



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:47 PM GMT

PDB ID : 4G70  
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant V236T from *Thermus thermophilus*  
Authors : Li, Y.; Chen, Y.; Stout, C.D.  
Deposited on : 2012-07-19  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

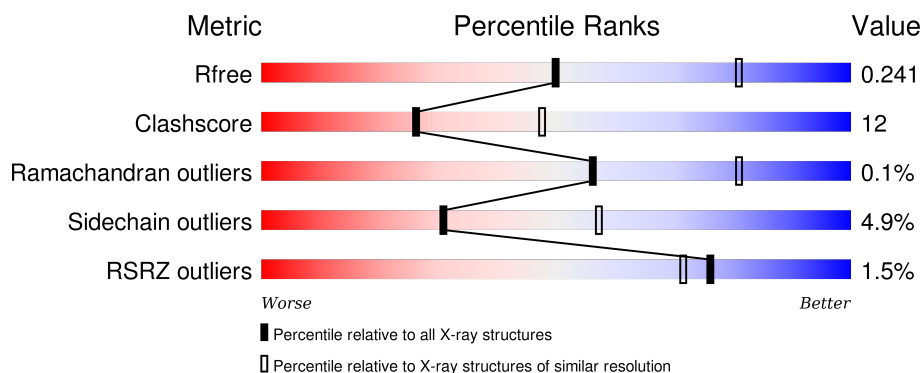
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	569	 2% 72% 22% . .
2	B	168	 77% 20% . .
3	C	34	 62% 26% . 9%

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
5	HAS	A	602	-	-	-	X
7	PER	A	604	-	-	-	X
8	OLC	A	605	-	-	-	X
8	OLC	A	606	-	-	-	X
8	OLC	A	607	-	-	-	X
8	OLC	A	608	-	-	-	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	B	202	-	-	-	X
8	OLC	B	203	-	-	-	X
8	OLC	B	204	-	-	-	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 6374 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	0	0
			4346	2950	692	688	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	THR	VAL	engineered mutation	UNP Q5SJ79

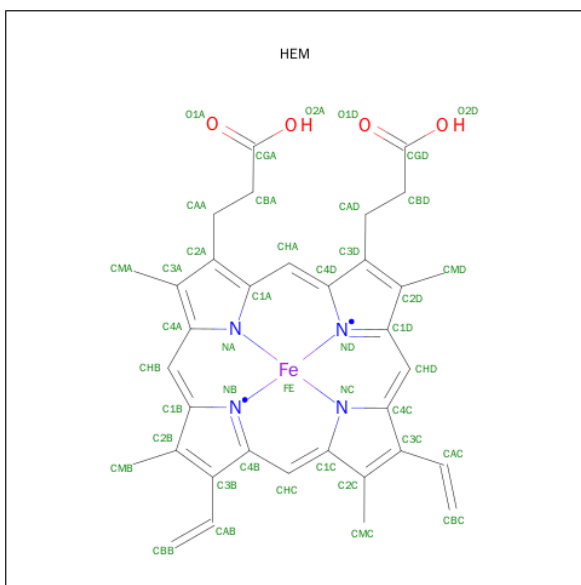
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1275	829	211	231	4			

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

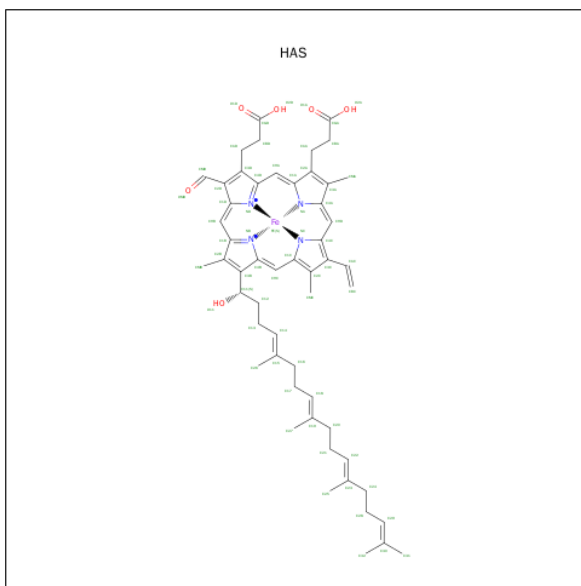
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	0	0	0
			237	166	36	35			

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 5 is HEME-AS (three-letter code: HAS) (formula:  $\text{C}_{54}\text{H}_{64}\text{FeN}_4\text{O}_6$ ).

