



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:09 am BST

PDB ID : 3MX2
Title : Lassa fever virus Nucleoprotein complexed with dTTP
Authors : Qi, X.; Lan, S.; Wang, W.; Schelde, L.M.; Dong, H.; Wallat, G.; Liang, Y.;
Ly, H.; Dong, C.; Scottish Structural Proteomics Facility (SSPF)
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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
buster-report : 1.1.7 (2018)
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

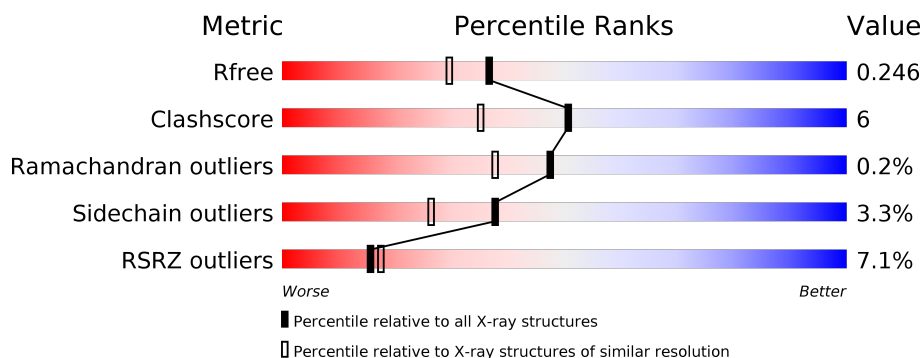
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (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 ≥ 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	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	C	800	-	-	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:

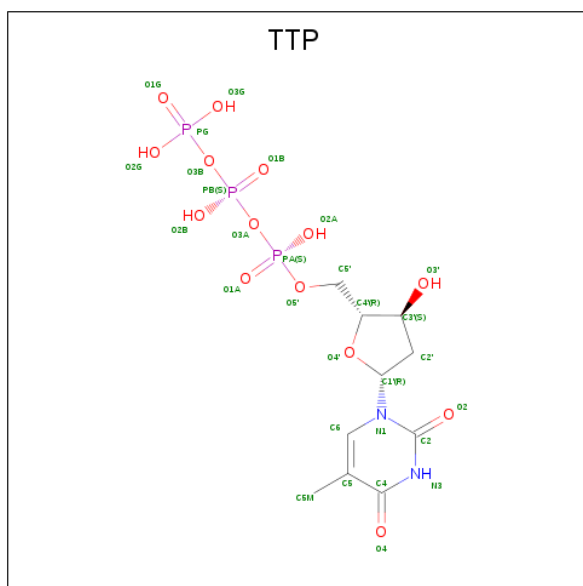
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP P13699
A	-6	ALA	-	EXPRESSION TAG	UNP P13699
A	-5	MET	-	EXPRESSION TAG	UNP P13699
A	-4	ASP	-	EXPRESSION TAG	UNP P13699
A	-3	HIS	-	EXPRESSION TAG	UNP P13699
A	-2	VAL	-	EXPRESSION TAG	UNP P13699
A	-1	GLU	-	EXPRESSION TAG	UNP P13699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

