



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:46 am GMT

PDB ID : 3MX2  
Title : Lassa fever virus Nucleoprotein complexed with dTTP  
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Deposited on : 2010-05-06  
Resolution : 1.98 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

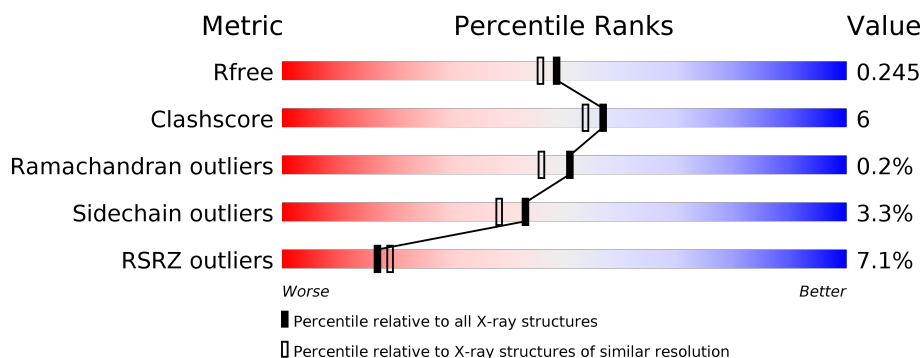
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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))
$R_{free}$	100719	9293 (2.00-1.96)
Clashscore	112137	10621 (2.00-1.96)
Ramachandran outliers	110173	10502 (2.00-1.96)
Sidechain outliers	110143	10501 (2.00-1.96)
RSRZ outliers	101464	9395 (2.00-1.96)

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	577	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	577	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div></div> <div>10%</div> </div> </div>
1	C	577	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>•</div> <div>11%</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
2	TTP	A	800	-	-	-	X
2	TTP	B	800	-	-	-	X
2	TTP	C	800	-	-	X	X
3	ZN	A	570	-	-	-	X
3	ZN	B	570	-	-	-	X
3	ZN	C	570	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12638 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4020	2525	699	769	27			
1	B	517	Total	C	N	O	S	0	0	0
			4041	2536	706	772	27			
1	C	513	Total	C	N	O	S	0	0	0
			4012	2519	698	768	27			

There are 24 discrepancies between the modelled and reference sequences:

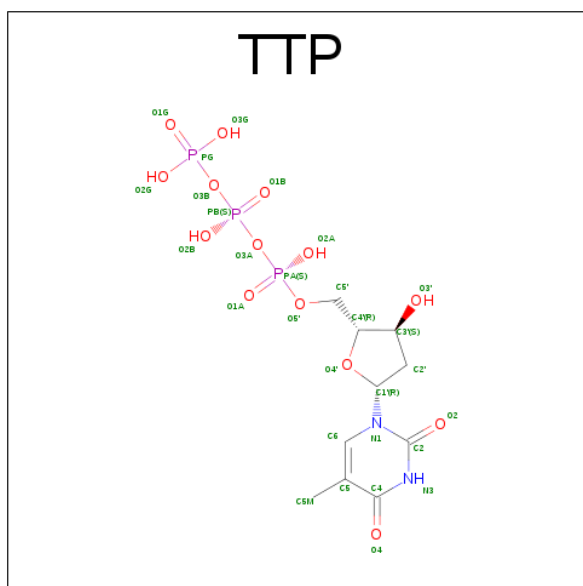
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP P13699
A	-6	ALA	-	EXPRESSION TAG	UNP P13699
A	-5	MET	-	EXPRESSION TAG	UNP P13699
A	-4	ASP	-	EXPRESSION TAG	UNP P13699
A	-3	HIS	-	EXPRESSION TAG	UNP P13699
A	-2	VAL	-	EXPRESSION TAG	UNP P13699
A	-1	GLU	-	EXPRESSION TAG	UNP P13699
A	0	PHE	-	EXPRESSION TAG	UNP P13699
B	-7	GLY	-	EXPRESSION TAG	UNP P13699
B	-6	ALA	-	EXPRESSION TAG	UNP P13699
B	-5	MET	-	EXPRESSION TAG	UNP P13699
B	-4	ASP	-	EXPRESSION TAG	UNP P13699
B	-3	HIS	-	EXPRESSION TAG	UNP P13699
B	-2	VAL	-	EXPRESSION TAG	UNP P13699
B	-1	GLU	-	EXPRESSION TAG	UNP P13699
B	0	PHE	-	EXPRESSION TAG	UNP P13699
C	-7	GLY	-	EXPRESSION TAG	UNP P13699
C	-6	ALA	-	EXPRESSION TAG	UNP P13699
C	-5	MET	-	EXPRESSION TAG	UNP P13699
C	-4	ASP	-	EXPRESSION TAG	UNP P13699
C	-3	HIS	-	EXPRESSION TAG	UNP P13699
C	-2	VAL	-	EXPRESSION TAG	UNP P13699
C	-1	GLU	-	EXPRESSION TAG	UNP P13699