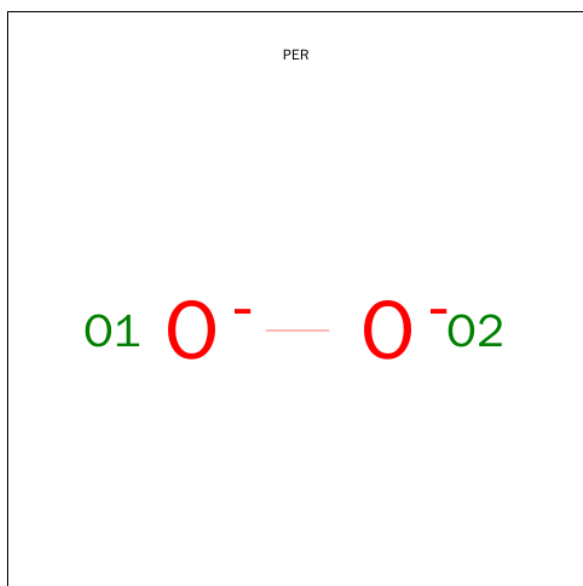


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

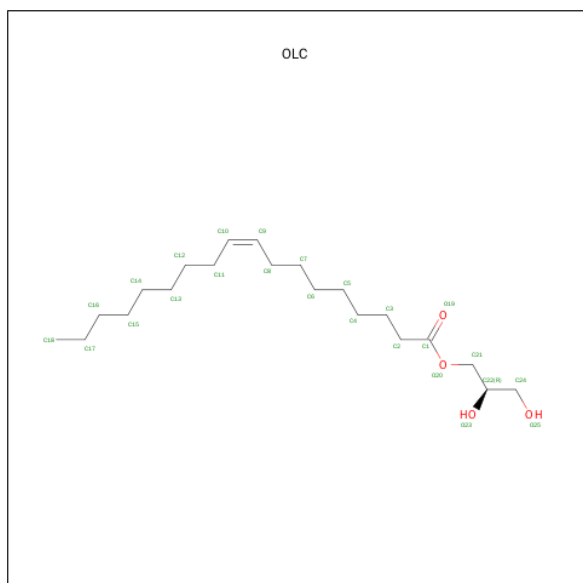
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cu	0	0
			1	1		

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



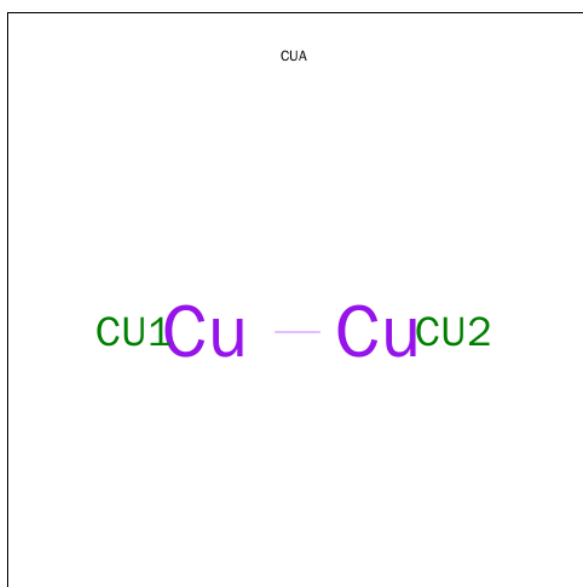
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			2	2		

- 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
			20	18	2		
8	A	1	Total	C	O	0	0
			22	18	4		
8	A	1	Total	C	O	0	0
			20	18	2		
8	A	1	Total	C	O	0	0
			18	14	4		
8	A	1	Total	C	O	0	0
			13	9	4		
8	A	1	Total	C	O	0	0
			8	4	4		
8	A	1	Total	C	O	0	0
			12	8	4		
8	A	1	Total	C	O	0	0
			9	7	2		
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			13	9	4		
8	A	1	Total	C	O	0	0
			24	20	4		
8	B	1	Total	C	O	0	0
			24	20	4		
8	B	1	Total	C	O	0	0
			23	19	4		
8	B	1	Total	C	O	0	0
			16	12	4		
8	C	1	Total	C	O	0	0
			23	19	4		
8	C	1	Total	C		0	0
			13	13			

- 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.

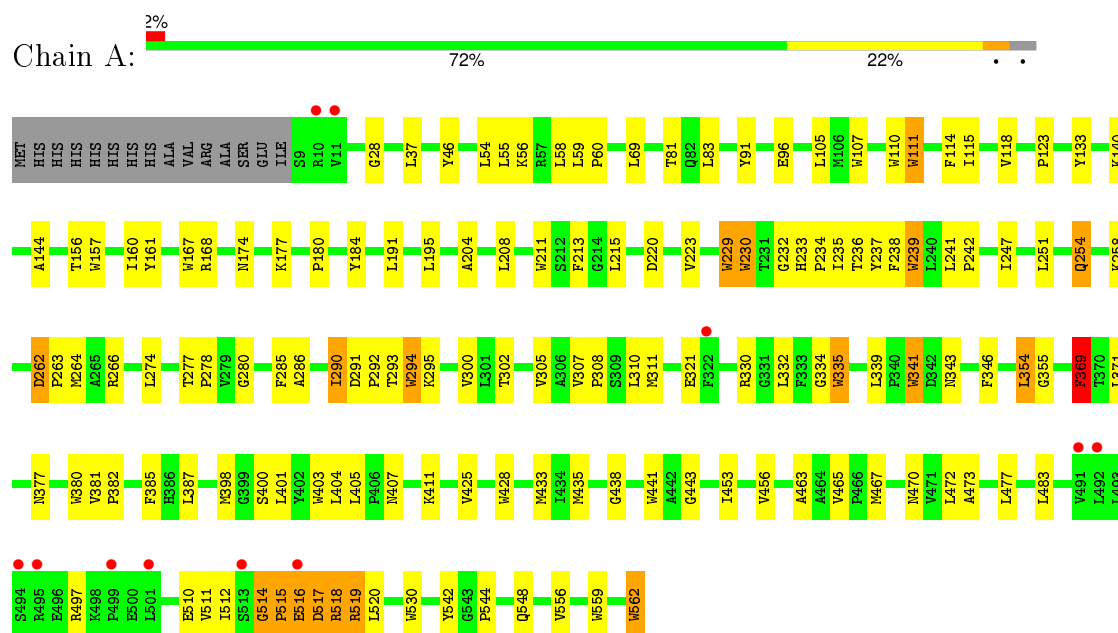
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	71	Total O 71 71	0	0
10	B	44	Total O 44 44	0	0
10	C	5	Total O 5 5	0	0