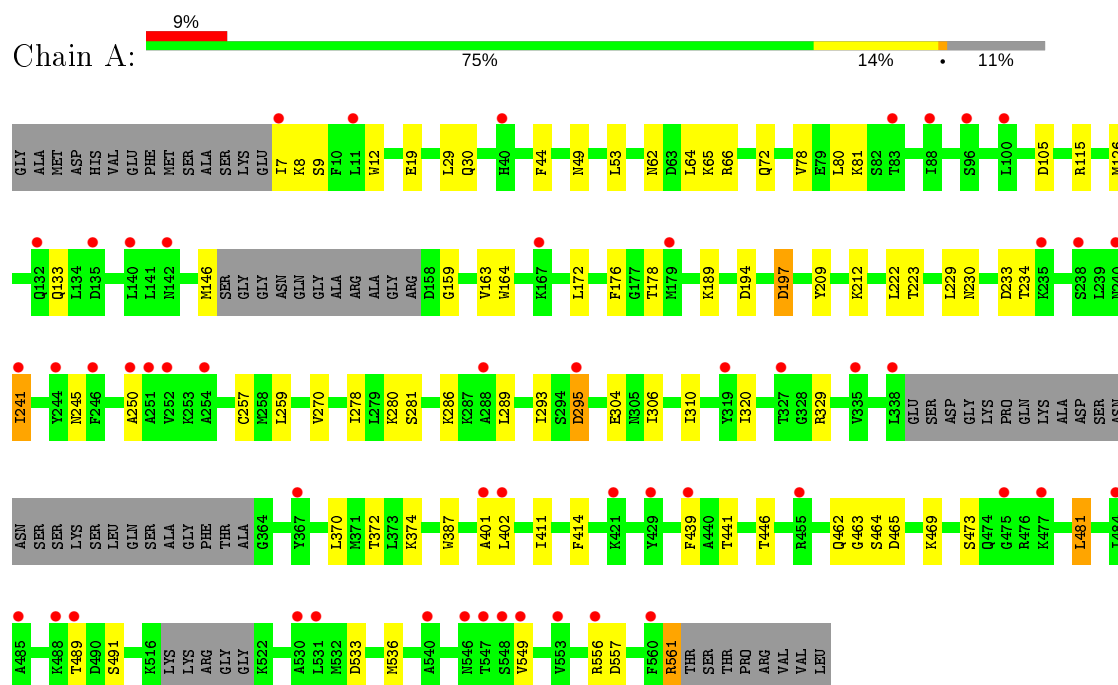
- Molecule 4 is water.

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

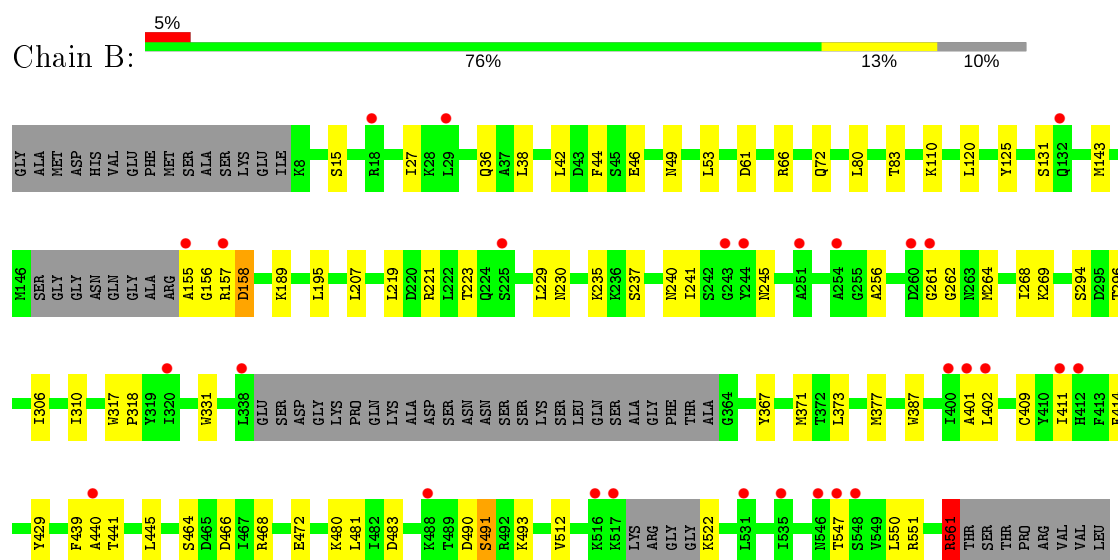
3 Residue-property plots [i](#)

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.

