



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:31 PM GMT

PDB ID : 4FAA  
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant A120F+A204F  
from *Thermus thermophilus*  
Authors : Li, Y.; Chen, Y.; Stout, C.D.  
Deposited on : 2012-05-21  
Resolution : 2.80 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  
<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

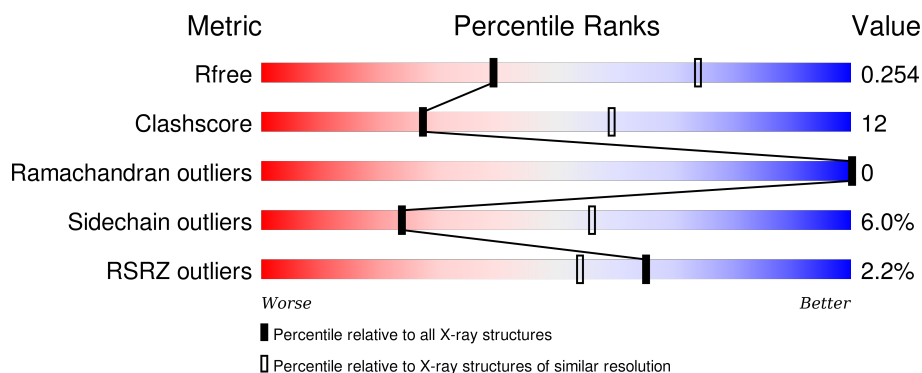
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

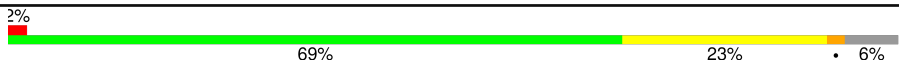
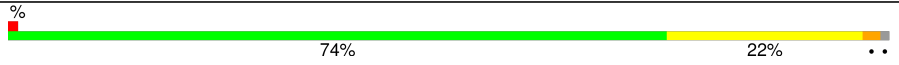

The reported resolution of this entry is 2.80 Å.

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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	568	
2	B	168	
3	C	34	

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
8	OLC	A	605	-	-	-	X
8	OLC	A	606	-	-	-	X
8	OLC	A	608	-	-	-	X
8	OLC	A	609	-	-	-	X
8	OLC	A	610	-	-	-	X
8	OLC	A	612	-	-	-	X
8	OLC	A	613	-	-	-	X
8	OLC	A	614	-	-	-	X
8	OLC	A	616	-	-	-	X
8	OLC	B	203	-	-	-	X
8	OLC	B	204	-	-	-	X
8	OLC	C	101	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6278 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	535	Total	C	N	O	S	0	0	0
			4203	2863	663	661	16			

There are 9 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	120	PHE	ALA	ENGINEERED MUTATION	UNP Q5SJ79
A	204	PHE	ALA	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
			1281	833	212	232	4			

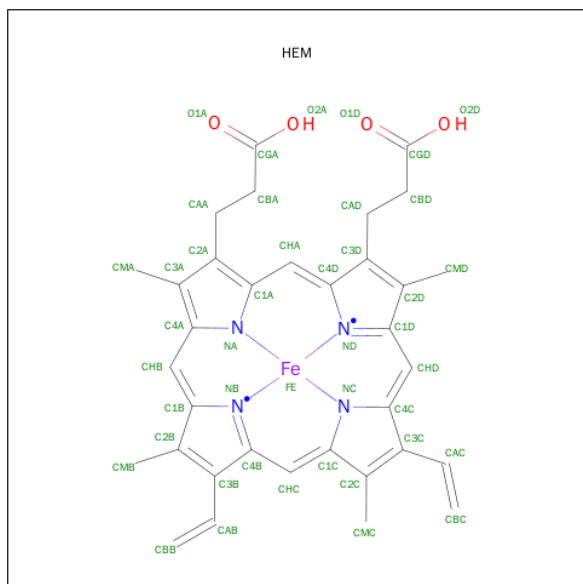
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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).

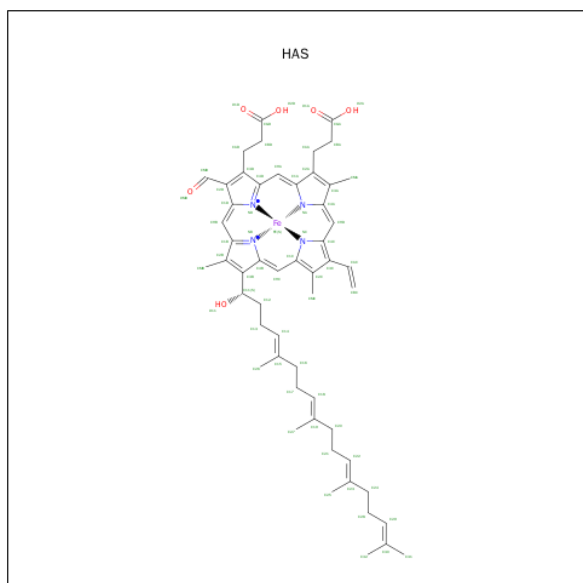
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cu 1 1	0	0