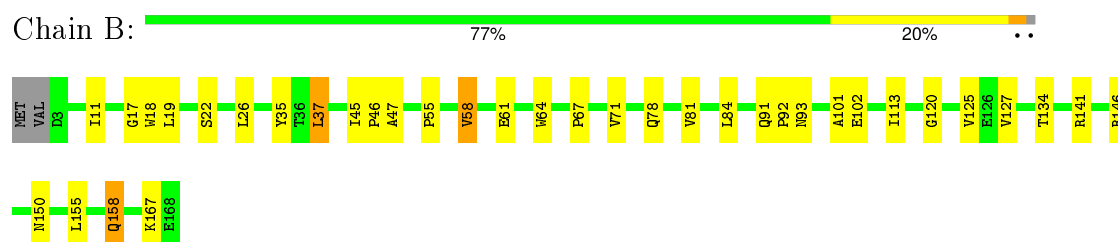
### 3 Residue-property plots

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

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



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.48 Å   98.36 Å   94.78 Å 90.00°   127.39°   90.00°	Depositor
Resolution (Å)	75.30 – 2.60 75.30 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (75.30-2.60) 97.9 (75.30-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.62 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.194   ,   0.252 0.186   ,   0.241	Depositor DCC
$R_{free}$ test set	1603 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 31639 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.14	18/4503 (0.4%)	1.07	7/6186 (0.1%)
2	B	0.83	0/1311	0.88	1/1795 (0.1%)
3	C	0.88	0/243	0.91	1/331 (0.3%)
All	All	1.08	18/6057 (0.3%)	1.03	9/8312 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	LEU	CA-CB	35.81	2.36	1.53
1	A	354	LEU	CG-CD2	26.95	2.51	1.51
1	A	530	TRP	CD2-CE2	6.81	1.49	1.41
1	A	157	TRP	CD2-CE2	6.21	1.48	1.41
1	A	294	TRP	CD2-CE2	6.02	1.48	1.41
1	A	230	TRP	CD2-CE2	6.00	1.48	1.41
1	A	559	TRP	CD2-CE2	5.94	1.48	1.41
1	A	229	TRP	CD2-CE2	5.75	1.48	1.41
1	A	110	TRP	CD2-CE2	5.75	1.48	1.41
1	A	341	TRP	CD2-CE2	5.70	1.48	1.41
1	A	335	TRP	CD2-CE2	5.61	1.48	1.41
1	A	380	TRP	CD2-CE2	5.57	1.48	1.41
1	A	441	TRP	CD2-CE2	5.43	1.47	1.41
1	A	107	TRP	CD2-CE2	5.30	1.47	1.41
1	A	239	TRP	CD2-CE2	5.28	1.47	1.41
1	A	562	TRP	CD2-CE2	5.25	1.47	1.41
1	A	428	TRP	CD2-CE2	5.18	1.47	1.41
1	A	111	TRP	CD2-CE2	5.06	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	LEU	CB-CG-CD2	-44.71	35.00	111.00
1	A	354	LEU	CB-CA-C	18.11	144.62	110.20
1	A	514	GLY	N-CA-C	-8.55	91.72	113.10
1	A	354	LEU	CA-CB-CG	-8.11	96.66	115.30
1	A	291	ASP	CB-CG-OD2	6.89	124.51	118.30
1	A	332	LEU	CA-CB-CG	6.45	130.13	115.30
2	B	146	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	515	PRO	N-CA-C	-5.15	98.71	112.10
3	C	13	LEU	CA-CB-CG	5.03	126.87	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	4346	0	4417	111	0
2	B	1275	0	1234	28	0
3	C	237	0	256	7	0
4	A	43	0	30	5	0
5	A	65	0	62	3	0
6	A	1	0	0	0	0
7	A	2	0	0	1	0
8	A	184	0	245	26	0
8	B	63	0	89	10	0
8	C	36	0	53	6	0
9	B	2	0	0	0	0
10	A	71	0	0	6	0
10	B	44	0	0	6	2
10	C	5	0	0	0	0
All	All	6374	0	6386	155	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (155) 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:CE1	1.70	1.56
1:A:233:HIS:NE2	1:A:237:TYR:HE1	0.78	1.26
7:A:604:PER:O1	7:A:604:PER:O2	1.52	1.23
1:A:233:HIS:CD2	1:A:237:TYR:HE1	1.74	1.05
1:A:354:LEU:CA	1:A:354:LEU:CB	2.36	1.04
8:B:203:OLC:H6	3:C:33:ARG:HE	1.39	0.87
2:B:120:GLY:HA2	8:B:203:OLC:H2	1.59	0.85
1:A:233:HIS:CD2	1:A:237:TYR:CE1	2.55	0.84
10:A:705:HOH:O	8:B:203:OLC:H4A	1.79	0.83
1:A:517:ASP:HA	1:A:519:ARG:HH21	1.43	0.82
8:A:605:OLC:H12	8:A:613:OLC:H14A	1.65	0.78
1:A:411:LYS:HE3	1:A:497:ARG:HH21	1.49	0.76
1:A:517:ASP:HB2	1:A:519:ARG:HE	1.50	0.76
8:A:613:OLC:H21A	10:A:706:HOH:O	1.84	0.76
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.68	0.75
