



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:14 am BST

PDB ID : 3N9M  
Title : ceKDM7A from C.elegans, alone  
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Deposited on : 2010-05-31  
Resolution : 2.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

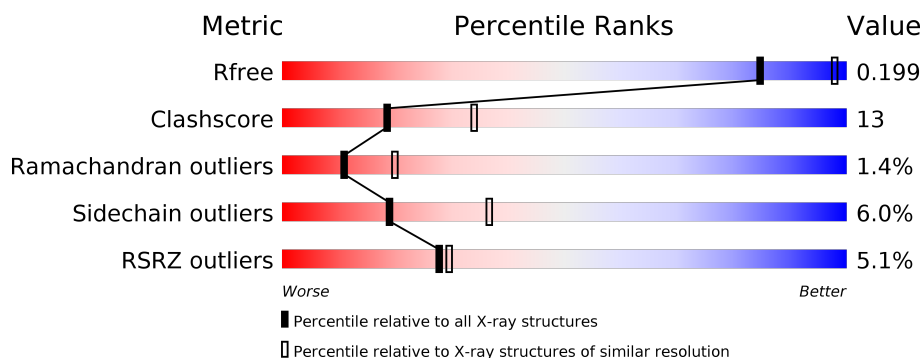
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 respectively. 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	528	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>• 5%</div> </div> </div>
1	C	528	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>• 9%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8332 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			4142	2645	701	768	28			
1	C	481	Total	C	N	O	S	0	0	0
			3964	2532	673	731	28			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	GLU	-	EXPRESSION TAG	UNP Q9GYI0
A	185	PHE	-	EXPRESSION TAG	UNP Q9GYI0
A	186	HIS	-	EXPRESSION TAG	UNP Q9GYI0
A	187	MET	-	EXPRESSION TAG	UNP Q9GYI0
C	184	GLU	-	EXPRESSION TAG	UNP Q9GYI0
C	185	PHE	-	EXPRESSION TAG	UNP Q9GYI0
C	186	HIS	-	EXPRESSION TAG	UNP Q9GYI0
C	187	MET	-	EXPRESSION TAG	UNP Q9GYI0

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

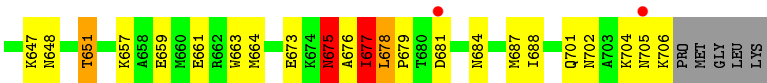
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total 112	O 112	0	0
4	C	108	Total 108	O 108	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.00 Å 144.51 Å 78.41 Å 90.00° 106.69° 90.00°	Depositor
Resolution (Å)	32.69 – 2.49 32.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.1 (32.69-2.49) 98.4 (32.69-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 2.51 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.201 , 0.247 0.201 , 0.199	Depositor DCC
$R_{free}$ test set	2421 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8332	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FE2

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	0.28	0/4249	0.50	2/5732 (0.0%)
1	C	0.27	0/4068	0.46	1/5486 (0.0%)
All	All	0.28	0/8317	0.48	3/11218 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	677	ILE	CB-CA-C	-9.40	92.80	111.60
1	C	677	ILE	CB-CA-C	-7.42	96.75	111.60
1	A	455	ASP	CB-CA-C	-5.68	99.03	110.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4142	0	4017	113	0
1	C	3964	0	3835	97	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	112	0	0	0	0
4	C	108	0	0	3	0
All	All	8332	0	7852	210	0

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 13.