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	PHE	-	EXPRESSION TAG	UNP P13699

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula:  $C_{10}H_{17}N_2O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	C	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

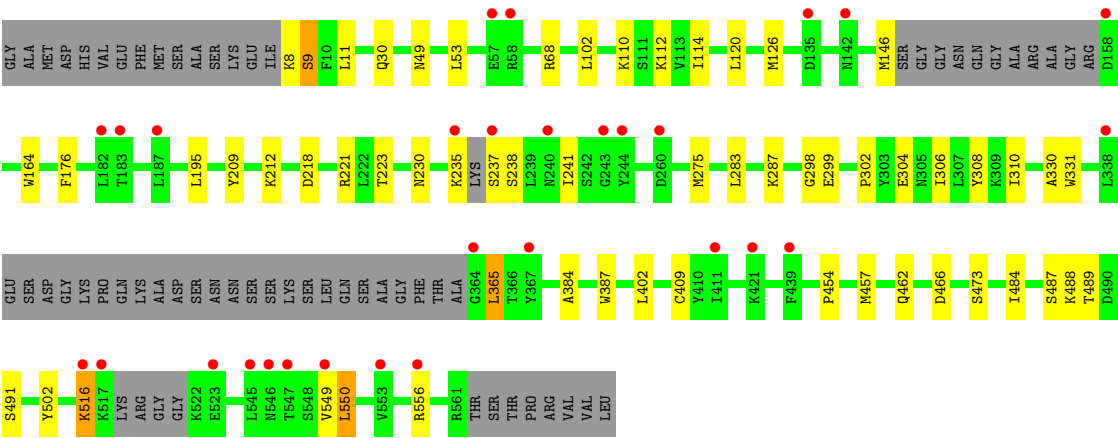
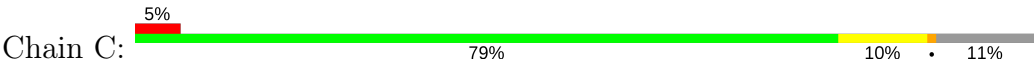
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total 106	O 106	0	0
4	B	204	Total 204	O 204	0	0
4	C	165	Total 165	O 165	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.15Å 176.15Å 56.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	152.55 – 1.98 29.75 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.1 (152.55-1.98) 99.5 (29.75-1.98)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.6.0081	Depositor
R, $R_{free}$	0.180 , 0.208 0.213 , 0.245	Depositor DCC
$R_{free}$ test set	6873 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.017 for h,-h-k,-l 0.003 for -k,-h,-l	Xtriage
Reported twinning fraction	0.606 for H, K, L 0.394 for K, H, -L	Depositor
Outliers	0 of 135046 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12638	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 2.55% 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, TTP

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	0.57	0/4077	0.67	1/5505 (0.0%)
1	B	0.76	2/4098 (0.0%)	0.78	1/5531 (0.0%)
1	C	0.68	1/4068 (0.0%)	0.74	1/5491 (0.0%)
All	All	0.67	3/12243 (0.0%)	0.73	3/16527 (0.0%)

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	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	409	CYS	CB-SG	-6.34	1.71	1.82
1	B	125	TYR	CD2-CE2	5.62	1.47	1.39
1	C	409	CYS	CB-SG	-5.03	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	GLY	N-CA-C	7.29	131.34	113.10
1	C	68	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	481	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	261	GLY	Peptide
1	B	561	ARG	Sidechain

## 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	4020	0	4091	48	0
1	B	4041	0	4114	51	0
1	C	4012	0	4079	39	0
2	A	29	0	13	4	0
2	B	29	0	13	0	0
2	C	29	0	13	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	106	0	0	8	0
4	B	204	0	0	9	0
4	C	165	0	0	6	0
All	All	12638	0	12323	139	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 6.