1:A:514:GLY:O	1:A:515:PRO:C	2.20	0.75
2:B:101:ALA:O	10:B:314:HOH:O	2.05	0.74
2:B:47:ALA:O	10:B:341:HOH:O	2.07	0.73
5:A:602:HAS:HBC1	5:A:602:HAS:HMC1	1.72	0.71
1:A:465:VAL:HG13	8:A:612:OLC:H5A	1.73	0.71
2:B:35:TYR:OH	8:B:202:OLC:H24A	1.91	0.70
2:B:141:ARG:HH12	8:B:203:OLC:H24A	1.57	0.69
1:A:168:ARG:HH11	8:A:610:OLC:C22	2.08	0.67
4:A:601:HEM:O2A	10:A:717:HOH:O	2.13	0.67
1:A:167:TRP:CZ3	8:A:611:OLC:H22	2.29	0.67
4:A:601:HEM:HBC2	4:A:601:HEM:HMC1	1.76	0.66
1:A:167:TRP:CH2	8:A:611:OLC:H22	2.31	0.65
8:C:101:OLC:H10	8:C:102:OLC:H8	1.79	0.65
1:A:161:TYR:CE2	8:A:610:OLC:H21	2.32	0.65
1:A:123:PRO:HG3	1:A:144:ALA:HB3	1.80	0.64
1:A:443:GLY:O	10:A:737:HOH:O	2.15	0.63
1:A:233:HIS:CE1	1:A:237:TYR:CE1	2.75	0.63
1:A:293:THR:HG23	8:A:607:OLC:H8	1.82	0.61
1:A:463:ALA:O	1:A:467:MET:HG3	1.99	0.61
2:B:17:GLY:HA3	8:B:204:OLC:H3	1.84	0.60
1:A:156:THR:O	1:A:160:ILE:HG13	2.01	0.59
1:A:174:ASN:HB3	1:A:177:LYS:HD2	1.85	0.59
1:A:111:TRP:HE3	1:A:115:ILE:CD1	2.16	0.58
8:A:606:OLC:H13A	8:A:613:OLC:H12	1.84	0.58
1:A:69:LEU:HD11	4:A:601:HEM:HBD2	1.86	0.58
1:A:232:GLY:O	1:A:235:ILE:HG22	2.04	0.58
1:A:233:HIS:NE2	1:A:237:TYR:CZ	2.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.39	0.58
1:A:401:LEU:O	1:A:405:LEU:HB2	2.04	0.58
8:B:203:OLC:H7A	8:C:101:OLC:O25	2.04	0.57
1:A:168:ARG:NH1	8:A:610:OLC:C22	2.68	0.57
1:A:403:TRP:CZ3	1:A:404:LEU:HD13	2.40	0.57
3:C:18:THR:HG23	8:C:102:OLC:H12A	1.86	0.56
8:A:613:OLC:H13A	8:A:613:OLC:C8	2.34	0.56
1:A:277:THR:N	1:A:278:PRO:CD	2.69	0.55
1:A:229:TRP:CE3	1:A:232:GLY:HA3	2.43	0.54
3:C:18:THR:HG23	8:C:102:OLC:C12	2.38	0.54
1:A:339:LEU:HD13	1:A:346:PHE:HZ	1.73	0.54
1:A:398:MET:O	1:A:401:LEU:HB2	2.08	0.53
2:B:58:VAL:O	10:B:344:HOH:O	2.17	0.53
1:A:341:TRP:CZ2	8:A:615:OLC:H3	2.44	0.53
1:A:341:TRP:CE2	8:A:615:OLC:H3	2.43	0.53
2:B:91:GLN:OE1	10:B:319:HOH:O	2.19	0.53
4:A:601:HEM:HBC2	4:A:601:HEM:CMC	2.38	0.52
1:A:517:ASP:CA	1:A:519:ARG:HH21	2.20	0.52
2:B:93:ASN:O	10:B:309:HOH:O	2.19	0.52
10:A:705:HOH:O	8:B:203:OLC:H6A	2.09	0.52
8:B:203:OLC:H6	3:C:33:ARG:NE	2.19	0.52
1:A:562:TRP:HA	2:B:155:LEU:HG	1.92	0.52
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.45	0.52
1:A:55:LEU:HD11	1:A:59:LEU:HD12	1.92	0.52
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.46	0.51
1:A:465:VAL:HG22	8:A:612:OLC:H3A	1.91	0.51
1:A:355:GLY:HA3	1:A:433:MET:HE1	1.93	0.51
1:A:400:SER:HB2	1:A:403:TRP:CZ2	2.46	0.50
1:A:377:ASN:HB3	2:B:150:ASN:HB2	1.93	0.50
2:B:11:ILE:HA	3:C:5:PRO:HG3	1.92	0.50
1:A:292:PRO:CB	8:A:607:OLC:H3A	2.41	0.50
1:A:518:ARG:NH2	10:A:760:HOH:O	2.44	0.50
1:A:111:TRP:HE3	1:A:115:ILE:HD11	1.75	0.50
1:A:290:ILE:HB	1:A:295:LYS:HE3	1.93	0.50
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.48	0.49
1:A:280:GLY:HA3	1:A:542:TYR:OH	2.13	0.49
1:A:371:LEU:HD21	3:C:27:TYR:HD1	1.77	0.49
8:A:613:OLC:H13A	8:A:613:OLC:H8A	1.93	0.49
1:A:341:TRP:HB3	8:A:606:OLC:H24A	1.95	0.49
2:B:18:TRP:CE3	3:C:12:ILE:HD13	2.47	0.49
2:B:158:GLN:NE2	2:B:158:GLN:H	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLN:HG2	1:A:343:ASN:HD21	1.78	0.48
1:A:263:PRO:HG2	1:A:516:GLU:HB3	1.94	0.48
