



Full wwPDB X-ray Structure Validation Report

Sep 29, 2014 – 09:13 PM EDT

PDB ID : 4N4Y
Title : Structure of Recombinant Cytochrome ba3 Oxidase mutant G232V from *Thermus thermophilus*
Authors : Li, Y.; Chen, Y.; Stout, C.D.
Deposited on : 2013-10-08
Resolution : 2.90 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>

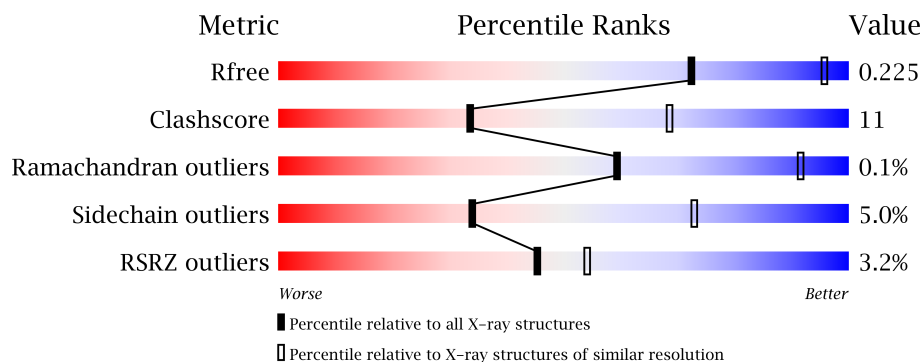
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23828
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) : stable23828

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	607	-	X
8	OLC	A	608	-	X
8	OLC	A	609	-	X
8	OLC	A	610	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
8	OLC	A	611	-	X
8	OLC	A	612	-	X
8	OLC	A	613	-	X
8	OLC	A	614	-	X
8	OLC	A	615	-	X
8	OLC	B	202	-	X
8	OLC	B	203	-	X
8	OLC	B	204	-	X
8	OLC	C	101	-	X
8	OLC	C	102	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6549 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	551	Total	C	N	O	S	0	4	0
			4371	2970	696	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	232	VAL	GLY	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			

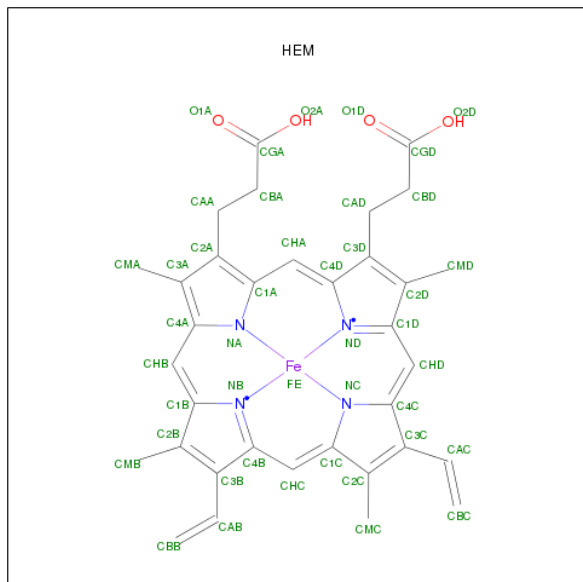
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

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).

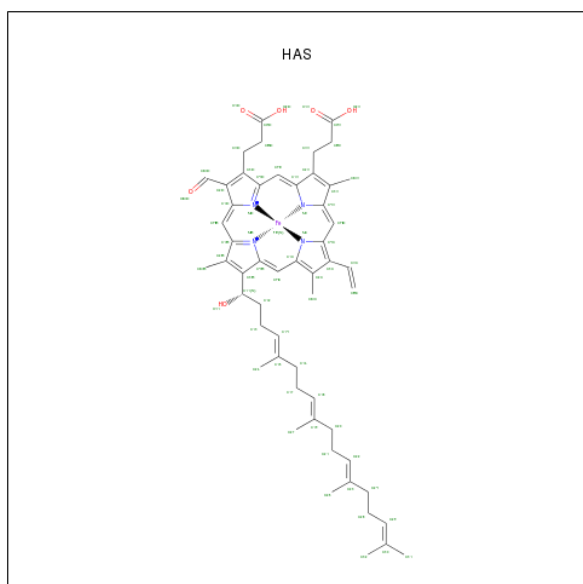
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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