All (139) 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:C:238:SER:O	2:C:800:TTP:H3'	1.63	0.98
1:B:445:LEU:HB2	4:B:645:HOH:O	1.63	0.96
1:B:155:ALA:HB1	1:B:156:GLY:HA3	1.55	0.86
1:A:164:TRP:NE1	2:A:800:TTP:O4	2.18	0.77
1:B:256:ALA:HB1	1:B:264:MET:CG	2.20	0.72
1:B:155:ALA:HB3	4:B:669:HOH:O	1.89	0.71
1:C:238:SER:O	2:C:800:TTP:C3'	2.36	0.71
1:A:66:ARG:O	4:A:627:HOH:O	2.09	0.71
1:A:446:THR:HB	4:A:608:HOH:O	1.91	0.70
1:A:19:GLU:HG3	1:A:281:SER:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ALA:HB1	1:B:264:MET:HG2	1.74	0.70
1:B:36:GLN:OE1	1:B:195:LEU:HD22	1.91	0.69
2:C:800:TTP:H2'1	2:C:800:TTP:O2	1.91	0.68
1:C:164:TRP:NE1	2:C:800:TTP:O4	2.25	0.68
1:A:439:PHE:O	1:A:561:ARG:NH1	2.28	0.67
1:C:237:SER:O	1:C:241:ILE:HG12	1.95	0.66
1:A:133:GLN:HG2	4:A:644:HOH:O	1.96	0.66
2:C:800:TTP:C2'	2:C:800:TTP:O2	2.45	0.65
1:A:280:LYS:NZ	4:A:628:HOH:O	1.95	0.65
1:B:522:LYS:N	4:B:697:HOH:O	2.29	0.65
1:C:8:LYS:HG3	1:C:11:LEU:H	1.62	0.65
1:C:384:ALA:HB1	4:C:655:HOH:O	1.97	0.64
1:B:468:ARG:O	1:B:472:GLU:HG3	1.98	0.64
1:A:105:ASP:OD2	1:A:286:LYS:HE3	1.97	0.63
1:B:551:ARG:HG2	1:B:551:ARG:HH11	1.62	0.63
1:A:293:ILE:HG23	1:A:304:GLU:HG2	1.81	0.62
1:B:237:SER:H	1:B:240:ASN:HD22	1.48	0.61
1:C:110:LYS:HD2	1:C:331:TRP:CD1	2.35	0.61
1:A:146:MET:CE	1:A:163:VAL:HG23	2.32	0.60
1:B:110:LYS:HG3	1:B:331:TRP:CE2	2.37	0.58
1:C:176:PHE:HB2	2:C:800:TTP:H1'	1.86	0.57
1:C:30:GLN:HG2	4:C:703:HOH:O	2.04	0.57
1:A:133:GLN:CG	4:A:644:HOH:O	2.51	0.57
1:B:414:PHE:HB2	1:B:441:THR:HG21	1.87	0.57
1:B:491:SER:CB	4:B:738:HOH:O	2.52	0.57
1:B:464:SER:HB2	1:B:483:ASP:HB2	1.87	0.56
1:A:29:LEU:HD23	1:A:29:LEU:O	2.05	0.56
1:B:46:GLU:OE2	1:B:66:ARG:HD2	2.05	0.56
1:B:155:ALA:CB	4:B:669:HOH:O	2.52	0.56
1:A:194:ASP:O	1:A:197:ASP:HB2	2.07	0.55
1:B:256:ALA:HB1	1:B:264:MET:HG3	1.87	0.55
1:C:110:LYS:O	1:C:114:ILE:HG13	2.07	0.55
1:A:44:PHE:CG	1:A:189:LYS:HG2	2.42	0.54
1:B:551:ARG:HG2	1:B:551:ARG:NH1	2.23	0.54
1:B:268:ILE:O	1:B:318:PRO:HD2	2.08	0.53
1:C:218:ASP:OD1	1:C:221:ARG:NH2	2.41	0.53
