



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 12:28 am GMT

PDB ID : 3S8F  
Title : 1.8 Å structure of ba3 cytochrome c oxidase from *Thermus thermophilus* in lipid environment  
Authors : Tiefenbrunn, T.; Liu, W.; Chen, Y.; Katritch, V.; Stout, C.D.; Fee, J.A.; Cherezov, V.  
Deposited on : 2011-05-27  
Resolution : 1.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

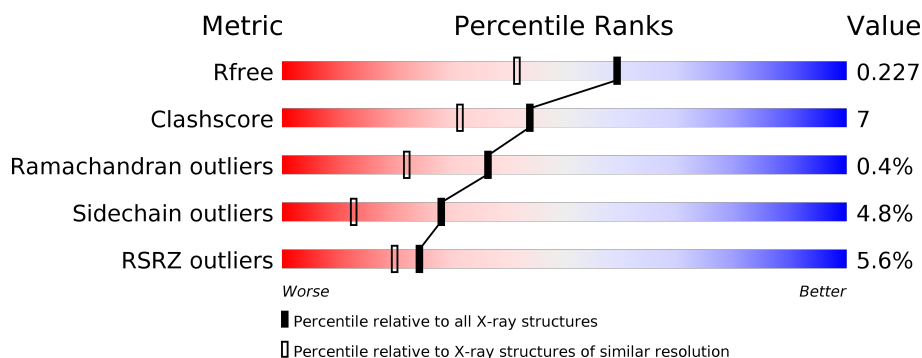
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	5253 (1.80-1.80)
Clashscore	122126	6077 (1.80-1.80)
Ramachandran outliers	120053	6011 (1.80-1.80)
Sidechain outliers	120020	6010 (1.80-1.80)
RSRZ outliers	108989	5157 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>6%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• •</div> </div> </div>
2	B	168	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>• •</div> </div> </div>
3	C	34	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>21%</div> <div>15%</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6567 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	5	0
			4389	2979	699	695	16			

There are 8 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

- 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).

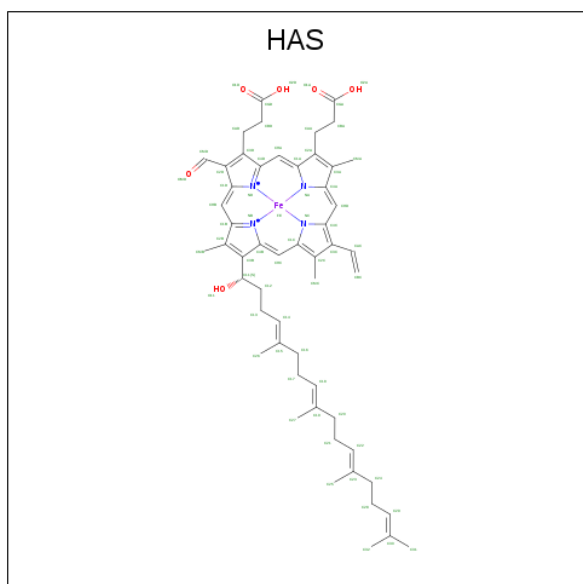
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



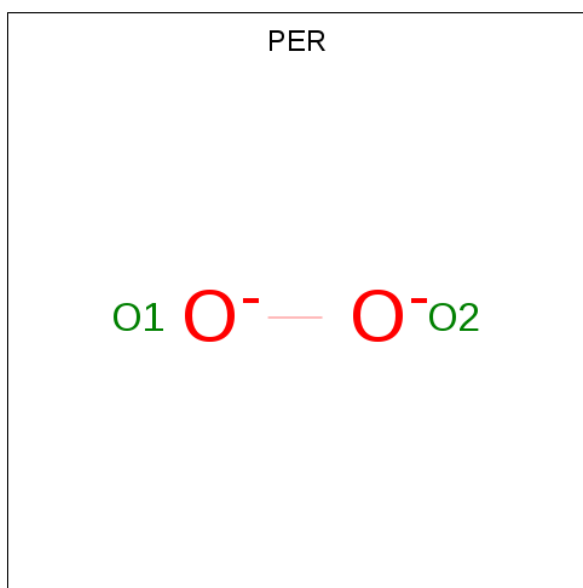
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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



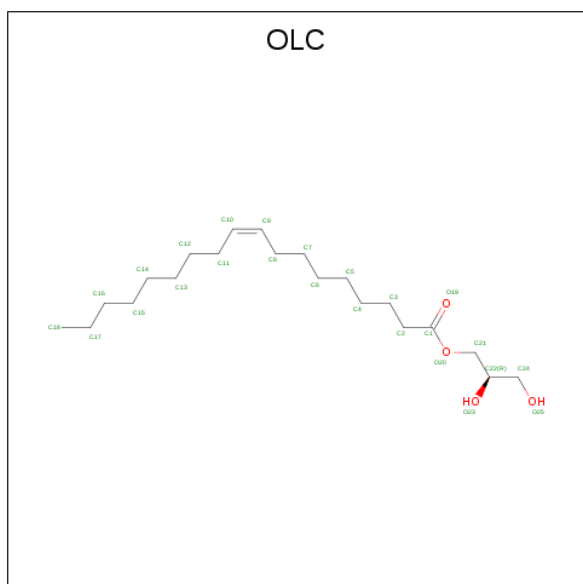
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	
			65	54	1	4	6	

- 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>).