1:A:247:ILE:HA	1:A:251:LEU:HB2	1.96	0.48
1:A:213:PHE:CD2	8:A:608:OLC:H4	2.48	0.48
1:A:472:LEU:HD22	8:A:613:OLC:H11	1.95	0.48
1:A:300:VAL:HG11	8:A:607:OLC:H16	1.94	0.47
8:C:101:OLC:C10	8:C:102:OLC:H7A	2.44	0.47
1:A:517:ASP:N	1:A:517:ASP:OD1	2.37	0.47
8:A:607:OLC:H4A	2:B:37:LEU:HG	1.96	0.47
1:A:140:LYS:HE3	1:A:211:TRP:NE1	2.29	0.47
1:A:330:ARG:O	1:A:334:GLY:HA3	2.14	0.47
1:A:292:PRO:HB2	8:A:607:OLC:H3A	1.96	0.47
1:A:277:THR:N	1:A:278:PRO:HD2	2.30	0.47
1:A:435:MET:HB2	1:A:473:ALA:HB1	1.96	0.47
1:A:233:HIS:CD2	1:A:237:TYR:CD1	3.01	0.47
2:B:120:GLY:CA	8:B:203:OLC:H2	2.37	0.47
1:A:28:GLY:HA2	1:A:83:LEU:HD12	1.97	0.46
1:A:91:TYR:OH	1:A:407:ASN:ND2	2.48	0.46
1:A:556:VAL:CG1	2:B:55:PRO:HG3	2.45	0.46
1:A:263:PRO:HG2	1:A:516:GLU:CB	2.44	0.46
1:A:511:VAL:HG12	1:A:512:ILE:N	2.31	0.46
2:B:45:ILE:O	10:B:302:HOH:O	2.20	0.46
1:A:277:THR:H	1:A:278:PRO:CD	2.28	0.46
1:A:305:VAL:O	1:A:308:PRO:HD2	2.16	0.45
1:A:310:LEU:HD13	2:B:22:SER:HB3	1.97	0.45
2:B:67:PRO:O	2:B:92:PRO:HG3	2.17	0.45
1:A:381:VAL:HB	1:A:382:PRO:HD3	1.97	0.45
1:A:300:VAL:HG11	8:A:607:OLC:C16	2.47	0.45
1:A:241:LEU:N	1:A:242:PRO:CD	2.80	0.45
1:A:548:GLN:HG2	1:A:548:GLN:O	2.16	0.45
1:A:286:ALA:HB1	2:B:125:VAL:HA	1.98	0.45
1:A:111:TRP:CE3	1:A:115:ILE:HD11	2.53	0.44
1:A:254:GLN:CG	1:A:343:ASN:HD21	2.30	0.44
1:A:302:THR:O	1:A:305:VAL:HG12	2.18	0.44
1:A:354:LEU:CG	1:A:354:LEU:CA	2.96	0.44
1:A:236:THR:HB	5:A:602:HAS:CAC	2.48	0.44
1:A:387:LEU:CD2	1:A:433:MET:HE2	2.48	0.44
1:A:514:GLY:C	1:A:515:PRO:O	2.50	0.44
1:A:339:LEU:HD13	1:A:346:PHE:CZ	2.51	0.44
8:A:607:OLC:H14A	8:A:607:OLC:H11A	1.79	0.43
2:B:64:TRP:HB3	2:B:84:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:HB3	1:A:510:GLU:O	2.18	0.43
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.82	0.43
1:A:114:PHE:O	1:A:118:VAL:HG23	2.18	0.43
2:B:113:ILE:HA	2:B:127:VAL:O	2.19	0.43
1:A:311:MET:HG3	2:B:19:LEU:HD21	2.01	0.43
1:A:96:GLU:OE2	1:A:180:PRO:HB2	2.19	0.43
1:A:438:GLY:HA3	1:A:470:ASN:OD1	2.19	0.43
1:A:233:HIS:C	1:A:233:HIS:CD2	2.93	0.43
1:A:477:LEU:HD13	4:A:601:HEM:HMB3	2.01	0.43
1:A:369:PHE:C	1:A:369:PHE:CD2	2.92	0.43
1:A:262:ASP:C	1:A:262:ASP:OD2	2.57	0.42
1:A:81:THR:HB	1:A:239:TRP:CD1	2.54	0.42
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.76	0.42
1:A:285:PHE:CZ	1:A:369:PHE:HA	2.54	0.42
1:A:184:TYR:CE2	1:A:266:ARG:HB3	2.55	0.42
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.96	0.42
1:A:233:HIS:N	1:A:234:PRO:HD2	2.35	0.42
8:A:615:OLC:H13	8:A:615:OLC:H10	1.58	0.42
1:A:46:TYR:HA	1:A:453:ILE:HD11	2.01	0.42
1:A:264:MET:HE1	2:B:19:LEU:HD11	2.02	0.42
1:A:307:VAL:N	1:A:308:PRO:HD2	2.35	0.41
2:B:46:PRO:HA	2:B:134:THR:O	2.20	0.41
2:B:78:GLN:HG3	2:B:102:GLU:HB3	2.03	0.41
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.85	0.41
8:C:101:OLC:H10	8:C:102:OLC:C8	2.48	0.41
1:A:235:ILE:O	1:A:238:PHE:HB3	2.21	0.41
5:A:602:HAS:CBC	5:A:602:HAS:HMC1	2.44	0.41
1:A:191:LEU:HD11	8:A:611:OLC:H3	2.04	0.40
1:A:56:LYS:O	1:A:60:PRO:HA	2.22	0.40
1:A:204:ALA:HA	1:A:208:LEU:HB2	2.04	0.40
2:B:71:VAL:HG22	2:B:81:VAL:HG22	2.04	0.40