1:B:306:ILE:HG12	1:B:310:ILE:HD12	1.90	0.53
1:B:143:MET:CE	1:B:296:THR:HB	2.39	0.52
1:C:164:TRP:CD1	2:C:800:TTP:O4	2.63	0.52
1:B:490:ASP:HA	4:B:672:HOH:O	2.08	0.52
1:A:62:ASN:O	1:A:65:LYS:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LEU:HD13	2:C:800:TTP:C4	2.44	0.51
1:B:367:TYR:CZ	1:B:371:MET:SD	3.03	0.51
1:A:49:ASN:O	1:A:53:LEU:HG	2.11	0.51
1:A:146:MET:HE2	1:A:163:VAL:HG23	1.91	0.50
1:A:270:VAL:HG22	1:A:278:ILE:HD13	1.94	0.50
1:A:280:LYS:CE	4:A:628:HOH:O	2.52	0.50
1:C:306:ILE:HG12	1:C:310:ILE:HD12	1.94	0.50
1:B:547:THR:HG22	1:B:547:THR:O	2.12	0.49
1:C:223:THR:HG21	1:C:230:ASN:HB3	1.93	0.49
1:A:115:ARG:NH2	1:A:295:ASP:O	2.46	0.49
1:C:466:ASP:HB3	4:C:637:HOH:O	2.12	0.49
1:A:414:PHE:HB2	1:A:441:THR:HG21	1.95	0.49
1:A:146:MET:HE3	1:A:163:VAL:HG23	1.94	0.48
1:C:110:LYS:HD2	1:C:331:TRP:NE1	2.28	0.48
1:B:155:ALA:HB1	1:B:156:GLY:CA	2.35	0.48
1:B:373:LEU:O	1:B:377:MET:HG2	2.13	0.48
1:A:64:LEU:HD13	1:A:172:LEU:HD23	1.95	0.48
1:A:257:CYS:SG	1:A:320:ILE:HG21	2.54	0.48
1:B:429:TYR:HB2	4:B:753:HOH:O	2.13	0.48
1:C:195:LEU:HB2	4:C:641:HOH:O	2.14	0.47
1:C:454:PRO:O	1:C:457:MET:HG3	2.13	0.47
1:A:387:TRP:O	1:A:402:LEU:HA	2.14	0.47
1:A:209:TYR:HA	1:A:212:LYS:O	2.13	0.47
1:C:9:SER:HB2	1:C:302:PRO:HD3	1.97	0.47
1:B:223:THR:HG21	1:B:230:ASN:OD1	2.15	0.46
1:A:178:THR:HG21	1:A:250:ALA:HB2	1.98	0.46
1:A:259:LEU:O	1:B:221:ARG:HD2	2.14	0.46
1:B:561:ARG:HA	4:B:776:HOH:O	2.16	0.46
1:C:112:LYS:HE3	1:C:304:GLU:OE1	2.16	0.46
1:A:306:ILE:O	1:A:310:ILE:HG13	2.15	0.46
2:A:800:TTP:H2'1	2:A:800:TTP:O2	2.15	0.46
1:C:120:LEU:HD23	1:C:146:MET:HG2	1.97	0.46
1:A:241:ILE:N	2:A:800:TTP:O2	2.48	0.45
1:B:439:PHE:O	1:B:561:ARG:NH2	2.49	0.45
1:C:487:SER:O	1:C:491:SER:HB2	2.15	0.45
1:C:235:LYS:O	1:C:237:SER:N	2.49	0.45
1:A:115:ARG:HD3	1:A:372:THR:HA	1.97	0.45
1:B:466:ASP:N	1:B:466:ASP:OD1	2.46	0.45
1:B:464:SER:HB2	1:B:483:ASP:OD2	2.16	0.45
1:C:176:PHE:CB	2:C:800:TTP:H1'	2.47	0.45
1:B:440:ALA:O	1:B:561:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:THR:HG21	1:A:230:ASN:HB3	2.00	0.44