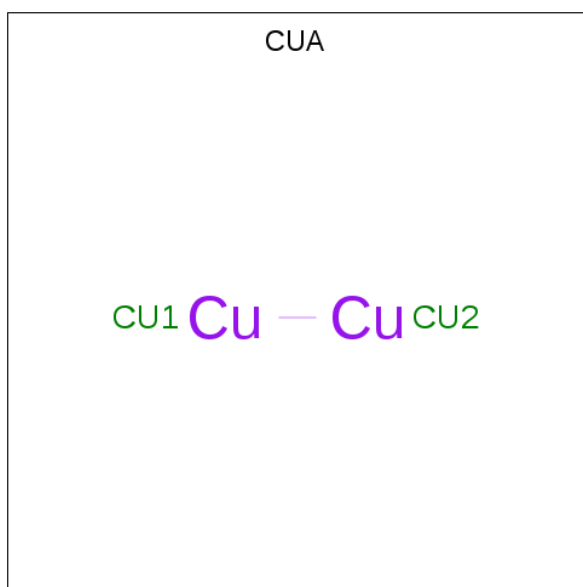
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			25	21	4		

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

- 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		

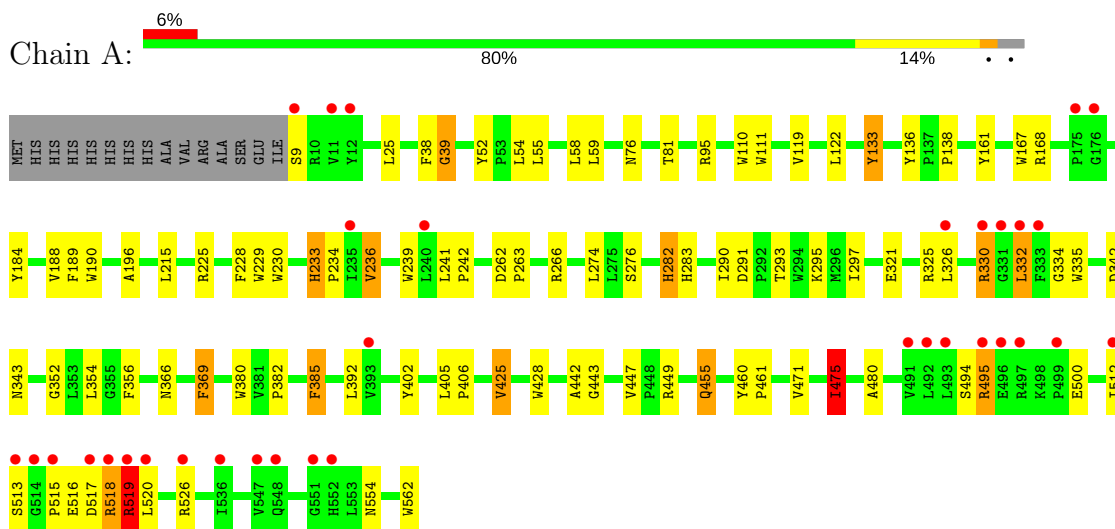
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	117	Total	O	0	0
			117	117		
10	B	71	Total	O	0	0
			71	71		
10	C	5	Total	O	0	0
			5	5		

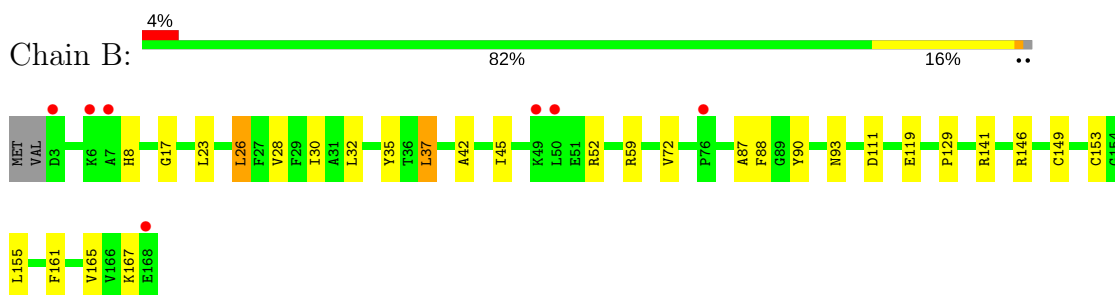
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

