



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:07 PM GMT

PDB ID : 4GP5
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant Y133W from
Thermus thermophilus
Authors : Li, Y.; Chen, Y.; Stout, C.D.
Deposited on : 2012-08-20
Resolution : 2.70 Å(reported)

This is a full wwPDB 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>

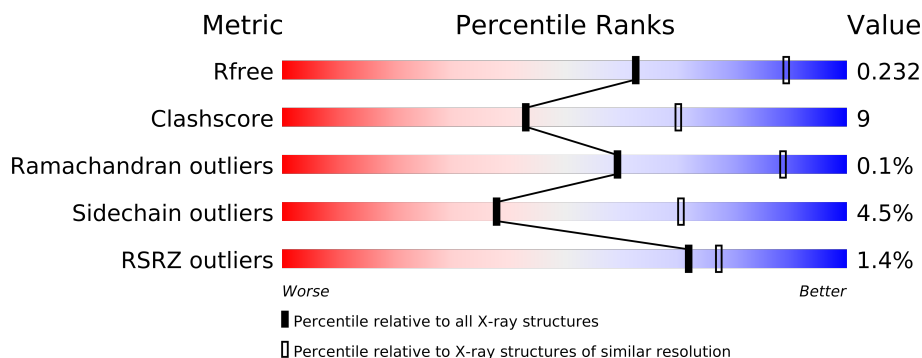
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	568	
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	605	-	X
8	OLC	A	606	-	X
8	OLC	A	607	-	X
8	OLC	A	608	-	X
8	OLC	A	609	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
8	OLC	A	610	-	X
8	OLC	A	611	-	X
8	OLC	A	612	-	X
8	OLC	A	613	-	X
8	OLC	A	614	-	X
8	OLC	B	202	-	X
8	OLC	B	203	-	X
8	OLC	B	204	-	X
8	OLC	B	205	-	X
8	OLC	C	101	-	X
8	OLC	C	102	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6429 atoms, of which 0 are 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	552	Total	C	N	O	S	0	4	0
			4377	2974	698	689	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP Q5SJ79
A	-4	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-3	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-2	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	0	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	133	TRP	TYR	engineered mutation	UNP Q5SJ79

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	1	0
			1288	837	214	233	4			

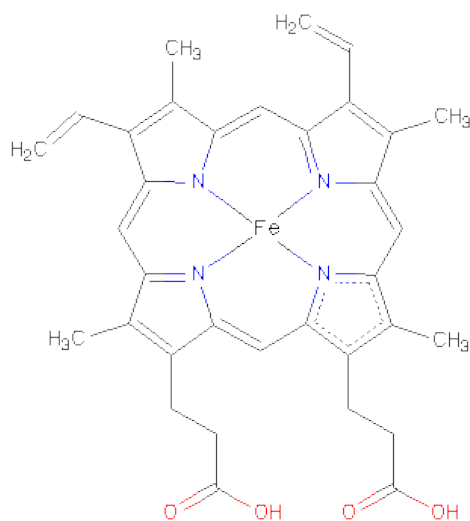
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

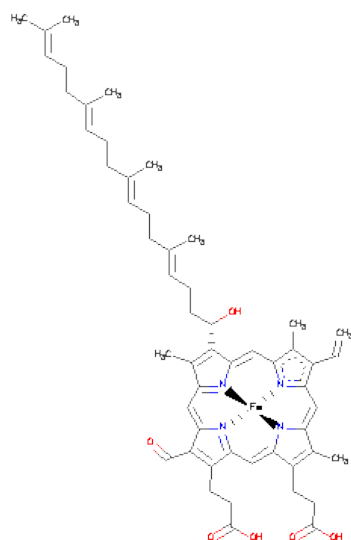
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



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

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



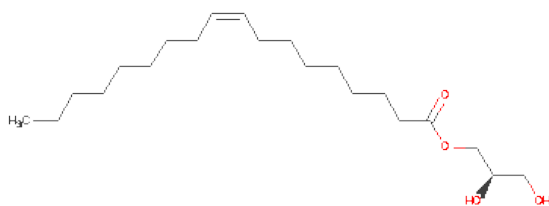
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
6	A	1	65	54	1	4	6	0	0

- 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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			23	19	4		
8	A	1	Total	C	O	0	0
			18	14	4		
8	A	1	Total	C	O	0	0
			17	13	4		
8	A	1	Total	C	O	0	0
			8	4	4		
8	A	1	Total	C	O	0	0
			15	11	4		
8	A	1	Total	C	O	0	0
			20	16	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			21	17	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			21	19	2		
8	C	1	Total	C	O	0	0
			25	21	4		
8	C	1	Total	C	O	0	0
			25	21	4		

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



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

- Molecule 10 is water.