1:C:502:TYR:CE1	1:C:550:LEU:HD22	2.52	0.44
1:A:78:VAL:O	1:A:81:LYS:HE2	2.17	0.44
1:B:561:ARG:H	1:B:561:ARG:HG3	1.55	0.44
1:B:72:GLN:HB3	4:B:721:HOH:O	2.17	0.44
1:C:387:TRP:O	1:C:402:LEU:HA	2.17	0.44
1:C:308:TYR:CE1	1:C:330:ALA:HB3	2.52	0.44
1:A:241:ILE:HA	1:A:241:ILE:HD12	1.76	0.44
1:C:112:LYS:NZ	1:C:298:GLY:O	2.50	0.44
1:C:466:ASP:N	4:C:637:HOH:O	2.50	0.43
1:C:49:ASN:O	1:C:53:LEU:HG	2.17	0.43
1:A:30:GLN:HG3	1:A:80:LEU:HG	1.99	0.43
1:B:235:LYS:NZ	1:B:235:LYS:HB2	2.33	0.43
1:A:12:TRP:CD1	1:A:289:LEU:HD13	2.54	0.43
1:B:401:ALA:HA	1:B:411:ILE:O	2.19	0.43
1:A:533:ASP:HA	1:A:536:MET:HG2	2.00	0.43
1:B:219:LEU:HD11	1:B:229:LEU:HB3	2.00	0.42
1:A:72:GLN:NE2	4:A:620:HOH:O	2.52	0.42
1:B:27:ILE:HD11	1:B:80:LEU:CD2	2.49	0.42
1:C:102:LEU:HG	1:C:283:LEU:HD11	2.01	0.42
1:A:241:ILE:HG13	1:A:245:ASN:CB	2.50	0.42
1:C:516:LYS:CD	1:C:516:LYS:H	2.30	0.42
1:A:133:GLN:HB3	4:A:644:HOH:O	2.18	0.42
1:A:469:LYS:HE3	1:A:469:LYS:HB2	1.81	0.42
1:C:556:ARG:NH2	4:C:590:HOH:O	2.53	0.42
1:B:223:THR:HG21	1:B:230:ASN:CG	2.40	0.42
1:C:237:SER:HB2	1:C:299:GLU:OE2	2.20	0.41
1:B:27:ILE:HD11	1:B:80:LEU:HD22	2.01	0.41
1:C:209:TYR:HA	1:C:212:LYS:O	2.20	0.41
1:A:370:LEU:O	1:A:374:LYS:HG3	2.20	0.41
1:A:401:ALA:HA	1:A:411:ILE:O	2.21	0.41
1:B:223:THR:HG22	1:B:223:THR:O	2.20	0.41
1:A:126:MET:N	1:A:159:GLY:O	2.36	0.41
1:A:176:PHE:HB2	2:A:800:TTP:H1'	2.01	0.41
1:C:516:LYS:HD2	1:C:516:LYS:H	1.86	0.41
1:B:49:ASN:O	1:B:53:LEU:HG	2.21	0.41
1:B:38:LEU:HD22	1:B:42:LEU:HD22	2.03	0.41
1:B:44:PHE:CG	1:B:189:LYS:HG2	2.56	0.41
1:B:269:LYS:HD2	1:B:317:TRP:CE2	2.56	0.41
1:B:241:ILE:HB	1:B:245:ASN:HB2	2.04	0.40
1:C:126:MET:HB3	1:C:126:MET:HE3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:HG21	1:A:310:ILE:HG23	2.03	0.40
1:B:157:ARG:HA	1:B:158:ASP:CB	2.51	0.40
1:C:488:LYS:O	1:C:491:SER:HB3	2.22	0.40
1:A:222:LEU:HD23	1:B:207:LEU:HD13	2.03	0.40
1:A:222:LEU:HB3	1:A:229:LEU:HD12	2.04	0.40
1:B:387:TRP:O	1:B:402:LEU:HA	2.21	0.40