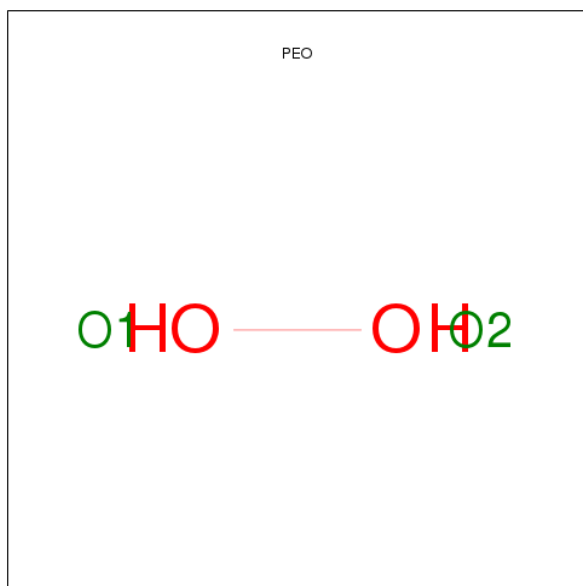
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is HEME-AS (three-letter code: HAS) (formula: $\text{C}_{54}\text{H}_{64}\text{FeN}_4\text{O}_6$).



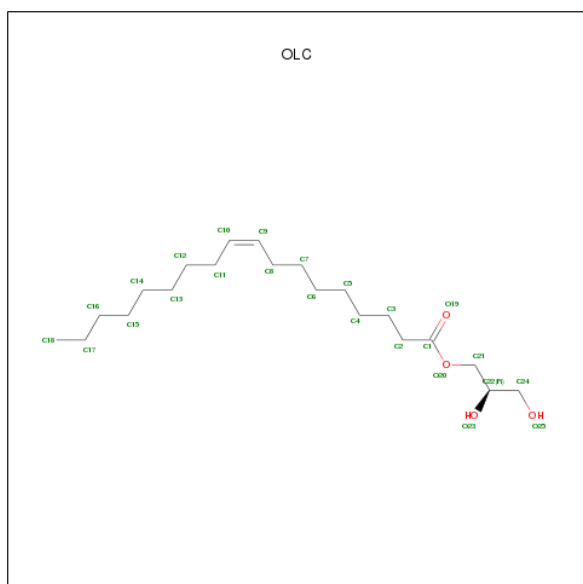
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 7 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_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: $\text{C}_{21}\text{H}_{40}\text{O}_4$).



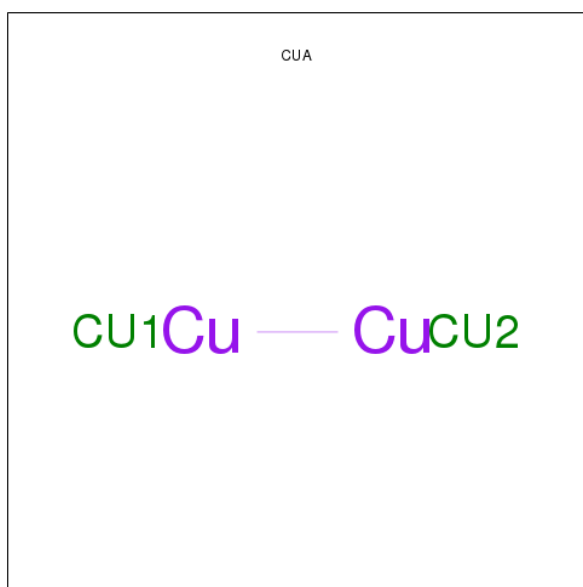
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			25	21	4		

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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
			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		
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 2	Cu 2	0	0

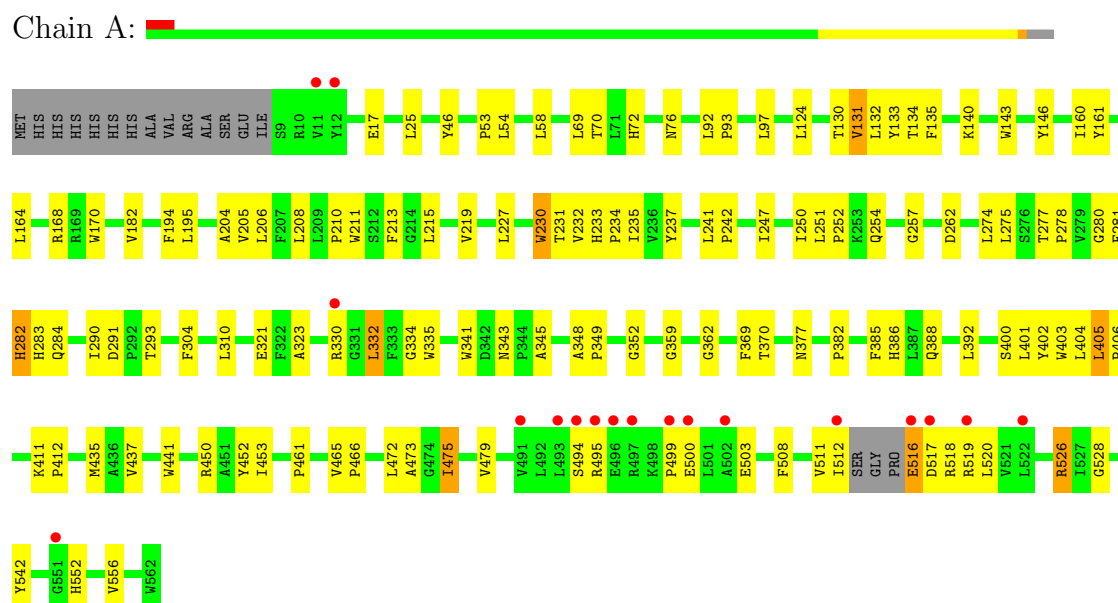
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	118	Total 118	O 118	0	0
10	B	72	Total 72	O 72	0	0
10	C	3	Total 3	O 3	0	0

