



Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 07:34 PM GMT

PDB ID : 3S8G
Title : 1.8 Å structure of ba3 cytochrome c oxidase mutant (A120F) 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

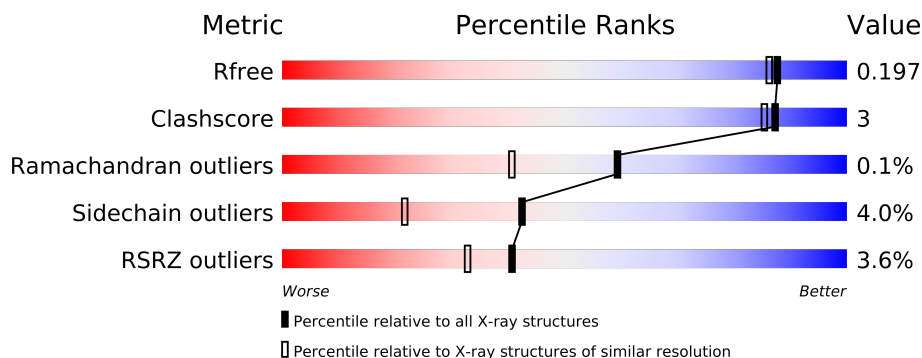
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 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}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	569	
2	B	168	
3	C	34	

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

Mol	Type	Chain	Res	Geometry	Electron density
8	OLC	A	564	-	X
8	OLC	A	565	-	X
8	OLC	A	566	-	X
8	OLC	A	567	-	X
8	OLC	A	569	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
8	OLC	A	570	-	X
8	OLC	A	571	-	X
8	OLC	A	572	-	X
8	OLC	A	573	-	X
8	OLC	A	574	-	X
8	OLC	A	575	-	X
8	OLC	A	576	-	X
8	OLC	A	577	-	X
8	OLC	A	578	-	X
8	OLC	B	169	-	X
8	OLC	B	170	-	X
8	OLC	B	171	-	X
8	OLC	B	172	-	X
8	OLC	C	35	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6695 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	7	0
			4399	2988	700	694	17			

There are 9 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	CONFLICT	UNP Q5SJ79

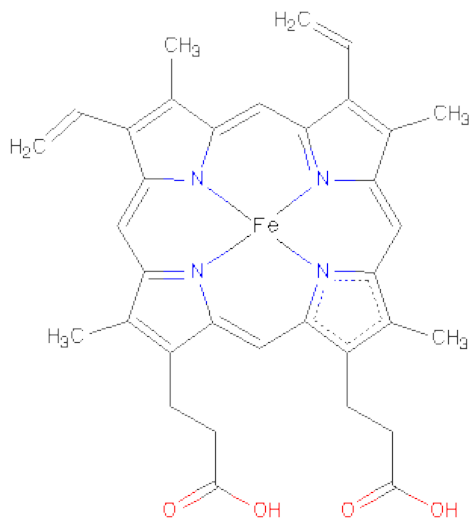
- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	5	0
			1307	846	219	238	4			

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

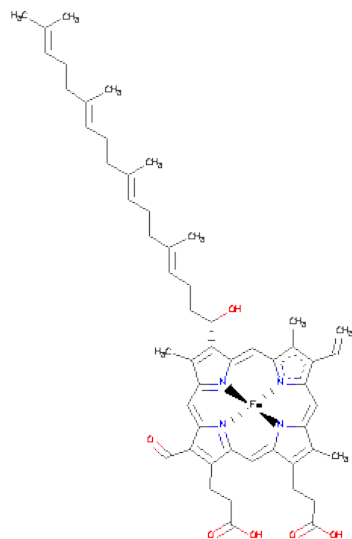
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	0	0	0
			241	169	37	35			

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 5 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



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).