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



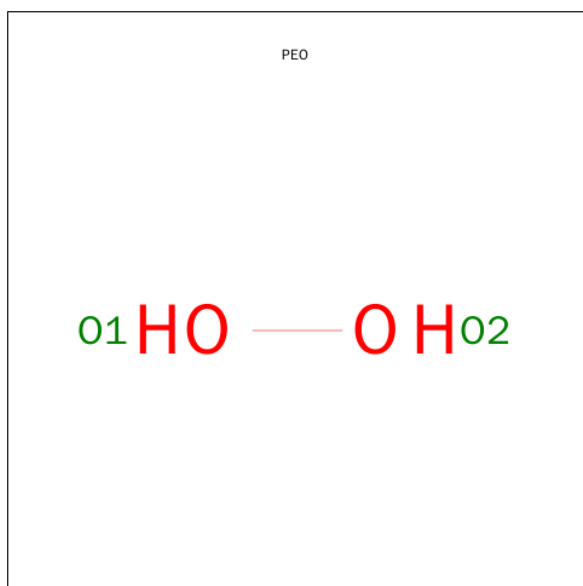
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Fe N O 43 34 1 4 4	0	0

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



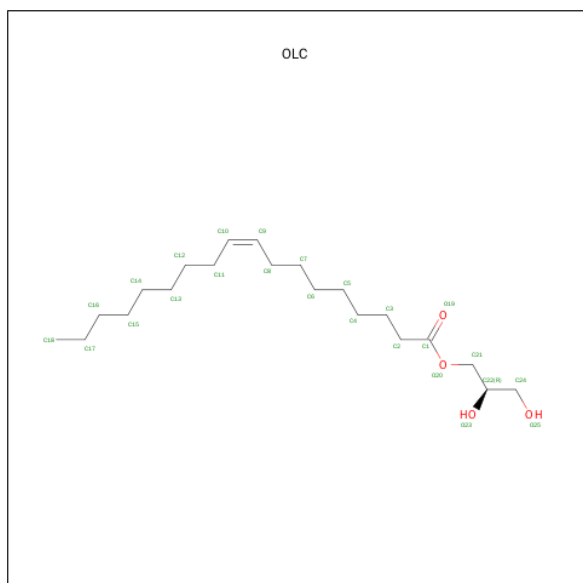
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 7 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula:  $\text{H}_2\text{O}_2$ ).



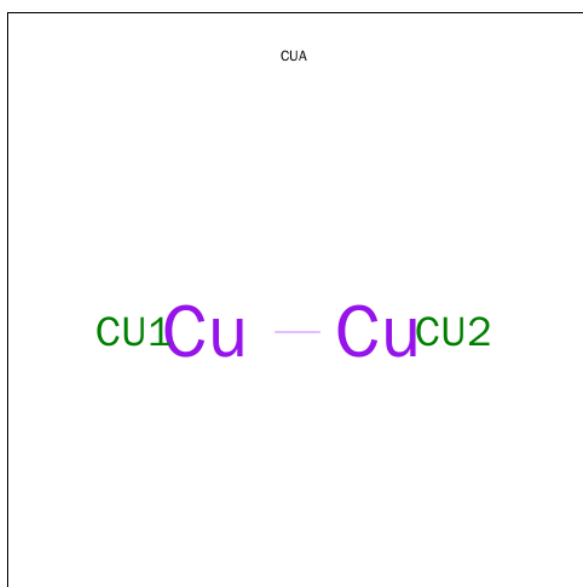
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			2	2		

- Molecule 8 is (2R)-2,3-DIHYDROXYPROPYL (9Z)-OCTADEC-9-ENOATE (three-letter code: OLC) (formula:  $\text{C}_{21}\text{H}_{40}\text{O}_4$ ).



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
			23	19	4		
8	A	1	Total	C	O	0	0
			21	19	2		
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	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 2 2	0	0

- Molecule 10 is water.