All (210) 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:206:HIS:HB2	1:A:207:GLU:HA	1.41	1.03
1:C:675:ASN:ND2	1:C:675:ASN:H	1.56	1.02
1:A:675:ASN:HD22	1:A:675:ASN:N	1.55	1.02
1:C:676:ALA:O	1:C:677:ILE:HG13	1.60	1.00
1:C:283:ARG:HH22	1:C:418:LEU:HD22	1.25	0.98
1:A:206:HIS:CB	1:A:207:GLU:HA	1.95	0.94
1:C:430:ASN:HD22	1:C:433:MET:H	1.14	0.91
1:C:676:ALA:O	1:C:677:ILE:CG1	2.20	0.90
1:C:470:TYR:N	1:C:471:LEU:HA	1.89	0.85
1:A:675:ASN:H	1:A:675:ASN:HD22	1.24	0.83
1:A:430:ASN:ND2	1:A:433:MET:H	1.77	0.82
1:C:675:ASN:ND2	1:C:675:ASN:N	2.30	0.80
1:A:430:ASN:HD22	1:A:433:MET:H	1.28	0.79
1:A:461:TYR:HA	1:A:464:LEU:HD22	1.65	0.77
1:A:675:ASN:ND2	1:A:675:ASN:N	2.30	0.76
1:A:677:ILE:HG22	1:A:677:ILE:O	1.84	0.76
1:A:200:GLY:HA3	1:A:255:CYS:HB3	1.67	0.76
1:A:283:ARG:HH22	1:A:418:LEU:HD22	1.50	0.75
1:C:430:ASN:ND2	1:C:433:MET:H	1.84	0.75
1:C:702:ASN:O	1:C:705:ASN:HB2	1.87	0.74
1:C:678:LEU:HD22	1:C:679:PRO:HD2	1.69	0.74
1:A:464:LEU:O	1:A:469:GLU:HB3	1.88	0.74
1:A:369:PRO:HG3	1:A:436:ILE:CG2	2.19	0.73
1:A:441:ARG:HA	1:A:444:GLN:HE21	1.52	0.73
1:C:596:HIS:HE1	1:C:659:GLU:OE1	1.72	0.73
1:C:283:ARG:NH2	1:C:418:LEU:HD22	2.03	0.72
1:A:206:HIS:HB2	1:A:207:GLU:CA	2.20	0.71
1:C:275:VAL:HA	1:C:278:THR:HG22	1.72	0.71
1:A:618:LEU:HD22	1:A:677:ILE:HG21	1.73	0.70
1:A:230:LYS:HG3	1:A:423:LEU:HD11	1.74	0.70
1:A:228:LYS:HE2	1:A:498:PHE:HE2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:ILE:O	1:A:677:ILE:CG2	2.33	0.69
1:C:677:ILE:HG22	1:C:677:ILE:O	1.90	0.69
1:C:247:CYS:SG	1:C:249:THR:HG23	2.32	0.69
1:C:193:LYS:HE3	1:C:241:TRP:CD2	2.27	0.69
1:A:456:VAL:O	1:A:458:GLY:N	2.26	0.69
1:A:260:GLN:HE21	1:A:399:TYR:HA	1.57	0.69
1:C:369:PRO:HG3	1:C:436:ILE:CG2	2.22	0.68
1:A:676:ALA:O	1:A:677:ILE:HB	1.94	0.67
1:A:283:ARG:HH22	1:A:418:LEU:CD2	2.07	0.67
1:A:193:LYS:O	1:A:194:GLU:HB2	1.96	0.66
1:C:676:ALA:O	1:C:677:ILE:CB	2.43	0.66
1:A:513:ILE:HD12	1:A:570:LEU:HD23	1.78	0.66
1:A:705:ASN:N	1:A:705:ASN:HD22	1.93	0.66
1:A:206:HIS:N	1:A:207:GLU:HG3	2.12	0.65
1:C:641:ASP:OD1	1:C:643:ARG:HD3	1.96	0.65
1:A:607:SER:HB2	1:A:610:LYS:HB2	1.80	0.64
1:A:456:VAL:HG13	1:A:460:GLU:HB2	1.80	0.64
1:A:675:ASN:ND2	1:A:675:ASN:H	1.91	0.63
1:A:229:LYS:HE2	1:A:232:HIS:HB3	1.80	0.63
1:A:678:LEU:HD22	1:A:679:PRO:HD2	1.81	0.62
1:C:193:LYS:NZ	1:C:205:THR:HB	2.13	0.62