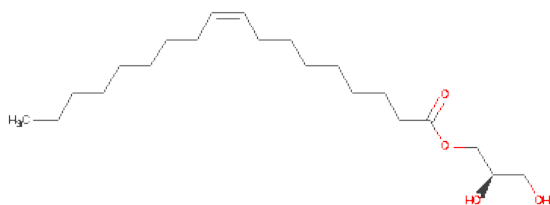
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cu	0	0
			1	1		

- Molecule 7 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



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: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			23	19	4		
8	A	1	Total	C	O	0	0
			25	21	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
			16	12	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			12	8	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
			14	10	4		

- Molecule 9 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

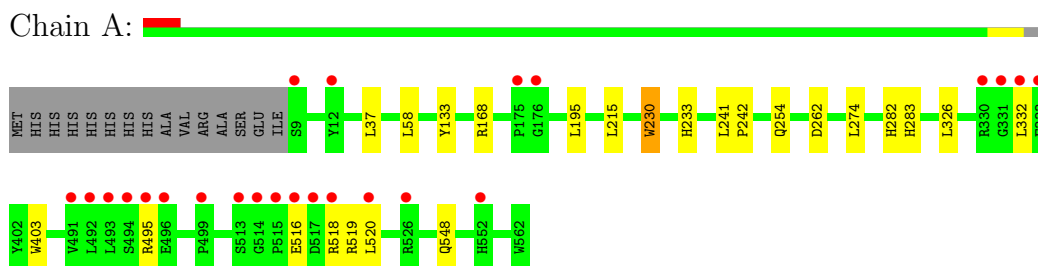
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	137	Total O 137 137	0	0
10	B	81	Total O 81 81	0	0
10	C	7	Total O 7 7	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.

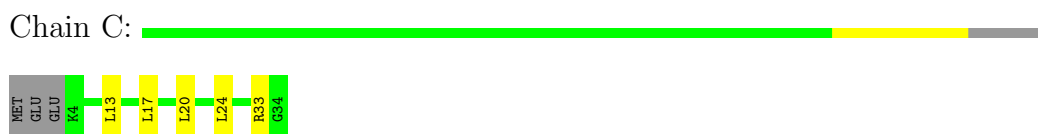
- Molecule 1: Cytochrome c oxidase subunit 1



- 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, α , β , γ	144.96Å 98.64Å 95.06Å 90.00° 128.07° 90.00°	Depositor
Resolution (Å)	39.48 – 1.80 39.48 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (39.48-1.80) 97.8 (39.48-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.196 0.176 , 0.197	Depositor DCC
R_{free} test set	4759 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.5	EDS
Estimated twinning fraction	0.017 for -h+k-l,-l,-k 0.002 for -h-k-l,l,k 0.018 for -h-2*l,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 95350 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6695	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.68	0/4584	0.64	1/6292 (0.0%)
2	B	0.69	0/1364	0.61	0/1862
3	C	0.73	0/247	0.72	0/335
All	All	0.69	0/6195	0.64	1/8489 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	HIS	N-CA-CB	5.24	120.04	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4399	0	0	7	0
2	B	1307	0	0	3	0
3	C	241	0	0	2	0
4	A	43	0	30	2	0
5	A	65	0	62	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
7	A	2	0	0	0	0
8	A	300	0	434	4	0
8	B	96	0	153	2	0
8	C	14	0	17	0	0
9	B	2	0	0	0	0
10	A	137	0	0	2	0
10	B	81	0	0	2	1
10	C	7	0	0	2	0
All	All	6695	0	696	18	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (18) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:168:ARG:NH2	8:A:572:OLC:H6A	2.02	0.75
2:B:141:ARG:NH1	8:B:170:OLC:H24A	2.02	0.75
2:B:93:ASN:O	10:B:1083:HOH:O	2.15	0.64
3:C:33:ARG:CD	10:C:36:HOH:O	2.48	0.61
8:A:578:OLC:H21A	8:B:170:OLC:H14	1.83	0.60
4:A:800:HEM:HBC2	4:A:800:HEM:CMC	2.36	0.56
3:C:33:ARG:NH2	10:C:36:HOH:O	2.41	0.53
4:A:800:HEM:HBC2	4:A:800:HEM:HMC2	1.90	0.53
1:A:254[B]:GLN:OE1	10:A:1077:HOH:O	2.19	0.51
1:A:282:HIS:CD2	1:A:283:HIS:CD2	3.00	0.50
5:A:801:HAS:HBC1	5:A:801:HAS:HMC1	1.94	0.48
8:A:575:OLC:H8	8:A:575:OLC:H11	1.85	0.43
2:B:93:ASN:ND2	10:B:1135:HOH:O	2.52	0.43
1:A:254[A]:GLN:NE2	1:A:403:TRP:CD1	2.88	0.42
1:A:548:GLN:NE2	10:A:1201:HOH:O	2.52	0.42
1:A:230:TRP:C	1:A:230:TRP:CD1	2.93	0.41
1:A:241:LEU:N	1:A:242:PRO:CD	2.83	0.41
8:A:574:OLC:H8A	8:A:574:OLC:H13A	2.03	0.41