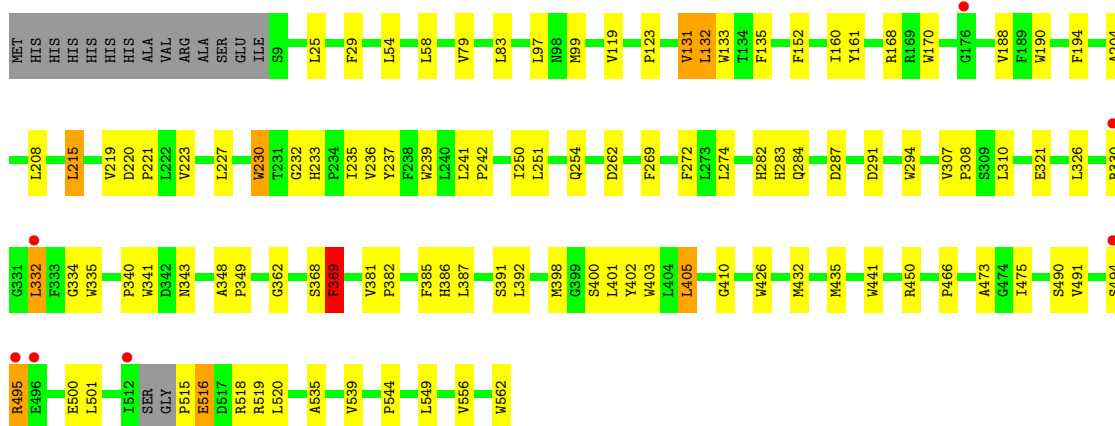
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	47	Total O 47 47	0	0
10	B	17	Total O 17 17	0	0
10	C	3	Total O 3 3	0	0

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.

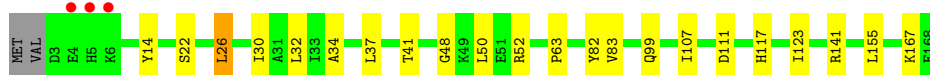
- Molecule 1: Cytochrome c oxidase subunit 1

Chain A: 



- Molecule 2: Cytochrome c oxidase subunit 2

Chain B: 



- Molecule 3: Cytochrome c oxidase polypeptide 2A

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.09Å 97.96Å 94.65Å 90.00° 127.99° 90.00°	Depositor
Resolution (Å)	74.60 – 2.70 56.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (74.60-2.70) 97.4 (56.78-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.173 , 0.230 0.176 , 0.232	Depositor DCC
R_{free} test set	1401 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 23.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 27874 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6429	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.83	2/4545 (0.0%)	0.80	3/6239 (0.0%)
2	B	0.88	0/1330	0.76	0/1817
3	C	0.88	0/247	0.85	1/335 (0.3%)
All	All	0.84	2/6122 (0.0%)	0.79	4/8391 (0.0%)

All (2) bond length outliers are listed below:

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

All (4) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 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	4377	0	4476	87	0
2	B	1288	0	1260	15	0
3	C	241	0	267	5	0
4	A	1	0	0	0	0
5	A	43	0	30	5	0
6	A	65	0	62	1	0
7	A	2	0	0	0	0
8	A	197	0	280	13	0
8	B	96	0	153	9	0
8	C	50	0	80	5	0
9	B	2	0	0	0	0
10	A	47	0	0	13	0
10	B	17	0	0	2	1
10	C	3	0	0	1	0
All	All	6429	0	6608	114	1

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 9.