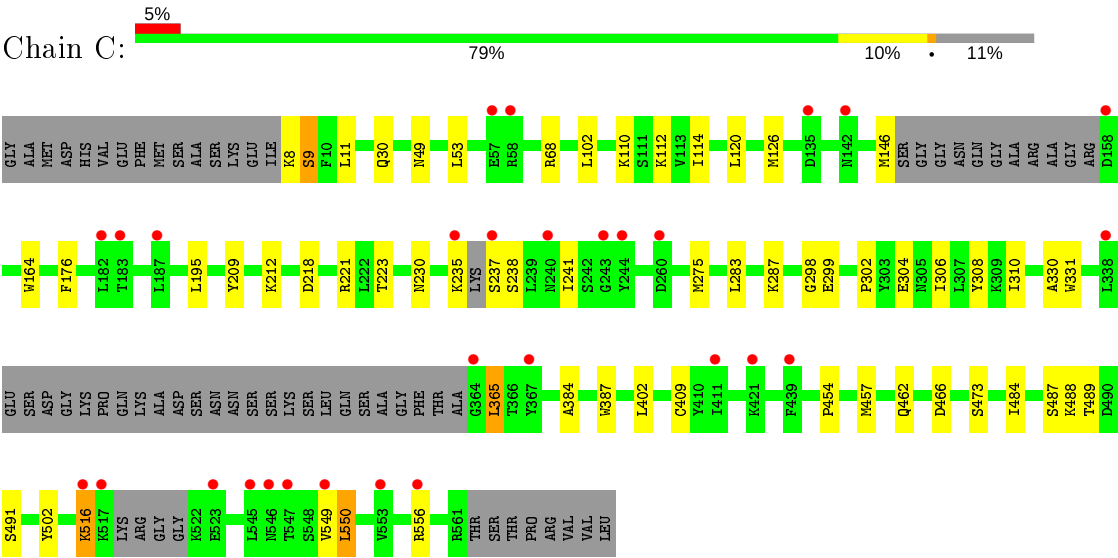
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein



● Molecule 1: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.180 , 0.208 0.213 , 0.246	Depositor DCC
R_{free} test set	6871 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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%)	34	22
1	B	509/577 (88%)	497 (98%)	12 (2%)	0	100	100
1	C	503/577 (87%)	495 (98%)	7 (1%)	1 (0%)	47	38
All	All	1518/1731 (88%)	1485 (98%)	30 (2%)	3 (0%)	47	38

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%)	30	17
1	B	452/498 (91%)	438 (97%)	14 (3%)	40	28
1	C	450/498 (90%)	439 (98%)	11 (2%)	49	41
All	All	1353/1494 (91%)	1309 (97%)	44 (3%)	38	26

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	-	23,30,30	1.17	1 (4%)	29,47,47	2.35	10 (34%)
2	TTP	B	800	-	23,30,30	1.36	2 (8%)	29,47,47	2.22	8 (27%)
2	TTP	C	800	-	23,30,30	1.20	1 (4%)	29,47,47	2.47	10 (34%)

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	-	-	7/19/34/34	0/2/2/2
2	TTP	B	800	-	-	3/19/34/34	0/2/2/2
2	TTP	C	800	-	-	8/19/34/34	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	TTP	C4-N3	3.95	1.39	1.33
2	B	800	TTP	C4-N3	3.70	1.39	1.33
2	A	800	TTP	C4-N3	3.28	1.38	1.33
2	B	800	TTP	PB-O1B	-2.02	1.43	1.50