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	Distance(Å)	Clash(Å)
10:B:1062:HOH:O	10:B:1063:HOH:O[2_556]	1.54	0.66

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	558/569 (98%)	542 (97%)	15 (3%)	1 (0%)	56	38
2	B	169/168 (101%)	167 (99%)	2 (1%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	756/771 (98%)	738 (98%)	17 (2%)	1 (0%)	59	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	516	GLU

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	453/464 (98%)	437 (96%)	16 (4%)	48	28
2	B	138/138 (100%)	133 (96%)	5 (4%)	47	27
3	C	24/27 (89%)	20 (83%)	4 (17%)	3	0
All	All	615/629 (98%)	590 (96%)	25 (4%)	42	21

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	58	LEU
1	A	133	TYR
1	A	195	LEU
1	A	215	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	230	TRP
1	A	262	ASP
1	A	274	LEU
1	A	326	LEU
1	A	332	LEU
1	A	369	PHE
1	A	401	LEU
1	A	495	ARG
1	A	518	ARG
1	A	519	ARG
1	A	520	LEU
2	B	26	LEU
2	B	37	LEU
2	B	158[A]	GLN
2	B	158[B]	GLN
2	B	167	LYS
3	C	13	LEU
3	C	17	LEU
3	C	20	LEU
3	C	24	LEU

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 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	5,6	1,1,1	1.56	0	0,0,0	0.00	-
8	OLC	A	564	-	24,24,24	0.43	0	25,25,25	0.70	0
8	OLC	A	565	-	24,24,24	0.43	0	25,25,25	0.58	0
8	OLC	A	566	-	24,24,24	0.44	0	25,25,25	0.63	0
8	OLC	A	567	-	22,22,24	1.05	1 (4%)	23,23,25	0.79	1 (4%)
8	OLC	A	568	-	24,24,24	0.44	0	25,25,25	0.58	0
8	OLC	A	569	-	16,17,24	0.55	0	17,18,25	0.66	0
8	OLC	A	570	-	15,16,24	0.46	0	16,17,25	0.57	0
8	OLC	A	571	-	6,7,24	0.23	0	5,7,25	0.43	0
8	OLC	A	572	-	14,14,24	1.50	1 (7%)	15,15,25	0.66	0
8	OLC	A	573	-	19,19,24	1.52	1 (5%)	20,20,25	1.52	1 (5%)
8	OLC	A	574	-	24,24,24	0.40	0	25,25,25	0.69	0
8	OLC	A	575	-	20,20,24	1.46	1 (5%)	21,21,25	0.87	1 (4%)
8	OLC	A	576	-	14,15,24	0.53	0	15,16,25	0.65	0
8	OLC	A	577	-	24,24,24	0.42	0	25,25,25	0.65	0
8	OLC	A	578	-	11,11,24	1.73	1 (9%)	12,12,25	0.73	0
4	HEM	A	800	1	49,50,50	6.49	22 (44%)	46,82,82	3.03	13 (28%)
5	HAS	A	801	1,7	72,72,72	2.45	25 (34%)	86,109,109	2.15	20 (23%)
8	OLC	B	169	-	24,24,24	0.44	0	25,25,25	0.64	0
8	OLC	B	170	-	24,24,24	0.51	0	25,25,25	0.65	1 (4%)
8	OLC	B	171	-	24,24,24	0.45	0	25,25,25	0.56	0
8	OLC	B	172	-	19,20,24	0.35	0	19,20,25	0.60	0
9	CUA	B	802	2	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	C	35	-	13,13,24	1.69	1 (7%)	14,14,25	0.76	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	5,6	-	0/0/0/0	0/0/0/0
8	OLC	A	564	-	-	0/24/24/24	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	A	565	-	-	0/24/24/24	0/0/0/0
8	OLC	A	566	-	-	0/24/24/24	0/0/0/0
8	OLC	A	567	-	-	0/22/22/24	0/0/0/0
8	OLC	A	568	-	-	0/24/24/24	0/0/0/0
8	OLC	A	569	-	-	0/17/17/24	0/0/0/0
8	OLC	A	570	-	-	0/16/16/24	0/0/0/0
8	OLC	A	571	-	-	0/5/6/24	0/0/0/0
8	OLC	A	572	-	-	0/14/14/24	0/0/0/0
8	OLC	A	573	-	-	0/19/19/24	0/0/0/0
8	OLC	A	574	-	-	0/24/24/24	0/0/0/0
8	OLC	A	575	-	-	0/20/20/24	0/0/0/0
8	OLC	A	576	-	-	0/15/15/24	0/0/0/0
8	OLC	A	577	-	-	0/24/24/24	0/0/0/0
8	OLC	A	578	-	-	0/11/11/24	0/0/0/0
4	HEM	A	800	1	-	0/14/114/114	0/0/8/8
5	HAS	A	801	1,7	-	0/36/82/82	0/0/8/8
8	OLC	B	169	-	-	0/24/24/24	0/0/0/0
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	-	-	0/13/13/24	0/0/0/0