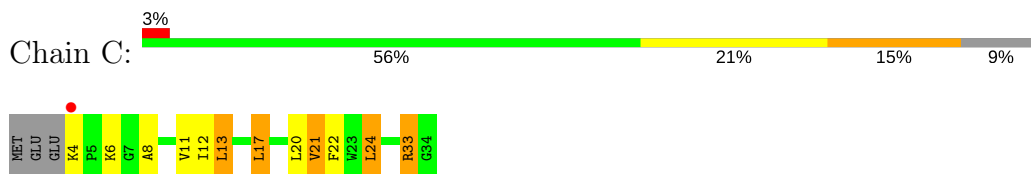
#### • Molecule 1: Cytochrome c oxidase subunit 1



#### • 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, $\alpha$ , $\beta$ , $\gamma$	143.59Å 97.82Å 94.95Å 90.00° 128.30° 90.00°	Depositor
Resolution (Å)	37.26 – 1.80 37.26 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (37.26-1.80) 97.2 (37.26-1.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.184 , 0.215 0.198 , 0.227	Depositor DCC
$R_{free}$ test set	4656 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 61.8	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	0.96	EDS
Total number of atoms	6567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% 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	1.42	29/4562 (0.6%)	1.09	14/6263 (0.2%)
2	B	1.48	8/1330 (0.6%)	1.11	5/1817 (0.3%)
3	C	1.50	4/247 (1.6%)	1.25	3/335 (0.9%)
All	All	1.44	41/6139 (0.7%)	1.11	22/8415 (0.3%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	PHE	CE2-CZ	8.17	1.52	1.37
1	A	133	TYR	CD1-CE1	7.43	1.50	1.39
2	B	161	PHE	CE2-CZ	7.36	1.51	1.37
1	A	449	ARG	CZ-NH1	7.29	1.42	1.33
2	B	119	GLU	CB-CG	-7.24	1.38	1.52
1	A	38	PHE	CD2-CE2	6.99	1.53	1.39
1	A	229	TRP	CE3-CZ3	6.59	1.49	1.38
2	B	165	VAL	CB-CG2	6.40	1.66	1.52
1	A	119	VAL	CB-CG2	6.32	1.66	1.52
1	A	480	ALA	CA-CB	6.15	1.65	1.52
2	B	153	CYS	CB-SG	6.12	1.92	1.82
3	C	11	VAL	CB-CG1	6.06	1.65	1.52
2	B	111	ASP	CB-CG	6.05	1.64	1.51
1	A	442	ALA	CA-CB	5.91	1.64	1.52
1	A	136	TYR	CE2-CZ	5.90	1.46	1.38
1	A	39	GLY	N-CA	5.84	1.54	1.46
1	A	352	GLY	CA-C	5.80	1.61	1.51
3	C	8	ALA	CA-CB	-5.74	1.40	1.52
1	A	447	VAL	CB-CG2	5.68	1.64	1.52
1	A	188	VAL	CB-CG1	5.55	1.64	1.52
1	A	52	TYR	CD2-CE2	5.54	1.47	1.39
1	A	110	TRP	CB-CG	5.53	1.60	1.50
1	A	236	VAL	CB-CG2	5.49	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	TRP	CE3-CZ3	5.49	1.47	1.38
1	A	356	PHE	CE1-CZ	5.47	1.47	1.37
3	C	22	PHE	CE1-CZ	5.43	1.47	1.37
1	A	111	TRP	CB-CG	-5.37	1.40	1.50
1	A	461	PRO	N-CA	5.32	1.56	1.47
1	A	228	PHE	CD1-CE1	5.29	1.49	1.39
1	A	460	TYR	CG-CD1	5.28	1.46	1.39
1	A	228	PHE	CE2-CZ	5.25	1.47	1.37
1	A	428	TRP	CG-CD1	5.20	1.44	1.36
2	B	28	VAL	CB-CG2	5.19	1.63	1.52
1	A	276	SER	CB-OG	5.13	1.49	1.42
1	A	380	TRP	CZ3-CH2	5.12	1.48	1.40
1	A	184	TYR	CD1-CE1	5.12	1.47	1.39
1	A	443	GLY	N-CA	5.11	1.53	1.46
2	B	72	VAL	CB-CG1	5.07	1.63	1.52
3	C	21	VAL	CB-CG2	5.05	1.63	1.52
2	B	90	TYR	CD1-CE1	-5.02	1.31	1.39
1	A	385	PHE	CE1-CZ	5.02	1.46	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	59	ARG	NE-CZ-NH1	-9.75	115.42	120.30
1	A	266	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	266	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	95	ARG	NE-CZ-NH2	7.75	124.18	120.30
1	A	425	VAL	CG1-CB-CG2	7.75	123.30	110.90
1	A	25	LEU	CB-CG-CD1	-7.46	98.31	111.00
2	B	37	LEU	CA-CB-CG	7.42	132.37	115.30
1	A	95	ARG	NE-CZ-NH1	-6.92	116.84	120.30
2	B	146	ARG	NE-CZ-NH1	-6.60	117.00	120.30
2	B	23	LEU	CB-CG-CD2	-6.56	99.85	111.00
2	B	149	CYS	CA-CB-SG	-6.40	102.48	114.00
3	C	24	LEU	CB-CG-CD1	6.33	121.75	111.00
3	C	33	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	A	425	VAL	CA-CB-CG1	6.05	119.98	110.90
3	C	13	LEU	CA-CB-CG	5.91	128.89	115.30
1	A	233	HIS	N-CA-CB	5.78	121.00	110.60
1	A	54	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	332	LEU	CA-CB-CG	5.64	128.27	115.30
1	A	475	ILE	CG1-CB-CG2	5.50	123.49	111.40
1	A	342	ASP	CB-CG-OD1	5.36	123.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	TYR	CA-CB-CG	-5.21	103.51	113.40
1	A	297	ILE	CG1-CB-CG2	-5.20	99.97	111.40