All (2) 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:306:HOH:O	10:B:320:HOH:O[2_556]	1.32	0.88
10:B:323:HOH:O	10:B:323:HOH:O[2_556]	1.41	0.79



## 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	552/569 (97%)	522 (95%)	29 (5%)	1 (0%)	52	77
2	B	164/168 (98%)	158 (96%)	6 (4%)	0	100	100
3	C	29/34 (85%)	28 (97%)	1 (3%)	0	100	100
All	All	745/771 (97%)	708 (95%)	36 (5%)	1 (0%)	56	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	PHE

### 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	440/464 (95%)	422 (96%)	18 (4%)	37	66
2	B	131/138 (95%)	125 (95%)	6 (5%)	33	61
3	C	23/27 (85%)	18 (78%)	5 (22%)	1	2
All	All	594/629 (94%)	565 (95%)	29 (5%)	31	57

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	54	LEU

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Mol	Chain	Res	Type
1	A	58	LEU
1	A	133	TYR
1	A	215	LEU
1	A	230	TRP
1	A	254	GLN
1	A	262	ASP
1	A	274	LEU
1	A	290	ILE
1	A	369	PHE
1	A	425	VAL
1	A	456	VAL
1	A	516	GLU
1	A	517	ASP
1	A	518	ARG
1	A	519	ARG
1	A	520	LEU
2	B	26	LEU
2	B	37	LEU
2	B	58	VAL
2	B	61	GLU
2	B	158	GLN
2	B	167	LYS
3	C	13	LEU
3	C	17	LEU
3	C	20	LEU
3	C	23	TRP
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
1	A	407	ASN
2	B	93	ASN
2	B	158	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z  > 2$
4	HEM	A	601	1	30,50,50	3.69	13 (43%)	24,82,82	2.65	11 (45%)
5	HAS	A	602	1,7	45,72,72	2.61	12 (26%)	47,109,109	1.79	11 (23%)
7	PER	A	604	5,6	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	A	605	-	19,19,24	0.48	0	19,19,25	0.84	0
8	OLC	A	606	-	21,21,24	0.56	0	22,22,25	1.26	3 (13%)
8	OLC	A	607	-	19,19,24	0.63	1 (5%)	19,19,25	0.63	1 (5%)
8	OLC	A	608	-	17,17,24	0.54	0	18,18,25	0.53	0
8	OLC	A	609	-	12,12,24	0.71	0	13,13,25	0.69	0
8	OLC	A	610	-	7,7,24	0.65	0	6,7,25	0.79	0
8	OLC	A	611	-	11,11,24	0.70	0	12,12,25	0.58	0
8	OLC	A	612	-	5,8,24	0.15	0	5,8,25	1.39	1 (20%)
8	OLC	A	613	-	24,24,24	0.64	1 (4%)	25,25,25	0.95	1 (4%)
8	OLC	A	614	-	12,12,24	0.60	0	13,13,25	0.93	1 (7%)
8	OLC	A	615	-	23,23,24	0.49	0	24,24,25	0.92	1 (4%)
9	CUA	B	201	2	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	B	202	-	23,23,24	0.49	0	24,24,25	0.73	0
8	OLC	B	203	-	22,22,24	0.81	1 (4%)	23,23,25	1.59	3 (13%)
8	OLC	B	204	-	15,15,24	0.50	0	16,16,25	0.63	0
8	OLC	C	101	-	22,22,24	0.53	0	23,23,25	0.80	0
8	OLC	C	102	-	12,12,24	0.13	0	10,11,25	0.72	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
4	HEM	A	601	1	-	0/10/54/54	0/0/8/8
5	HAS	A	602	1,7	-	0/30/82/82	0/0/8/8
7	PER	A	604	5,6	-	0/0/0/0	0/0/0/0
8	OLC	A	605	-	-	0/18/18/24	0/0/0/0
8	OLC	A	606	-	-	0/21/21/24	0/0/0/0
8	OLC	A	607	-	-	0/18/18/24	0/0/0/0
8	OLC	A	608	-	-	0/17/17/24	0/0/0/0
8	OLC	A	609	-	-	0/12/12/24	0/0/0/0
8	OLC	A	610	-	-	0/6/6/24	0/0/0/0
8	OLC	A	611	-	-	0/11/11/24	0/0/0/0
8	OLC	A	612	-	-	0/4/6/24	0/0/0/0
8	OLC	A	613	-	-	0/24/24/24	0/0/0/0
8	OLC	A	614	-	-	0/12/12/24	0/0/0/0
8	OLC	A	615	-	-	0/23/23/24	0/0/0/0
9	CUA	B	201	2	-	0/0/0/0	0/0/0/0
8	OLC	B	202	-	-	0/23/23/24	0/0/0/0
8	OLC	B	203	-	-	0/22/22/24	0/0/0/0
8	OLC	B	204	-	-	0/15/15/24	0/0/0/0
8	OLC	C	101	-	-	0/22/22/24	0/0/0/0
8	OLC	C	102	-	-	0/10/10/24	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	HEM	C3B-CAB	-10.41	1.31	1.51
4	A	601	HEM	C2C-C1C	-9.53	1.34	1.52
4	A	601	HEM	C2D-C3D	-6.96	1.33	1.54
5	A	602	HAS	C3C-CAC	-6.60	1.33	1.47
