



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 05:08 AM EDT

PDB ID : 1VS0  
Title : Crystal Structure of the Ligase Domain from M. tuberculosis LigD at 2.4Å  
Authors : Akey, D.; Martins, A.; Aniukwu, J.; Glickman, M.S.; Shuman, S.; Berger, J.M.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2006-01-27  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

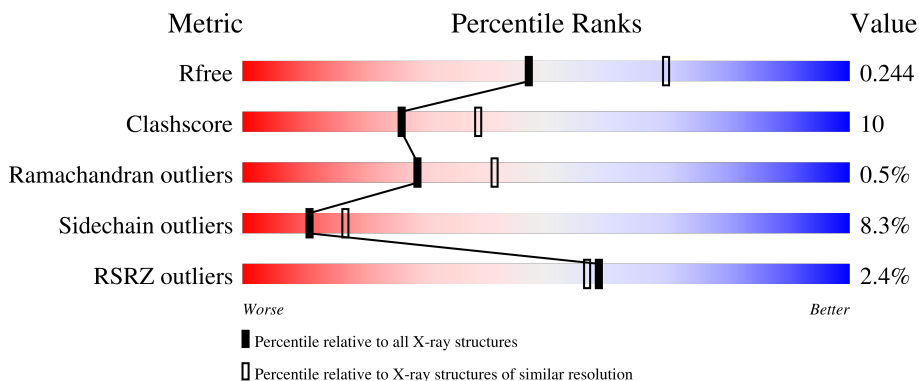
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of 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	310	<div> <div>3%</div> <div>79%</div> <div>15%</div> <div>• •</div> </div>
1	B	310	<div> <div>2%</div> <div>72%</div> <div>21%</div> <div>5%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	9005	-	-	X	-
3	CL	A	9007	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5287 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 DNA ligase-like protein Rv0938/MT0965.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	P	S	Se	26	4	0
			2409	1507	452	442	1	3	4			
1	B	305	Total	C	N	O	P	S	Se	46	7	0
			2462	1536	460	457	1	3	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	450	GLY	-	CLONING ARTIFACT	UNP P71571
A	451	ALA	-	CLONING ARTIFACT	UNP P71571
A	461	MSE	MET	MODIFIED RESIDUE	UNP P71571
A	481	APK	LYS	MODIFIED RESIDUE	UNP P71571
A	545	MSE	MET	MODIFIED RESIDUE	UNP P71571
A	665	MSE	MET	MODIFIED RESIDUE	UNP P71571
A	694	MSE	MET	MODIFIED RESIDUE	UNP P71571
B	450	GLY	-	CLONING ARTIFACT	UNP P71571
B	451	ALA	-	CLONING ARTIFACT	UNP P71571
B	461	MSE	MET	MODIFIED RESIDUE	UNP P71571
B	481	APK	LYS	MODIFIED RESIDUE	UNP P71571
B	545	MSE	MET	MODIFIED RESIDUE	UNP P71571
B	665	MSE	MET	MODIFIED RESIDUE	UNP P71571
B	694	MSE	MET	MODIFIED RESIDUE	UNP P71571

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	2	Total	Cl	0	0
			2	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

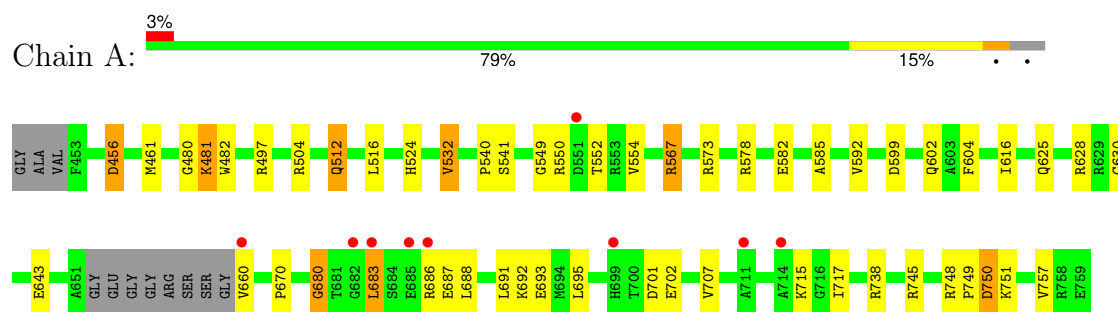
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total	O	0	0
			223	223		
5	B	184	Total	O	0	0
			184	184		