1:C:421:ASN:ND2	1:C:487:MET:H	1.97	0.62
1:C:570:LEU:O	1:C:572:PRO:HD3	1.98	0.62
1:A:325:PRO:HB2	1:A:330:VAL:HG13	1.80	0.62
1:A:352:TRP:NE1	1:A:562:PRO:HG3	2.15	0.62
1:A:228:LYS:HE2	1:A:498:PHE:CE2	2.35	0.62
1:A:456:VAL:O	1:A:457:SER:C	2.38	0.62
1:A:420:TYR:C	1:A:421:ASN:HD22	2.04	0.62
1:C:643:ARG:HD2	1:C:701:GLN:CD	2.21	0.61
1:A:455:ASP:O	1:A:457:SER:N	2.34	0.60
1:A:648:ASN:H	1:A:648:ASN:ND2	2.00	0.60
1:A:643:ARG:NH1	1:A:701:GLN:HB3	2.17	0.60
1:C:391:ILE:HG12	1:C:398:THR:HG22	1.82	0.60
1:C:625:ARG:HD2	1:C:626:ASN:OD1	2.04	0.58
1:A:206:HIS:H	1:A:207:GLU:HG3	1.68	0.58
1:C:370:LYS:HD3	4:C:64:HOH:O	2.03	0.58
1:A:421:ASN:N	1:A:421:ASN:HD22	2.01	0.57
1:C:675:ASN:HD22	1:C:675:ASN:N	1.98	0.57
1:A:228:LYS:HB3	1:A:424:SER:HB2	1.87	0.57
1:A:305:GLU:OE2	1:A:536:THR:HG21	2.04	0.57
1:C:687:MET:HE3	1:C:687:MET:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:563:ALA:H	1:C:587:ASN:ND2	2.04	0.56
1:A:330:VAL:HB	1:A:355:VAL:HG22	1.88	0.56
1:C:507:ILE:HG13	1:C:553:ILE:HG22	1.87	0.56
1:A:588:LEU:HD21	1:A:656:MET:HB2	1.88	0.55
1:A:375:LEU:O	1:A:379:VAL:HG12	2.05	0.55
1:A:377:ASP:HA	1:A:380:LYS:HD2	1.88	0.55
1:A:369:PRO:HG3	1:A:436:ILE:HG23	1.89	0.55
1:C:193:LYS:HD3	1:C:193:LYS:C	2.28	0.54
1:A:461:TYR:HA	1:A:464:LEU:CD2	2.34	0.54
1:A:241:TRP:HA	1:A:251:TYR:O	2.07	0.54
1:A:605:ILE:O	1:A:605:ILE:HD12	2.07	0.53
1:C:370:LYS:N	1:C:370:LYS:HD2	2.23	0.53
1:A:271:CYS:HB2	1:A:272:PRO:HD2	1.91	0.53
1:C:507:ILE:HD13	1:C:577:VAL:HG22	1.91	0.53
1:A:376:GLU:O	1:A:380:LYS:HG3	2.09	0.53
1:A:667:GLU:HG3	1:A:672:PRO:HA	1.91	0.53
1:C:421:ASN:HD21	1:C:487:MET:H	1.56	0.53
1:A:430:ASN:HD22	1:A:433:MET:N	2.02	0.52
1:C:607:SER:C	1:C:609:GLU:H	2.12	0.52
1:A:206:HIS:HB3	1:A:207:GLU:HA	1.87	0.52
1:A:461:TYR:O	1:A:465:LEU:HD22	2.09	0.51
1:C:678:LEU:HD22	1:C:679:PRO:CD	2.39	0.51
1:C:664:MET:HG3	1:C:687:MET:HG3	1.91	0.51
1:A:511:GLU:O	1:A:572:PRO:HD2	2.10	0.51
1:C:482:PHE:HE2	1:C:484:LEU:HD22	1.74	0.51
1:C:270:PHE:HB3	1:C:278:THR:HG21	1.91	0.51
1:A:469:GLU:O	1:A:469:GLU:HG3	2.10	0.51
1:C:266:TYR:HA	1:C:283:ARG:HA	1.93	0.51
1:A:457:SER:HA	1:A:461:TYR:HB2	1.92	0.51
1:A:469:GLU:O	1:A:469:GLU:CG	2.59	0.50
1:C:452:LEU:C	1:C:454:PRO:HD3	2.31	0.50
1:A:617:GLU:HG2	1:A:663:TRP:CZ3	2.46	0.50
1:A:231:SER:HB2	1:A:260:GLN:HE22	1.76	0.50