4	A	601	HEM	C2B-C1B	-5.50	1.33	1.51
5	A	602	HAS	C2D-C3D	-4.22	1.34	1.40
5	A	602	HAS	C4A-CHD	-3.30	1.30	1.39
5	A	602	HAS	C1A-CHA	-2.75	1.32	1.39
4	A	601	HEM	C3B-C4B	-2.41	1.49	1.51
4	A	601	HEM	CHD-C1D	-2.29	1.32	1.38
4	A	601	HEM	C3D-C4D	-2.21	1.48	1.51
4	A	601	HEM	C4A-CHB	-2.07	1.34	1.39
5	A	602	HAS	C2A-C3A	-2.01	1.31	1.37
8	A	613	OLC	O20-C1	2.03	1.39	1.33
8	A	607	OLC	O20-C1	2.07	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HAS	C2D-CMD	2.33	1.52	1.46
8	B	203	OLC	O20-C1	2.47	1.40	1.33
4	A	601	HEM	FE-NC	2.80	2.06	1.95
5	A	602	HAS	CBC-CAC	3.08	1.51	1.28
5	A	602	HAS	C1C-CHC	3.23	1.48	1.39
4	A	601	HEM	C1A-CHA	3.78	1.50	1.39
5	A	602	HAS	C1D-CHB	3.91	1.50	1.39
4	A	601	HEM	CBB-CAB	3.95	1.52	1.29
4	A	601	HEM	CHD-C4C	5.04	1.48	1.36
4	A	601	HEM	CHC-C1C	5.56	1.49	1.36
5	A	602	HAS	C4C-NC	5.78	1.44	1.36
5	A	602	HAS	C4D-ND	7.30	1.46	1.36
5	A	602	HAS	C3C-C2C	8.81	1.51	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	HEM	CAA-C2A-C1A	-5.05	121.52	127.01
5	A	602	HAS	CAA-CBA-CGA	-4.63	104.25	112.75
5	A	602	HAS	CAD-CBD-CGD	-4.57	104.36	112.75
4	A	601	HEM	CMA-C3A-C4A	-4.55	120.83	128.36
4	A	601	HEM	C3B-C4B-NB	-3.45	105.03	111.63
5	A	602	HAS	C21-C22-C23	-3.17	120.86	127.76
5	A	602	HAS	C20-C19-C18	-3.01	115.35	121.05
8	A	612	OLC	C4-C3-C2	-2.99	101.25	113.90
5	A	602	HAS	CAA-C2A-C1A	-2.95	123.80	127.01
8	A	606	OLC	O20-C21-C22	-2.66	91.56	106.10
4	A	601	HEM	CBA-CAA-C2A	-2.62	107.84	112.53
8	A	615	OLC	C3-C2-C1	-2.22	104.85	113.59
5	A	602	HAS	C16-C17-C18	-2.00	106.44	111.69
8	A	607	OLC	C21-O20-C1	2.01	123.63	116.21
8	A	614	OLC	C21-O20-C1	2.04	122.56	116.85
8	A	606	OLC	C21-C22-C24	2.17	119.84	111.08
5	A	602	HAS	C25-C23-C24	2.34	118.98	115.41
8	A	613	OLC	C21-O20-C1	2.36	123.46	116.85
4	A	601	HEM	CMB-C2B-C3B	2.59	123.01	116.53
5	A	602	HAS	C12-C13-C14	2.65	119.82	112.40
5	A	602	HAS	CMA-C3A-C2A	2.66	130.80	125.24
5	A	602	HAS	C12-C11-C3B	2.69	118.16	112.59
4	A	601	HEM	CMC-C2C-C3C	2.82	123.58	116.53
4	A	601	HEM	CMD-C2D-C3D	2.84	126.89	114.35
4	A	601	HEM	C2D-C3D-C4D	3.09	106.74	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	HEM	CHC-C4B-NB	3.12	132.05	124.52
8	A	606	OLC	C21-O20-C1	3.20	125.79	116.85
8	B	203	OLC	C21-C22-C24	3.30	124.40	111.08
8	B	203	OLC	O20-C21-C22	3.47	125.10	106.10
4	A	601	HEM	CAD-C3D-C4D	3.68	125.46	112.47
5	A	602	HAS	C27-C19-C20	4.18	121.80	115.41
4	A	601	HEM	CAD-C3D-C2D	4.93	127.40	113.22
8	B	203	OLC	C21-O20-C1	4.97	130.74	116.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	HEM	5	0
5	A	602	HAS	3	0
7	A	604	PER	1	0
8	A	605	OLC	1	0
8	A	606	OLC	2	0
8	A	607	OLC	7	0
8	A	608	OLC	1	0
8	A	610	OLC	3	0
8	A	611	OLC	3	0
8	A	612	OLC	2	0
8	A	613	OLC	6	0
8	A	615	OLC	3	0
8	B	202	OLC	1	0
8	B	203	OLC	8	0
8	B	204	OLC	1	0
8	C	101	OLC	4	0
8	C	102	OLC	5	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	554/569 (97%)	-0.00	11 (1%) 68 63	19, 30, 61, 95	1 (0%)
2	B	166/168 (98%)	-0.13	0 100 100	21, 31, 50, 70	0
3	C	31/34 (91%)	-0.39	0 100 100	24, 30, 42, 55	0
All	All	751/771 (97%)	-0.05	11 (1%) 76 71	19, 30, 57, 95	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	SER	3.5
1	A	501	LEU	3.5
1	A	495	ARG	3.3
1	A	494	SER	2.9
1	A	499	PRO	2.8
1	A	516	GLU	2.5
1	A	322	PHE	2.4
1	A	491	VAL	2.4
1	A	492	LEU	2.2
1	A	10	ARG	2.2
1	A	11	VAL	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

