



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:04 AM GMT

PDB ID : 3H38  
Title : The structure of CCA-adding enzyme apo form II  
Authors : Toh, Y.; Tomita, K.  
Deposited on : 2009-04-16  
Resolution : 2.37 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

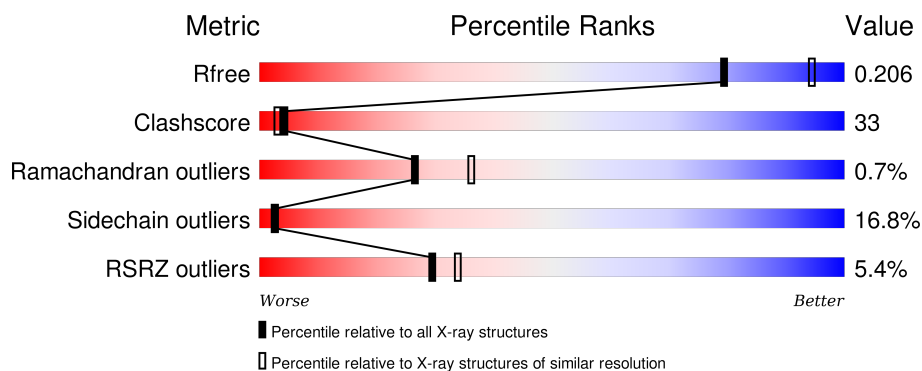
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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	441	<div> <div>5%</div> <div>48%</div> <div>39%</div> <div>10%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3576 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 TRNA nucleotidyl transferase-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3493	2259	590	633	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q9WZH4
A	429	LYS	-	EXPRESSION TAG	UNP Q9WZH4
A	430	LEU	-	EXPRESSION TAG	UNP Q9WZH4
A	431	ALA	-	EXPRESSION TAG	UNP Q9WZH4
A	432	ALA	-	EXPRESSION TAG	UNP Q9WZH4
A	433	ALA	-	EXPRESSION TAG	UNP Q9WZH4
A	434	LEU	-	EXPRESSION TAG	UNP Q9WZH4
A	435	GLU	-	EXPRESSION TAG	UNP Q9WZH4
A	436	HIS	-	EXPRESSION TAG	UNP Q9WZH4
A	437	HIS	-	EXPRESSION TAG	UNP Q9WZH4
A	438	HIS	-	EXPRESSION TAG	UNP Q9WZH4
A	439	HIS	-	EXPRESSION TAG	UNP Q9WZH4
A	440	HIS	-	EXPRESSION TAG	UNP Q9WZH4
A	441	HIS	-	EXPRESSION TAG	UNP Q9WZH4

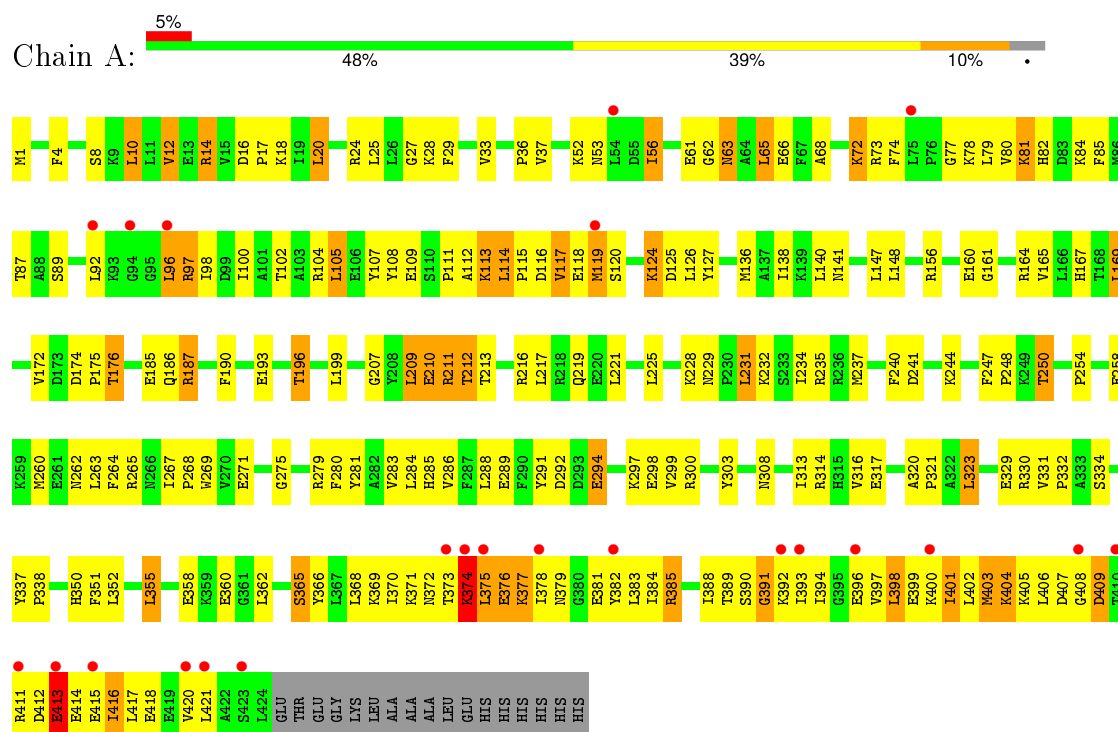
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	83	Total	O	0	0
			83	83		

