



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:19 am BST

PDB ID : 6N0V  
Title : tRNA ligase  
Authors : Banerjee, A.; Goldgur, Y.; Shuman, S.  
Deposited on : 2018-11-07  
Resolution : 2.50 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

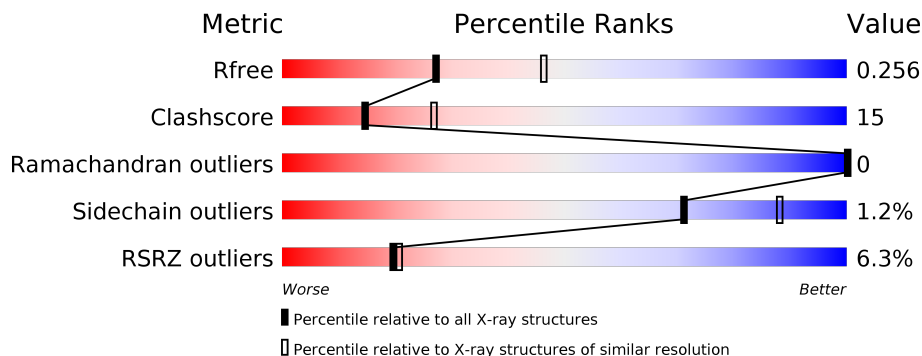
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


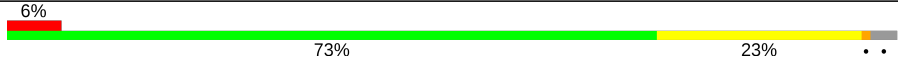
The reported resolution of this entry is 2.50 Å.

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	407	
1	B	407	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6506 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 ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	395	3178	2013	554	603	1	7	0	0	0
1	B	395	3178	2013	554	603	1	7	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

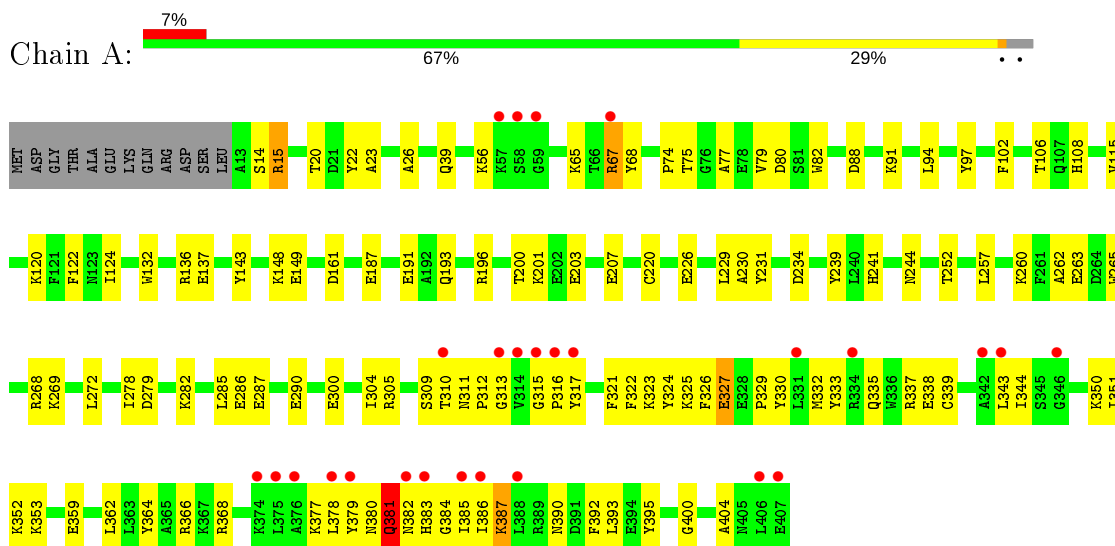
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	94	Total	O	0	0
			94	94		