1:A:453:TRP:CD1	1:A:476:ARG:HB2	2.47	0.50
1:C:283:ARG:NH2	1:C:417:PRO:HB2	2.27	0.50
1:A:252:HIS:HB2	1:A:255:CYS:SG	2.52	0.49
1:C:647:LYS:O	1:C:651:THR:HG23	2.12	0.49
1:C:333:VAL:HB	1:C:338:GLU:HB2	1.93	0.49
1:A:607:SER:C	1:A:609:GLU:H	2.16	0.49
1:C:617:GLU:HG2	1:C:663:TRP:CH2	2.48	0.49
1:A:431:ASN:HA	1:A:434:LYS:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ASN:ND2	1:A:487:MET:H	2.11	0.49
1:A:258:LEU:HD13	1:A:269:PHE:HE2	1.77	0.49
1:C:617:GLU:HG2	1:C:663:TRP:CZ3	2.48	0.49
1:A:697:GLN:O	1:A:701:GLN:HG3	2.13	0.48
1:C:482:PHE:CE2	1:C:484:LEU:HD22	2.48	0.48
1:A:596:HIS:HE1	1:A:659:GLU:OE1	1.96	0.48
1:A:260:GLN:HB3	1:A:400:SER:HB2	1.95	0.48
1:C:274:CYS:O	1:C:278:THR:HG22	2.14	0.48
1:C:607:SER:O	1:C:609:GLU:HG2	2.12	0.48
1:A:570:LEU:O	1:A:572:PRO:HD3	2.13	0.48
1:A:376:GLU:OE1	1:A:407:ARG:HD2	2.14	0.48
1:C:238:ASP:HB3	1:C:254:LEU:HG	1.96	0.48
1:A:563:ALA:H	1:A:587:ASN:ND2	2.11	0.47
1:C:605:ILE:O	1:C:605:ILE:HD12	2.14	0.47
1:C:283:ARG:HH22	1:C:418:LEU:CD2	2.11	0.47
1:C:341:ARG:O	1:C:345:LYS:HB2	2.15	0.47
1:C:624:MET:O	1:C:629:LEU:HB2	2.15	0.47
1:A:464:LEU:HD23	1:A:465:LEU:N	2.30	0.47
1:A:233:HIS:NE2	1:A:609:GLU:HA	2.30	0.47
1:A:309:LYS:HE3	1:A:313:GLU:OE1	2.14	0.47
1:A:411:ARG:HD3	1:A:411:ARG:HA	1.69	0.47
1:A:678:LEU:HB3	1:A:683:LYS:HE3	1.97	0.47
1:A:507:ILE:HG13	1:A:553:ILE:HG22	1.97	0.46
1:C:677:ILE:CG2	1:C:677:ILE:O	2.57	0.46
1:C:312:ILE:O	1:C:316:ILE:HG13	2.16	0.45
1:C:609:GLU:HG2	1:C:609:GLU:H	1.65	0.45
1:C:641:ASP:OD1	1:C:701:GLN:HG2	2.14	0.45
1:C:553:ILE:N	1:C:553:ILE:HD12	2.32	0.45
1:A:394:TYR:CZ	1:A:419:LEU:HG	2.51	0.45
1:C:470:TYR:N	1:C:471:LEU:CA	2.71	0.45
1:C:681:ASP:HA	4:C:79:HOH:O	2.16	0.45
1:A:241:TRP:N	1:A:252:HIS:O	2.49	0.45
1:C:375:LEU:O	1:C:379:VAL:HG12	2.16	0.45
1:C:427:PHE:CD1	1:C:433:MET:HB3	2.52	0.45
1:C:675:ASN:H	1:C:675:ASN:HD22	1.45	0.45
1:A:306:VAL:O	1:A:311:TRP:CE3	2.70	0.44
1:C:515:TYR:O	1:C:567:HIS:HA	2.17	0.44
1:C:657:LYS:O	1:C:661:GLU:HG2	2.16	0.44
1:A:238:ASP:HB3	1:A:254:LEU:HG	1.99	0.44
1:C:559:LEU:HA	1:C:559:LEU:HD12	1.85	0.44
1:A:619:LEU:HD23	1:A:619:LEU:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:GLU:O	1:C:355:VAL:HG13	2.17	0.44
1:C:514:PHE:HB2	1:C:551:VAL:HG13	2.00	0.44
1:C:515:TYR:CE1	1:C:550:ARG:HG3	2.53	0.44
1:A:384:SER:HB3	1:A:404:ASP:HB2	2.00	0.44