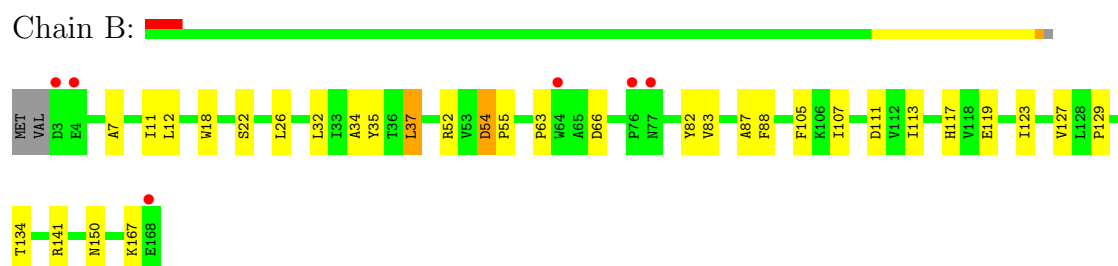
3 Residue-property plots

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



• 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	144.15Å 98.40Å 114.10Å 90.00° 138.93° 90.00°	Depositor
Resolution (Å)	74.96 – 2.90 49.20 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (74.96-2.90) 98.5 (49.20-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.177 , 0.225 0.179 , 0.225	Depositor DCC
R_{free} test set	1191 reflections (5.46%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 23015 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6549	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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, 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	0.78	0/4537	0.77	2/6228 (0.0%)
2	B	0.80	0/1330	0.74	1/1817 (0.1%)
3	C	0.84	0/247	0.82	1/335 (0.3%)
All	All	0.79	0/6114	0.77	4/8380 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	VAL	N-CA-C	-6.50	93.46	111.00
2	B	54	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	332	LEU	CA-CB-CG	5.27	127.43	115.30
3	C	13	LEU	CA-CB-CG	5.27	127.43	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	4371	0	4473	110	0
2	B	1288	0	1260	21	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	241	0	267	3	0
4	A	1	0	0	0	0
5	A	43	0	30	6	0
6	A	65	0	62	1	0
7	A	2	0	0	0	0
8	A	218	0	313	23	0
8	B	75	0	120	8	0
8	C	50	0	80	5	0
9	B	2	0	0	0	0
10	A	118	0	0	6	1
10	B	72	0	0	2	1
10	C	3	0	0	0	0
All	All	6549	0	6605	142	2

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 11.