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	800	TTP	C4'-O4'-C1'	-7.00	92.54	109.45
2	C	800	TTP	O5'-PA-O1A	-6.78	82.59	109.07
2	B	800	TTP	C4-N3-C2	5.92	120.14	115.14
2	A	800	TTP	C4'-O4'-C1'	-5.56	96.04	109.45
2	B	800	TTP	PB-O3A-PA	-5.22	114.91	132.83
2	A	800	TTP	O5'-PA-O1A	-4.66	90.87	109.07
2	B	800	TTP	O5'-PA-O1A	-4.63	90.99	109.07
2	A	800	TTP	O2A-PA-O5'	-4.45	87.08	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	TTP	C4-N3-C2	4.30	118.77	115.14
2	C	800	TTP	C4-N3-C2	4.13	118.63	115.14
2	A	800	TTP	PB-O3A-PA	-3.73	120.02	132.83
2	A	800	TTP	O4'-C1'-C2'	-3.69	99.28	106.25
2	B	800	TTP	O2A-PA-O5'	-3.56	91.20	107.75
2	A	800	TTP	PB-O3B-PG	-3.29	121.54	132.83
2	C	800	TTP	O2A-PA-O5'	-3.23	92.76	107.75
2	B	800	TTP	C2'-C1'-N1	-3.20	106.90	114.27
2	C	800	TTP	C5-C6-N1	-3.10	118.86	122.19
2	A	800	TTP	C5-C6-N1	-3.01	118.95	122.19
2	C	800	TTP	O4'-C1'-C2'	-2.99	100.61	106.25
2	B	800	TTP	PB-O3B-PG	-2.79	123.25	132.83
2	C	800	TTP	PB-O3A-PA	-2.72	123.50	132.83
2	B	800	TTP	C5-C6-N1	-2.50	119.50	122.19
2	C	800	TTP	O2A-PA-O1A	2.35	123.88	112.24
2	A	800	TTP	O2A-PA-O1A	2.27	123.47	112.24
2	C	800	TTP	PB-O3B-PG	-2.16	125.41	132.83
2	C	800	TTP	O4'-C4'-C5'	2.15	116.43	109.37
2	A	800	TTP	C3'-C2'-C1'	-2.11	97.26	102.54
2	B	800	TTP	O2A-PA-O1A	2.02	122.23	112.24

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	800	TTP	O4'-C1'-N1-C6
2	C	800	TTP	PB-O3B-PG-O2G
2	A	800	TTP	C5'-O5'-PA-O1A
2	A	800	TTP	C5'-O5'-PA-O2A
2	A	800	TTP	C5'-O5'-PA-O3A
2	C	800	TTP	O4'-C4'-C5'-O5'
2	C	800	TTP	C3'-C4'-C5'-O5'
2	A	800	TTP	PB-O3B-PG-O1G
2	A	800	TTP	C4'-C5'-O5'-PA
2	C	800	TTP	C5'-O5'-PA-O1A
2	C	800	TTP	C5'-O5'-PA-O2A
2	A	800	TTP	PB-O3A-PA-O1A
2	C	800	TTP	PB-O3B-PG-O3G
2	C	800	TTP	C5'-O5'-PA-O3A
2	A	800	TTP	O4'-C4'-C5'-O5'
2	B	800	TTP	C5'-O5'-PA-O1A
2	B	800	TTP	PB-O3B-PG-O1G