1:A:664:MET:HG3	1:A:687:MET:HG3	1.99	0.44
1:C:407:ARG:NH2	1:C:411:ARG:HB2	2.33	0.44
1:C:648:ASN:ND2	1:C:648:ASN:H	2.16	0.44
1:C:275:VAL:HA	1:C:278:THR:CG2	2.44	0.43
1:A:592:MET:SD	1:A:659:GLU:HG2	2.57	0.43
1:C:490:SER:O	1:C:570:LEU:HD12	2.17	0.43
1:C:676:ALA:O	1:C:677:ILE:HB	2.17	0.43
1:A:607:SER:HB3	1:A:610:LYS:HD2	2.00	0.43
1:C:325:PRO:HB2	1:C:330:VAL:HG13	2.00	0.43
1:C:411:ARG:HA	1:C:411:ARG:HD3	1.60	0.43
1:A:461:TYR:CA	1:A:464:LEU:HD22	2.43	0.43
1:A:465:LEU:C	1:A:467:ARG:H	2.21	0.43
1:C:228:LYS:CD	1:C:423:LEU:HD22	2.48	0.43
1:C:414:LYS:HG2	1:C:415:ASN:OD1	2.19	0.43
1:A:471:LEU:HB3	1:A:472:PRO:HD2	2.01	0.43
1:A:228:LYS:HD2	1:A:423:LEU:HD22	2.00	0.43
1:C:293:ARG:HD3	1:C:299:GLU:OE2	2.19	0.43
1:C:497:ASP:OD1	1:C:581:ASN:ND2	2.51	0.43
1:C:319:GLU:OE1	1:C:550:ARG:HD2	2.19	0.43
1:A:515:TYR:O	1:A:567:HIS:HA	2.19	0.43
1:A:634:GLU:O	1:A:638:GLU:HG2	2.19	0.43
1:A:320:ASN:HD22	1:A:320:ASN:H	1.68	0.42
1:C:228:LYS:HE2	1:C:498:PHE:HE2	1.85	0.42
1:A:468:GLU:C	1:A:470:TYR:H	2.22	0.42
1:C:275:VAL:N	1:C:276:PRO:CD	2.83	0.42
1:C:335:ASP:HB2	1:C:362:ASP:O	2.19	0.42
1:C:518:ALA:HA	1:C:519:PRO:HD3	1.79	0.42
1:C:367:THR:O	1:C:437:ALA:HA	2.19	0.42
1:A:231:SER:HB2	1:A:260:GLN:NE2	2.34	0.42
1:C:520:THR:HB	4:C:59:HOH:O	2.18	0.42
1:A:561:ILE:HA	1:A:562:PRO:HD3	1.83	0.42
1:C:704:LYS:HA	1:C:706:LYS:HE3	2.01	0.42
1:C:377:ASP:HA	1:C:380:LYS:HD2	2.02	0.41
1:A:296:SER:HA	1:A:297:PRO:HD3	1.84	0.41
1:A:705:ASN:N	1:A:705:ASN:ND2	2.65	0.41
1:C:386:TYR:CE2	1:C:425:LEU:HD13	2.55	0.41
1:A:195:SER:O	1:A:204:PHE:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:490:SER:HB2	1:C:571:THR:HB	2.02	0.41
1:A:450:ASN:O	1:A:454:PRO:HA	2.20	0.41
1:C:381:ILE:HG21	1:C:433:MET:HG2	2.03	0.41
1:C:421:ASN:ND2	1:C:486:GLY:HA2	2.36	0.41
1:C:641:ASP:O	1:C:644:GLU:HG2	2.21	0.41
1:C:322:VAL:HA	1:C:323:PRO:HD3	1.91	0.41
1:A:455:ASP:OD1	1:A:455:ASP:C	2.58	0.41
1:C:271:CYS:HB2	1:C:272:PRO:HD2	2.03	0.41
1:A:507:ILE:HD13	1:A:577:VAL:HG22	2.03	0.41
1:A:381:ILE:HG21	1:A:433:MET:HG2	2.03	0.40
1:A:461:TYR:CZ	1:A:465:LEU:HD13	2.56	0.40
1:A:227:SER:HB3	1:A:478:LYS:HB3	2.04	0.40
1:A:421:ASN:HD21	1:A:487:MET:H	1.69	0.40
1:A:678:LEU:HA	1:A:679:PRO:HD2	1.70	0.40
1:A:687:MET:O	1:A:691:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