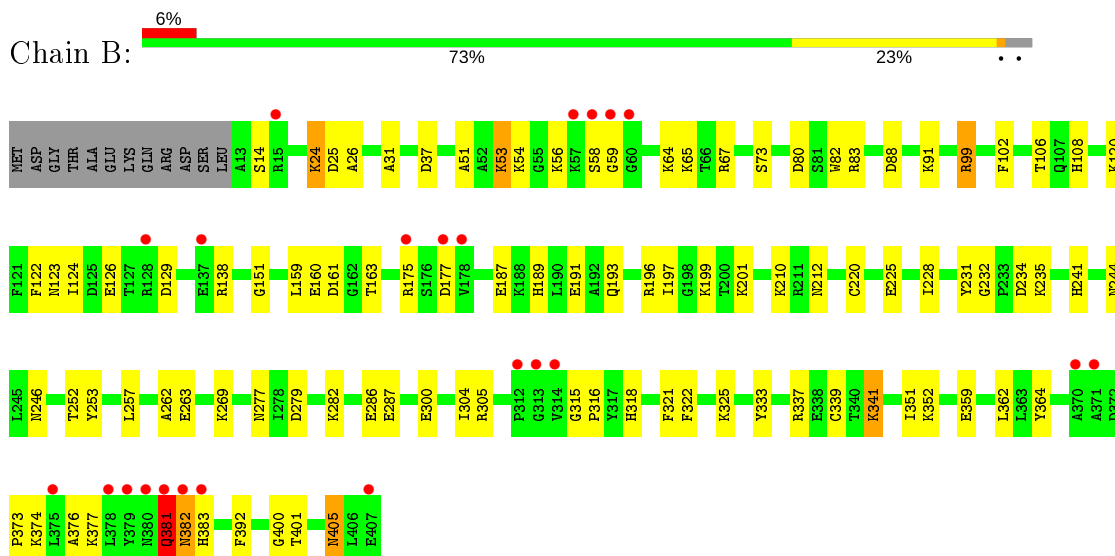
### 3 Residue-property plots [i](#)

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



- Molecule 1: tRNA ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.23Å 114.07Å 68.20Å 90.00° 100.36° 90.00°	Depositor
Resolution (Å)	46.48 – 2.50 45.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (46.48-2.50) 85.5 (45.69-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, $R_{free}$	0.212 , 0.256 0.212 , 0.256	Depositor DCC
$R_{free}$ test set	1927 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.2	Xtrriage
Anisotropy	0.425	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6506	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.90% 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: APK, MN

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	0.47	0/3218	0.71	3/4343 (0.1%)
1	B	0.52	2/3218 (0.1%)	0.71	2/4343 (0.0%)
All	All	0.50	2/6436 (0.0%)	0.71	5/8686 (0.1%)

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
1	A	0	2
1	B	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	GLN	CG-CD	-5.06	1.39	1.51
1	B	99	ARG	CZ-NH2	-5.04	1.26	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	53	LYS	CB-CG-CD	-7.68	91.64	111.60
1	A	327	GLU	CA-CB-CG	6.08	126.78	113.40
1	B	99	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	67	ARG	CG-CD-NE	5.41	123.16	111.80
1	A	327	GLU	N-CA-CB	-5.38	100.93	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	PHE	Peptide
1	A	381	GLN	Peptide
1	B	382	ASN	Peptide
1	B	405	ASN	Peptide

## 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	3178	0	3124	118	1
1	B	3178	0	3125	77	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	54	0	0	7	0
3	B	94	0	0	9	0
All	All	6506	0	6249	193	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 15.