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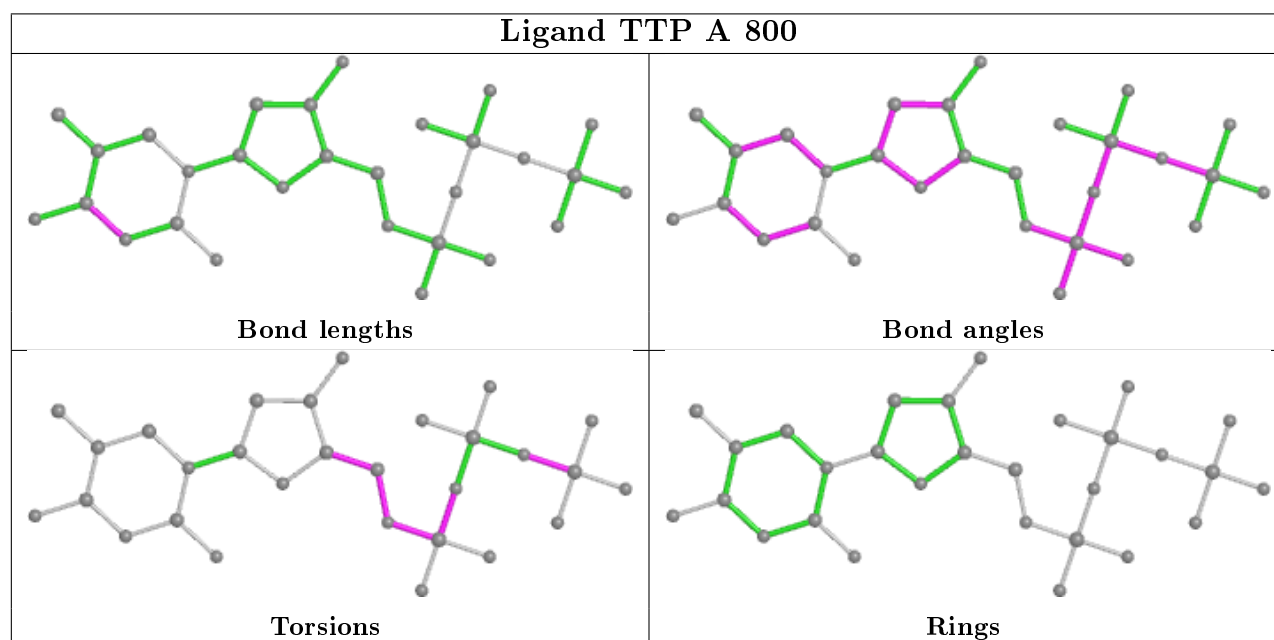
Mol	Chain	Res	Type	Atoms