## 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	499/528 (94%)	453 (91%)	35 (7%)	11 (2%)	6	10
1	C	475/528 (90%)	440 (93%)	32 (7%)	3 (1%)	25	43
All	All	974/1056 (92%)	893 (92%)	67 (7%)	14 (1%)	11	20

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	ASP
1	A	205	THR
1	A	206	HIS

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Mol	Chain	Res	Type
1	A	253	PHE
1	A	456	VAL
1	A	457	SER
1	C	253	PHE
1	C	677	ILE
1	A	194	GLU
1	A	241	TRP
1	A	677	ILE
1	A	608	GLU
1	A	208	ASP
1	C	675	ASN

### 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	452/475 (95%)	429 (95%)	23 (5%)	24	45
1	C	432/475 (91%)	402 (93%)	30 (7%)	15	30
All	All	884/950 (93%)	831 (94%)	53 (6%)	19	37

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	SER
1	A	196	ASP
1	A	234	HIS
1	A	252	HIS
1	A	253	PHE
1	A	258	LEU
1	A	283	ARG
1	A	330	VAL
1	A	379	VAL
1	A	423	LEU
1	A	442	PHE
1	A	464	LEU

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Mol	Chain	Res	Type
1	A	465	LEU
1	A	490	SER
1	A	536	THR
1	A	604	GLU
1	A	628	LEU
1	A	629	LEU
1	A	648	ASN
1	A	664	MET
1	A	675	ASN
1	A	678	LEU
1	A	705	ASN
1	C	196	ASP
1	C	226	MET
1	C	234	HIS
1	C	237	ASN
1	C	249	THR
1	C	253	PHE
1	C	254	LEU
1	C	258	LEU
1	C	273	LYS
1	C	330	VAL
1	C	344	GLU
1	C	355	VAL
1	C	370	LYS
1	C	379	VAL
1	C	407	ARG
1	C	418	LEU
1	C	423	LEU
1	C	441	ARG
1	C	484	LEU
1	C	585	LEU
1	C	604	GLU
1	C	628	LEU
1	C	629	LEU
1	C	651	THR
1	C	673	GLU
1	C	675	ASN
1	C	677	ILE
1	C	678	LEU
1	C	684	ASN
1	C	688	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	A	260	GLN
1	A	320	ASN
1	A	395	ASN
1	A	396	GLN
1	A	421	ASN
1	A	430	ASN
1	A	444	GLN
1	A	587	ASN
1	A	596	HIS
1	A	648	ASN
1	A	675	ASN
1	A	684	ASN
1	A	705	ASN
1	C	237	ASN
1	C	351	ASN
1	C	395	ASN
1	C	421	ASN
1	C	430	ASN
1	C	444	GLN
1	C	581	ASN
1	C	587	ASN
1	C	596	HIS
1	C	615	ASN
1	C	648	ASN
1	C	675	ASN
1	C	684	ASN

### 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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	503/528 (95%)	0.16	31 (6%)	20 21	29, 54, 90, 127	0
1	C	481/528 (91%)	0.09	19 (3%)	38 41	28, 53, 81, 114	0
All	All	984/1056 (93%)	0.12	50 (5%)	28 29	28, 53, 86, 127	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	PHE	5.3
1	C	239	PHE	4.0
1	C	236	LYS	3.9
1	A	210	LEU	3.9
1	A	459	ALA	3.9
1	A	457	SER	3.9
1	A	211	ILE	3.8
1	A	233	HIS	3.8
1	C	705	ASN	3.8
1	C	233	HIS	3.7
1	A	469	GLU	3.6
1	A	705	ASN	3.6
1	C	232	HIS	3.5
1	C	234	HIS	3.4
1	C	607	SER	3.4
1	C	206	HIS	3.3
1	A	462	ILE	3.2
1	C	194	GLU	3.2
1	A	606	ARG	3.2
1	A	677	ILE	3.1
1	A	223	LYS	3.1
1	A	607	SER	3.1
1	A	461	TYR	3.1
1	A	241	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	204	PHE	2.8
1	A	195	SER	2.8
1	C	606	ARG	2.8
1	A	206	HIS	2.8
1	A	456	VAL	2.7
1	C	470	TYR	2.6
1	A	234	HIS	2.6
1	C	422	PHE	2.5
1	C	681	ASP	2.5
1	A	470	TYR	2.4
1	A	224	PRO	2.4
1	C	237	ASN	2.4
1	C	205	THR	2.3
1	C	424	SER	2.3
1	A	302	LEU	2.3
1	A	668	LEU	2.2
1	A	608	GLU	2.2
1	A	237	ASN	2.2
1	A	422	PHE	2.2
1	A	463	LYS	2.1
1	A	699	LYS	2.1
1	C	423	LEU	2.1
1	A	424	SER	2.1
1	A	703	ALA	2.0
1	C	610	LYS	2.0
1	C	207	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FE2	A	1	1/1	0.96	0.25	72,72,72,72	0
3	ZN	A	3	1/1	0.97	0.10	64,64,64,64	0
3	ZN	A	2	1/1	0.97	0.07	86,86,86,86	0
2	FE2	C	1	1/1	0.97	0.19	66,66,66,66	0
3	ZN	C	2	1/1	0.98	0.07	73,73,73,73	0
3	ZN	C	3	1/1	0.99	0.10	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.