All (114) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:HIS:NE2	1:A:237:TYR:HE2	0.87	1.36
1:A:233:HIS:NE2	1:A:237:TYR:CE2	1.78	1.32
8:A:607:OLC:H2	10:A:713:HOH:O	1.35	1.24
10:A:744:HOH:O	8:B:203:OLC:H17	1.45	1.16
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:HG2	0.94	1.07
1:A:330[B]:ARG:NH1	1:A:330[B]:ARG:HG2	1.64	1.03
1:A:168:ARG:HH22	8:A:610:OLC:H6A	1.24	1.03
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:CG	1.70	1.01
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.81	0.98
1:A:515:PRO:HA	1:A:516:GLU:HB2	1.44	0.95
8:B:204:OLC:H3	10:B:313:HOH:O	1.71	0.90
10:A:744:HOH:O	8:C:101:OLC:H11	1.86	0.76
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.63	0.76
3:C:4:LYS:HG3	3:C:6:LYS:HG2	1.70	0.72
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.76	0.71
1:A:133:TRP:CD1	10:A:709:HOH:O	2.46	0.67
1:A:168:ARG:NH2	8:A:610:OLC:H6A	2.06	0.66
1:A:381:VAL:HB	1:A:382:PRO:HD3	1.78	0.66
5:A:602:HEM:HBC2	5:A:602:HEM:HMC1	1.78	0.65
1:A:341:TRP:O	8:A:606:OLC:H24A	1.97	0.63
2:B:141:ARG:HH12	8:B:203:OLC:H22	1.63	0.63
1:A:161:TYR:CE2	8:A:609:OLC:H21	2.34	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:233:HIS:O	1:A:236:VAL:HG22	2.01	0.60
1:A:160:ILE:HG12	1:A:190:TRP:HB3	1.85	0.59
3:C:18:THR:HG23	8:C:102:OLC:H12	1.85	0.59
1:A:133:TRP:HD1	10:A:709:HOH:O	1.85	0.58
1:A:362:GLY:HA3	10:A:721:HOH:O	2.02	0.58
1:A:450:ARG:NH1	10:A:709:HOH:O	2.37	0.57
2:B:14:TYR:CD2	3:C:9:LEU:HD11	2.40	0.56
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.40	0.56
1:A:204:ALA:HA	1:A:208:LEU:HB2	1.89	0.55
8:A:606:OLC:H15	8:A:611:OLC:H12	1.89	0.55
1:A:562:TRP:HA	2:B:155:LEU:HG	1.88	0.54
8:B:204:OLC:H7	10:B:312:HOH:O	2.07	0.54
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.43	0.54
1:A:220:ASP:HB3	1:A:223:VAL:HG12	1.91	0.53
8:B:204:OLC:C10	10:C:201:HOH:O	2.57	0.53
10:A:744:HOH:O	8:C:101:OLC:C11	2.52	0.53
2:B:26:LEU:O	2:B:30:ILE:HG13	2.09	0.52
1:A:232:GLY:O	1:A:235:ILE:HG22	2.10	0.52
1:A:219:VAL:O	1:A:221:PRO:HD3	2.10	0.52
1:A:450:ARG:HB2	10:A:726:HOH:O	2.10	0.51
1:A:535:ALA:O	1:A:539:VAL:HG23	2.09	0.51
1:A:168:ARG:HH11	8:A:609:OLC:H22	1.75	0.51
1:A:400:SER:HA	1:A:403:TRP:NE1	2.26	0.51
1:A:307:VAL:N	1:A:308:PRO:HD2	2.25	0.51
1:A:168:ARG:NH2	8:A:610:OLC:H3A	2.26	0.51
1:A:385:PHE:CG	6:A:603:HAS:HMA2	2.46	0.50
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.94	0.50
2:B:141:ARG:NH2	8:B:203:OLC:O19	2.44	0.50
1:A:348:ALA:HB3	1:A:349:PRO:CD	2.42	0.50
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.99	0.50
1:A:432:MET:HE2	5:A:602:HEM:HAB	1.94	0.50
1:A:387:LEU:O	1:A:391:SER:HB3	2.12	0.49
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.46	0.49