2	C	800	TTP	PB-O3B-PG-O1G

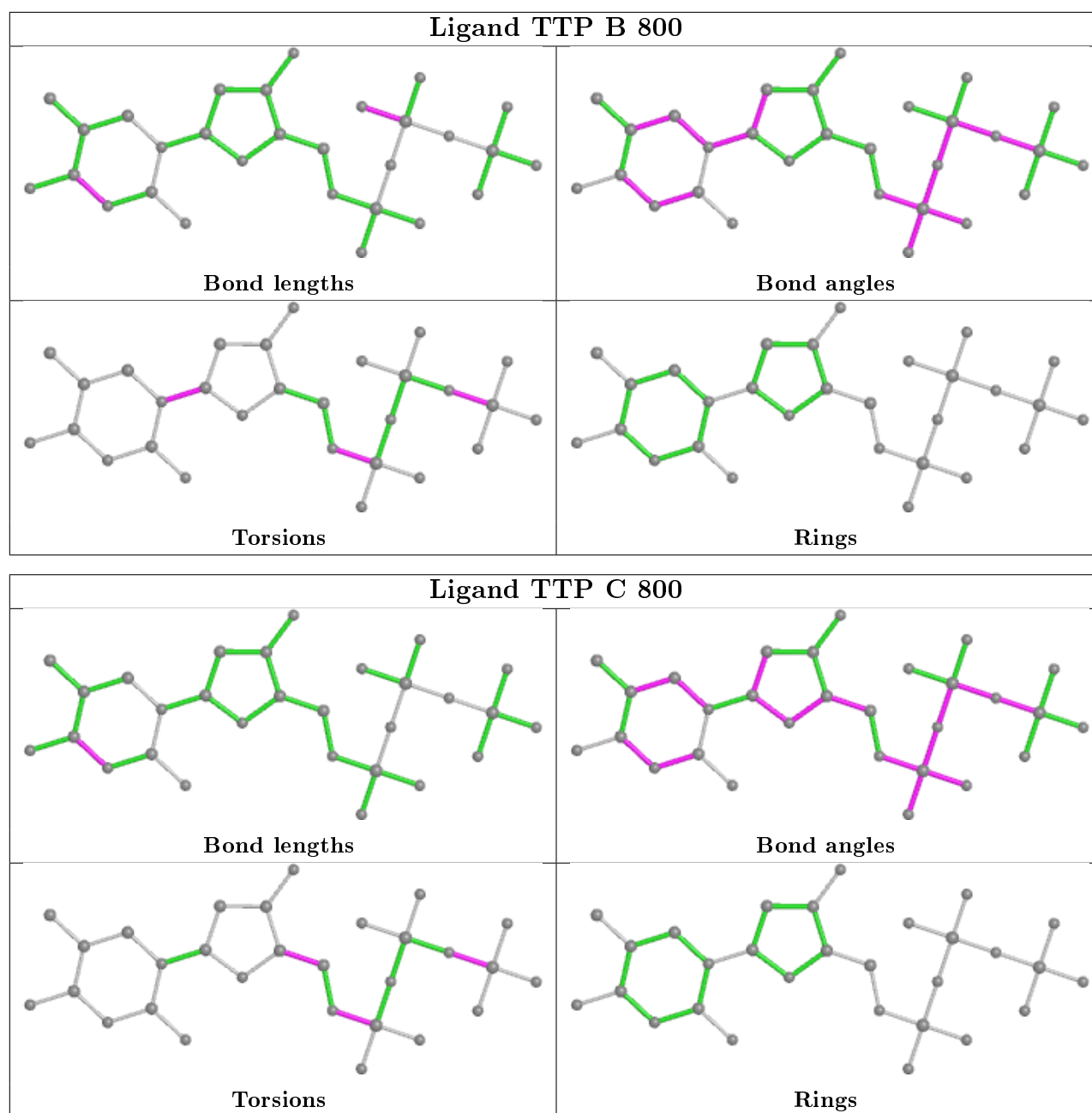
There are no ring outliers.