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	4389	0	4484	54	0
2	B	1288	0	1260	20	0
3	C	241	0	267	7	0
4	A	1	0	0	0	0
5	A	43	0	30	3	0
6	A	65	0	62	4	0
7	A	2	0	0	1	0
8	A	222	0	320	21	0
8	B	96	0	153	16	0
8	C	25	0	40	1	0
9	B	2	0	0	0	0
10	A	117	0	0	5	0
10	B	71	0	0	1	1
10	C	5	0	0	0	0
All	All	6567	0	6616	94	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 7.

All (94) 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)
7:A:563:PER:O1	7:A:563:PER:O2	1.54	1.23
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:CG	1.49	1.21
1:A:330[B]:ARG:NH1	1:A:330[B]:ARG:HG2	1.41	1.13
1:A:516[A]:GLU:HG3	1:A:517:ASP:H	1.08	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516[A]:GLU:HG3	1:A:517:ASP:N	1.55	1.11
2:B:141:ARG:HH12	8:B:170:OLC:H24A	1.28	0.98
1:A:263:PRO:HG2	1:A:516[A]:GLU:HG2	1.42	0.98
1:A:554:ASN:HB2	2:B:52:ARG:HD2	1.45	0.96
2:B:141:ARG:NH1	8:B:170:OLC:H24A	1.82	0.94
1:A:495:ARG:HH21	1:A:495:ARG:HA	1.32	0.94
8:A:565:OLC:H12	8:A:572:OLC:H14A	1.48	0.92
1:A:516[A]:GLU:CG	1:A:517:ASP:H	1.86	0.89
1:A:168:ARG:HH22	8:A:570:OLC:C6	1.90	0.85
1:A:518:ARG:O	1:A:519:ARG:HB3	1.82	0.79
2:B:141:ARG:HH12	8:B:170:OLC:C24	1.96	0.78
1:A:330[B]:ARG:NH1	1:A:330[B]:ARG:CG	2.20	0.78
2:B:35:TYR:OH	8:B:169:OLC:H24A	1.84	0.76
2:B:93:ASN:O	10:B:201:HOH:O	2.06	0.74
1:A:168:ARG:HH22	8:A:570:OLC:H6A	1.54	0.71
1:A:495:ARG:HA	1:A:495:ARG:NH2	2.07	0.69
8:B:170:OLC:H6	3:C:33:ARG:HE	1.59	0.67
8:A:565:OLC:C12	8:A:572:OLC:H14A	2.22	0.65
2:B:17:GLY:HA3	8:B:171:OLC:H3	1.79	0.64
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:HG2	0.59	0.63
8:A:569:OLC:O19	8:A:570:OLC:C8	2.48	0.62
1:A:168:ARG:HH22	8:A:570:OLC:H6	1.62	0.61
1:A:518:ARG:O	1:A:519:ARG:CB	2.49	0.61
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.36	0.60
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.88	0.60
8:A:564:OLC:O25	8:B:170:OLC:H7A	2.03	0.58
8:B:170:OLC:H4	3:C:33:ARG:HG2	1.86	0.57
6:A:801:HAS:HBC1	6:A:801:HAS:HMC1	1.87	0.57
8:A:572:OLC:C8	8:A:572:OLC:H13A	2.36	0.56
1:A:161:TYR:CE2	8:A:569:OLC:H21	2.42	0.55
2:B:32:LEU:HD21	8:B:169:OLC:H7A	1.90	0.54
2:B:141:ARG:HH12	8:B:170:OLC:C22	2.21	0.52
3:C:21:VAL:HG11	8:C:35:OLC:H9	1.90	0.52
2:B:141:ARG:NH1	8:B:170:OLC:C24	2.62	0.52
1:A:516[B]:GLU:OE1	1:A:517:ASP:N	2.44	0.50
1:A:475:ILE:CG1	8:A:565:OLC:H13A	2.41	0.50
10:A:583:HOH:O	8:B:170:OLC:H4A	2.10	0.50
1:A:241:LEU:N	1:A:242:PRO:CD	2.75	0.50