All (193) 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:148:APK:C1'	1:A:148:APK:O4'	1.64	1.12
1:B:374:LYS:HA	1:B:377:LYS:HD3	1.49	0.93
1:A:382:ASN:ND2	3:A:601:HOH:O	2.02	0.92
1:A:106:THR:HG22	1:A:108:HIS:H	1.37	0.87
1:B:106:THR:HG22	1:B:108:HIS:H	1.44	0.83
1:B:373:PRO:O	1:B:376:ALA:N	2.11	0.82
1:B:99:ARG:NH2	3:B:601:HOH:O	2.01	0.81
1:B:305:ARG:HG2	1:B:321:PHE:CE2	2.18	0.78
1:A:120:LYS:HD3	1:A:122:PHE:CZ	2.19	0.77
1:A:39:GLN:NE2	1:B:315:GLY:O	2.17	0.76
1:B:53:LYS:HE3	1:B:54:LYS:H	1.50	0.76
1:A:379:TYR:CE1	1:A:385:ILE:HD13	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ARG:NE	1:A:15:ARG:HA	2.00	0.76
1:B:300:GLU:OE2	1:B:325:LYS:NZ	2.19	0.75
1:A:230:ALA:HB2	1:A:386:ILE:HD13	1.67	0.75
1:A:364:TYR:CD1	1:A:392:PHE:HB2	2.24	0.73
1:B:88:ASP:HA	1:B:91:LYS:HE3	1.72	0.72
1:A:379:TYR:CZ	1:A:385:ILE:HD13	2.26	0.70
1:B:129:ASP:OD1	1:B:138:ARG:NH1	2.24	0.69
1:A:68:TYR:N	1:A:79:VAL:O	2.22	0.69
1:B:99:ARG:NH1	3:B:604:HOH:O	2.24	0.69
1:B:26:ALA:HB1	1:B:257:LEU:HD23	1.74	0.68
1:A:387:LYS:HD2	1:A:387:LYS:H	1.59	0.67
1:A:290:GLU:OE1	3:A:603:HOH:O	2.13	0.66
1:A:387:LYS:NZ	3:A:605:HOH:O	2.16	0.66
1:A:310:THR:HG23	1:A:316:PRO:CG	2.26	0.66
1:A:392:PHE:HA	1:A:395:TYR:HB3	1.77	0.66
1:A:379:TYR:OH	3:A:602:HOH:O	2.11	0.65
1:A:94:LEU:HB2	1:A:97:TYR:CZ	2.31	0.65
1:B:161:ASP:OD1	1:B:163:THR:HG22	1.96	0.65
1:A:343:LEU:HD21	1:A:366:ARG:HG3	1.80	0.64
1:B:65:LYS:HD2	1:B:82:TRP:CH2	2.33	0.64
1:A:310:THR:HG23	1:A:316:PRO:HG3	1.80	0.64
1:A:75:THR:HG22	1:A:161:ASP:OD2	1.97	0.64
1:A:187:GLU:O	1:A:191:GLU:HG3	1.98	0.63
1:A:88:ASP:HA	1:A:91:LYS:HE3	1.81	0.62
1:A:377:LYS:HZ3	1:A:377:LYS:HB2	1.65	0.62
1:A:120:LYS:HD3	1:A:122:PHE:CE2	2.35	0.61
1:A:310:THR:OG1	1:A:311:ASN:N	2.34	0.61
1:A:207:GLU:OE1	3:A:604:HOH:O	2.15	0.60
1:B:67:ARG:NE	1:B:80:ASP:OD1	2.29	0.60
1:B:316:PRO:HG2	1:B:318:HIS:CE1	2.36	0.60
1:A:193:GLN:HA	1:A:196:ARG:NH1	2.16	0.60
1:B:53:LYS:CE	1:B:54:LYS:H	2.15	0.60
1:A:339:CYS:HB3	1:A:362:LEU:HD21	1.83	0.59
1:B:122:PHE:HB3	1:B:126:GLU:HG2	1.84	0.59
1:B:263:GLU:HG3	1:B:269:LYS:HE2	1.85	0.59
1:B:175:ARG:HH11	1:B:175:ARG:HG2	1.68	0.58
1:A:14:SER:O	1:A:14:SER:OG	2.20	0.58
1:B:123:ASN:OD1	1:B:124:ILE:N	2.37	0.57
1:A:14:SER:HB2	1:A:287:GLU:OE2	2.06	0.56
1:B:287:GLU:HG2	3:B:616:HOH:O	2.05	0.56
1:A:230:ALA:HB2	1:A:386:ILE:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:HB3	1:A:383:HIS:HB3	1.86	0.56
1:A:67:ARG:HA	1:A:80:ASP:HA	1.88	0.56
1:A:384:GLY:N	3:A:605:HOH:O	2.38	0.55
1:B:401:THR:O	1:B:405:ASN:ND2	2.39	0.55
1:A:120:LYS:HE3	1:A:122:PHE:HE2	1.71	0.54
1:A:364:TYR:OH	1:A:368:ARG:NH1	2.40	0.54
1:A:382:ASN:HB3	1:A:385:ILE:HG13	1.89	0.54
1:A:325:LYS:O	1:A:327:GLU:OE2	2.26	0.54
1:B:151:GLY:O	3:B:602:HOH:O	2.19	0.54
1:B:53:LYS:HE3	1:B:54:LYS:N	2.19	0.54
1:A:137:GLU:OE1	1:A:312:PRO:HG3	2.07	0.53