10:A:744:HOH:O	8:C:101:OLC:C12	2.60	0.49
1:A:343:ASN:OD1	1:A:402[B]:TYR:CE2	2.66	0.49
1:A:426:TRP:CB	8:A:606:OLC:H3A	2.42	0.48
1:A:132:LEU:HB2	10:A:709:HOH:O	2.13	0.48
1:A:241:LEU:N	1:A:242:PRO:CD	2.76	0.48
1:A:79:VAL:HA	1:A:152:PHE:CZ	2.48	0.48
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.49	0.47
8:A:613:OLC:H11	8:A:613:OLC:H8	1.70	0.47
1:A:401:LEU:HG	1:A:405:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:168:ARG:HH11	8:A:609:OLC:C22	2.27	0.47
1:A:435:MET:HB2	1:A:473:ALA:HB1	1.97	0.47
1:A:251:LEU:HA	1:A:254:GLN:HG3	1.97	0.46
1:A:119:VAL:O	1:A:123:PRO:HD2	2.15	0.46
1:A:221:PRO:HD3	1:A:556:VAL:HG22	1.98	0.46
1:A:220:ASP:O	1:A:223:VAL:HG12	2.15	0.46
1:A:495:ARG:HH21	1:A:495:ARG:HA	1.81	0.46
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.85	0.45
1:A:432:MET:CE	5:A:602:HEM:HAB	2.47	0.45
10:A:744:HOH:O	8:C:101:OLC:H12A	2.17	0.45
1:A:310:LEU:HD13	2:B:22:SER:HB2	1.99	0.45
2:B:32:LEU:HD21	8:B:202:OLC:H7A	1.99	0.45
1:A:227:LEU:O	1:A:230:TRP:HB3	2.17	0.44
1:A:188:VAL:HG21	1:A:269:PHE:HB3	2.00	0.44
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.52	0.44
1:A:291:ASP:HA	2:B:48:GLY:HA3	2.00	0.44
1:A:168:ARG:NH1	8:A:609:OLC:H22	2.32	0.44
1:A:369:PHE:CD2	1:A:369:PHE:C	2.90	0.44
1:A:386:HIS:CE1	5:A:602:HEM:C1A	3.06	0.44
1:A:405:LEU:HD23	1:A:491:VAL:HG11	2.00	0.44
2:B:63:PRO:HB2	2:B:82:TYR:CG	2.53	0.44
1:A:386:HIS:CE1	5:A:602:HEM:NA	2.86	0.43
1:A:410:GLY:HA2	1:A:501:LEU:HB2	2.00	0.43
1:A:233:HIS:NE2	1:A:237:TYR:CZ	2.66	0.43
1:A:519:ARG:HB2	1:A:519:ARG:HE	1.63	0.43
1:A:29:PHE:CE1	1:A:401:LEU:CD1	3.02	0.42
2:B:83:VAL:HB	2:B:107:ILE:HG23	2.01	0.42
2:B:117:HIS:HD2	2:B:123:ILE:O	2.02	0.42
8:A:607:OLC:H4A	10:A:706:HOH:O	2.18	0.42
1:A:330[B]:ARG:NH1	1:A:330[B]:ARG:CG	2.42	0.42
1:A:215:LEU:HD12	1:A:215:LEU:HA	1.86	0.42
8:B:203:OLC:H6	3:C:33:ARG:HH11	1.84	0.42
1:A:284:GLN:HG2	1:A:287:ASP:OD1	2.19	0.42
2:B:34:ALA:O	2:B:37:LEU:HB2	2.20	0.42
1:A:398:MET:O	1:A:401:LEU:HB2	2.20	0.42
1:A:97:LEU:O	1:A:99:MET:HG3	2.19	0.41
1:A:272:PHE:CE1	1:A:308:PRO:HB2	2.55	0.41
2:B:41:THR:HG21	3:C:31:PHE:CE1	2.55	0.41
1:A:549:LEU:HD23	2:B:50:LEU:HD11	2.03	0.41
2:B:141:ARG:NH1	8:B:203:OLC:H22	2.33	0.41
1:A:441:TRP:CG	1:A:466:PRO:HG3	2.56	0.41
1:A:25:LEU:HA	1:A:25:LEU:HD23	1.90	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:254:GLN:O	1:A:340:PRO:HG2	2.21	0.40
1:A:250:ILE:HG22	1:A:254:GLN:HE21	1.86	0.40
1:A:230:TRP:C	1:A:230:TRP:CD1	2.95	0.40
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.56	0.40
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.97	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:B:303:HOH:O	10:B:303:HOH:O[2.554]	1.73	0.47