### 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: TRNA nucleotidyl transferase-related protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.35Å 50.45Å 69.87Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	43.33 – 2.37 43.33 – 2.37	Depositor EDS
% Data completeness (in resolution range)	95.3 (43.33-2.37) 95.3 (43.33-2.37)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.211 , 0.266 0.206 , 0.206	Depositor DCC
$R_{free}$ test set	1193 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 49.6	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23735 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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 [i](#)

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

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	0.72	0/3559	0.82	2/4786 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	413	GLU	CB-CA-C	-13.33	83.75	110.40
1	A	374	LYS	N-CA-C	-5.69	95.63	111.00

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	3493	0	3590	235	1
2	A	83	0	0	8	0
All	All	3576	0	3590	235	1

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 33.

All (235) 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:377:LYS:CD	1:A:377:LYS:H	1.50	1.22
1:A:377:LYS:HD3	1:A:377:LYS:N	1.45	1.20
1:A:114:LEU:H	1:A:114:LEU:HD13	0.94	1.08
1:A:114:LEU:HD13	1:A:114:LEU:N	1.69	1.06
1:A:114:LEU:CD1	1:A:114:LEU:H	1.63	1.04
1:A:108:TYR:CE2	1:A:114:LEU:HD12	1.93	1.03
1:A:412:ASP:O	1:A:414:GLU:HG3	1.64	0.95
1:A:405:LYS:O	1:A:408:GLY:HA2	1.66	0.95
1:A:186:GLN:OE1	1:A:232:LYS:HE3	1.66	0.95
1:A:85:PHE:HZ	1:A:118:GLU:HB3	1.30	0.94
1:A:85:PHE:CZ	1:A:118:GLU:HB3	2.00	0.94
1:A:375:LEU:HD13	1:A:376:GLU:O	1.68	0.93
1:A:164:ARG:HA	1:A:196:THR:HG21	1.48	0.93
1:A:211:ARG:HG2	1:A:211:ARG:HH21	1.30	0.92
1:A:56:ILE:HD11	1:A:98:ILE:HG12	1.51	0.91
1:A:37:VAL:H	1:A:141:ASN:HD21	1.11	0.89
1:A:331:VAL:HG13	1:A:332:PRO:HD2	1.52	0.89
1:A:262:ASN:ND2	1:A:265:ARG:HH12	1.70	0.88
1:A:105:LEU:HD12	1:A:119:MET:O	1.79	0.82
1:A:396:GLU:O	1:A:400:LYS:HD3	1.80	0.81
1:A:369:LYS:HE2	1:A:406:LEU:O	1.80	0.81
1:A:37:VAL:H	1:A:141:ASN:ND2	1.78	0.80
1:A:412:ASP:O	1:A:414:GLU:CG	2.30	0.80
1:A:374:LYS:O	1:A:375:LEU:HB3	1.80	0.80
1:A:376:GLU:HA	1:A:376:GLU:OE1	1.81	0.79