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	HEM	C2B-C1B	-30.95	1.36	1.44
4	A	800	HEM	C3D-C4D	21.52	1.49	1.44
4	A	800	HEM	C2D-C1D	15.76	1.48	1.44
4	A	800	HEM	CHB-C1B	8.54	1.48	1.35
5	A	801	HAS	C2D-C1D	6.85	1.51	1.40
8	A	573	OLC	C13-C12	-6.28	1.52	1.55
5	A	801	HAS	C3C-CAC	-6.28	1.35	1.48
4	A	800	HEM	C4A-C3A	6.23	1.47	1.40
8	A	575	OLC	C14-C13	-6.23	1.52	1.55
5	A	801	HAS	C4A-C3A	6.21	1.47	1.40
4	A	800	HEM	CHD-C4C	6.08	1.47	1.36
5	A	801	HAS	C4D-ND	5.80	1.45	1.37
8	C	35	OLC	C7-C6	-5.74	1.52	1.55
4	A	800	HEM	CHC-C1C	5.67	1.47	1.36
4	A	800	HEM	C3D-C2D	-5.67	1.33	1.43
8	A	578	OLC	C5-C4	-5.41	1.53	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	572	OLC	C8-C7	-5.23	1.53	1.55
5	A	801	HAS	C4C-C3C	5.14	1.48	1.41
5	A	801	HAS	C4C-NC	4.86	1.44	1.37
8	A	567	OLC	C16-C15	-4.45	1.53	1.55
5	A	801	HAS	C3C-C2C	4.44	1.49	1.41
5	A	801	HAS	C2D-C3D	-4.41	1.33	1.41
5	A	801	HAS	C1D-ND	4.32	1.45	1.36
4	A	800	HEM	C1A-NA	4.30	1.45	1.36
5	A	801	HAS	C1C-C2C	-4.17	1.34	1.40
5	A	801	HAS	C1C-CHC	3.95	1.50	1.39
4	A	800	HEM	C1A-CHA	3.86	1.50	1.39
4	A	800	HEM	CBB-CAB	3.85	1.51	1.28
4	A	800	HEM	FE-NB	3.57	2.10	1.97
4	A	800	HEM	C1A-C2A	3.47	1.49	1.43
5	A	801	HAS	C1D-CHB	3.34	1.49	1.39
5	A	801	HAS	C4D-CHA	3.29	1.48	1.38
5	A	801	HAS	C1A-C2A	3.24	1.49	1.43
4	A	800	HEM	C2C-C1C	-3.20	1.33	1.43
5	A	801	HAS	C4C-CHD	3.04	1.47	1.38
4	A	800	HEM	C3B-C4B	3.03	1.48	1.44
5	A	801	HAS	FE-NA	2.98	2.05	1.92
4	A	800	HEM	C3C-CAC	2.94	1.49	1.40
5	A	801	HAS	O1D-CGD	2.83	1.32	1.22
5	A	801	HAS	CBC-CAC	2.77	1.49	1.28
5	A	801	HAS	C4A-CHD	-2.76	1.32	1.39
4	A	800	HEM	CHD-C1D	-2.63	1.33	1.39
5	A	801	HAS	FE-NB	2.62	2.03	1.92
4	A	800	HEM	C3B-C2B	2.60	1.48	1.43
4	A	800	HEM	FE-NA	2.49	2.03	1.92
4	A	800	HEM	C4D-ND	-2.48	1.34	1.39
5	A	801	HAS	FE-NC	2.41	2.02	1.92
5	A	801	HAS	C4B-C3B	2.32	1.51	1.43
4	A	800	HEM	CHC-C4B	-2.31	1.33	1.39
4	A	800	HEM	C4A-CHB	-2.30	1.33	1.39
5	A	801	HAS	C1A-CHA	-2.21	1.33	1.39
5	A	801	HAS	O2D-CGD	-2.06	1.23	1.30
5	A	801	HAS	C3B-C2B	-2.06	1.33	1.40