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/568 (97%)	525 (95%)	25 (4%)	1 (0%)	56	86
2	B	165/168 (98%)	161 (98%)	4 (2%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	745/770 (97%)	715 (96%)	29 (4%)	1 (0%)	59	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	448/462 (97%)	429 (96%)	19 (4%)	40	73
2	B	134/138 (97%)	129 (96%)	5 (4%)	45	78
3	C	24/27 (89%)	21 (88%)	3 (12%)	7	16
All	All	606/627 (97%)	579 (96%)	27 (4%)	38	70

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

Mol	Chain	Res	Type
1	A	54	LEU
1	A	58	LEU
1	A	132	LEU
1	A	215	LEU
1	A	230	TRP
1	A	262	ASP
1	A	274	LEU
1	A	326	LEU
1	A	332	LEU
1	A	369	PHE
1	A	405	LEU
1	A	475	ILE
1	A	490	SER
1	A	494	SER
1	A	495	ARG
1	A	500	GLU
1	A	516	GLU
1	A	518	ARG
1	A	520	LEU
2	B	26	LEU
2	B	52	ARG
2	B	99	GLN
2	B	111	ASP
2	B	167	LYS
3	C	13	LEU
3	C	20	LEU
3	C	24	LEU

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

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

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Mol	Chain	Res	Type
2	B	117	HIS

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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	HEM	A	602	1	49,50,50	8.46	26 (53%)	46,82,82	3.29	17 (36%)
6	HAS	A	603	1,7	72,72,72	2.65	25 (34%)	86,109,109	2.32	27 (31%)
7	PER	A	604	4,6	1,1,1	1.29	0	0,0,0	0.00	-
8	OLC	A	605	-	24,24,24	0.53	0	25,25,25	0.82	1 (4%)
8	OLC	A	606	-	22,22,24	1.02	1 (4%)	23,23,25	0.66	1 (4%)
8	OLC	A	607	-	16,17,24	0.66	0	17,18,25	0.59	0
8	OLC	A	608	-	15,16,24	0.87	1 (6%)	16,17,25	0.80	1 (6%)
8	OLC	A	609	-	6,7,24	0.31	0	5,7,25	0.72	0
8	OLC	A	610	-	14,14,24	1.66	1 (7%)	15,15,25	0.80	0
8	OLC	A	611	-	19,19,24	1.07	1 (5%)	20,20,25	1.29	2 (10%)
8	OLC	A	612	-	24,24,24	0.61	1 (4%)	25,25,25	0.99	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	OLC	A	613	-	20,20,24	1.10	1 (5%)	21,21,25	0.80	0
8	OLC	A	614	-	24,24,24	0.53	0	25,25,25	0.68	0
9	CUA	B	201	2	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	B	202	-	24,24,24	0.53	0	25,25,25	0.50	0
8	OLC	B	203	-	24,24,24	0.65	1 (4%)	25,25,25	1.10	2 (8%)
8	OLC	B	204	-	24,24,24	0.54	0	25,25,25	0.43	0
8	OLC	B	205	-	19,20,24	0.49	0	19,20,25	0.50	0
8	OLC	C	101	-	24,24,24	0.53	0	25,25,25	0.95	1 (4%)
8	OLC	C	102	-	24,24,24	0.44	0	25,25,25	0.56	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	-	0/14/114/114	0/0/8/8
6	HAS	A	603	1,7	-	0/36/82/82	0/0/8/8
7	PER	A	604	4,6	-	0/0/0/0	0/0/0/0
8	OLC	A	605	-	-	0/24/24/24	0/0/0/0
8	OLC	A	606	-	-	0/22/22/24	0/0/0/0
8	OLC	A	607	-	-	0/17/17/24	0/0/0/0
8	OLC	A	608	-	-	0/16/16/24	0/0/0/0
8	OLC	A	609	-	-	0/5/6/24	0/0/0/0
8	OLC	A	610	-	-	0/14/14/24	0/0/0/0
8	OLC	A	611	-	-	0/19/19/24	0/0/0/0
8	OLC	A	612	-	-	0/24/24/24	0/0/0/0
8	OLC	A	613	-	-	0/20/20/24	0/0/0/0
8	OLC	A	614	-	-	0/24/24/24	0/0/0/0
9	CUA	B	201	2	-	0/0/0/0	0/0/0/0
8	OLC	B	202	-	-	0/24/24/24	0/0/0/0
8	OLC	B	203	-	-	0/24/24/24	0/0/0/0
8	OLC	B	204	-	-	0/24/24/24	0/0/0/0
8	OLC	B	205	-	-	0/19/19/24	0/0/0/0
8	OLC	C	101	-	-	0/24/24/24	0/0/0/0
8	OLC	C	102	-	-	0/24/24/24	0/0/0/0