1:A:233:HIS:O	1:A:236:VAL:HG22	2.12	0.49
10:A:592:HOH:O	2:B:8:HIS:HE1	1.96	0.48
1:A:39:GLY:C	5:A:800:HEM:HMB3	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ILE:HB	1:A:295:LYS:HE3	1.95	0.48
1:A:168:ARG:HH11	8:A:569:OLC:C22	2.27	0.47
2:B:52:ARG:HG3	2:B:52:ARG:HH11	1.80	0.47
2:B:32:LEU:CD2	8:B:169:OLC:H7A	2.45	0.47
3:C:4:LYS:HG3	3:C:6:LYS:HG2	1.96	0.46
8:A:566:OLC:H13A	8:A:572:OLC:H12	1.97	0.46
8:A:572:OLC:H13A	8:A:572:OLC:H8A	1.97	0.46
1:A:168:ARG:HD2	8:A:569:OLC:O23	2.15	0.46
1:A:225:ARG:HG3	10:A:609:HOH:O	2.16	0.45
1:A:138:PRO:HG2	2:B:129:PRO:HG2	1.99	0.45
1:A:526:ARG:NH2	10:A:658:HOH:O	2.42	0.45
1:A:455:GLN:NE2	10:A:580:HOH:O	2.50	0.45
1:A:167:TRP:CH2	8:A:570:OLC:H22	2.51	0.45
3:C:13:LEU:HD13	3:C:17:LEU:HD22	1.98	0.45
2:B:35:TYR:HE2	8:B:169:OLC:H21A	1.82	0.44
2:B:26:LEU:O	2:B:30:ILE:HG13	2.16	0.44
2:B:141:ARG:HH12	8:B:170:OLC:H22	1.82	0.44
8:B:172:OLC:H11A	8:B:172:OLC:H14A	1.90	0.44
1:A:405:LEU:HB3	1:A:406:PRO:HD3	2.00	0.44
1:A:168:ARG:NH2	8:A:570:OLC:H6A	2.28	0.43
2:B:42:ALA:HB1	2:B:45:ILE:HD12	2.00	0.43
1:A:562:TRP:HA	2:B:155:LEU:HG	2.01	0.43
1:A:366:ASN:HB3	6:A:801:HAS:C2D	2.48	0.43
1:A:168:ARG:NH2	8:A:570:OLC:H3A	2.34	0.43
1:A:475:ILE:HG12	8:A:565:OLC:H13A	2.00	0.43
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.81	0.43
1:A:516[A]:GLU:CG	1:A:517:ASP:N	2.41	0.43
1:A:196:ALA:CB	1:A:234:PRO:HB2	2.49	0.42
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.54	0.42
1:A:55:LEU:HD11	1:A:59:LEU:HD12	2.01	0.42
2:B:87:ALA:HA	2:B:88:PHE:HA	1.80	0.42
3:C:12:ILE:C	3:C:12:ILE:HD12	2.40	0.41
1:A:196:ALA:HB1	1:A:234:PRO:HB2	2.02	0.41
8:A:571:OLC:O19	8:A:572:OLC:O23	2.38	0.41
1:A:325:ARG:HG2	1:A:325:ARG:HH21	1.84	0.41
6:A:801:HAS:HHA	6:A:801:HAS:HAA2	1.81	0.41
1:A:291:ASP:OD2	1:A:293:THR:HB	2.19	0.41
5:A:800:HEM:HBC2	5:A:800:HEM:CMC	2.51	0.41
3:C:17:LEU:HA	3:C:17:LEU:HD12	1.91	0.41
1:A:471:VAL:O	1:A:475:ILE:HG23	2.20	0.41
1:A:354:LEU:HD21	6:A:801:HAS:H323	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASN:OD1	1:A:402[B]:TYR:CE2	2.74	0.41
8:A:566:OLC:H15	8:A:571:OLC:H12	2.01	0.40
1:A:76:ASN:HB3	5:A:800:HEM:CAC	2.52	0.40
1:A:81:THR:HB	1:A:239:TRP:CD1	2.57	0.40
8:A:574:OLC:H10	8:A:574:OLC:H13	1.57	0.40
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.56	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:175:HOH:O	10:B:201:HOH:O[2_556]	2.08	0.12