1:A:305:ARG:HG2	1:A:321:PHE:CE2	2.43	0.53
1:A:20:THR:O	1:A:269:LYS:NZ	2.38	0.53
1:B:24:LYS:NZ	1:B:25:ASP:OD1	2.41	0.53
1:A:65:LYS:HB2	1:A:82:TRP:CZ3	2.44	0.53
1:B:197:ILE:HD12	1:B:199:LYS:HD2	1.89	0.53
1:A:120:LYS:HE3	1:A:122:PHE:CE2	2.43	0.53
1:A:22:TYR:CD2	1:A:272:LEU:HD23	2.43	0.53
1:A:382:ASN:HB3	1:A:385:ILE:CG1	2.39	0.53
1:B:65:LYS:NZ	3:B:607:HOH:O	2.31	0.53
1:A:379:TYR:CE2	1:A:385:ILE:HA	2.44	0.52
1:A:311:ASN:O	1:A:313:GLY:N	2.42	0.52
1:B:123:ASN:HD21	1:B:325:LYS:HB2	1.74	0.52
1:B:304:ILE:HD13	1:B:322:PHE:CE1	2.45	0.52
1:B:339:CYS:HB3	1:B:362:LEU:HD21	1.92	0.51
1:A:26:ALA:HB1	1:A:257:LEU:HD23	1.92	0.51
1:B:225:GLU:HA	1:B:382:ASN:ND2	2.25	0.51
1:A:191:GLU:HG2	1:A:201:LYS:HE3	1.92	0.51
1:B:263:GLU:CG	1:B:269:LYS:HE2	2.41	0.51
1:A:377:LYS:HA	1:A:380:ASN:OD1	2.10	0.51
1:B:160:GLU:OE1	3:B:603:HOH:O	2.19	0.50
1:B:212:ASN:ND2	1:B:246:ASN:HB2	2.26	0.50
1:A:386:ILE:HG12	1:A:390:ASN:ND2	2.27	0.50
1:A:102:PHE:HB2	1:A:115:VAL:HB	1.94	0.50
1:A:382:ASN:ND2	1:A:385:ILE:HD11	2.27	0.50
1:A:333:TYR:OH	1:A:400:GLY:HA3	2.10	0.50
1:A:80:ASP:O	1:A:102:PHE:HA	2.12	0.50
1:B:228:ILE:HD13	1:B:337:ARG:NH1	2.27	0.50
1:A:244:ASN:ND2	1:A:252:THR:OG1	2.45	0.50
1:A:207:GLU:HG2	1:A:265:TRP:CZ2	2.47	0.50
1:A:310:THR:HG23	1:A:316:PRO:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LYS:NZ	1:B:83:ARG:HD3	2.27	0.50
1:B:189:HIS:HD2	3:B:680:HOH:O	1.93	0.50
1:A:377:LYS:O	1:A:377:LYS:HG2	2.12	0.49
1:A:241:HIS:O	1:A:305:ARG:NH2	2.45	0.49
1:A:300:GLU:OE2	1:A:325:LYS:HG2	2.12	0.49
1:A:364:TYR:HD1	1:A:392:PHE:HB2	1.75	0.49
1:A:230:ALA:CB	1:A:386:ILE:HD13	2.41	0.49
1:A:300:GLU:OE2	1:A:325:LYS:HE3	2.13	0.49
1:B:31:ALA:HB1	1:B:253:TYR:CZ	2.47	0.49
1:A:200:THR:CG2	1:A:203:GLU:HG3	2.43	0.48
1:A:200:THR:HG22	1:A:203:GLU:OE1	2.13	0.48
1:A:304:ILE:HD13	1:A:322:PHE:CE1	2.49	0.48
1:B:282:LYS:O	1:B:286:GLU:HG3	2.13	0.48
1:A:120:LYS:CE	1:A:122:PHE:CE2	2.96	0.48
1:B:234:ASP:O	1:B:235:LYS:HB2	2.14	0.48
1:A:65:LYS:NZ	3:A:607:HOH:O	2.30	0.47
1:B:364:TYR:CD2	1:B:392:PHE:HB2	2.49	0.47
1:B:80:ASP:O	1:B:102:PHE:HA	2.13	0.47
1:B:341:LYS:HG3	1:B:381:GLN:H	1.79	0.47
1:A:124:ILE:HD12	1:A:323:LYS:O	2.14	0.47
1:B:175:ARG:HB3	1:B:177:ASP:OD1	2.15	0.47
1:A:200:THR:HG22	1:A:203:GLU:HG3	1.97	0.46
1:B:234:ASP:OD1	1:B:234:ASP:N	2.48	0.46
1:B:381:GLN:HG2	1:B:382:ASN:N	2.26	0.46
1:B:73:SER:HB2	1:B:163:THR:HG21	1.96	0.46
1:A:220:CYS:HB3	1:A:231:TYR:CG	2.50	0.46
1:A:239:TYR:CZ	1:A:268:ARG:HD2	2.51	0.46
1:B:159:LEU:HD12	1:B:163:THR:HG23	1.97	0.46
1:A:234:ASP:N	1:A:234:ASP:OD2	2.48	0.46
1:A:15:ARG:HE	1:A:15:ARG:HA	1.80	0.46
1:A:393:LEU:HA	1:A:393:LEU:HD23	1.69	0.46
1:A:75:THR:HG23	1:A:77:ALA:HB2	1.98	0.45
1:B:123:ASN:ND2	1:B:325:LYS:HB2	2.30	0.45
1:A:263:GLU:CG	1:A:269:LYS:HE2	2.46	0.45
1:B:210:LYS:NZ	3:B:620:HOH:O	2.48	0.45
1:A:338:GLU:OE1	1:A:350:LYS:NZ	2.48	0.45