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	HEM	C3B-C4B-NB	-10.57	106.44	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	801	HAS	C4C-C3C-C2C	-10.29	99.68	106.87
5	A	801	HAS	C2C-C1C-NC	8.80	116.06	109.41
4	A	800	HEM	CHC-C4B-NB	8.32	131.50	124.58
4	A	800	HEM	C1B-NB-C4B	6.60	111.92	105.16
4	A	800	HEM	CHD-C1D-ND	5.94	129.52	124.58
8	A	573	OLC	C13-C12-C11	-5.84	111.88	117.97
4	A	800	HEM	C1A-CHA-C4D	-5.50	120.23	127.47
4	A	800	HEM	C4D-ND-C1D	4.94	110.22	105.16
4	A	800	HEM	CHA-C4D-ND	4.61	130.64	124.31
4	A	800	HEM	C2D-C1D-ND	-4.60	107.50	112.93
5	A	801	HAS	C3A-C4A-NA	4.34	112.69	109.41
5	A	801	HAS	C4D-ND-C1D	-4.20	101.23	106.76
5	A	801	HAS	C3D-C4D-ND	3.73	112.43	109.64
5	A	801	HAS	C2A-C1A-CHA	-3.21	119.92	126.00
5	A	801	HAS	C3A-C4A-CHD	-3.12	120.09	126.00
5	A	801	HAS	C2C-C3C-CAC	3.11	133.69	127.33
5	A	801	HAS	CHB-C1D-ND	-3.04	119.51	124.58
5	A	801	HAS	CHC-C1C-NC	-2.96	119.64	124.58
5	A	801	HAS	C4A-C3A-C2A	-2.89	104.98	107.00
5	A	801	HAS	C4C-NC-C1C	-2.85	103.00	106.76
5	A	801	HAS	C3C-C2C-C1C	2.78	108.62	107.00
4	A	800	HEM	C4A-CHB-C1B	-2.63	124.01	127.47
5	A	801	HAS	C2D-C1D-ND	2.57	111.14	108.64
4	A	800	HEM	CMA-C3A-C4A	-2.55	124.69	128.62
5	A	801	HAS	C4B-C3B-C2B	-2.52	105.10	106.87
5	A	801	HAS	C2B-C1B-NB	2.52	111.31	109.41
4	A	800	HEM	O2D-CGD-O1D	-2.46	117.03	123.30
5	A	801	HAS	C4D-CHA-C1A	-2.43	124.28	127.47
4	A	800	HEM	C2A-C1A-NA	-2.42	106.37	109.73
5	A	801	HAS	CHA-C1A-NA	2.31	128.44	124.58
8	A	567	OLC	C21-O20-C1	2.27	123.77	117.13
5	A	801	HAS	C4B-C3B-C11	2.21	128.65	124.67
8	A	575	OLC	C14-C13-C12	-2.15	109.64	114.46
8	B	170	OLC	O20-C21-C22	2.13	116.30	105.69
5	A	801	HAS	O2D-CGD-CBD	2.03	121.40	114.22
4	A	800	HEM	CHA-C1A-NA	2.03	127.96	124.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	554/569 (97%)	-0.12	24 (4%) 34 27	11, 21, 43, 67	0
2	B	166/168 (98%)	-0.27	3 (1%) 65 60	12, 22, 38, 53	0