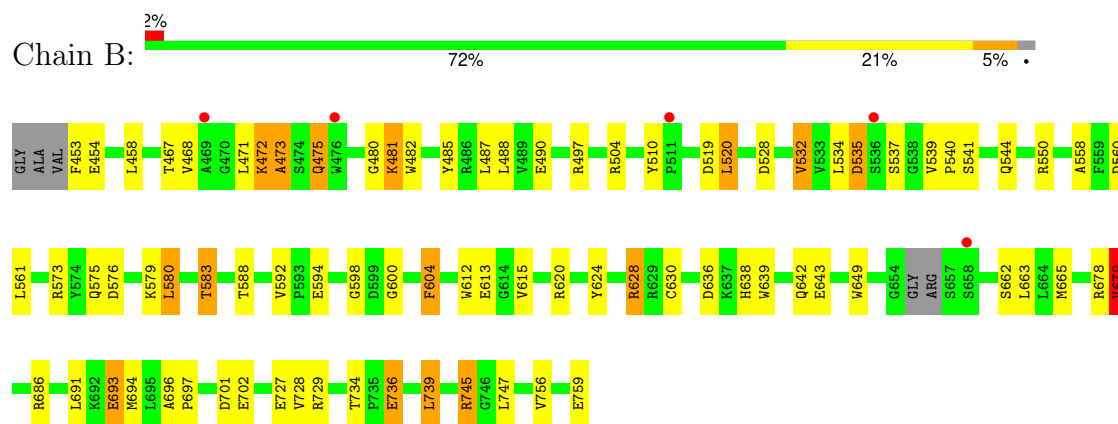
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Putative DNA ligase-like protein Rv0938/MT0965



- Molecule 1: Putative DNA ligase-like protein Rv0938/MT0965



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.10Å 57.10Å 368.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.40 28.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.40) 99.2 (28.55-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	19.74 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.192 , 0.248 0.186 , 0.244	Depositor DCC
$R_{free}$ test set	1453 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5287	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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

### 5.1 Standard geometry

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

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	2/2428 (0.1%)	0.81	2/3278 (0.1%)
1	B	1.06	6/2483 (0.2%)	0.95	8/3350 (0.2%)
All	All	0.91	8/4911 (0.2%)	0.88	10/6628 (0.2%)

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	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	504	ARG	CD-NE	-31.17	0.93	1.46
1	B	472	LYS	CD-CE	-17.76	1.06	1.51
1	B	693	GLU	CG-CD	-12.24	1.33	1.51
1	B	686	ARG	CD-NE	10.50	1.64	1.46
1	A	550	ARG	CB-CG	9.69	1.78	1.52
1	B	454	GLU	CG-CD	-9.04	1.38	1.51
1	B	628	ARG	CG-CD	-8.38	1.30	1.51
1	A	504	ARG	CG-CD	-5.71	1.37	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	504	ARG	CG-CD-NE	19.33	152.40	111.80
1	B	472	LYS	CD-CE-NZ	14.06	144.04	111.70
1	B	472	LYS	CG-CD-CE	12.16	148.39	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	504	ARG	CD-NE-CZ	9.76	137.26	123.60
1	B	679	VAL	CB-CA-C	-6.42	99.20	111.40
1	B	686	ARG	CG-CD-NE	-5.82	99.58	111.80
1	B	487	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	739	LEU	CA-CB-CG	5.12	127.09	115.30
1	A	715	LYS	CB-CG-CD	-5.08	98.40	111.60
1	A	504	ARG	CG-CD-NE	5.04	122.38	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	GLY	Mainchain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2409	0	2360	38	2
1	B	2462	0	2399	56	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	3	1
3	B	2	0	0	1	1
4	A	1	0	0	0	0
5	A	223	0	0	13	1
5	B	184	0	0	10	2
All	All	5287	0	4759	96	5

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 10.