All (142) 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	1.34
1:A:233:HIS:NE2	1:A:237:TYR:CE2	1.79	1.26
1:A:168:ARG:HH22	8:A:611:OLC:H6A	1.18	1.05
1:A:330[B]:ARG:NH1	1:A:330[B]:ARG:HG2	1.61	1.04
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:CG	1.73	1.01
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:HG2	0.83	1.00
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.85	0.94
8:A:606:OLC:H11	8:A:613:OLC:H14	1.57	0.84
1:A:168:ARG:NH2	8:A:611:OLC:H6A	1.98	0.78
1:A:168:ARG:HH22	8:A:611:OLC:C6	1.97	0.77
1:A:516:GLU:OE2	1:A:517:ASP:N	2.18	0.76
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.67	0.74
8:A:606:OLC:H13A	8:A:613:OLC:H12	1.70	0.74
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.74	0.73
1:A:17:GLU:OE2	10:A:732:HOH:O	2.07	0.72
8:A:613:OLC:H13A	8:A:613:OLC:H8	1.71	0.72
1:A:46:TYR:HA	1:A:453:ILE:HD11	1.73	0.69
1:A:400:SER:HA	1:A:403:TRP:NE1	2.08	0.68
10:A:714:HOH:O	8:B:203:OLC:H8A	1.96	0.66
2:B:35:TYR:CE2	8:B:202:OLC:H2A	2.34	0.63
1:A:511:VAL:HG12	1:A:512:ILE:O	1.98	0.63
8:A:606:OLC:H13	8:A:612:OLC:H12	1.78	0.63
1:A:168:ARG:HH21	8:A:611:OLC:H3A	1.63	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:231:THR:O	1:A:234:PRO:HG2	1.99	0.62
5:A:602:HEM:CMC	5:A:602:HEM:HBC2	2.31	0.61
1:A:526:ARG:NH2	10:A:785:HOH:O	2.33	0.61
1:A:359:GLY:HA3	1:A:388:GLN:OE1	2.01	0.60
1:A:499:PRO:O	1:A:503:GLU:HG3	2.01	0.60
1:A:131:VAL:HB	1:A:135:PHE:HA	1.85	0.58
1:A:168:ARG:NH2	8:A:611:OLC:H3A	2.19	0.57
8:B:203:OLC:H7	8:C:101:OLC:O25	2.05	0.56
1:A:310:LEU:HD13	2:B:22:SER:HB2	1.87	0.56
1:A:204:ALA:HA	1:A:208:LEU:HB2	1.87	0.55
1:A:280:GLY:HA3	1:A:542:TYR:OH	2.05	0.55
1:A:76:ASN:HB3	5:A:602:HEM:CAC	2.36	0.55
8:A:613:OLC:H8	8:A:613:OLC:C13	2.36	0.55
1:A:552:HIS:HB3	2:B:52:ARG:NH1	2.22	0.55
1:A:281:PHE:O	1:A:283:HIS:N	2.39	0.54
1:A:461:PRO:HA	10:A:726:HOH:O	2.06	0.54
1:A:72:HIS:O	1:A:76:ASN:HB2	2.07	0.54
1:A:341:TRP:CE2	8:A:615:OLC:H3	2.43	0.54
1:A:281:PHE:C	1:A:283:HIS:N	2.62	0.54
1:A:400:SER:HA	1:A:403:TRP:CD1	2.44	0.53
2:B:35:TYR:CZ	8:B:202:OLC:H2A	2.43	0.53
2:B:18:TRP:CE3	3:C:12:ILE:HD13	2.44	0.53
8:C:101:OLC:H2A	8:C:102:OLC:H21A	1.91	0.52
1:A:435:MET:HB2	1:A:473:ALA:HB1	1.91	0.52
1:A:281:PHE:C	1:A:283:HIS:H	2.13	0.52
1:A:131:VAL:HG21	1:A:135:PHE:HB3	1.91	0.52
1:A:251:LEU:HB3	1:A:252:PRO:HD3	1.92	0.51
1:A:25:LEU:HD11	1:A:404:LEU:HD23	1.92	0.51
3:C:4:LYS:HG3	3:C:6:LYS:HG2	1.92	0.51
1:A:277:THR:N	1:A:278:PRO:HD2	2.26	0.51
1:A:472:LEU:HD22	8:A:613:OLC:H11	1.93	0.50
1:A:232:VAL:HG13	1:A:235:ILE:HG21	1.93	0.50
1:A:352:GLY:C	1:A:392[A]:LEU:HD23	2.31	0.50
1:A:168:ARG:NH1	8:A:610:OLC:O23	2.44	0.50
1:A:343:ASN:OD1	1:A:402[B]:TYR:CE2	2.65	0.50
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.93	0.50
5:A:602:HEM:HBC2	5:A:602:HEM:HMC2	1.94	0.50
1:A:516:GLU:CD	1:A:517:ASP:N	2.65	0.50
2:B:32:LEU:HD21	8:B:202:OLC:H7A	1.92	0.50
1:A:241:LEU:N	1:A:242:PRO:CD	2.75	0.50
1:A:69:LEU:HD11	5:A:602:HEM:HBD2	1.94	0.50
8:B:203:OLC:H10	8:C:102:OLC:H24	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:247:ILE:O	1:A:252:PRO:HD3	2.12	0.49
1:A:70:THR:OG1	1:A:131:VAL:O	2.23	0.49
1:A:341:TRP:CZ2	8:A:615:OLC:H3	2.47	0.49
1:A:146:TYR:CD1	1:A:208:LEU:HD13	2.47	0.49
1:A:140:LYS:HE3	1:A:211:TRP:CE2	2.48	0.49
1:A:275:LEU:HD13	1:A:304:PHE:HB3	1.95	0.48