There are no symmetry-related clashes.

## 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	506/577 (88%)	493 (97%)	11 (2%)	2 (0%)	38	30
1	B	509/577 (88%)	497 (98%)	12 (2%)	0	100	100
1	C	503/577 (87%)	495 (98%)	7 (1%)	1 (0%)	51	46
All	All	1518/1731 (88%)	1485 (98%)	30 (2%)	3 (0%)	51	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	557	ASP
1	C	365	LEU
1	A	463	GLY

### 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	451/498 (91%)	432 (96%)	19 (4%)	34	28
1	B	452/498 (91%)	438 (97%)	14 (3%)	45	41
1	C	450/498 (90%)	439 (98%)	11 (2%)	54	53
All	All	1353/1494 (91%)	1309 (97%)	44 (3%)	43	38

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	8	LYS
1	A	9	SER
1	A	197	ASP
1	A	233	ASP
1	A	234	THR
1	A	241	ILE
1	A	295	ASP
1	A	329	ARG
1	A	462	GLN
1	A	464	SER
1	A	465	ASP
1	A	473	SER
1	A	481	LEU
1	A	489	THR
1	A	491	SER
1	A	549	VAL
1	A	556	ARG
1	A	561	ARG
1	B	15	SER
1	B	61	ASP
1	B	83	THR
1	B	120	LEU
1	B	131	SER
1	B	158	ASP
1	B	294	SER
1	B	480	LYS
1	B	481	LEU
1	B	491	SER
1	B	493	LYS
1	B	512	VAL
1	B	550	LEU

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Mol	Chain	Res	Type
1	B	561	ARG
1	C	9	SER
1	C	275	MET
1	C	287	LYS
1	C	365	LEU
1	C	462	GLN
1	C	473	SER
1	C	484	ILE
1	C	489	THR
1	C	516	LYS
1	C	549	VAL
1	C	550	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	B	132	GLN
1	B	224	GLN
1	B	240	ASN
1	B	379	GLN
1	C	442	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	TTP	A	800	-	22,30,30	1.14	1 (4%)	25,47,47	3.23	10 (40%)
2	TTP	B	800	-	22,30,30	1.50	2 (9%)	25,47,47	2.26	7 (28%)
2	TTP	C	800	-	22,30,30	1.17	1 (4%)	25,47,47	3.14	10 (40%)

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
2	TTP	A	800	-	-	0/18/34/34	0/2/2/2
2	TTP	B	800	-	-	0/18/34/34	0/2/2/2
2	TTP	C	800	-	-	0/18/34/34	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	TTP	PG-O3B	-3.14	1.55	1.60
2	A	800	TTP	C4-N3	3.14	1.38	1.33
2	B	800	TTP	C4-N3	3.56	1.39	1.33
2	C	800	TTP	C4-N3	3.79	1.39	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	TTP	C4'-O4'-C1'	-6.90	92.54	109.42
2	C	800	TTP	O5'-PA-O1A	-6.61	82.59	109.25
2	A	800	TTP	C4'-O4'-C1'	-5.47	96.04	109.42
2	A	800	TTP	O5'-PA-O1A	-4.56	90.87	109.25
2	B	800	TTP	O5'-PA-O1A	-4.53	90.99	109.25
2	A	800	TTP	O2A-PA-O5'	-4.46	87.08	108.14
2	B	800	TTP	C5-C4-N3	-3.72	121.13	125.24
2	A	800	TTP	O4'-C1'-C2'	-3.63	99.28	106.25
2	A	800	TTP	C5-C4-N3	-3.62	121.25	125.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	TTP	O2A-PA-O5'	-3.59	91.20	108.14
2	C	800	TTP	C5-C4-N3	-3.34	121.56	125.24
2	C	800	TTP	O2A-PA-O5'	-3.26	92.76	108.14
2	B	800	TTP	C2'-C1'-N1	-3.10	106.90	114.23
2	C	800	TTP	C5-C6-N1	-3.04	118.86	122.15
2	A	800	TTP	C5-C6-N1	-2.96	118.95	122.15
2	C	800	TTP	O4'-C1'-C2'	-2.94	100.61	106.25
2	B	800	TTP	C5-C6-N1	-2.44	119.50	122.15
2	A	800	TTP	C3'-C2'-C1'	-2.04	97.26	102.48
2	C	800	TTP	O4'-C4'-C5'	2.08	116.43	109.40
2	A	800	TTP	O2A-PA-O1A	2.16	123.47	112.28
2	C	800	TTP	O2A-PA-O1A	2.24	123.88	112.28
2	B	800	TTP	O4'-C1'-N1	3.30	113.33	107.78
2	C	800	TTP	C4-N3-C2	3.97	118.63	115.16
2	A	800	TTP	C4-N3-C2	4.13	118.77	115.16
2	B	800	TTP	C4-N3-C2	5.70	120.14	115.16
2	C	800	TTP	O4'-C1'-N1	8.91	122.80	107.78
2	A	800	TTP	O4'-C1'-N1	10.99	126.30	107.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	TTP	4	0
2	C	800	TTP	9	0