1:A:377:LYS:HG2	1:A:378:ILE:H	1.47	0.79
1:A:393:ILE:HD12	1:A:393:ILE:H	1.47	0.78
1:A:37:VAL:N	1:A:141:ASN:HD21	1.82	0.78
1:A:371:LYS:O	1:A:374:LYS:HE2	1.84	0.78
1:A:82:HIS:HD2	1:A:87:THR:HG22	1.47	0.78
1:A:105:LEU:HD11	1:A:117:VAL:HG23	1.66	0.78
1:A:113:LYS:NZ	1:A:216:ARG:HD2	1.98	0.78
1:A:376:GLU:OE1	1:A:376:GLU:CA	2.30	0.78
1:A:82:HIS:CD2	1:A:87:THR:HG22	2.19	0.77
1:A:289:GLU:OE1	1:A:350:HIS:HE1	1.66	0.77
1:A:397:VAL:O	1:A:401:ILE:HG22	1.85	0.77
1:A:108:TYR:CZ	1:A:114:LEU:HD12	2.21	0.76
1:A:375:LEU:HD13	1:A:375:LEU:C	2.07	0.75
1:A:262:ASN:HD22	1:A:265:ARG:NH1	1.84	0.74
1:A:211:ARG:HH21	1:A:211:ARG:CG	2.01	0.73
1:A:260:MET:HE2	1:A:286:VAL:HG11	1.71	0.72
1:A:331:VAL:CG1	1:A:332:PRO:HD2	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:MET:HA	1:A:403:MET:HE2	1.73	0.71
1:A:207:GLY:O	1:A:210:GLU:HG2	1.90	0.71
1:A:271:GLU:HA	1:A:275:GLY:O	1.90	0.71
1:A:370:ILE:O	1:A:374:LYS:HB3	1.92	0.70
1:A:260:MET:CE	1:A:286:VAL:HG11	2.22	0.70
1:A:331:VAL:HG13	1:A:332:PRO:CD	2.20	0.69
1:A:63:ASN:ND2	1:A:66:GLU:H	1.90	0.69
1:A:193:GLU:HG3	1:A:196:THR:HG23	1.73	0.69
1:A:96:LEU:HD23	1:A:97:ARG:H	1.55	0.69
1:A:29:PHE:O	1:A:33:VAL:HG22	1.92	0.68
1:A:8:SER:O	1:A:12:VAL:HG13	1.93	0.68
1:A:174:ASP:OD2	1:A:176:THR:HB	1.93	0.68
1:A:118:GLU:O	1:A:120:SER:N	2.26	0.68
1:A:372:ASN:C	1:A:374:LYS:H	1.98	0.68
1:A:260:MET:HE1	1:A:286:VAL:HB	1.75	0.67
1:A:120:SER:OG	1:A:124:LYS:HB3	1.95	0.66
1:A:175:PRO:HG2	1:A:212:THR:HG22	1.77	0.66
1:A:104:ARG:HD3	1:A:116:ASP:OD2	1.94	0.66
1:A:405:LYS:O	1:A:408:GLY:CA	2.41	0.66
1:A:211:ARG:HG2	1:A:211:ARG:NH2	2.02	0.66
1:A:80:VAL:HG12	1:A:81:LYS:O	1.95	0.66
1:A:375:LEU:CD1	1:A:376:GLU:O	2.44	0.66
1:A:254:PRO:O	1:A:258:GLU:HG3	1.96	0.66
1:A:414:GLU:O	1:A:418:GLU:HB2	1.96	0.65
1:A:105:LEU:CD1	1:A:119:MET:O	2.44	0.65
1:A:377:LYS:HD3	1:A:377:LYS:H	0.60	0.65
1:A:262:ASN:HD22	1:A:265:ARG:HH12	1.35	0.65
1:A:107:TYR:O	1:A:115:PRO:HD2	1.96	0.65
1:A:331:VAL:CG1	1:A:332:PRO:CD	2.74	0.65
1:A:247:PHE:HB2	1:A:250:THR:HG23	1.77	0.65
1:A:314:ARG:HA	1:A:317:GLU:HG2	1.78	0.65
1:A:292:ASP:HB2	1:A:294:GLU:OE1	1.97	0.65
1:A:193:GLU:OE2	1:A:196:THR:HG22	1.97	0.64
1:A:175:PRO:HB2	1:A:212:THR:HG21	1.79	0.64
1:A:234:ILE:HA	1:A:237:MET:HE3	1.78	0.64