1:A:330[B]:ARG:NH1	1:A:330[B]:ARG:CG	2.46	0.48
1:A:386:HIS:CE1	5:A:602:HEM:C1A	3.01	0.48
1:A:132:LEU:C	1:A:134:THR:H	2.17	0.48
2:B:7:ALA:O	2:B:11:ILE:HG13	2.14	0.47
1:A:130:THR:HG22	1:A:130:THR:O	2.14	0.47
1:A:134:THR:O	1:A:135:PHE:C	2.53	0.47
1:A:362:GLY:HA3	10:A:748:HOH:O	2.14	0.47
2:B:113:ILE:HG23	2:B:127:VAL:O	2.15	0.47
1:A:53:PRO:HD3	10:A:801:HOH:O	2.14	0.46
2:B:35:TYR:OH	8:B:202:OLC:H24A	2.15	0.46
1:A:386:HIS:HE1	5:A:602:HEM:C1A	2.34	0.46
1:A:232:VAL:HG12	1:A:232:VAL:O	2.16	0.46
2:B:141:ARG:NH2	8:B:203:OLC:O19	2.49	0.46
1:A:348:ALA:N	1:A:349:PRO:HD2	2.31	0.45
1:A:132:LEU:C	1:A:134:THR:N	2.69	0.45
1:A:227:LEU:O	1:A:230:TRP:HB3	2.17	0.45
1:A:161:TYR:CE2	8:A:610:OLC:H21	2.51	0.45
1:A:556:VAL:HG21	2:B:129:PRO:HB2	1.99	0.45
6:A:603:HAS:HBC1	6:A:603:HAS:HMC1	1.97	0.45
2:B:119:GLU:HB3	10:B:347:HOH:O	2.17	0.45
1:A:400:SER:O	1:A:404:LEU:N	2.46	0.45
2:B:117:HIS:HD2	2:B:123:ILE:O	1.99	0.45
1:A:517:ASP:OD1	1:A:519:ARG:HG2	2.17	0.45
1:A:230:TRP:C	1:A:230:TRP:CD1	2.91	0.44
1:A:293:THR:HG23	8:A:607:OLC:H8	1.99	0.44
1:A:377:ASN:HB3	2:B:150:ASN:O	2.17	0.44
1:A:341:TRP:HB3	8:A:606:OLC:H24A	1.98	0.44
1:A:528:GLY:HA2	8:A:611:OLC:H2	1.99	0.44
2:B:105:PHE:O	2:B:134:THR:HA	2.17	0.44
1:A:479:VAL:HG21	8:A:605:OLC:H17A	2.00	0.43
1:A:291:ASP:OD2	1:A:293:THR:HB	2.18	0.43
2:B:63:PRO:HB2	2:B:82:TYR:CD2	2.53	0.43
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.53	0.43
1:A:475:ILE:HD11	8:A:605:OLC:H15	2.00	0.43
1:A:277:THR:H	1:A:278:PRO:HD2	1.84	0.43
2:B:34:ALA:HA	2:B:37:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:281:PHE:O	1:A:284:GLN:N	2.27	0.43
1:A:25:LEU:HA	1:A:25:LEU:HD23	1.87	0.43
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.54	0.42
1:A:250:ILE:HD13	1:A:403:TRP:CH2	2.54	0.42
1:A:411:LYS:HA	1:A:412:PRO:HD3	1.96	0.42
1:A:257:GLY:HA3	1:A:323:ALA:HB2	2.01	0.42
1:A:277:THR:N	1:A:278:PRO:CD	2.82	0.42
1:A:450:ARG:HB2	10:B:345:HOH:O	2.19	0.42
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.55	0.42
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.80	0.42
8:A:607:OLC:H4A	2:B:37:LEU:HG	2.02	0.42
1:A:401:LEU:O	1:A:405:LEU:HB2	2.20	0.42
1:A:92:LEU:N	1:A:93:PRO:HD2	2.34	0.42
2:B:54:ASP:HA	2:B:55:PRO:HD2	1.83	0.42
1:A:182:VAL:HG21	1:A:508:PHE:CE1	2.55	0.41
1:A:465:VAL:HB	1:A:466:PRO:HD3	2.02	0.41
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.89	0.41
3:C:25:GLY:HA3	8:C:101:OLC:H6	2.03	0.41
1:A:210:PRO:HD3	8:A:614:OLC:H11A	2.01	0.41
1:A:143:TRP:HB2	1:A:213:PHE:CE1	2.55	0.41
1:A:97:LEU:HD22	1:A:170:TRP:CD1	2.56	0.41
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.78	0.41
1:A:251:LEU:HA	1:A:254:GLN:HG3	2.03	0.41
2:B:83:VAL:HB	2:B:107:ILE:HG23	2.02	0.41
1:A:437:VAL:HG22	8:C:101:OLC:H15A	2.03	0.41
8:A:606:OLC:H11	8:A:613:OLC:C14	2.39	0.41
1:A:205:VAL:HG12	1:A:206:LEU:HD23	2.02	0.40
1:A:211:TRP:CG	1:A:219:VAL:HG23	2.56	0.40
1:A:519:ARG:HB3	1:A:519:ARG:CZ	2.50	0.40
2:B:87:ALA:HA	2:B:88:PHE:HA	1.79	0.40
1:A:140:LYS:HE3	1:A:211:TRP:NE1	2.35	0.40
1:A:345:ALA:HB2	1:A:402[B]:TYR:HB3	2.03	0.40
1:A:405:LEU:CB	1:A:406:PRO:HD3	2.51	0.40
1:A:441:TRP:HB3	1:A:466:PRO:HB3	2.03	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	Distance(Å)	Clash(Å)
10:B:317:HOH:O	10:B:340:HOH:O[2_656]	2.06	0.14
2:B:66:ASP:OD2	10:A:716:HOH:O[2_656]	2.13	0.07