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 95th 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 ²)	Q<0.9
1	A	514/577 (89%)	0.69	52 (10%) 7 7	36, 49, 70, 81	0
1	B	517/577 (89%)	0.45	28 (5%) 25 28	28, 38, 56, 90	0
1	C	513/577 (88%)	0.43	29 (5%) 23 25	28, 40, 62, 80	0
All	All	1544/1731 (89%)	0.52	109 (7%) 16 17	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	5.1
1	C	364	GLY	5.0
1	B	548	SER	4.5
1	A	338	LEU	4.3
1	B	547	THR	4.0
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	C	545	LEU	3.7
1	A	548	SER	3.7
1	A	429	TYR	3.7
1	A	546	ASN	3.7
1	C	517	LYS	3.7
1	A	402	LEU	3.5
1	C	260	ASP	3.5
1	A	547	THR	3.5
1	A	132	GLN	3.5
1	C	516	LYS	3.4
1	B	516	LYS	3.4
1	B	411	ILE	3.4
1	C	547	THR	3.2

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

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

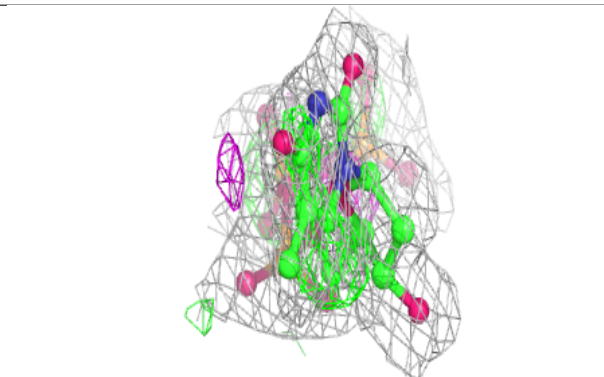
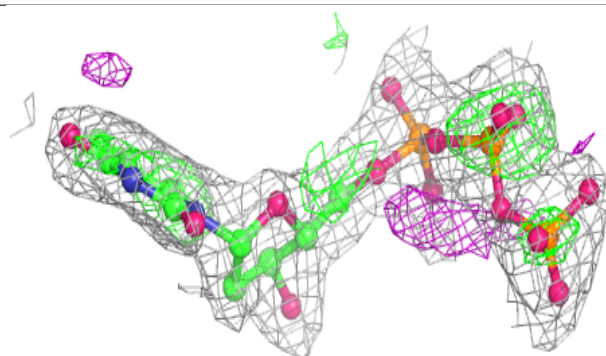
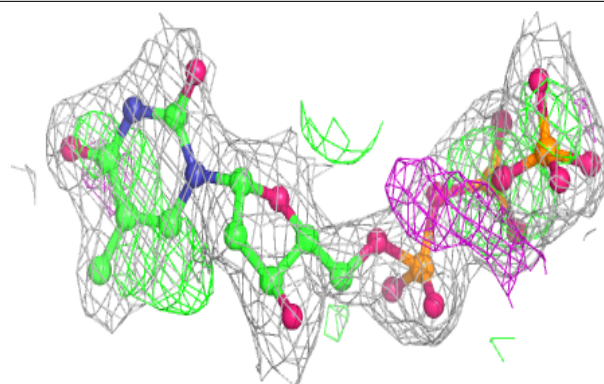
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	C	570	1/1	0.01	0.95	0,0,0,0	0
3	ZN	B	570	1/1	0.07	0.79	625,625,625,625	0
3	ZN	A	570	1/1	0.43	1.04	0,0,0,0	0
2	TTP	B	800	29/29	0.88	0.28	69,78,92,94	0
2	TTP	A	800	29/29	0.89	0.43	75,109,141,165	7
2	TTP	C	800	29/29	0.89	0.30	56,85,117,125	6

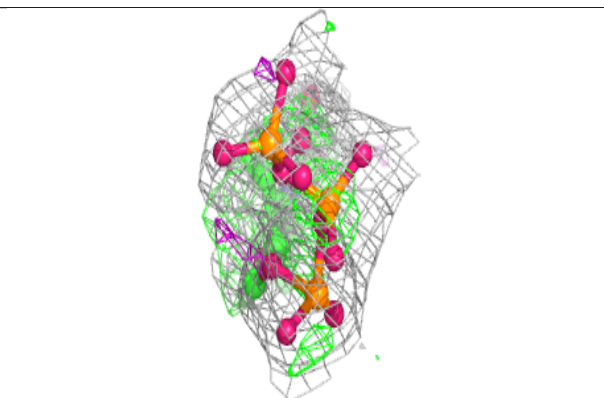
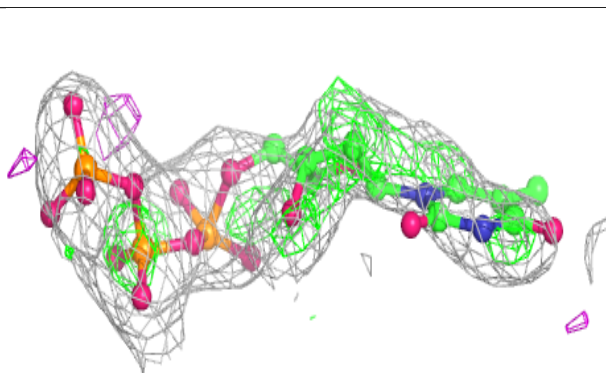
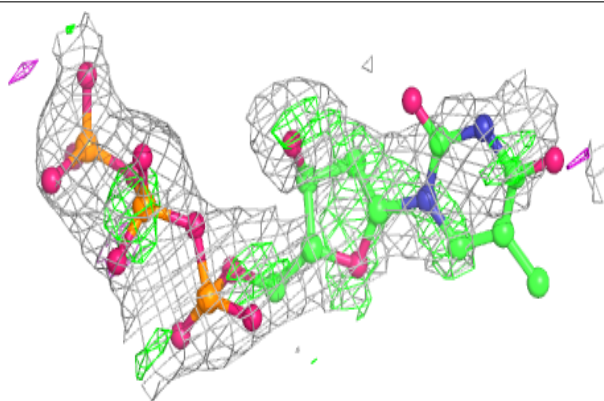
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