All (96) 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:481:APK:HC	1:A:482:TRP:N	0.98	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:APK:HC	1:A:482:TRP:CA	1.81	1.10
1:B:480:GLY:C	1:B:481:APK:H2	1.63	0.93
1:A:582:GLU:OE2	5:A:9022:HOH:O	1.88	0.92
1:B:532:VAL:HG22	1:B:540:PRO:HB3	1.54	0.90
1:B:612:TRP:O	1:B:638:HIS:HE1	1.57	0.87
1:B:453:PHE:N	5:B:9083:HOH:O	2.08	0.84
1:B:643[B]:GLU:HG3	1:B:756:VAL:HG13	1.61	0.83
1:B:665:MSE:SE	1:B:679:VAL:HG22	2.31	0.81
1:A:512:GLN:NE2	1:A:554:VAL:HB	1.97	0.79
1:B:481:APK:C	1:B:482:TRP:CA	2.60	0.79
1:A:497:ARG:HD2	5:A:9064:HOH:O	1.81	0.79
1:A:628:ARG:HG2	1:A:628:ARG:HH11	1.47	0.79
1:B:480:GLY:C	1:B:481:APK:H	1.84	0.79
1:A:670:PRO:HA	5:A:9175:HOH:O	1.83	0.78
1:B:612:TRP:O	1:B:638:HIS:CE1	2.36	0.78
1:A:512:GLN:HE22	1:A:554:VAL:HB	1.46	0.78
1:A:524:HIS:ND1	5:A:9220:HOH:O	2.16	0.76
1:B:458:LEU:HD23	1:B:488:LEU:HD13	1.66	0.76
1:A:532:VAL:HG22	1:A:540:PRO:HB3	1.66	0.75
1:B:575:GLN:HG2	1:B:620:ARG:HB3	1.68	0.74
1:A:738:ARG:HD3	5:A:9193:HOH:O	1.88	0.73
1:B:639:TRP:CE3	1:B:729:ARG:HD3	2.27	0.70
1:B:535:ASP:OD2	1:B:539:VAL:HB	1.90	0.70
1:B:535:ASP:HB3	1:B:537:SER:H	1.57	0.69
1:A:481:APK:C	1:A:482:TRP:CA	2.56	0.68
1:A:745[B]:ARG:NH2	5:A:9181:HOH:O	2.27	0.67
1:A:660:VAL:HG21	1:A:692:LYS:HB2	1.76	0.67
1:B:535:ASP:HB2	1:B:539:VAL:H	1.60	0.66
1:A:549:GLY:H	1:A:552:THR:CG2	2.08	0.65
1:A:628:ARG:HG2	1:A:628:ARG:NH1	2.14	0.62
1:A:643:GLU:OE2	1:A:751:LYS:HD3	2.00	0.62
1:A:549:GLY:H	1:A:552:THR:HG23	1.64	0.61
1:B:481:APK:H2'	5:B:9188:HOH:O	2.00	0.60
1:A:749:PRO:HD2	5:A:9150:HOH:O	2.01	0.59
1:B:745:ARG:HD2	5:B:9103:HOH:O	2.02	0.58
1:A:578:ARG:O	1:A:582:GLU:HG2	2.02	0.58
1:B:473:ALA:O	1:B:620:ARG:NH1	2.36	0.58
1:B:642:GLN:HE22	1:B:759:GLU:H	1.51	0.57
3:B:9006:CL:CL	5:B:9188:HOH:O	2.54	0.57
1:B:579:LYS:O	1:B:583:THR:HG23	2.05	0.56
1:B:480:GLY:O	1:B:481:APK:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:745:ARG:CD	5:B:9103:HOH:O	2.54	0.56
1:B:535:ASP:HB3	1:B:537:SER:N	2.20	0.55
1:B:481:APK:CA	1:B:482:TRP:N	2.64	0.55
1:B:485:TYR:HD2	1:B:510:TYR:OH	1.90	0.55
1:B:630:CYS:HB3	5:B:9182:HOH:O	2.06	0.55
1:A:599:ASP:H	1:A:602[B]:GLN:NE2	2.05	0.53
1:A:481:APK:CA	1:A:482:TRP:N	2.65	0.53
1:B:678[A]:ARG:NH1	5:B:9041:HOH:O	2.42	0.52
1:B:541:SER:HB3	1:B:544:GLN:HB2	1.92	0.52
1:A:748:ARG:HB3	1:A:751:LYS:HD2	1.93	0.50
1:B:662:SER:OG	1:B:678[B]:ARG:HD2	2.11	0.50
1:B:468:VAL:O	1:B:600:GLY:HA3	2.11	0.50
1:B:745:ARG:HH11	1:B:745:ARG:HG3	1.76	0.50
1:B:696:ALA:N	1:B:697:PRO:HD2	2.28	0.49
1:B:520:LEU:HD12	1:B:588:THR:HG21	1.95	0.49
1:B:665:MSE:SE	1:B:679:VAL:CG2	3.08	0.49
1:A:481:APK:C	1:A:482:TRP:HA	2.41	0.48
3:A:9005:CL:CL	5:A:9163:HOH:O	2.58	0.48
1:B:467:THR:HA	1:B:636:ASP:OD2	2.15	0.47
1:A:680:GLY:HA2	1:A:683:LEU:HD11	1.95	0.47
1:B:579:LYS:HB2	1:B:579:LYS:HE2	1.59	0.47
1:A:567:ARG:HD2	5:A:9160:HOH:O	2.14	0.46
1:A:630:CYS:HB3	5:A:9124:HOH:O	2.15	0.46
1:A:481:APK:H8	1:A:482:TRP:O	2.16	0.46
1:A:687:GLU:O	1:A:691:LEU:HD23	2.16	0.46
1:B:472:LYS:HB2	5:B:9160:HOH:O	2.16	0.46
1:B:490:GLU:OE1	1:B:497:ARG:HD3	2.16	0.46
1:A:573:ARG:HG2	5:A:9101:HOH:O	2.16	0.45
1:B:558:ALA:HB3	1:B:592:VAL:HG22	1.99	0.45
1:B:727:GLU:OE2	1:B:745:ARG:NH1	2.50	0.45
1:B:473:ALA:HB2	1:B:598:GLY:O	2.15	0.45
1:B:468:VAL:HA	1:B:471:LEU:HD12	1.98	0.44
1:B:649:TRP:HB3	1:B:663:LEU:HD23	1.98	0.44
1:A:549:GLY:H	1:A:552:THR:HG21	1.79	0.44
1:B:482:TRP:HB3	1:B:540:PRO:HG2	1.99	0.44
1:B:573:ARG:HG2	1:B:576:ASP:OD2	2.17	0.44
1:B:736:GLU:HG2	5:B:9067:HOH:O	2.18	0.44
1:B:561:LEU:HD23	1:B:580:LEU:HB3	2.00	0.44
1:A:573:ARG:HD3	5:A:9153:HOH:O	2.18	0.43
1:A:585:ALA:HB2	1:A:592:VAL:HG21	1.99	0.43
1:A:481:APK:O3'	3:A:9005:CL:CL	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:ASP:OD2	1:B:624:TYR:OH	2.28	0.43
1:B:663:LEU:HD11	1:B:691:LEU:HD13	2.00	0.43
1:A:748:ARG:NH2	3:A:9007:CL:CL	2.83	0.42
1:B:485:TYR:CD2	1:B:510:TYR:OH	2.71	0.42
1:B:604:PHE:HD2	1:B:604:PHE:HA	1.68	0.42
1:B:736:GLU:CG	5:B:9067:HOH:O	2.68	0.42
1:A:628:ARG:HD2	5:A:9162:HOH:O	2.20	0.42
1:B:475:GLN:O	1:B:620:ARG:HG3	2.19	0.41
1:B:693:GLU:HB3	1:B:694[A]:MSE:HE2	2.03	0.41
1:A:585:ALA:HB2	1:A:592:VAL:CG2	2.51	0.41
1:B:561:LEU:CD2	1:B:580:LEU:HB3	2.51	0.40
1:A:461:MSE:SE	1:A:625:GLN:H	2.54	0.40
1:B:734:THR:OG1	1:B:736:GLU:HG2	2.21	0.40