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	550/568 (97%)	519 (94%)	30 (6%)	1 (0%)	56	89
2	B	165/168 (98%)	163 (99%)	2 (1%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	744/770 (97%)	711 (96%)	32 (4%)	1 (0%)	59	91

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	HIS

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	448/463 (97%)	426 (95%)	22 (5%)	35	73
2	B	134/138 (97%)	129 (96%)	5 (4%)	45	84
3	C	24/27 (89%)	21 (88%)	3 (12%)	7	19
All	All	606/628 (96%)	576 (95%)	30 (5%)	34	73

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

Mol	Chain	Res	Type
1	A	54	LEU
1	A	58	LEU
1	A	133	TYR
1	A	215	LEU

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Mol	Chain	Res	Type
1	A	230	TRP
1	A	262	ASP
1	A	274	LEU
1	A	282	HIS
1	A	290	ILE
1	A	332	LEU
1	A	369	PHE
1	A	370	THR
1	A	405	LEU
1	A	452	TYR
1	A	475	ILE
1	A	494	SER
1	A	495	ARG
1	A	500	GLU
1	A	516	GLU
1	A	518	ARG
1	A	520	LEU
1	A	526	ARG
2	B	12	LEU
2	B	26	LEU
2	B	37	LEU
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	446	ASN
2	B	69	GLN
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	42,50,50	4.27	21 (50%)	27,82,82	1.55	6 (22%)
6	HAS	A	603	1,7	66,72,72	2.72	20 (30%)	66,109,109	2.57	18 (27%)
7	PEO	A	604	4,6	1,1,1	0.56	0	0,0,0	0.00	-
8	OLC	A	605	-	24,24,24	0.47	0	25,25,25	0.64	0
8	OLC	A	606	-	22,22,24	1.61	1 (4%)	23,23,25	0.83	1 (4%)
8	OLC	A	607	-	19,20,24	0.55	0	19,20,25	0.45	0
8	OLC	A	608	-	16,17,24	0.65	0	17,18,25	0.64	0
8	OLC	A	609	-	15,16,24	0.72	0	16,17,25	0.92	1 (6%)
8	OLC	A	610	-	6,7,24	0.54	0	5,7,25	0.87	0
8	OLC	A	611	-	14,14,24	1.66	1 (7%)	15,15,25	0.64	0
8	OLC	A	612	-	19,19,24	1.14	1 (5%)	20,20,25	1.34	1 (5%)
8	OLC	A	613	-	24,24,24	0.63	1 (4%)	25,25,25	1.07	3 (12%)
8	OLC	A	614	-	20,20,24	1.51	1 (5%)	21,21,25	0.69	0
8	OLC	A	615	-	24,24,24	0.51	0	25,25,25	0.70	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	0.77	0
8	OLC	B	203	-	24,24,24	0.73	1 (4%)	25,25,25	1.10	2 (8%)
8	OLC	B	204	-	24,24,24	0.47	0	25,25,25	0.72	0
8	OLC	C	101	-	24,24,24	0.48	0	25,25,25	0.83	1 (4%)
8	OLC	C	102	-	24,24,24	0.55	0	25,25,25	0.60	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	-	0/40/122/122	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	-	-	0/22/22/24	0/0/0/0
8	OLC	A	607	-	-	0/19/19/24	0/0/0/0
8	OLC	A	608	-	-	0/17/17/24	0/0/0/0
8	OLC	A	609	-	-	0/16/16/24	0/0/0/0
8	OLC	A	610	-	-	0/5/6/24	0/0/0/0
8	OLC	A	611	-	-	0/14/14/24	0/0/0/0
8	OLC	A	612	-	-	0/19/19/24	0/0/0/0
8	OLC	A	613	-	-	0/24/24/24	0/0/0/0
8	OLC	A	614	-	-	0/20/20/24	0/0/0/0
8	OLC	A	615	-	-	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
8	OLC	C	102	-	-	0/24/24/24	0/0/0/0

