.10	103.65	114.45
8	A	611	OLC	O20-C1-O19	2.02	128.58	123.55
6	A	603	HAS	CAD-C3D-C4D	2.03	126.65	122.52
8	B	203	OLC	C6-C7-C8	2.03	121.55	113.74
8	A	606	OLC	C21-C22-C24	2.24	120.62	111.51
6	A	603	HAS	C27-C19-C20	2.26	119.21	115.29
8	A	609	OLC	C21-O20-C1	2.47	124.55	117.13
8	A	611	OLC	O20-C21-C22	2.49	117.93	105.72
6	A	603	HAS	CHB-C1B-C2B	2.62	122.88	114.70
8	A	611	OLC	C21-O20-C1	2.68	125.19	117.13
8	B	203	OLC	C21-C22-C24	2.73	122.65	111.51
8	C	101	OLC	C21-O20-C1	2.76	125.44	117.13
5	A	602	HEM	C4A-C3A-C2A	3.29	109.29	107.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C1B-CHB-C1D	3.51	126.84	116.30
8	B	203	OLC	O20-C21-C22	3.92	124.94	105.72
8	A	609	OLC	O20-C1-C2	4.44	124.82	111.90
6	A	603	HAS	C4A-CHD-C4C	4.51	122.92	112.83
8	B	203	OLC	C21-O20-C1	5.04	132.29	117.13
6	A	603	HAS	CHA-C4D-ND	5.95	121.97	110.75
6	A	603	HAS	CHC-C4B-NB	8.42	126.62	110.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	HEM	2	0
6	A	603	HAS	5	0
8	A	605	OLC	3	0
8	A	606	OLC	3	0
8	A	609	OLC	19	0
8	A	610	OLC	1	0
8	A	611	OLC	9	0
8	A	612	OLC	1	0
8	A	613	OLC	1	0
8	B	202	OLC	1	0
8	B	203	OLC	7	0
8	B	204	OLC	3	0
8	B	205	OLC	1	0
8	C	101	OLC	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	554/569 (97%)	-0.32	24 (4%) 36 36	15, 25, 49, 100	0
2	B	166/168 (98%)	-0.44	4 (2%) 59 59	16, 26, 45, 64	0
3	C	31/34 (91%)	-0.66	0 100 100	20, 26, 37, 59	0
All	All	751/771 (97%)	-0.36	28 (3%) 42 43	15, 26, 49, 100	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	ARG	8.1
1	A	494	SER	5.1
1	A	515	PRO	5.0
1	A	513	SER	5.0
1	A	330[A]	ARG	4.9
1	A	491	VAL	4.7
1	A	516	GLU	4.6
1	A	493	LEU	4.5
1	A	496	GLU	3.8
1	A	492	LEU	3.3
2	B	6	LYS	3.2
1	A	11	VAL	3.1
1	A	514	GLY	3.0
1	A	332	LEU	2.9
1	A	176	GLY	2.9
1	A	500	GLU	2.9
2	B	7	ALA	2.8
1	A	175	PRO	2.6
1	A	499	PRO	2.4
1	A	12	TYR	2.4
1	A	512	ILE	2.3
2	B	76	PRO	2.3
1	A	333	PHE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	168	GLU	2.2
1	A	504	ALA	2.1
1	A	57	ARG	2.1
1	A	322	PHE	2.0
1	A	489	PHE	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	OLC	C	102	9/25	0.78	0.24	10.81	56,60,62,66	0
8	OLC	A	607	14/25	0.77	0.22	7.25	46,55,74,79	0
8	OLC	B	205	20/25	0.77	0.22	5.95	47,55,80,82	0
8	OLC	C	101	23/25	0.81	0.20	5.36	37,53,73,79	0
8	OLC	A	610	20/25	0.83	0.19	4.79	46,66,86,87	0
8	OLC	A	605	19/25	0.88	0.19	4.25	43,57,83,84	0
8	OLC	B	204	16/25	0.81	0.20	4.17	49,60,80,93	0
8	OLC	A	611	25/25	0.78	0.19	3.97	42,59,71,76	0
8	OLC	A	613	25/25	0.80	0.18	3.66	47,57,69,87	0
8	OLC	A	609	15/25	0.56	0.24	3.58	50,62,84,92	0
8	OLC	B	203	24/25	0.67	0.23	3.13	46,62,86,100	0
8	OLC	B	202	20/25	0.82	0.16	3.04	46,57,65,67	0
7	PER	A	604	2/2	0.94	0.12	2.90	21,21,21,23	0
8	OLC	A	612	21/25	0.80	0.15	1.53	46,57,86,96	0
8	OLC	A	606	23/25	0.88	0.14	1.45	29,40,58,68	0
6	HAS	A	603	65/65	0.98	0.10	0.40	14,18,33,36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
9	CUA	B	201	2/2	1.00	0.09	0.19	19,19,19,19	0
5	HEM	A	602	43/43	0.99	0.07	-0.52	12,15,18,19	0
4	CU	A	601	1/1	1.00	0.10	-	21,21,21,21	0
8	OLC	A	608	12/25	0.86	0.14	-	48,54,71,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.