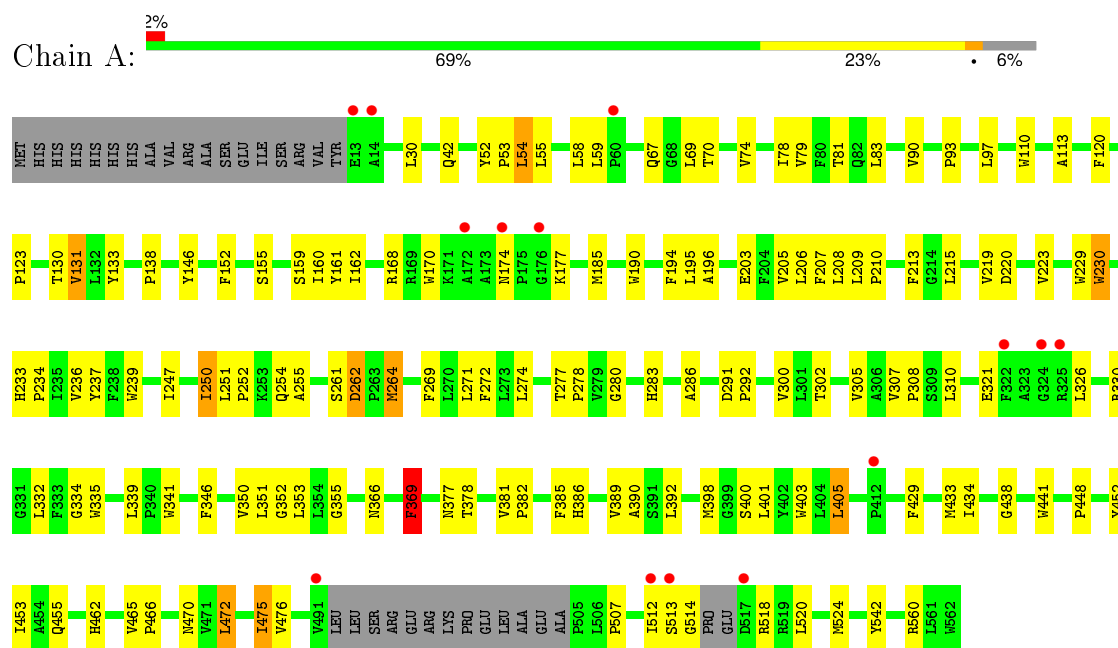
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	51	Total O 51 51	0	0
10	B	44	Total O 44 44	0	0
10	C	2	Total O 2 2	0	0



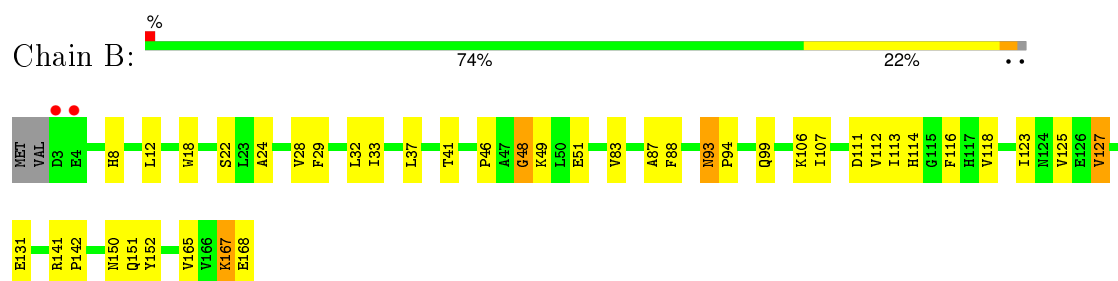
### 3 Residue-property plots [i](#)

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

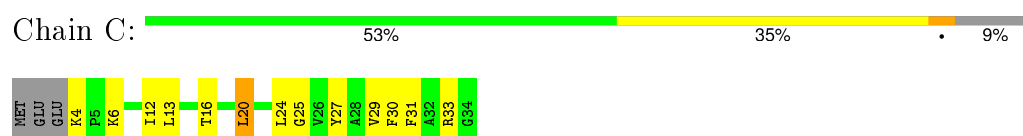
#### • Molecule 1: Cytochrome c oxidase subunit 1



#### • 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, $\alpha$ , $\beta$ , $\gamma$	143.28Å 98.29Å 95.05Å 90.00° 127.50° 90.00°	Depositor
Resolution (Å)	56.84 – 2.80 56.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (56.84-2.80) 97.3 (56.84-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 2011_01_25_1225)	Depositor
R, $R_{free}$	0.194 , 0.254 0.197 , 0.254	Depositor DCC
$R_{free}$ test set	1290 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 61.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 25172 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% 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, PEO, 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	0.50	0/4356	0.57	2/5982 (0.0%)
2	B	0.53	0/1317	0.58	0/1801
3	C	0.48	0/247	0.52	0/335
All	All	0.51	0/5920	0.57	2/8118 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	VAL	N-CA-C	-5.83	95.26	111.00
1	A	369	PHE	N-CA-CB	-5.34	100.98	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	48	GLY	Peptide