1:A:350:LYS:HD3	1:A:352:LYS:HE3	1.98	0.45
1:A:226:GLU:OE1	1:A:387:LYS:NZ	2.50	0.45
1:A:316:PRO:O	1:A:317:TYR:CD2	2.70	0.45
1:B:120:LYS:HD2	3:B:601:HOH:O	2.16	0.45
1:A:120:LYS:CD	1:A:122:PHE:CE2	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:LEU:HD23	1:A:383:HIS:CG	2.52	0.44
1:B:187:GLU:O	1:B:191:GLU:HG3	2.16	0.44
1:A:335:GLN:NE2	1:A:352:LYS:H	2.15	0.44
1:A:335:GLN:HE22	1:A:352:LYS:H	1.64	0.44
1:B:212:ASN:HD21	1:B:246:ASN:HB2	1.82	0.44
1:B:51:ALA:C	1:B:53:LYS:H	2.20	0.44
1:A:309:SER:HB3	1:A:316:PRO:O	2.18	0.44
1:A:337:ARG:HG3	1:A:385:ILE:HD12	1.98	0.44
1:A:23:ALA:HB1	1:A:260:LYS:HA	1.99	0.44
1:B:193:GLN:HA	1:B:196:ARG:NH1	2.33	0.44
1:B:64:LYS:HE3	1:B:64:LYS:HB3	1.75	0.44
1:A:220:CYS:HB3	1:A:231:TYR:CD1	2.53	0.43
1:A:234:ASP:O	1:A:268:ARG:NH2	2.51	0.43
1:B:351:ILE:HD13	1:B:359:GLU:HG2	1.99	0.43
1:B:382:ASN:HB3	1:B:383:HIS:CD2	2.54	0.43
1:B:333:TYR:OH	1:B:400:GLY:HA3	2.19	0.43
1:B:262:ALA:HB3	1:B:269:LYS:HG2	2.01	0.43
1:A:136:ARG:NH1	1:A:279:ASP:OD1	2.45	0.43
1:B:305:ARG:HG2	1:B:321:PHE:CZ	2.53	0.43
1:B:56:LYS:HB2	1:B:56:LYS:HE2	1.81	0.43
1:B:232:GLY:O	1:B:234:ASP:O	2.37	0.42
1:B:58:SER:OG	1:B:59:GLY:N	2.52	0.42
1:B:362:LEU:HD23	1:B:362:LEU:HA	1.84	0.42
1:A:344:ILE:CD1	1:A:379:TYR:HB3	2.50	0.42
1:A:262:ALA:HB3	1:A:269:LYS:HG2	2.01	0.42
1:A:282:LYS:O	1:A:286:GLU:HG3	2.20	0.42
1:B:244:ASN:ND2	1:B:252:THR:OG1	2.52	0.42
1:A:229:LEU:HD11	1:A:300:GLU:HB2	2.00	0.42
1:A:351:ILE:HD13	1:A:359:GLU:HG2	2.02	0.42
1:A:381:GLN:OE1	1:A:382:ASN:N	2.53	0.42
1:A:384:GLY:HA2	1:A:387:LYS:HD3	2.02	0.42
1:A:200:THR:HG23	1:A:203:GLU:H	1.84	0.42
1:B:382:ASN:HB3	1:B:383:HIS:HD2	1.83	0.42
1:B:277:ASN:OD1	1:B:279:ASP:HB2	2.20	0.42
1:B:123:ASN:HD21	1:B:325:LYS:H	1.68	0.42
1:B:54:LYS:HD2	1:B:54:LYS:HA	1.79	0.41
1:A:74:PRO:HD2	1:A:161:ASP:OD2	2.20	0.41
1:A:315:GLY:HA3	1:A:316:PRO:HD3	1.89	0.41
1:A:335:GLN:HE22	1:A:353:LYS:H	1.67	0.41
1:B:220:CYS:HB3	1:B:231:TYR:CD2	2.55	0.41
1:A:124:ILE:H	1:A:124:ILE:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ASN:C	1:A:313:GLY:H	2.24	0.41
1:A:132:TRP:CZ3	1:A:282:LYS:HB2	2.55	0.41
1:A:143:TYR:CE2	1:A:278:ILE:HD13	2.56	0.41
1:A:191:GLU:OE2	1:A:201:LYS:NZ	2.37	0.41
1:A:329:PRO:HD2	1:A:330:TYR:CE1	2.56	0.41
1:A:332:MET:CE	1:A:404:ALA:HA	2.51	0.41
1:B:191:GLU:HG2	1:B:201:LYS:HE3	2.02	0.41
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.93	0.41
1:B:374:LYS:HG2	1:B:377:LYS:HD3	2.03	0.40
1:B:64:LYS:HZ1	1:B:83:ARG:HD3	1.86	0.40
1:A:200:THR:OG1	1:A:201:LYS:N	2.55	0.40
1:A:317:TYR:HB2	1:B:37:ASP:OD2	2.20	0.40
1:A:383:HIS:CG	1:A:384:GLY:N	2.89	0.40
1:A:56:LYS:HB2	1:A:56:LYS:HE2	1.91	0.40
1:B:241:HIS:O	1:B:305:ARG:NH2	2.54	0.40
1:A:148:APK:H8	1:A:149:GLU:O	2.20	0.40
1:A:285:LEU:HD13	1:A:324:TYR:CD2	2.56	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:67:ARG:O	1:B:53:LYS:NZ[4_556]	2.00	0.20