## 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	556/569 (98%)	536 (96%)	17 (3%)	3 (0%)	31	16
2	B	165/168 (98%)	162 (98%)	3 (2%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	750/771 (97%)	727 (97%)	20 (3%)	3 (0%)	36	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	PRO
1	A	519	ARG
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	450/463 (97%)	426 (95%)	24 (5%)	25	10
2	B	134/138 (97%)	131 (98%)	3 (2%)	55	42
3	C	24/27 (89%)	21 (88%)	3 (12%)	5	1
All	All	608/628 (97%)	578 (95%)	30 (5%)	28	12

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

Mol	Chain	Res	Type
1	A	9	SER
1	A	58	LEU
1	A	133	TYR
1	A	215	LEU
1	A	230	TRP
1	A	262	ASP
1	A	274	LEU
1	A	282	HIS
1	A	326	LEU
1	A	330[A]	ARG
1	A	330[B]	ARG
1	A	332	LEU
1	A	369	PHE
1	A	425	VAL
1	A	455	GLN
1	A	475	ILE
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	519	ARG
1	A	520	LEU
2	B	26	LEU
2	B	37	LEU

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Mol	Chain	Res	Type
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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	GLN
2	B	8	HIS
2	B	40	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 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	$\# Z  > 2$
7	PER	A	563	4,6	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	A	564	-	24,24,24	0.53	0	25,25,25	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	OLC	A	565	-	24,24,24	0.47	0	25,25,25	0.82	0
8	OLC	A	566	-	22,22,24	0.53	0	23,23,25	1.25	4 (17%)
8	OLC	A	567	-	17,17,24	0.58	0	18,18,25	0.66	0
8	OLC	A	568	-	16,16,24	0.74	0	17,17,25	0.74	0
8	OLC	A	569	-	7,7,24	0.59	0	6,7,25	0.84	0
8	OLC	A	570	-	14,14,24	0.69	1 (7%)	15,15,25	0.58	0
8	OLC	A	571	-	19,19,24	0.50	0	20,20,25	1.12	1 (5%)
8	OLC	A	572	-	24,24,24	0.68	1 (4%)	25,25,25	0.99	2 (8%)
8	OLC	A	573	-	20,20,24	0.54	0	21,21,25	0.90	1 (4%)
8	OLC	A	574	-	24,24,24	0.49	0	25,25,25	0.92	1 (4%)
5	HEM	A	800	1	27,50,50	2.47	9 (33%)	17,82,82	3.90	8 (47%)
6	HAS	A	801	1,7	56,72,72	4.11	18 (32%)	49,109,109	3.48	22 (44%)
8	OLC	B	169	-	24,24,24	0.50	0	25,25,25	0.80	0
8	OLC	B	170	-	24,24,24	0.84	1 (4%)	25,25,25	1.16	2 (8%)
8	OLC	B	171	-	24,24,24	0.50	0	25,25,25	0.52	0
8	OLC	B	172	-	20,20,24	0.63	1 (5%)	20,20,25	0.70	1 (5%)
9	CUA	B	802	2	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	C	35	-	24,24,24	0.51	0	25,25,25	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PER	A	563	4,6	-	0/0/0/0	0/0/0/0
8	OLC	A	564	-	-	0/24/24/24	0/0/0/0
8	OLC	A	565	-	-	0/24/24/24	0/0/0/0
8	OLC	A	566	-	-	0/22/22/24	0/0/0/0
8	OLC	A	567	-	-	0/17/17/24	0/0/0/0
8	OLC	A	568	-	-	0/16/16/24	0/0/0/0
8	OLC	A	569	-	-	0/6/6/24	0/0/0/0
8	OLC	A	570	-	-	0/14/14/24	0/0/0/0
8	OLC	A	571	-	-	0/19/19/24	0/0/0/0
8	OLC	A	572	-	-	0/24/24/24	0/0/0/0
8	OLC	A	573	-	-	0/20/20/24	0/0/0/0
8	OLC	A	574	-	-	0/24/24/24	0/0/0/0
5	HEM	A	800	1	-	0/6/54/54	0/0/8/8
6	HAS	A	801	1,7	-	0/35/122/122	0/0/8/8
8	OLC	B	169	-	-	0/24/24/24	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	B	170	-	-	0/24/24/24	0/0/0/0
8	OLC	B	171	-	-	0/24/24/24	0/0/0/0
8	OLC	B	172	-	-	0/19/19/24	0/0/0/0
9	CUA	B	802	2	-	0/0/0/0	0/0/0/0
8	OLC	C	35	-	-	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	801	HAS	CHD-C4A	-17.80	1.33	1.51
6	A	801	HAS	C1B-NB	-11.43	1.33	1.49
6	A	801	HAS	C4B-NB	-11.32	1.33	1.49