## 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	4203	0	4278	108	0
2	B	1281	0	1249	27	0
3	C	241	0	267	9	0
4	A	1	0	0	0	0
5	A	43	0	30	0	0
6	A	65	0	62	2	0
7	A	2	0	0	0	0
8	A	243	0	353	28	0
8	B	75	0	120	10	0
8	C	25	0	40	3	0
9	B	2	0	0	0	0
10	A	51	0	0	4	0
10	B	44	0	0	2	2
10	C	2	0	0	0	0
All	All	6278	0	6399	150	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 (150) 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:HE2	1.26	1.30
1:A:233:HIS:NE2	1:A:237:TYR:CE2	2.10	1.19
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.76	1.04
1:A:174:ASN:HB3	1:A:177:LYS:HD2	1.49	0.94
2:B:51:GLU:OE2	10:B:309:HOH:O	1.89	0.90
8:A:605:OLC:H11	8:B:203:OLC:H17	1.55	0.88
1:A:168:ARG:HH22	8:A:612:OLC:H6A	1.40	0.86
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.60	0.85
8:A:605:OLC:H12	8:B:203:OLC:H18	1.62	0.82
1:A:261:SER:HB3	1:A:264:MET:HB2	1.69	0.74
1:A:161:TYR:CZ	8:A:611:OLC:H24A	2.27	0.69
1:A:310:LEU:HD13	2:B:22:SER:HB2	1.75	0.69
8:B:203:OLC:H18A	8:C:101:OLC:H7A	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:TRP:CE3	1:A:283:HIS:CD2	2.81	0.68
8:A:605:OLC:H2A	8:C:101:OLC:H21A	1.76	0.68
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.76	0.66
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.31	0.65
1:A:381:VAL:HB	1:A:382:PRO:HD3	1.78	0.63
1:A:434:ILE:HG12	8:A:616:OLC:H18A	1.80	0.62
1:A:514:GLY:HA3	2:B:8:HIS:CD2	2.35	0.61
2:B:46:PRO:O	10:B:340:HOH:O	2.16	0.61
8:B:203:OLC:H7A	3:C:29:VAL:HG13	1.81	0.61
1:A:280:GLY:HA3	1:A:542:TYR:OH	2.00	0.61
1:A:74:VAL:O	1:A:79:VAL:HG23	2.02	0.59
1:A:160:ILE:HG12	1:A:190:TRP:HB3	1.86	0.58
8:A:605:OLC:H12	8:B:203:OLC:C18	2.34	0.57
1:A:67:GLN:HA	1:A:130:THR:HG23	1.87	0.56
2:B:29:PHE:O	2:B:33:ILE:HG13	2.05	0.56
1:A:209:LEU:HB2	1:A:210:PRO:HD3	1.88	0.56
2:B:32:LEU:HD21	8:B:202:OLC:H7A	1.85	0.56
1:A:462:HIS:HB2	10:A:725:HOH:O	2.06	0.56
1:A:250:ILE:HG23	1:A:507:PRO:HG2	1.88	0.56
8:B:203:OLC:H5A	3:C:33:ARG:HE	1.71	0.55
8:A:605:OLC:H6	3:C:25:GLY:HA3	1.88	0.55
3:C:16:THR:HG22	3:C:20:LEU:HD22	1.87	0.55
1:A:366:ASN:HB3	6:A:603:HAS:HBD2	1.89	0.55
8:A:605:OLC:C11	8:B:203:OLC:H17	2.34	0.55
1:A:278:PRO:HD3	10:A:718:HOH:O	2.05	0.55
1:A:152:PHE:O	1:A:155:SER:HB3	2.06	0.54
1:A:251:LEU:HB3	1:A:252:PRO:HD3	1.89	0.54
1:A:398:MET:O	1:A:401:LEU:HB2	2.07	0.54
8:A:606:OLC:H13A	8:A:614:OLC:H14A	1.90	0.54
1:A:261:SER:CB	1:A:264:MET:HB2	2.38	0.53
1:A:352:GLY:HA3	1:A:392:LEU:HA	1.90	0.53
1:A:378:THR:HA	1:A:448:PRO:HA	1.91	0.53
1:A:291:ASP:HB2	10:A:730:HOH:O	2.08	0.53