## 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	392/407 (96%)	374 (95%)	18 (5%)	0	100	100
1	B	392/407 (96%)	373 (95%)	19 (5%)	0	100	100
All	All	784/814 (96%)	747 (95%)	37 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	329/339 (97%)	326 (99%)	3 (1%)	78	92
1	B	329/339 (97%)	324 (98%)	5 (2%)	65	85
All	All	658/678 (97%)	650 (99%)	8 (1%)	71	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	381	GLN
1	A	387	LYS
1	B	14	SER
1	B	24	LYS
1	B	341	LYS
1	B	352	LYS
1	B	381	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	A	244	ASN
1	A	335	GLN
1	B	189	HIS
1	B	212	ASN
1	B	244	ASN
1	B	354	HIS
1	B	382	ASN
1	B	383	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	APK	B	148	1,2	29,33,33	2.75	8 (27%)	28,47,47	1.46	3 (10%)
1	APK	A	148	1,2	29,33,33	5.21	14 (48%)	28,47,47	1.55	2 (7%)

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
1	APK	B	148	1,2	-	7/15/37/37	0/3/3/3
1	APK	A	148	1,2	-	7/15/37/37	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	APK	O4'-C1'	16.48	1.64	1.41
1	A	148	APK	C2'-C1'	-15.03	1.30	1.53
1	A	148	APK	P-NZ	11.77	1.74	1.61
1	B	148	APK	P-NZ	11.23	1.73	1.61
1	A	148	APK	O4'-C4'	-5.59	1.32	1.45
1	A	148	APK	CB-CA	5.08	1.60	1.53
1	B	148	APK	CB-CA	4.82	1.60	1.53
1	B	148	APK	P-O1P	4.21	1.52	1.46
1	A	148	APK	P-O1P	3.71	1.52	1.46
1	B	148	APK	C6-N6	3.63	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	APK	C6-N6	3.54	1.47	1.34
1	A	148	APK	P-O5'	3.03	1.69	1.57
1	B	148	APK	P-O2P	-3.01	1.48	1.56
1	A	148	APK	O2'-C2'	2.95	1.49	1.43
1	A	148	APK	O3'-C3'	-2.88	1.36	1.43
1	A	148	APK	P-O2P	-2.79	1.49	1.56
1	B	148	APK	C2-N3	2.57	1.36	1.32
1	A	148	APK	C5'-C4'	2.36	1.59	1.51
1	B	148	APK	C6-C5	-2.21	1.35	1.43
1	A	148	APK	C2-N3	2.17	1.35	1.32
1	A	148	APK	C5-C4	-2.07	1.35	1.40
1	B	148	APK	C5-C4	-2.00	1.35	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	APK	N3-C2-N1	-5.62	119.89	128.68
1	B	148	APK	N3-C2-N1	-5.17	120.59	128.68
1	A	148	APK	C3'-C2'-C1'	4.20	107.31	100.98
1	B	148	APK	O2P-P-O1P	3.45	117.16	109.92
1	B	148	APK	O5'-P-O1P	-2.00	106.54	114.24