6	A	801	HAS	CHC-C4B	-9.65	1.34	1.53
6	A	801	HAS	CHA-C1A	-5.67	1.37	1.51
5	A	800	HEM	C3B-CAB	-5.43	1.37	1.47
5	A	800	HEM	C1C-C2C	-4.85	1.31	1.42
6	A	801	HAS	CHD-C4C	-3.85	1.47	1.51
6	A	801	HAS	CHB-C1B	-3.54	1.38	1.53
6	A	801	HAS	C3C-CAC	-3.53	1.40	1.47
6	A	801	HAS	CHA-C4D	-3.07	1.47	1.53
6	A	801	HAS	C2B-C3B	-2.71	1.31	1.34
5	A	800	HEM	CAA-C2A	-2.63	1.47	1.52
5	A	800	HEM	C4B-CHC	-2.50	1.33	1.40
6	A	801	HAS	C1C-C2C	-2.18	1.35	1.38
5	A	800	HEM	C1D-CHD	-2.17	1.34	1.40
8	A	570	OLC	O20-C1	2.09	1.39	1.33
8	A	572	OLC	O20-C1	2.16	1.39	1.33
8	B	172	OLC	O20-C1	2.18	1.40	1.32
6	A	801	HAS	CMA-C3A	2.36	1.56	1.51
8	B	170	OLC	O20-C1	2.71	1.41	1.33
6	A	801	HAS	CBC-CAC	2.94	1.49	1.29
5	A	800	HEM	CBB-CAB	3.11	1.50	1.29
6	A	801	HAS	CMB-C2B	3.36	1.56	1.50
5	A	800	HEM	C4A-NA	3.85	1.44	1.36
5	A	800	HEM	C1A-CHA	4.20	1.51	1.40
6	A	801	HAS	C4A-C3A	4.41	1.44	1.38
5	A	800	HEM	C1A-NA	4.78	1.46	1.36
6	A	801	HAS	CMD-C2D	5.11	1.54	1.44
6	A	801	HAS	C3C-C2C	6.27	1.49	1.40
6	A	801	HAS	C1A-C2A	6.56	1.47	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	HEM	C4C-C3C-C2C	-11.91	98.58	106.90
6	A	801	HAS	CAA-C2A-C1A	-11.82	118.99	127.30
6	A	801	HAS	CHD-C4A-C3A	-5.85	119.75	129.53
6	A	801	HAS	CAA-CBA-CGA	-4.83	104.41	112.66
6	A	801	HAS	CBD-CAD-C3D	-4.60	106.09	114.28
6	A	801	HAS	CHD-C4C-C3C	-4.26	124.02	129.61
5	A	800	HEM	CMD-C2D-C1D	-4.23	121.97	128.46
6	A	801	HAS	OMD-CMD-C2D	-3.97	119.45	124.28
6	A	801	HAS	C4C-C3C-C2C	-3.96	98.21	104.13
5	A	800	HEM	CBD-CAD-C3D	-3.51	105.78	112.47
8	A	571	OLC	C4-C3-C2	-3.37	100.99	113.23
5	A	800	HEM	CMA-C3A-C4A	-3.08	123.74	128.46
8	A	566	OLC	O20-C21-C22	-3.05	91.03	105.77
6	A	801	HAS	C20-C19-C18	-2.83	115.33	121.10
6	A	801	HAS	CHC-C1C-C2C	-2.75	124.70	129.45
6	A	801	HAS	CAD-CBD-CGD	-2.56	108.29	112.66
5	A	800	HEM	CAD-CBD-CGD	-2.48	108.42	112.66
6	A	801	HAS	CMB-C2B-C3B	-2.23	124.12	129.74
6	A	801	HAS	C24-C23-C22	-2.20	116.62	121.10
8	A	574	OLC	C3-C2-C1	-2.18	105.73	113.60
8	A	566	OLC	C3-C2-C1	-2.12	105.95	113.60
8	A	573	OLC	O20-C1-O19	2.07	128.64	123.58
8	A	566	OLC	C21-C22-C24	2.14	120.06	111.62
8	A	572	OLC	C21-O20-C1	2.15	123.55	117.13
8	A	572	OLC	O20-C21-C22	2.18	116.31	105.77
8	B	172	OLC	C21-O20-C1	2.30	123.97	116.14
6	A	801	HAS	CHB-C1B-C2B	2.34	122.02	114.70
8	A	566	OLC	C21-O20-C1	2.45	124.44	117.13
6	A	801	HAS	CAA-C2A-C3A	2.47	136.07	129.00
6	A	801	HAS	C12-C13-C14	2.49	118.84	112.33
8	B	170	OLC	O20-C21-C22	2.52	117.92	105.77
6	A	801	HAS	CMB-C2B-C1B	2.86	128.59	120.24
5	A	800	HEM	CAA-CBA-CGA	3.28	118.26	112.66
8	B	170	OLC	C21-O20-C1	3.40	127.29	117.13
6	A	801	HAS	C27-C19-C20	3.45	121.23	115.29
6	A	801	HAS	O11-C11-C12	3.55	119.65	109.54
5	A	800	HEM	C3C-C4C-NC	3.73	117.98	110.94
6	A	801	HAS	C1B-CHB-C1D	3.73	127.49	116.30
5	A	800	HEM	C1D-C2D-C3D	6.13	111.26	107.00
6	A	801	HAS	CHA-C4D-ND	6.21	122.45	110.75
6	A	801	HAS	C4A-CHD-C4C	7.60	130.45	112.66
6	A	801	HAS	CHC-C4B-NB	10.43	130.42	110.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	563	PER	1	0
8	A	564	OLC	1	0
8	A	565	OLC	4	0
8	A	566	OLC	2	0
8	A	569	OLC	4	0
8	A	570	OLC	7	0
8	A	571	OLC	2	0
8	A	572	OLC	6	0
8	A	574	OLC	1	0
5	A	800	HEM	3	0
6	A	801	HAS	4	0
8	B	169	OLC	4	0
8	B	170	OLC	10	0
8	B	171	OLC	1	0
8	B	172	OLC	1	0
8	C	35	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