1:A:341:TRP:CE2	8:A:616:OLC:H3A	2.44	0.53
1:A:205:VAL:HG12	1:A:206:LEU:HD23	1.91	0.52
2:B:18:TRP:CE3	3:C:12:ILE:HD13	2.45	0.52
1:A:230:TRP:C	1:A:230:TRP:CD1	2.82	0.52
1:A:233:HIS:O	1:A:236:VAL:HG22	2.10	0.52
1:A:161:TYR:CE2	8:A:611:OLC:H21	2.45	0.52
2:B:41:THR:HG1	3:C:30:PHE:HE2	1.57	0.52
1:A:475:ILE:HD11	8:A:606:OLC:H12A	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TYR:N	1:A:53:PRO:HD2	2.26	0.51
2:B:107:ILE:HG22	2:B:127:VAL:HG11	1.92	0.51
1:A:55:LEU:HD11	1:A:59:LEU:HD12	1.93	0.50
1:A:400:SER:HA	1:A:403:TRP:NE1	2.26	0.50
1:A:233:HIS:HB3	1:A:234:PRO:CD	2.42	0.50
1:A:351:LEU:HB3	1:A:429:PHE:CD2	2.47	0.49
2:B:165:VAL:HG12	2:B:167:LYS:HD3	1.95	0.49
1:A:291:ASP:CB	10:A:730:HOH:O	2.60	0.49
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.48	0.49
1:A:353:LEU:N	1:A:392:LEU:HD23	2.27	0.49
1:A:330:ARG:O	1:A:334:GLY:HA3	2.13	0.49
1:A:196:ALA:HB1	1:A:234:PRO:CG	2.43	0.49
1:A:401:LEU:O	1:A:405:LEU:HB2	2.12	0.49
2:B:32:LEU:CD2	8:B:202:OLC:H7A	2.43	0.49
1:A:213:PHE:CD2	8:A:609:OLC:H4	2.48	0.49
1:A:254:GLN:NE2	1:A:507:PRO:HG3	2.28	0.48
1:A:386:HIS:HA	1:A:390:ALA:HB3	1.96	0.48
1:A:302:THR:HA	1:A:305:VAL:HG12	1.95	0.48
1:A:74:VAL:HA	1:A:78:ILE:HD12	1.95	0.48
1:A:476:VAL:HG22	8:A:606:OLC:H16A	1.96	0.47
1:A:254:GLN:HE22	1:A:507:PRO:HG3	1.79	0.47
1:A:159:SER:HA	1:A:162:ILE:HD12	1.96	0.47
1:A:352:GLY:C	1:A:392:LEU:HD23	2.35	0.47
8:A:605:OLC:O25	8:B:203:OLC:H7	2.15	0.46
2:B:113:ILE:HA	2:B:127:VAL:O	2.15	0.46
2:B:118:VAL:HB	2:B:123:ILE:HB	1.97	0.46
2:B:93:ASN:HA	2:B:94:PRO:HA	1.64	0.46
1:A:168:ARG:NH2	8:A:612:OLC:H6A	2.21	0.46
1:A:90:VAL:O	1:A:93:PRO:HG2	2.16	0.46
8:A:614:OLC:H5	8:A:614:OLC:H2A	1.54	0.45
2:B:111:ASP:OD2	2:B:112:VAL:N	2.37	0.45
8:A:605:OLC:H24A	3:C:29:VAL:HG22	1.99	0.45
1:A:341:TRP:CZ2	8:A:616:OLC:H3A	2.51	0.45
1:A:438:GLY:HA3	1:A:470:ASN:OD1	2.16	0.45
2:B:114:HIS:O	2:B:127:VAL:HG23	2.16	0.45
8:A:607:OLC:H15A	8:A:613:OLC:H12	1.99	0.45
1:A:247:ILE:O	1:A:252:PRO:HD3	2.16	0.45
1:A:300:VAL:HG11	8:A:608:OLC:H16A	1.98	0.45
1:A:441:TRP:HB3	1:A:466:PRO:HB3	1.99	0.45
8:C:101:OLC:H15	8:C:101:OLC:H18A	1.56	0.45
1:A:277:THR:N	1:A:278:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:PHE:CE1	1:A:350:VAL:HG21	2.52	0.44
1:A:70:THR:OG1	1:A:131:VAL:O	2.29	0.44
1:A:520:LEU:O	1:A:524:MET:HG3	2.18	0.44
1:A:292:PRO:HD3	2:B:48:GLY:CA	2.47	0.44
1:A:369:PHE:CD2	1:A:369:PHE:C	2.90	0.44
1:A:161:TYR:CE2	8:A:611:OLC:H24A	2.53	0.44
1:A:271:LEU:HA	1:A:271:LEU:HD23	1.71	0.44