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	148	APK	C5'-O5'-P-NZ
1	B	148	APK	C5'-O5'-P-O2P
1	B	148	APK	C4'-C5'-O5'-P
1	A	148	APK	C5'-O5'-P-NZ
1	A	148	APK	C5'-O5'-P-O2P
1	A	148	APK	C4'-C5'-O5'-P
1	B	148	APK	C3'-C4'-C5'-O5'
1	A	148	APK	C3'-C4'-C5'-O5'
1	B	148	APK	O4'-C4'-C5'-O5'
1	A	148	APK	O4'-C4'-C5'-O5'
1	B	148	APK	C5'-O5'-P-O1P
1	A	148	APK	C5'-O5'-P-O1P
1	B	148	APK	CE-CD-CG-CB
1	A	148	APK	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	148	APK	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [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	394/407 (96%)	0.39	27 (6%) 16 17	31, 63, 119, 169	0
1	B	394/407 (96%)	0.13	23 (5%) 23 24	26, 49, 115, 179	0
All	All	788/814 (96%)	0.26	50 (6%) 20 21	26, 57, 118, 179	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	379	TYR	8.3
1	B	382	ASN	7.9
1	B	381	GLN	7.5
1	A	376	ALA	6.0
1	A	59	GLY	5.8
1	A	379	TYR	5.5
1	B	378	LEU	5.2
1	A	407	GLU	5.1
1	A	58	SER	5.1
1	B	60	GLY	4.6
1	A	383	HIS	4.6
1	B	383	HIS	4.3
1	A	378	LEU	4.3
1	B	57	LYS	3.7
1	A	314	VAL	3.6
1	A	374	LYS	3.5
1	B	371	ALA	3.4
1	B	58	SER	3.3
1	A	386	ILE	3.3
1	B	380	ASN	3.2
1	A	57	LYS	3.2
1	A	343	LEU	3.2
1	B	15	ARG	3.2
1	B	312	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	406	LEU	3.1
1	A	346	GLY	3.1
1	A	334	ARG	3.1
1	A	316	PRO	3.0
1	A	67	ARG	3.0
1	B	375	LEU	3.0
1	B	313	GLY	2.8
1	B	59	GLY	2.8
1	A	382	ASN	2.7
1	B	137	GLU	2.7
1	B	175	ARG	2.7
1	A	317	TYR	2.6
1	B	314	VAL	2.6
1	A	375	LEU	2.6
1	B	407	GLU	2.6
1	A	315	GLY	2.6
1	A	331	LEU	2.6
1	B	177	ASP	2.5
1	B	370	ALA	2.5
1	A	310	THR	2.4
1	A	388	LEU	2.4
1	A	342	ALA	2.3
1	B	178	VAL	2.2
1	A	385	ILE	2.1
1	A	313	GLY	2.1
1	B	128	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	APK	A	148	31/31	0.94	0.15	38,53,66,74	0
1	APK	B	148	31/31	0.97	0.13	26,35,49,69	0

## 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(Å <sup>2</sup> )	Q<0.9
2	MN	A	501	1/1	0.75	0.35	130,130,130,130	0
2	MN	B	501	1/1	0.94	0.14	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.