1:A:185:GLU:HG2	1:A:190:PHE:O	1.98	0.64
1:A:209:LEU:HB2	2:A:448:HOH:O	1.96	0.64
1:A:393:ILE:O	1:A:397:VAL:HG23	1.98	0.63
1:A:113:LYS:HZ2	1:A:216:ARG:HD2	1.60	0.63
1:A:412:ASP:O	1:A:414:GLU:N	2.30	0.63
1:A:408:GLY:C	1:A:409:ASP:OD1	2.37	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:HD22	1:A:66:GLU:H	1.47	0.62
1:A:412:ASP:C	1:A:414:GLU:H	2.02	0.62
1:A:417:LEU:O	1:A:421:LEU:HD13	1.99	0.61
1:A:377:LYS:HG2	1:A:378:ILE:N	2.14	0.61
1:A:412:ASP:OD1	1:A:413:GLU:N	2.27	0.61
1:A:84:LYS:HB3	1:A:87:THR:HB	1.83	0.60
1:A:352:LEU:HD23	1:A:355:LEU:HD21	1.83	0.60
1:A:247:PHE:CB	1:A:250:THR:HG23	2.32	0.60
1:A:24:ARG:NH2	2:A:510:HOH:O	2.36	0.59
1:A:289:GLU:OE1	1:A:350:HIS:CE1	2.54	0.59
1:A:393:ILE:HD12	1:A:393:ILE:N	2.16	0.59
1:A:65:LEU:HD23	1:A:65:LEU:N	2.16	0.59
1:A:404:LYS:HB2	1:A:415:GLU:OE1	2.02	0.59
1:A:294:GLU:CD	1:A:294:GLU:H	2.05	0.58
1:A:108:TYR:HE2	1:A:114:LEU:HD12	1.62	0.58
1:A:378:ILE:HG13	1:A:379:ASN:N	2.19	0.57
1:A:161:GLY:HA2	1:A:190:PHE:CE2	2.40	0.57
1:A:211:ARG:NH2	2:A:518:HOH:O	2.26	0.57
1:A:416:ILE:O	1:A:420:VAL:HG22	2.05	0.57
1:A:231:LEU:HD13	1:A:235:ARG:NH2	2.20	0.56
1:A:120:SER:OG	1:A:124:LYS:CB	2.54	0.56
1:A:72:LYS:HE3	1:A:77:GLY:O	2.05	0.56
1:A:113:LYS:HZ3	1:A:216:ARG:HD2	1.69	0.55
1:A:167:HIS:HD2	1:A:169:LEU:H	1.54	0.55
1:A:416:ILE:CG2	1:A:417:LEU:N	2.70	0.55
1:A:409:ASP:N	1:A:409:ASP:OD1	2.38	0.55
1:A:279:ARG:O	1:A:283:VAL:HG23	2.06	0.55
1:A:384:ILE:HG21	1:A:394:ILE:HG22	1.88	0.55
1:A:85:PHE:CE2	1:A:118:GLU:HB3	2.41	0.54
1:A:331:VAL:HG12	1:A:332:PRO:N	2.22	0.54
1:A:114:LEU:CD1	1:A:114:LEU:N	2.41	0.54
1:A:375:LEU:C	1:A:375:LEU:CD1	2.75	0.54
1:A:403:MET:HA	1:A:403:MET:CE	2.37	0.54
1:A:412:ASP:HB3	1:A:413:GLU:OE1	2.07	0.54
1:A:16:ASP:OD1	1:A:17:PRO:HD2	2.07	0.54
1:A:390:SER:HB2	1:A:391:GLY:HA3	1.90	0.54
1:A:260:MET:CE	1:A:286:VAL:CG1	2.86	0.54
1:A:213:THR:OG1	1:A:216:ARG:HG3	2.08	0.54
1:A:117:VAL:C	1:A:119:MET:H	2.10	0.54
1:A:373:THR:O	1:A:373:THR:HG22	2.08	0.53
1:A:334:SER:CB	1:A:403:MET:HG3	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:CD1	1:A:98:ILE:HG12	2.31	0.53
1:A:334:SER:HB2	1:A:403:MET:HG3	1.90	0.53
1:A:269:TRP:O	1:A:269:TRP:CE3	2.62	0.53
1:A:408:GLY:O	1:A:409:ASP:OD1	2.26	0.53
1:A:377:LYS:CG	1:A:378:ILE:H	2.18	0.53
1:A:393:ILE:H	1:A:393:ILE:CD1	2.20	0.52