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.52	0.43
1:A:277:THR:H	1:A:278:PRO:HD2	1.84	0.43
1:A:52:TYR:N	1:A:53:PRO:CD	2.81	0.43
2:B:87:ALA:HA	2:B:88:PHE:HA	1.60	0.43
1:A:120:PHE:O	1:A:123:PRO:HG2	2.18	0.43
8:A:606:OLC:H15A	8:A:606:OLC:H18B	1.65	0.43
8:A:616:OLC:H7	8:A:616:OLC:H4A	1.77	0.43
1:A:110:TRP:O	1:A:113:ALA:HB3	2.19	0.43
1:A:472:LEU:HD23	8:A:614:OLC:H8	2.00	0.43
1:A:254:GLN:NE2	1:A:507:PRO:CG	2.81	0.43
1:A:203:GLU:O	1:A:207:PHE:HB2	2.19	0.43
1:A:255:ALA:HB1	1:A:339:LEU:HD12	2.01	0.43
8:A:613:OLC:H5A	8:A:613:OLC:H2	1.74	0.43
2:B:24:ALA:O	2:B:28:VAL:HG23	2.19	0.43
1:A:138:PRO:HG2	2:B:111:ASP:O	2.19	0.42
2:B:99:GLN:OE1	2:B:142:PRO:HD3	2.19	0.42
1:A:220:ASP:O	1:A:223:VAL:HG12	2.20	0.42
1:A:262:ASP:C	1:A:262:ASP:OD2	2.57	0.42
1:A:512:ILE:HG23	2:B:8:HIS:HB2	2.00	0.42
1:A:465:VAL:N	1:A:466:PRO:HD2	2.35	0.42
1:A:185:MET:HG2	1:A:269:PHE:CG	2.55	0.42
1:A:54:LEU:HD22	1:A:54:LEU:O	2.20	0.42
1:A:286:ALA:HB1	2:B:125:VAL:HA	2.02	0.42
3:C:20:LEU:HD12	3:C:20:LEU:HA	1.89	0.42
1:A:146:TYR:CD2	1:A:208:LEU:HB3	2.55	0.42
1:A:81:THR:HB	1:A:239:TRP:CD1	2.55	0.42
1:A:307:VAL:N	1:A:308:PRO:HD2	2.34	0.42
3:C:27:TYR:CE2	3:C:31:PHE:HE2	2.37	0.42
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.54	0.42
1:A:272:PHE:CE1	1:A:308:PRO:HB2	2.55	0.41
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.55	0.41
1:A:453:ILE:C	1:A:455:GLN:N	2.73	0.41
1:A:389:VAL:HB	6:A:603:HAS:HBC2	2.01	0.41
1:A:185:MET:HG2	1:A:269:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:VAL:HG11	2:B:116:PHE:CE1	2.55	0.41
8:A:613:OLC:H6	8:A:613:OLC:H9	1.76	0.41
1:A:377:ASN:O	2:B:150:ASN:HB2	2.20	0.41
1:A:233:HIS:NE2	1:A:237:TYR:CZ	2.73	0.41
1:A:277:THR:N	1:A:278:PRO:CD	2.83	0.41
1:A:250:ILE:HD12	1:A:403:TRP:CH2	2.55	0.41
1:A:230:TRP:C	1:A:230:TRP:HD1	2.22	0.41
1:A:42:GLN:HE22	1:A:69:LEU:HA	1.85	0.41
2:B:51:GLU:N	2:B:131:GLU:OE2	2.52	0.41
1:A:42:GLN:NE2	1:A:69:LEU:HA	2.35	0.41
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.86	0.40
1:A:207:PHE:CD1	1:A:219:VAL:HG13	2.56	0.40
1:A:355:GLY:HA3	1:A:433:MET:HE1	2.03	0.40
2:B:151:GLN:O	2:B:152:TYR:C	2.59	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:330:HOH:O	10:B:330:HOH:O[2_554]	1.94	0.26
10:B:308:HOH:O	10:B:324:HOH:O[2_554]	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	529/568 (93%)	489 (92%)	40 (8%)	0	100	100
2	B	164/168 (98%)	154 (94%)	10 (6%)	0	100	100
3	C	29/34 (85%)	24 (83%)	5 (17%)	0	100	100
All	All	722/770 (94%)	667 (92%)	55 (8%)	0	100	100