All (5) 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:456:ASP:OD2	1:B:701:ASP:OD2[2_674]	1.94	0.26
3:B:9008:CL:CL	5:B:9178:HOH:O[4_456]	1.99	0.21
1:A:456:ASP:OD2	1:A:750:ASP:OD2[6_655]	2.06	0.14
5:B:9037:HOH:O	5:B:9124:HOH:O[4_566]	2.16	0.04
3:A:9007:CL:CL	5:A:9220:HOH:O[6_665]	2.17	0.03

## 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	298/310 (96%)	292 (98%)	5 (2%)	1 (0%)	41	55
1	B	307/310 (99%)	300 (98%)	5 (2%)	2 (1%)	22	32
All	All	605/620 (98%)	592 (98%)	10 (2%)	3 (0%)	29	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	535	ASP
1	B	473	ALA
1	A	680	GLY

### 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	244/241 (101%)	225 (92%)	19 (8%)	12	19
1	B	250/241 (104%)	229 (92%)	21 (8%)	11	16
All	All	494/482 (102%)	454 (92%)	40 (8%)	11	18

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	456	ASP
1	A	512	GLN
1	A	516	LEU
1	A	532	VAL
1	A	541	SER
1	A	567	ARG
1	A	604	PHE
1	A	616	ILE
1	A	683	LEU
1	A	686	ARG
1	A	688	LEU
1	A	693	GLU
1	A	695	LEU
1	A	701	ASP
1	A	702	GLU
1	A	707	VAL
1	A	717	ILE
1	A	750	ASP
1	A	757	VAL
1	B	475	GLN