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	C2B-C1B	-43.86	1.33	1.44
5	A	602	HEM	C2D-C1D	24.21	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	C3D-C4D	21.13	1.49	1.44
5	A	602	HEM	CHB-C1B	10.86	1.51	1.35
5	A	602	HEM	C4A-C3A	9.42	1.51	1.40
6	A	603	HAS	C4A-C3A	8.13	1.50	1.40
5	A	602	HEM	FE-NB	7.53	2.25	1.97
6	A	603	HAS	C3C-CAC	-7.46	1.33	1.48
6	A	603	HAS	C2D-C1D	7.27	1.52	1.40
6	A	603	HAS	C4C-C3C	6.49	1.49	1.41
5	A	602	HEM	CHC-C1C	6.24	1.48	1.36
5	A	602	HEM	CHD-C4C	6.14	1.48	1.36
8	A	610	OLC	C8-C7	-5.87	1.52	1.55
6	A	603	HAS	C4D-ND	5.64	1.45	1.37
5	A	602	HEM	C3D-C2D	-5.50	1.34	1.43
6	A	603	HAS	C1D-ND	4.76	1.45	1.36
6	A	603	HAS	C3C-C2C	4.43	1.49	1.41
6	A	603	HAS	C2D-C3D	-4.43	1.33	1.41
6	A	603	HAS	C1C-C2C	-4.35	1.34	1.40
8	A	613	OLC	C14-C13	-4.33	1.53	1.55
8	A	611	OLC	C13-C12	-4.25	1.53	1.55
8	A	606	OLC	C16-C15	-4.20	1.53	1.55
5	A	602	HEM	C1A-NA	4.16	1.44	1.36
6	A	603	HAS	C4D-CHA	3.87	1.50	1.38
6	A	603	HAS	C4C-NC	3.81	1.42	1.37
5	A	602	HEM	CBB-CAB	3.76	1.50	1.28
6	A	603	HAS	C4C-CHD	3.54	1.49	1.38
6	A	603	HAS	C1C-CHC	3.45	1.49	1.39
5	A	602	HEM	C1A-CHA	3.36	1.49	1.39
6	A	603	HAS	C1D-CHB	3.23	1.48	1.39
5	A	602	HEM	C3B-C2B	3.17	1.49	1.43
5	A	602	HEM	CHA-C4D	-3.11	1.31	1.35
5	A	602	HEM	C4D-ND	-3.08	1.33	1.39
5	A	602	HEM	CHC-C4B	-3.06	1.32	1.39
5	A	602	HEM	C1A-C2A	3.03	1.48	1.43
5	A	602	HEM	C3C-CAC	3.03	1.49	1.40
6	A	603	HAS	CBC-CAC	3.01	1.51	1.28
6	A	603	HAS	O1D-CGD	2.99	1.32	1.22
6	A	603	HAS	C1A-C2A	2.92	1.48	1.43
5	A	602	HEM	C2C-C1C	-2.89	1.34	1.43
5	A	602	HEM	C1C-NC	-2.81	1.34	1.38
5	A	602	HEM	CHD-C1D	-2.79	1.32	1.39
5	A	602	HEM	C3B-C4B	2.76	1.47	1.44
5	A	602	HEM	FE-NC	2.65	2.07	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	C1B-NB	-2.63	1.33	1.37
6	A	603	HAS	C1A-CHA	-2.50	1.33	1.39
6	A	603	HAS	FE-NC	2.48	2.03	1.92
6	A	603	HAS	O2D-CGD	-2.46	1.21	1.30
6	A	603	HAS	FE-NB	2.45	2.02	1.92
8	B	203	OLC	O20-C1	2.45	1.40	1.33
5	A	602	HEM	C3B-CAB	-2.38	1.32	1.40
6	A	603	HAS	FE-NA	2.38	2.02	1.92
6	A	603	HAS	C1B-CHB	-2.20	1.31	1.38
8	A	612	OLC	O20-C1	2.18	1.40	1.33
5	A	602	HEM	C4A-CHB	-2.14	1.33	1.39
5	A	602	HEM	FE-NA	2.12	2.01	1.92
6	A	603	HAS	C4A-CHD	-2.09	1.34	1.39
8	A	608	OLC	O20-C1	2.08	1.39	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEM	C3B-C4B-NB	-14.59	103.56	114.00
6	A	603	HAS	C2C-C1C-NC	9.82	116.82	109.41