There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	428/464 (92%)	407 (95%)	21 (5%)	31	65
2	B	132/138 (96%)	123 (93%)	9 (7%)	20	49
3	C	24/27 (89%)	19 (79%)	5 (21%)	1	4
All	All	584/629 (93%)	549 (94%)	35 (6%)	24	56

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	54	LEU
1	A	58	LEU
1	A	133	TYR
1	A	195	LEU
1	A	215	LEU
1	A	230	TRP
1	A	250	ILE
1	A	262	ASP
1	A	264	MET
1	A	274	LEU
1	A	326	LEU
1	A	332	LEU
1	A	369	PHE
1	A	405	LEU
1	A	452	TYR
1	A	472	LEU
1	A	475	ILE
1	A	513	SER
1	A	518	ARG
1	A	560	ARG
2	B	12	LEU
2	B	37	LEU

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Mol	Chain	Res	Type
2	B	49	LYS
2	B	93	ASN
2	B	106	LYS
2	B	127	VAL
2	B	141	ARG
2	B	167	LYS
2	B	168	GLU
3	C	4	LYS
3	C	6	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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	122	ASN
2	B	157	HIS

### 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	$\# Z  > 2$
5	HEM	A	602	1	30,50,50	3.96	13 (43%)	24,82,82	2.42	12 (50%)
6	HAS	A	603	1,7	45,72,72	2.69	12 (26%)	47,109,109	1.15	4 (8%)
7	PEO	A	604	4,6	1,1,1	0.59	0	0,0,0	0.00	-
8	OLC	A	605	-	24,24,24	0.47	0	25,25,25	0.83	0
8	OLC	A	606	-	24,24,24	0.47	0	25,25,25	0.87	0
8	OLC	A	607	-	22,22,24	0.53	0	23,23,25	0.52	0
8	OLC	A	608	-	20,20,24	0.55	0	20,20,25	0.63	0
8	OLC	A	609	-	17,17,24	0.63	0	18,18,25	0.76	0
8	OLC	A	610	-	16,16,24	0.74	1 (6%)	17,17,25	0.92	1 (5%)
8	OLC	A	611	-	7,7,24	0.57	0	6,7,25	0.18	0
8	OLC	A	612	-	14,14,24	0.54	0	15,15,25	0.80	1 (6%)
8	OLC	A	613	-	19,19,24	0.65	1 (5%)	19,20,25	0.78	0
8	OLC	A	614	-	24,24,24	0.55	1 (4%)	25,25,25	0.81	1 (4%)
8	OLC	A	615	-	20,20,24	0.50	0	20,21,25	0.75	0
8	OLC	A	616	-	24,24,24	0.54	1 (4%)	25,25,25	0.64	0
9	CUA	B	201	2	0,1,1	0.00	-	0,0,0	0.00	-
8	OLC	B	202	-	24,24,24	0.61	1 (4%)	25,25,25	0.76	1 (4%)
8	OLC	B	203	-	24,24,24	0.55	1 (4%)	25,25,25	0.92	1 (4%)
8	OLC	B	204	-	24,24,24	0.48	0	25,25,25	0.67	0
8	OLC	C	101	-	24,24,24	0.51	0	25,25,25	0.59	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	-	0/10/54/54	0/0/8/8
6	HAS	A	603	1,7	-	0/30/82/82	0/0/8/8
7	PEO	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	-	-	0/24/24/24	0/0/0/0
8	OLC	A	607	-	-	0/22/22/24	0/0/0/0
8	OLC	A	608	-	-	0/19/19/24	0/0/0/0
8	OLC	A	609	-	-	0/17/17/24	0/0/0/0
8	OLC	A	610	-	-	0/16/16/24	0/0/0/0
8	OLC	A	611	-	-	0/6/6/24	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	A	612	-	-	0/14/14/24	0/0/0/0
8	OLC	A	613	-	-	0/19/19/24	0/0/0/0
8	OLC	A	614	-	-	0/24/24/24	0/0/0/0
8	OLC	A	615	-	-	0/20/20/24	0/0/0/0
8	OLC	A	616	-	-	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	C	101	-	-	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)
5	A	602	HEM	C2C-C1C	-10.31	1.33	1.52
5	A	602	HEM	C3B-CAB	-10.28	1.32	1.51
6	A	603	HAS	C3C-CAC	-6.97	1.32	1.47
5	A	602	HEM	C2D-C3D	-6.96	1.33	1.54
5	A	602	HEM	C2B-C1B	-5.35	1.34	1.51
6	A	603	HAS	C2D-C3D	-5.06	1.33	1.40
5	A	602	HEM	C3B-C4B	-3.16	1.49	1.51
5	A	602	HEM	C4A-CHB	-2.67	1.32	1.39
6	A	603	HAS	C1A-CHA	-2.62	1.32	1.39
6	A	603	HAS	C4A-CHD	-2.56	1.32	1.39
6	A	603	HAS	C2A-C3A	-2.15	1.31	1.37
6	A	603	HAS	C3B-C2B	-2.11	1.33	1.41
5	A	602	HEM	CHC-C4B	-2.07	1.33	1.38
8	A	616	OLC	O20-C1	2.00	1.39	1.33
8	B	203	OLC	O20-C1	2.11	1.39	1.33
8	A	610	OLC	O20-C1	2.12	1.39	1.33
8	A	613	OLC	O20-C1	2.15	1.39	1.33
8	A	614	OLC	O20-C1	2.15	1.39	1.33
8	B	202	OLC	O20-C1	2.18	1.39	1.33
5	A	602	HEM	FE-NC	2.49	2.05	1.95
6	A	603	HAS	CBC-CAC	3.12	1.51	1.28