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEM	C1B-C2B	-15.52	1.33	1.45
5	A	602	HEM	C3C-C4C	-14.40	1.34	1.45
6	A	603	HAS	C3C-C2C	8.28	1.50	1.40
8	A	606	OLC	C16-C15	-7.11	1.52	1.55
6	A	603	HAS	CHB-C1B	-7.01	1.31	1.41
6	A	603	HAS	C3C-CAC	-6.59	1.33	1.47
8	A	614	OLC	C14-C13	-6.31	1.52	1.55
6	A	603	HAS	C3C-C4C	6.11	1.48	1.40
5	A	602	HEM	CHC-C4B	-6.06	1.32	1.39
8	A	611	OLC	C8-C7	-5.84	1.52	1.55
6	A	603	HAS	C1D-ND	5.83	1.48	1.33
5	A	602	HEM	FE-NB	5.71	2.16	1.95
6	A	603	HAS	CHB-C1D	5.56	1.48	1.41
6	A	603	HAS	C4D-ND	5.52	1.47	1.33
5	A	602	HEM	C1A-NA	5.30	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	HAS	C1A-C2A	4.60	1.50	1.43
6	A	603	HAS	C4C-NC	4.58	1.44	1.36
6	A	603	HAS	C4D-C3D	4.53	1.51	1.43
8	A	612	OLC	C13-C12	-4.52	1.53	1.55
6	A	603	HAS	C1C-C2C	-4.45	1.37	1.43
6	A	603	HAS	C4B-C3B	4.27	1.50	1.43
5	A	602	HEM	C3C-C2C	4.27	1.48	1.45
5	A	602	HEM	C3B-C2B	4.26	1.49	1.45
5	A	602	HEM	C1C-C2C	-4.23	1.32	1.43
5	A	602	HEM	C1A-C2A	4.13	1.50	1.43
5	A	602	HEM	CMD-C2D	4.09	1.52	1.45
5	A	602	HEM	C4A-C3A	3.94	1.49	1.43
5	A	602	HEM	CBB-CAB	3.90	1.51	1.29
5	A	602	HEM	CMC-C2C	3.89	1.51	1.45
5	A	602	HEM	CMB-C2B	3.69	1.51	1.45
6	A	603	HAS	C4A-C3A	3.61	1.49	1.43
5	A	602	HEM	C3D-C2D	-3.44	1.34	1.43
6	A	603	HAS	O1D-CGD	3.20	1.33	1.22
6	A	603	HAS	CBC-CAC	3.04	1.51	1.28
5	A	602	HEM	C1D-C2D	3.01	1.51	1.43
6	A	603	HAS	C1D-C2D	3.00	1.50	1.44
6	A	603	HAS	C1B-C2B	2.78	1.48	1.43
5	A	602	HEM	FE-NC	2.73	2.06	1.95
6	A	603	HAS	C11-C3B	2.71	1.54	1.50
5	A	602	HEM	C3C-CAC	2.62	1.49	1.40
6	A	603	HAS	C2A-C3A	-2.62	1.29	1.37
8	B	203	OLC	O20-C1	2.55	1.41	1.33
6	A	603	HAS	O2D-CGD	-2.41	1.22	1.30
8	A	613	OLC	O20-C1	2.39	1.40	1.33
5	A	602	HEM	C4D-C3D	2.35	1.49	1.43
5	A	602	HEM	FE-ND	2.30	2.05	1.95
5	A	602	HEM	C3B-CAB	-2.26	1.33	1.40
8	B	202	OLC	O20-C1	2.23	1.40	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C2C-C1C-NC	8.85	115.41	109.50
6	A	603	HAS	C3D-C4D-ND	6.74	111.68	109.67
6	A	603	HAS	C3B-C4B-NB	6.31	111.55	109.67
6	A	603	HAS	C3A-C4A-NA	6.27	113.69	109.50
6	A	603	HAS	C2D-C1D-ND	5.60	111.34	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	603	HAS	C2B-C1B-NB	5.57	111.33	109.67
6	A	603	HAS	C4C-C3C-C2C	-5.23	100.20	105.61
8	A	612	OLC	C13-C12-C11	-4.90	112.86	117.97
6	A	603	HAS	C4A-NA-C1A	-4.23	102.66	107.93
6	A	603	HAS	C4A-C3A-C2A	-4.19	104.08	107.00
5	A	602	HEM	CMA-C3A-C4A	-4.17	122.05	128.46
8	B	203	OLC	C21-O20-C1	3.97	128.33	116.99
6	A	603	HAS	C25-C23-C24	3.20	120.25	115.39
8	A	613	OLC	C21-O20-C1	3.18	126.06	116.99
5	A	602	HEM	CAD-C3D-C4D	-3.10	121.24	125.60
6	A	603	HAS	CAD-CBD-CGD	-3.06	107.76	113.53
6	A	603	HAS	C2C-C3C-CAC	3.02	133.50	127.33
8	A	609	OLC	C21-O20-C1	3.01	125.57	116.99
6	A	603	HAS	CAA-CBA-CGA	-2.99	103.92	113.66
6	A	603	HAS	C12-C11-C3B	2.78	118.13	113.58
6	A	603	HAS	C3C-CAC-CBC	2.76	131.68	125.95
5	A	602	HEM	CBA-CAA-C2A	-2.65	108.21	112.63
8	C	101	OLC	C21-O20-C1	2.56	124.29	116.99
8	A	606	OLC	C21-O20-C1	2.52	124.18	116.99
6	A	603	HAS	C4C-NC-C1C	-2.49	104.83	107.93
8	B	203	OLC	O20-C21-C22	2.44	119.46	106.10
5	A	602	HEM	C4A-C3A-C2A	2.42	108.68	107.00
8	A	613	OLC	O20-C1-O19	2.27	129.40	123.48
5	A	602	HEM	CMA-C3A-C2A	2.18	129.05	124.94
6	A	603	HAS	C24-C23-C22	-2.15	116.94	121.06
6	A	603	HAS	O1A-CGA-CBA	-2.10	115.94	123.06
5	A	602	HEM	O2A-CGA-O1A	-2.09	118.01	123.31
8	A	613	OLC	O20-C21-C22	2.04	117.27	106.10