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	613	25/25	0.73	0.39	12.41	48,59,64,67	0
8	OLC	A	605	20/25	0.74	0.38	10.74	45,65,84,87	0
8	OLC	A	615	24/25	0.58	0.45	10.38	52,59,67,69	0
8	OLC	A	607	20/25	0.69	0.38	9.83	57,62,75,77	0
8	OLC	A	611	12/25	0.46	0.56	9.24	48,73,75,75	0
8	OLC	B	204	16/25	0.71	0.27	9.16	65,66,70,72	0
8	OLC	C	101	23/25	0.77	0.37	8.86	46,56,71,74	0
8	OLC	A	612	9/25	0.63	0.39	7.89	53,55,62,64	0
8	OLC	B	202	24/25	0.69	0.28	6.87	53,66,71,73	0
8	OLC	A	608	18/25	0.67	0.36	6.56	47,60,72,72	0
8	OLC	B	203	23/25	0.57	0.35	6.27	57,63,72,76	0
8	OLC	A	614	13/25	0.59	0.54	5.08	62,75,81,81	0
8	OLC	C	102	13/25	0.81	0.23	3.78	63,70,79,81	0
8	OLC	A	606	22/25	0.84	0.27	2.91	30,45,62,64	0
7	PER	A	604	2/2	0.98	0.25	2.54	27,27,27,29	0
5	HAS	A	602	65/65	0.94	0.22	2.12	19,25,42,47	0
4	HEM	A	601	43/43	0.97	0.17	-0.30	18,21,23,26	0
9	CUA	B	201	2/2	1.00	0.15	-1.13	24,24,24,26	0
8	OLC	A	609	13/25	0.42	0.46	-	59,65,77,78	0
6	CU	A	603	1/1	1.00	0.14	-	27,27,27,27	0
8	OLC	A	610	8/25	0.80	0.31	-	67,68,70,70	0

## 6.5 Other polymers

There are no such residues in this entry.