### 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%)	0.06	34 (6%) 21 17	16, 29, 54, 84	0
2	B	166/168 (98%)	-0.17	7 (4%) 36 30	18, 30, 48, 65	0
3	C	31/34 (91%)	-0.54	1 (3%) 47 42	24, 30, 40, 55	0
All	All	751/771 (97%)	-0.02	42 (5%) 24 20	16, 29, 53, 84	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	SER	8.0
1	A	495	ARG	6.0
1	A	12	TYR	5.0
1	A	330[A]	ARG	4.9
1	A	515	PRO	4.6
1	A	496	GLU	4.2
1	A	499	PRO	4.2
1	A	514	GLY	4.1
1	A	332	LEU	4.1
2	B	6	LYS	4.0
1	A	333	PHE	3.9
1	A	519	ARG	3.8
1	A	9	SER	3.5
1	A	492	LEU	3.4
1	A	491	VAL	3.4
1	A	11	VAL	3.3
1	A	493	LEU	3.2
1	A	512	ILE	3.1
1	A	331	GLY	3.0
1	A	176	GLY	2.7
1	A	547	VAL	2.6
1	A	526	ARG	2.6
1	A	551	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	168	GLU	2.6
1	A	517	ASP	2.5
1	A	235	ILE	2.5
1	A	518	ARG	2.4
1	A	552	HIS	2.4
3	C	4	LYS	2.4
1	A	536	ILE	2.4
1	A	497	ARG	2.3
1	A	520	LEU	2.3
1	A	240	LEU	2.3
2	B	3	ASP	2.3
1	A	393	VAL	2.2
2	B	7	ALA	2.2
1	A	326	LEU	2.2
1	A	548	GLN	2.2
2	B	49	LYS	2.1
2	B	76	PRO	2.1
2	B	50	LEU	2.1
1	A	175	PRO	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
8	OLC	A	568	17/25	0.52	0.26	59,63,79,80	0
8	OLC	B	170	25/25	0.63	0.23	56,63,72,76	0
8	OLC	C	35	25/25	0.64	0.31	67,81,92,93	0
8	OLC	A	570	15/25	0.67	0.28	47,64,76,77	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	OLC	A	567	18/25	0.67	0.18	47,60,73,74	0
8	OLC	A	572	25/25	0.68	0.19	48,59,64,68	0
8	OLC	A	573	21/25	0.70	0.18	56,66,81,82	0
8	OLC	A	565	25/25	0.71	0.24	44,65,90,92	0
8	OLC	B	172	21/25	0.73	0.22	60,63,76,79	0
8	OLC	A	564	25/25	0.75	0.22	45,55,73,76	0
8	OLC	B	169	25/25	0.77	0.19	54,65,72,73	0
8	OLC	A	571	20/25	0.77	0.19	54,66,71,71	0
8	OLC	B	171	25/25	0.78	0.21	65,68,73,74	0
8	OLC	A	574	25/25	0.82	0.17	51,58,68,70	0
8	OLC	A	566	23/25	0.91	0.13	30,45,65,66	0
8	OLC	A	569	8/25	0.91	0.21	68,68,70,71	0
7	PER	A	563	2/2	0.98	0.13	19,19,19,21	0
6	HAS	A	801	65/65	0.98	0.13	11,20,34,39	0
4	CU	A	803	1/1	0.99	0.09	22,22,22,22	0
5	HEM	A	800	43/43	0.99	0.10	10,15,19,21	0
9	CUA	B	802	2/2	1.00	0.09	20,20,20,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.