6	A	603	HAS	C1D-CHB	3.83	1.50	1.39
5	A	602	HEM	CBB-CAB	3.89	1.51	1.29
6	A	603	HAS	C1C-CHC	3.93	1.50	1.39
5	A	602	HEM	C1A-CHA	4.17	1.51	1.39
5	A	602	HEM	CHC-C1C	5.59	1.49	1.36
5	A	602	HEM	CHD-C4C	5.76	1.49	1.36
6	A	603	HAS	C4C-NC	6.63	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	FE-NB	6.68	2.32	1.97
6	A	603	HAS	C4D-ND	8.22	1.47	1.36
6	A	603	HAS	C3C-C2C	8.29	1.51	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEM	C3B-CAB-CBB	-3.78	118.66	124.46
5	A	602	HEM	C3B-C4B-NB	-3.52	104.90	111.63
6	A	603	HAS	CAD-CBD-CGD	-2.82	107.57	112.75
5	A	602	HEM	C3C-CAC-CBC	-2.74	120.26	124.46
5	A	602	HEM	CBA-CAA-C2A	-2.51	108.03	112.53
6	A	603	HAS	CMC-C2C-C1C	-2.30	124.56	128.36
6	A	603	HAS	C21-C22-C23	-2.19	123.01	127.76
6	A	603	HAS	CAA-CBA-CGA	-2.17	108.77	112.75
5	A	602	HEM	CMA-C3A-C4A	-2.10	124.88	128.36
8	A	614	OLC	C21-O20-C1	2.02	122.49	116.85
8	A	612	OLC	C21-O20-C1	2.05	122.58	116.85
5	A	602	HEM	CHC-C4B-NB	2.39	130.27	124.52
8	B	202	OLC	C21-O20-C1	2.43	123.64	116.85
5	A	602	HEM	C2D-C3D-C4D	2.46	105.67	101.50
8	A	610	OLC	C21-O20-C1	2.55	123.97	116.85
5	A	602	HEM	CMD-C2D-C3D	2.58	125.78	114.35
8	B	203	OLC	C21-O20-C1	2.98	125.19	116.85
5	A	602	HEM	CMB-C2B-C3B	3.35	124.88	116.53
5	A	602	HEM	CMC-C2C-C3C	3.65	125.65	116.53
5	A	602	HEM	CAD-C3D-C4D	4.14	127.07	112.47
5	A	602	HEM	CAD-C3D-C2D	4.79	127.00	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	HAS	2	0
8	A	605	OLC	8	0
8	A	606	OLC	4	0
8	A	607	OLC	1	0
8	A	608	OLC	1	0
8	A	609	OLC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	611	OLC	3	0
8	A	612	OLC	2	0
8	A	613	OLC	3	0
8	A	614	OLC	3	0
8	A	616	OLC	4	0
8	B	202	OLC	2	0
8	B	203	OLC	8	0
8	C	101	OLC	3	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	535/568 (94%)	-0.32	14 (2%) 59 47	21, 29, 49, 77	1 (0%)
2	B	166/168 (98%)	-0.38	2 (1%) 81 73	22, 30, 46, 68	0
3	C	31/34 (91%)	-0.59	0 100 100	23, 28, 37, 49	0
All	All	732/770 (95%)	-0.35	16 (2%) 65 54	21, 29, 48, 77	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	SER	4.7
1	A	322	PHE	3.7
1	A	60	PRO	3.2
1	A	14	ALA	3.1
1	A	412	PRO	3.0
1	A	13	GLU	3.0
1	A	172	ALA	2.8
1	A	512	ILE	2.8
1	A	176	GLY	2.8
1	A	517	ASP	2.7
1	A	324	GLY	2.7
1	A	491	VAL	2.6
2	B	3	ASP	2.6
2	B	4	GLU	2.3
1	A	174	ASN	2.2
1	A	325	ARG	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, 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	B	204	25/25	0.76	0.30	7.32	35,46,73,78	0
8	OLC	A	613	20/25	0.73	0.33	6.28	39,49,65,66	0
8	OLC	A	608	21/25	0.76	0.30	6.00	38,50,58,66	0
8	OLC	A	610	17/25	0.64	0.31	5.72	39,50,74,74	0
8	OLC	C	101	25/25	0.80	0.24	4.84	39,61,77,81	0
8	OLC	A	605	25/25	0.82	0.26	3.17	27,44,64,71	0
8	OLC	A	616	25/25	0.82	0.29	3.14	38,49,56,58	0
8	OLC	A	612	15/25	0.80	0.54	2.89	47,59,73,74	0
8	OLC	B	203	25/25	0.69	0.31	2.88	41,53,74,85	0
8	OLC	A	614	25/25	0.82	0.25	2.76	38,45,54,61	0
8	OLC	A	606	25/25	0.77	0.26	2.74	34,43,82,92	0
8	OLC	A	609	18/25	0.83	0.23	2.07	30,47,69,69	0
8	OLC	B	202	25/25	0.81	0.22	1.79	31,39,56,62	0
8	OLC	A	607	23/25	0.88	0.21	1.12	34,40,53,56	0
8	OLC	A	615	21/25	0.82	0.25	1.00	39,51,65,73	0
6	HAS	A	603	65/65	0.96	0.16	0.43	17,23,34,39	0
5	HEM	A	602	43/43	0.96	0.14	-0.36	18,23,26,31	0
7	PEO	A	604	2/2	0.99	0.12	-1.09	19,19,19,25	0
9	CUA	B	201	2/2	0.99	0.11	-1.49	21,21,21,24	0
8	OLC	A	611	8/25	0.88	0.27	-	45,47,54,57	0
4	CU	A	601	1/1	0.99	0.12	-	25,25,25,25	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.