3	C	31/34 (91%)	-0.55	0 100 100	16, 21, 31, 41	0
All	All	751/771 (97%)	-0.17	27 (3%) 41 33	11, 21, 42, 67	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	PRO	5.9
1	A	495	ARG	4.8
1	A	496	GLU	4.3
1	A	333	PHE	4.0
1	A	513	SER	4.0
1	A	517	ASP	4.0
1	A	516	GLU	3.6
2	B	6	LYS	3.5
1	A	330[A]	ARG	3.4
2	B	168	GLU	3.4
1	A	12	TYR	3.1
1	A	331	GLY	2.9
1	A	491	VAL	2.9
1	A	493	LEU	2.8
1	A	176	GLY	2.8
1	A	332	LEU	2.8
1	A	9	SER	2.6
1	A	492	LEU	2.5
1	A	499	PRO	2.4
2	B	3	ASP	2.4
1	A	175	PRO	2.3
1	A	518	ARG	2.2
1	A	552	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	526	ARG	2.1
1	A	520	LEU	2.1
1	A	514	GLY	2.1
1	A	494	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	OLC	C	35	14/25	0.32	38.73	77,78,79,79	0
8	OLC	A	570	17/25	0.27	27.75	63,65,74,74	0
8	OLC	A	573	20/25	0.24	24.45	59,63,64,64	0
8	OLC	A	565	25/25	0.25	13.82	66,70,79,80	0
8	OLC	A	576	16/25	0.33	12.72	67,70,72,72	0
8	OLC	B	169	25/25	0.20	11.95	56,59,61,62	0
8	OLC	B	172	21/25	0.21	10.44	59,61,65,66	0
8	OLC	A	566	25/25	0.23	9.71	54,64,73,73	0
8	OLC	A	569	18/25	0.25	9.05	56,61,70,70	0
8	OLC	A	564	25/25	0.24	9.02	37,46,64,65	0
8	OLC	A	577	25/25	0.21	7.74	52,55,58,59	0
8	OLC	A	572	15/25	0.41	7.57	54,59,65,65	0
8	OLC	B	171	25/25	0.22	6.23	59,61,66,67	0
8	OLC	A	574	25/25	0.17	5.87	53,56,57,57	0
8	OLC	A	571	8/25	0.25	5.15	59,61,63,64	0
8	OLC	A	575	21/25	0.23	5.12	57,63,71,72	0
8	OLC	A	578	12/25	0.33	3.75	74,76,77,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	OLC	B	170	25/25	0.27	3.24	60,65,68,69	0
8	OLC	A	567	23/25	0.14	2.40	28,36,54,55	0
8	OLC	A	568	25/25	0.31	1.60	74,75,83,83	0
7	PER	A	563	2/2	0.13	0.78	14,14,14,15	0
5	HAS	A	801	65/65	0.11	0.25	8,13,26,30	0
4	HEM	A	800	43/43	0.08	-0.32	6,11,14,20	0
9	CUA	B	802	2/2	0.06	-2.88	14,14,14,14	0
6	CU	A	803	1/1	0.07	-4.23	15,15,15,15	0

6.5 Other polymers

There are no such residues in this entry.