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	551/568 (97%)	-0.35	18 (3%) 44 53	14, 26, 50, 80	0
2	B	166/168 (98%)	-0.18	6 (3%) 41 48	16, 27, 41, 65	0
3	C	31/34 (91%)	-0.53	0 100 100	19, 25, 38, 44	0
All	All	748/770 (97%)	-0.32	24 (3%) 45 54	14, 26, 46, 80	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	496	GLU	5.5
1	A	495	ARG	5.4
1	A	493	LEU	4.1
1	A	494	SER	3.8
1	A	517	ASP	3.7
2	B	4	GLU	3.5
1	A	11	VAL	3.3
1	A	12	TYR	3.2
1	A	499	PRO	2.9
1	A	512	ILE	2.8
2	B	76	PRO	2.7
1	A	330[A]	ARG	2.7
1	A	522	LEU	2.6
2	B	168	GLU	2.5
1	A	516	GLU	2.4
1	A	551	GLY	2.4
1	A	502	ALA	2.4
2	B	64	TRP	2.4
1	A	497	ARG	2.3
2	B	77	ASN	2.2
1	A	519	ARG	2.1
2	B	3	ASP	2.1
1	A	500	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	491	VAL	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	102	25/25	0.46	15.24	82,91,98,98	0
8	OLC	A	615	25/25	0.34	10.04	57,60,68,69	0
8	OLC	A	611	15/25	0.60	9.29	51,68,81,81	0
8	OLC	A	609	17/25	0.38	8.10	61,66,77,80	0
8	OLC	C	101	25/25	0.34	8.06	54,56,77,78	0
8	OLC	A	612	20/25	0.31	7.91	60,62,70,72	0
8	OLC	A	605	25/25	0.34	5.68	60,68,81,81	0
8	OLC	A	607	21/25	0.29	4.75	49,55,70,70	0
8	OLC	B	204	25/25	0.33	4.72	61,69,72,76	0
8	OLC	A	613	25/25	0.36	4.66	54,58,61,62	0
8	OLC	B	202	25/25	0.30	4.44	57,59,62,63	0
8	OLC	A	608	18/25	0.28	4.16	47,60,71,71	0
8	OLC	A	614	21/25	0.41	3.78	57,63,78,78	0
8	OLC	B	203	25/25	0.33	2.43	52,67,78,79	0
8	OLC	A	610	8/25	0.30	2.30	55,56,59,60	0
8	OLC	A	606	23/25	0.22	1.48	35,41,46,47	0
6	HAS	A	603	65/65	0.13	0.20	13,19,23,29	0
5	HEM	A	602	43/43	0.12	-0.42	7,14,17,20	0
9	CUA	B	201	2/2	0.08	-1.60	19,19,19,19	0
7	PEO	A	604	2/2	0.08	-1.81	18,18,18,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CU	A	601	1/1	0.06	-1.96	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.