1:A:294:GLU:O	1:A:298:GLU:HG3	2.09	0.52
1:A:10:LEU:HD22	1:A:14:ARG:HG3	1.90	0.52
1:A:104:ARG:O	1:A:125:ASP:HA	2.10	0.52
1:A:165:VAL:HG22	1:A:196:THR:HB	1.91	0.51
1:A:389:THR:OG1	1:A:390:SER:N	2.43	0.51
1:A:96:LEU:CD2	1:A:97:ARG:H	2.23	0.51
1:A:73:ARG:HG3	1:A:74:PHE:CE1	2.46	0.51
1:A:114:LEU:HD22	1:A:114:LEU:N	2.25	0.51
1:A:369:LYS:O	1:A:372:ASN:O	2.28	0.51
1:A:56:ILE:HD11	1:A:98:ILE:HG23	1.92	0.51
1:A:219:GLN:NE2	2:A:496:HOH:O	2.44	0.51
1:A:399:GLU:O	1:A:403:MET:HB2	2.11	0.50
1:A:105:LEU:CD1	1:A:117:VAL:HG23	2.40	0.50
1:A:156:ARG:O	1:A:160:GLU:HG3	2.10	0.50
1:A:355:LEU:HG	1:A:360:GLU:HA	1.94	0.50
1:A:210:GLU:CD	1:A:210:GLU:H	2.15	0.50
1:A:114:LEU:HD22	2:A:487:HOH:O	2.12	0.49
1:A:36:PRO:HD2	1:A:61:GLU:HB2	1.93	0.49
1:A:375:LEU:HD13	1:A:375:LEU:O	2.12	0.49
1:A:231:LEU:O	1:A:235:ARG:HG3	2.13	0.49
1:A:111:PRO:HB3	1:A:172:VAL:O	2.13	0.49
1:A:376:GLU:N	1:A:376:GLU:OE1	2.46	0.49
1:A:320:ALA:HB3	1:A:321:PRO:HD3	1.93	0.49
1:A:225:LEU:CD1	1:A:280:PHE:HA	2.42	0.49
1:A:375:LEU:HD13	1:A:376:GLU:C	2.30	0.49
1:A:56:ILE:HD11	1:A:98:ILE:CG1	2.36	0.49
1:A:337:TYR:N	1:A:338:PRO:CD	2.76	0.49
1:A:378:ILE:HG13	1:A:379:ASN:HD22	1.78	0.48
1:A:329:GLU:O	1:A:330:ARG:C	2.51	0.48
1:A:377:LYS:HZ2	1:A:412:ASP:CG	2.17	0.48
1:A:20:LEU:HA	1:A:20:LEU:HD23	1.67	0.48
1:A:398:LEU:O	1:A:401:ILE:HG23	2.13	0.48
1:A:27:GLY:HA3	1:A:140:LEU:O	2.13	0.48
1:A:374:LYS:O	1:A:375:LEU:CB	2.49	0.48
1:A:102:THR:HG21	1:A:118:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:VAL:CG1	1:A:332:PRO:N	2.76	0.48
1:A:391:GLY:H	1:A:393:ILE:CD1	2.27	0.47
1:A:377:LYS:CD	1:A:377:LYS:N	2.30	0.47
1:A:84:LYS:HB3	1:A:87:THR:CB	2.42	0.47
1:A:250:THR:HG22	1:A:291:TYR:CE2	2.49	0.47
1:A:63:ASN:HD21	1:A:65:LEU:HB2	1.79	0.47
1:A:167:HIS:CD2	1:A:169:LEU:H	2.32	0.47
1:A:36:PRO:HA	1:A:141:ASN:HD21	1.80	0.47
1:A:297:LYS:HG2	1:A:300:ARG:CZ	2.45	0.47
1:A:97:ARG:HG3	1:A:97:ARG:O	2.14	0.47
1:A:377:LYS:CG	1:A:378:ILE:N	2.77	0.46
1:A:92:LEU:HD11	1:A:98:ILE:HD11	1.97	0.46
1:A:358:GLU:OE1	1:A:358:GLU:HA	2.14	0.46
1:A:391:GLY:O	1:A:394:ILE:HG12	2.15	0.46
1:A:4:PHE:HB3	1:A:147:LEU:HD11	1.97	0.46
1:A:84:LYS:O	1:A:85:PHE:C	2.53	0.46
1:A:193:GLU:HG3	1:A:196:THR:CG2	2.41	0.46
1:A:416:ILE:HG23	1:A:417:LEU:N	2.31	0.46