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Mol	Chain	Res	Type
1	B	519	ASP
1	B	520	LEU
1	B	532	VAL
1	B	534	LEU
1	B	550	ARG
1	B	560	ASP
1	B	580	LEU
1	B	583	THR
1	B	594	GLU
1	B	604	PHE
1	B	613	GLU
1	B	615	VAL
1	B	628	ARG
1	B	679	VAL
1	B	702	GLU
1	B	728	VAL
1	B	736	GLU
1	B	739	LEU
1	B	745	ARG
1	B	747	LEU

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

Mol	Chain	Res	Type
1	A	512	GLN
1	A	586	ASN
1	A	610	HIS
1	A	640	ASN
1	B	544	GLN
1	B	638	HIS
1	B	642	GLN
1	B	699	HIS
1	B	741	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	481	2,1	28,33,33	1.24	4 (14%)	27,47,47	2.75	8 (29%)
1	APK	A	481	2,1	28,33,33	1.52	4 (14%)	27,47,47	2.47	4 (14%)

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	481	2,1	-	0/15/37/37	0/3/3/3
1	APK	A	481	2,1	-	1/15/37/37	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	481	APK	O4'-C1'	3.91	1.46	1.40
1	A	481	APK	P-O2P	-3.56	1.47	1.56
1	B	481	APK	P-O2P	-3.12	1.48	1.56
1	A	481	APK	P-NZ	2.84	1.65	1.61
1	B	481	APK	O4'-C1'	2.71	1.44	1.40
1	B	481	APK	P-NZ	-2.64	1.58	1.61
1	A	481	APK	P-O1P	2.37	1.49	1.46
1	B	481	APK	O5'-C5'	-2.10	1.36	1.44

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	APK	P-NZ-CE	-9.34	111.58	124.61
1	B	481	APK	O4'-C1'-N9	6.85	117.83	108.75
1	B	481	APK	P-NZ-CE	-6.80	115.12	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	APK	N3-C2-N1	-6.01	120.52	128.67
1	B	481	APK	O2P-P-O1P	5.41	121.48	109.87
1	A	481	APK	N3-C2-N1	-4.98	121.91	128.67
1	A	481	APK	O2P-P-O1P	4.08	118.63	109.87
1	A	481	APK	O3'-C3'-C2'	-3.43	100.82	111.82
1	B	481	APK	C4'-O4'-C1'	-2.93	107.24	109.92
1	B	481	APK	CD-CE-NZ	-2.72	104.27	111.63
1	B	481	APK	C4-C5-N7	-2.71	106.47	109.34
1	B	481	APK	O3'-C3'-C2'	-2.60	103.47	111.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	481	APK	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	481	APK	6	0
1	A	481	APK	7	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	480:GLY	C	481:APK	N	1.81
1	A	481:APK	C	482:TRP	N	1.75
1	B	481:APK	C	482:TRP	N	1.71

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	294/310 (94%)	-0.25	9 (3%)	49	47	15, 28, 54, 78	6 (2%)
1	B	300/310 (96%)	-0.20	5 (1%)	70	68	21, 33, 49, 65	12 (4%)
All	All	594/620 (95%)	-0.23	14 (2%)	59	57	15, 31, 52, 78	18 (3%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	685	GLU	4.1
1	A	682	GLY	3.9
1	B	476	TRP	3.7
1	A	699	HIS	3.3
1	A	686	ARG	3.0
1	B	469	ALA	3.0
1	B	658	SER	2.8
1	B	536	SER	2.6
1	A	714	ALA	2.6
1	A	683	LEU	2.4
1	A	711	ALA	2.3
1	A	551	ASP	2.2
1	B	511	PRO	2.2
1	A	660	VAL	2.1

### 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( $\text{\AA}^2$ )	Q<0.9
1	APK	B	481	31/31	0.97	0.20	24,32,36,38	0
1	APK	A	481	31/31	0.98	0.17	13,24,29,31	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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
3	CL	B	9006	1/1	0.94	0.06	54,54,54,54	0
2	ZN	B	9001	1/1	0.95	0.04	34,34,34,34	0
3	CL	A	9005	1/1	0.96	0.05	38,38,38,38	0
4	MG	A	9009	1/1	0.96	0.06	23,23,23,23	0
3	CL	A	9007	1/1	0.99	0.03	24,24,24,24	0
2	ZN	A	9002	1/1	0.99	0.04	21,21,21,21	0
3	CL	B	9008	1/1	0.99	0.02	26,26,26,26	0
2	ZN	A	9004	1/1	0.99	0.02	21,21,21,21	0
2	ZN	B	9003	1/1	1.00	0.01	23,23,23,23	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.