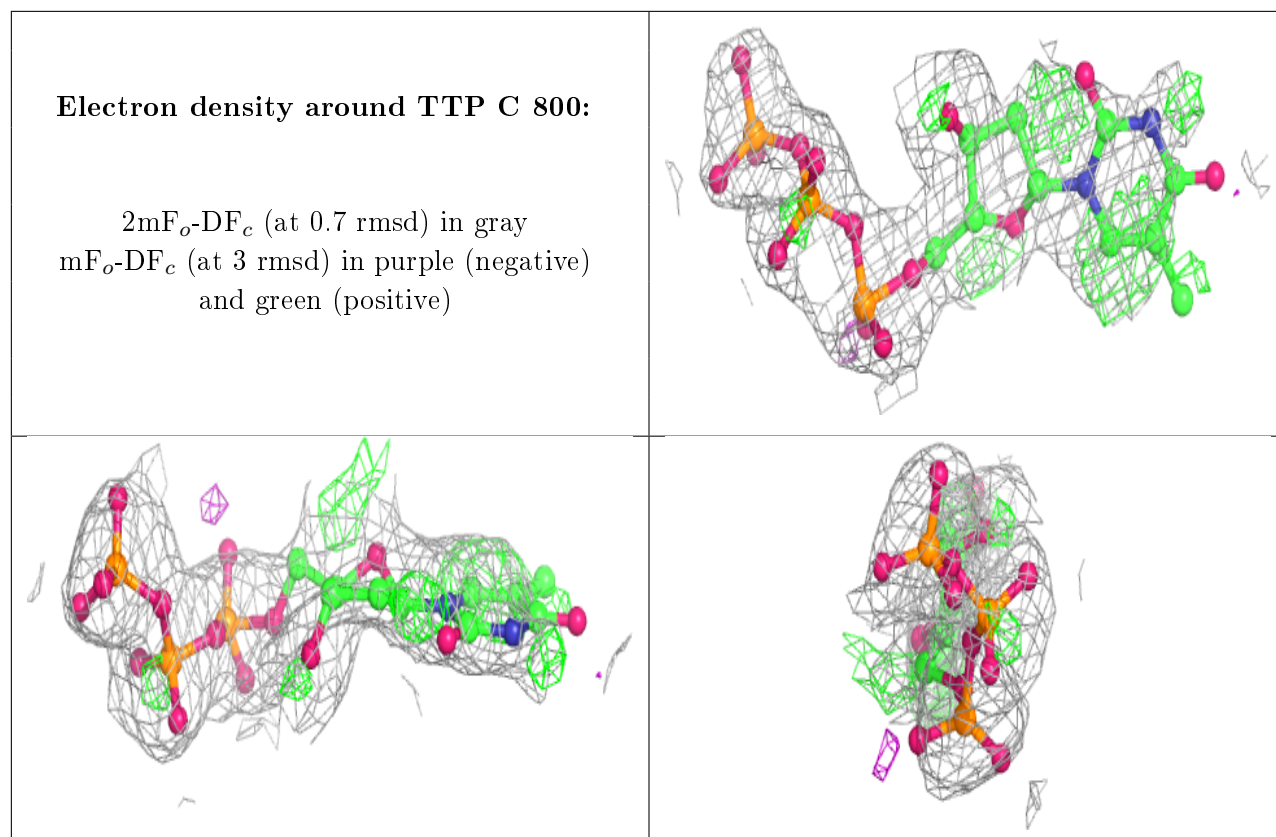
Electron density around TTP B 800:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around TTP A 800:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.