1:A:85:PHE:CE2	1:A:118:GLU:CB	2.99	0.46
1:A:375:LEU:O	1:A:375:LEU:CD1	2.64	0.45
1:A:267:ILE:N	1:A:268:PRO:CD	2.79	0.45
1:A:285:HIS:HB3	1:A:350:HIS:CG	2.51	0.45
1:A:63:ASN:HB3	1:A:66:GLU:HG3	1.99	0.44
1:A:280:PHE:O	1:A:284:LEU:HG	2.18	0.44
1:A:105:LEU:H	1:A:105:LEU:HD13	1.83	0.44
1:A:104:ARG:HB2	1:A:116:ASP:OD1	2.16	0.44
1:A:411:ARG:O	1:A:412:ASP:HB2	2.17	0.44
1:A:112:ALA:O	2:A:455:HOH:O	2.21	0.44
1:A:365:SER:O	1:A:366:TYR:C	2.55	0.44
1:A:117:VAL:C	1:A:119:MET:N	2.69	0.44
1:A:294:GLU:HG2	2:A:485:HOH:O	2.17	0.44
1:A:240:PHE:O	1:A:241:ASP:HB2	2.17	0.44
1:A:372:ASN:C	1:A:374:LYS:N	2.61	0.44
1:A:407:ASP:OD2	1:A:407:ASP:N	2.50	0.44
1:A:65:LEU:N	1:A:65:LEU:CD2	2.80	0.43
1:A:62:GLY:O	1:A:102:THR:HG23	2.18	0.43
1:A:187:ARG:O	1:A:228:LYS:HE2	2.17	0.43
1:A:405:LYS:O	1:A:408:GLY:N	2.51	0.43
1:A:371:LYS:O	1:A:371:LYS:HG2	2.19	0.43
1:A:316:VAL:HG11	1:A:350:HIS:CG	2.53	0.43
1:A:136:MET:HB2	2:A:447:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:SER:HB2	1:A:391:GLY:CA	2.49	0.43
1:A:161:GLY:HA2	1:A:190:PHE:CZ	2.54	0.43
1:A:416:ILE:HD13	1:A:416:ILE:O	2.18	0.42
1:A:225:LEU:HD12	1:A:280:PHE:HA	2.01	0.42
1:A:89:SER:HA	1:A:98:ILE:O	2.19	0.42
1:A:114:LEU:HD22	1:A:114:LEU:O	2.19	0.42
1:A:323:LEU:HD12	1:A:351:PHE:CD2	2.54	0.42
1:A:229:ASN:O	1:A:232:LYS:HB2	2.19	0.42
1:A:68:ALA:HB2	1:A:100:ILE:HD12	2.02	0.42
1:A:285:HIS:HA	1:A:313:ILE:HG12	2.02	0.42
1:A:385:ARG:HA	1:A:388:ILE:O	2.18	0.42
1:A:355:LEU:HD22	1:A:355:LEU:H	1.85	0.42
1:A:53:ASN:C	1:A:53:ASN:OD1	2.57	0.42
1:A:260:MET:CE	1:A:286:VAL:CB	2.98	0.42
1:A:368:LEU:HA	1:A:368:LEU:HD23	1.76	0.41
1:A:297:LYS:HG2	1:A:300:ARG:NH1	2.35	0.41
1:A:416:ILE:HD13	1:A:420:VAL:HG13	2.01	0.41
1:A:412:ASP:O	1:A:414:GLU:HG2	2.18	0.41
1:A:285:HIS:HB3	1:A:350:HIS:CD2	2.56	0.41
1:A:65:LEU:O	1:A:66:GLU:C	2.58	0.41
1:A:300:ARG:O	1:A:303:TYR:O	2.39	0.41
1:A:381:GLU:OE2	1:A:381:GLU:N	2.47	0.41
1:A:113:LYS:HA	1:A:114:LEU:HD13	2.02	0.41
1:A:394:ILE:O	1:A:398:LEU:HD22	2.21	0.41
1:A:262:ASN:ND2	1:A:265:ARG:NH1	2.44	0.40
1:A:247:PHE:HA	1:A:248:PRO:HD3	1.68	0.40
1:A:234:ILE:HD12	1:A:264:PHE:HE1	1.85	0.40
1:A:377:LYS:HD2	1:A:405:LYS:NZ	2.37	0.40
1:A:138:ILE:HA	1:A:147:LEU:O	2.21	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:TYR:OH	1:A:382:TYR:OH[2_556]	1.94	0.26