6	A	603	HAS	C4C-C3C-C2C	-8.83	100.70	106.87
5	A	602	HEM	C1B-NB-C4B	7.16	112.48	105.16
5	A	602	HEM	CHC-C4B-NB	6.88	130.30	124.58
6	A	603	HAS	C4D-ND-C1D	-5.24	99.86	106.76
5	A	602	HEM	C3A-C4A-NA	-4.77	105.81	109.41
8	A	611	OLC	C13-C12-C11	-4.61	113.17	117.97
6	A	603	HAS	C2A-C1A-CHA	-4.26	117.93	126.00
5	A	602	HEM	CHC-C1C-NC	-4.14	121.14	124.73
5	A	602	HEM	C1A-CHA-C4D	-4.03	122.17	127.47
6	A	603	HAS	C4B-C3B-C2B	-4.01	104.07	106.87
5	A	602	HEM	C4A-C3A-C2A	3.85	109.68	107.00
6	A	603	HAS	C3A-C4A-NA	3.74	112.23	109.41
5	A	602	HEM	CMA-C3A-C4A	-3.67	122.98	128.62
6	A	603	HAS	CHB-C1D-ND	-3.62	118.52	124.58
6	A	603	HAS	C2B-C1B-NB	3.61	112.13	109.41
5	A	602	HEM	C2D-C1D-ND	-3.51	108.78	112.93
8	B	203	OLC	C21-O20-C1	3.46	127.26	117.13
6	A	603	HAS	C4A-C3A-C2A	-3.36	104.66	107.00
6	A	603	HAS	CMC-C2C-C1C	-3.29	123.55	128.62
5	A	602	HEM	CHD-C1D-ND	3.24	127.28	124.58
6	A	603	HAS	C3B-C4B-NB	3.08	112.89	109.90
5	A	602	HEM	C4D-ND-C1D	3.00	108.23	105.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEM	C4A-CHB-C1B	-2.87	123.69	127.47
6	A	603	HAS	CHA-C1A-NA	2.87	129.37	124.58
6	A	603	HAS	C4B-C3B-C11	2.81	129.74	124.67
5	A	602	HEM	CBD-CAD-C3D	-2.78	108.31	114.37
6	A	603	HAS	C4A-NA-C1A	-2.77	103.12	106.76
6	A	603	HAS	C1D-C2D-C3D	-2.70	105.49	107.90
6	A	603	HAS	C2D-C1D-ND	2.69	111.26	108.64
6	A	603	HAS	C3A-C4A-CHD	-2.68	120.92	126.00
6	A	603	HAS	C3C-CAC-CBC	2.65	131.45	125.95
6	A	603	HAS	CMA-C3A-C4A	-2.64	124.56	128.62
8	C	101	OLC	C21-O20-C1	2.55	124.60	117.13
6	A	603	HAS	C1B-CHB-C1D	-2.51	124.16	127.47
8	A	612	OLC	C21-O20-C1	2.51	124.49	117.13
6	A	603	HAS	C4D-CHA-C1A	-2.49	124.19	127.47
8	B	203	OLC	O20-C21-C22	2.48	118.05	105.69
6	A	603	HAS	C4D-C3D-C2D	2.44	108.83	106.80
6	A	603	HAS	CHC-C1C-NC	-2.44	120.50	124.58
8	A	606	OLC	C21-O20-C1	2.42	124.23	117.13
5	A	602	HEM	O2D-CGD-CBD	2.39	122.67	114.22
5	A	602	HEM	O2A-CGA-O1A	-2.37	117.28	123.30
8	A	612	OLC	O20-C21-C22	2.29	117.09	105.69
5	A	602	HEM	C2A-C1A-NA	-2.27	106.58	109.73
8	A	611	OLC	O20-C21-C22	2.23	116.83	105.69
5	A	602	HEM	CHA-C4D-ND	2.23	127.37	124.31
8	A	605	OLC	O20-C21-C22	2.20	116.65	105.69
6	A	603	HAS	C2D-C1D-CHB	2.20	130.17	126.00
6	A	603	HAS	C2C-C1C-CHC	-2.18	121.87	126.00
8	A	608	OLC	C21-O20-C1	2.08	123.23	117.13
6	A	603	HAS	CAD-CBD-CGD	-2.03	106.94	113.47
6	A	603	HAS	C4C-NC-C1C	-2.01	104.12	106.76