## 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	514/577 (89%)	0.69	52 (10%) <b>8</b> <b>9</b>	36, 49, 70, 81	0
1	B	517/577 (89%)	0.45	28 (5%) <b>26</b> <b>29</b>	28, 38, 56, 90	0
1	C	513/577 (88%)	0.43	29 (5%) <b>24</b> <b>27</b>	28, 40, 62, 80	0
All	All	1544/1731 (89%)	0.52	109 (7%) <b>17</b> <b>19</b>	28, 43, 65, 90	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	157	ARG	5.7
1	C	546	ASN	5.0
1	C	364	GLY	5.0
1	B	548	SER	4.6
1	A	338	LEU	4.3
1	B	547	THR	3.9
1	A	439	PHE	3.9
1	A	288	ALA	3.8
1	A	475	GLY	3.8
1	A	556	ARG	3.8
1	A	548	SER	3.7
1	C	545	LEU	3.7
1	C	517	LYS	3.7
1	A	429	TYR	3.7
1	A	546	ASN	3.7
1	A	402	LEU	3.5
1	A	132	GLN	3.5
1	C	260	ASP	3.5
1	A	547	THR	3.5
1	C	516	LYS	3.4
1	B	411	ILE	3.4
1	B	516	LYS	3.4
1	C	547	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	155	ALA	3.2
1	C	367	TYR	3.2
1	A	238	SER	3.1
1	A	251	ALA	3.1
1	C	549	VAL	3.1
1	C	439	PHE	3.1
1	A	560	PHE	3.0
1	A	549	VAL	3.0
1	A	531	LEU	3.0
1	B	546	ASN	2.9
1	A	488	LYS	2.8
1	C	244	TYR	2.8
1	B	401	ALA	2.8
1	A	179	MET	2.8
1	A	254	ALA	2.8
1	C	235	LYS	2.7
1	B	243	GLY	2.7
1	C	556	ARG	2.7
1	C	57	GLU	2.7
1	A	96	SER	2.7
1	A	135	ASP	2.7
1	A	252	VAL	2.7
1	B	402	LEU	2.7
1	B	338	LEU	2.7
1	C	338	LEU	2.7
1	A	484	ILE	2.6
1	A	240	ASN	2.6
1	C	240	ASN	2.6
1	A	246	PHE	2.6
1	C	158	ASP	2.6
1	A	327	THR	2.5
1	A	235	LYS	2.5
1	B	260	ASP	2.5
1	C	135	ASP	2.5
1	B	531	LEU	2.5
1	A	250	ALA	2.4
1	A	319	TYR	2.4
1	B	244	TYR	2.4
1	B	225	SER	2.4
1	C	553	VAL	2.4
1	A	421	LYS	2.4
1	A	477	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	251	ALA	2.4
1	A	140	LEU	2.4
1	C	237	SER	2.4
1	A	455	ARG	2.4
1	A	7	ILE	2.4
1	A	40	HIS	2.3
1	A	244	TYR	2.3
1	B	400	ILE	2.3
1	B	261	GLY	2.3
1	A	241	ILE	2.3
1	B	320	ILE	2.3
1	A	540	ALA	2.3
1	A	142	ASN	2.3
1	A	367	TYR	2.2
1	A	485	ALA	2.2
1	B	440	ALA	2.2
1	A	167	LYS	2.2
1	B	488	LYS	2.2
1	B	254	ALA	2.2
1	C	243	GLY	2.2
1	A	100	LEU	2.2
1	B	18	ARG	2.2
1	A	83	THR	2.2
1	B	29	LEU	2.2
1	C	182	LEU	2.2
1	C	187	LEU	2.2
1	C	183	THR	2.2
1	A	11	LEU	2.1
1	C	421	LYS	2.1
1	C	411	ILE	2.1
1	B	132	GLN	2.1
1	B	535	ILE	2.1
1	A	401	ALA	2.1
1	A	335	VAL	2.1
1	A	489	THR	2.1
1	C	58	ARG	2.1
1	A	553	VAL	2.1
1	B	412	HIS	2.1
1	C	142	ASN	2.1
1	C	523	GLU	2.0
1	B	517	LYS	2.0
1	A	530	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	295	ASP	2.0
1	A	88	ILE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	C	570	1/1	0.01	0.95	28.91	0,0,0,0	0
3	ZN	A	570	1/1	0.43	1.04	19.90	0,0,0,0	0
3	ZN	B	570	1/1	0.07	0.79	15.25	625,625,625,625	0
2	TTP	A	800	29/29	0.89	0.43	4.77	75,109,141,165	7
2	TTP	C	800	29/29	0.89	0.30	3.63	56,85,117,125	6
2	TTP	B	800	29/29	0.88	0.28	3.61	69,78,92,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.