## 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	422/441 (96%)	405 (96%)	14 (3%)	3 (1%)	26	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	GLU
1	A	391	GLY
1	A	375	LEU

### 5.3.2 Protein sidechains [i](#)

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	382/395 (97%)	318 (83%)	64 (17%)	2	3

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	LEU
1	A	12	VAL
1	A	14	ARG
1	A	18	LYS
1	A	20	LEU
1	A	25	LEU
1	A	28	LYS

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Mol	Chain	Res	Type
1	A	52	LYS
1	A	56	ILE
1	A	63	ASN
1	A	65	LEU
1	A	72	LYS
1	A	78	LYS
1	A	79	LEU
1	A	81	LYS
1	A	96	LEU
1	A	97	ARG
1	A	105	LEU
1	A	109	GLU
1	A	113	LYS
1	A	114	LEU
1	A	117	VAL
1	A	119	MET
1	A	124	LYS
1	A	126	LEU
1	A	127	TYR
1	A	148	LEU
1	A	169	LEU
1	A	176	THR
1	A	187	ARG
1	A	196	THR
1	A	199	LEU
1	A	209	LEU
1	A	210	GLU
1	A	211	ARG
1	A	212	THR
1	A	217	LEU
1	A	221	LEU
1	A	231	LEU
1	A	244	LYS
1	A	250	THR
1	A	263	LEU
1	A	288	LEU
1	A	294	GLU
1	A	299	VAL
1	A	308	ASN
1	A	323	LEU
1	A	355	LEU
1	A	362	LEU

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Mol	Chain	Res	Type
1	A	365	SER
1	A	374	LYS
1	A	376	GLU
1	A	377	LYS
1	A	383	LEU
1	A	385	ARG
1	A	392	LYS
1	A	398	LEU
1	A	401	ILE
1	A	402	LEU
1	A	403	MET
1	A	404	LYS
1	A	409	ASP
1	A	416	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	141	ASN
1	A	167	HIS
1	A	202	GLN
1	A	262	ASN
1	A	345	ASN
1	A	350	HIS
1	A	379	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

There are no ligands in this entry.

## 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	424/441 (96%)	0.21	23 (5%)	29 34	20, 47, 106, 129	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	ARG	7.9
1	A	375	LEU	5.3
1	A	410	THR	5.2
1	A	119	MET	3.9
1	A	408	GLY	3.8
1	A	421	LEU	3.5
1	A	382	TYR	3.4
1	A	420	VAL	3.2
1	A	374	LYS	3.2
1	A	54	LEU	3.1
1	A	92	LEU	2.7
1	A	413	GLU	2.6
1	A	373	THR	2.5
1	A	378	ILE	2.5
1	A	75	LEU	2.4
1	A	393	ILE	2.4
1	A	396	GLU	2.3
1	A	392	LYS	2.2
1	A	400	LYS	2.2
1	A	415	GLU	2.1
1	A	94	GLY	2.1
1	A	96	LEU	2.1
1	A	423	SER	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.