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	552/568 (97%)	-0.45	7 (1%) 74 79	12, 24, 47, 74	0
2	B	166/168 (98%)	-0.43	3 (1%) 65 71	14, 25, 41, 68	0
3	C	31/34 (91%)	-0.67	0 100 100	19, 23, 40, 45	0
All	All	749/770 (97%)	-0.46	10 (1%) 72 79	12, 24, 45, 74	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	ARG	4.7
2	B	4	GLU	3.8
1	A	176	GLY	3.1
2	B	6	LYS	3.0
1	A	496	GLU	2.7
1	A	330[A]	ARG	2.5
1	A	494	SER	2.5
2	B	5	HIS	2.3
1	A	512	ILE	2.3
1	A	332	LEU	2.1

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	A	608	17/25	0.33	12.01	57,64,77,77	0
8	OLC	C	102	25/25	0.25	10.49	81,85,91,93	0
8	OLC	B	204	25/25	0.41	9.40	76,87,96,97	0
8	OLC	C	101	25/25	0.26	6.63	41,55,75,75	0
8	OLC	A	611	20/25	0.27	6.58	55,59,69,69	0
8	OLC	A	605	25/25	0.29	5.89	72,80,92,92	0
8	OLC	A	610	15/25	0.53	5.69	68,80,86,86	0
8	OLC	A	613	21/25	0.26	5.61	49,64,82,84	0
8	OLC	A	607	18/25	0.23	4.48	48,54,64,65	0
8	OLC	A	614	25/25	0.30	4.20	55,63,70,73	0
8	OLC	B	205	21/25	0.27	3.88	56,61,71,72	0
8	OLC	B	203	25/25	0.27	3.51	52,68,79,80	0
8	OLC	B	202	25/25	0.25	3.13	56,61,70,71	0
8	OLC	A	609	8/25	0.33	2.93	55,56,57,57	0
8	OLC	A	606	23/25	0.21	2.34	39,43,52,52	0
8	OLC	A	612	25/25	0.19	2.10	40,44,50,51	0
6	HAS	A	603	65/65	0.12	0.11	10,16,26,27	0
7	PER	A	604	2/2	0.10	-0.08	20,20,20,22	0
5	HEM	A	602	43/43	0.11	-0.11	10,15,19,26	0
4	CU	A	601	1/1	0.07	-1.45	19,19,19,19	0
9	CUA	B	201	2/2	0.07	-2.12	18,18,18,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.