



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:20 AM UTC

PDB ID : 8T3X / pdb_00008t3x
Title : TNA polymerase, closed ternary
Authors : Maola, V.; Chaput, J.; Chim, N.
Deposited on : 2023-06-07
Resolution : 2.73 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 types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

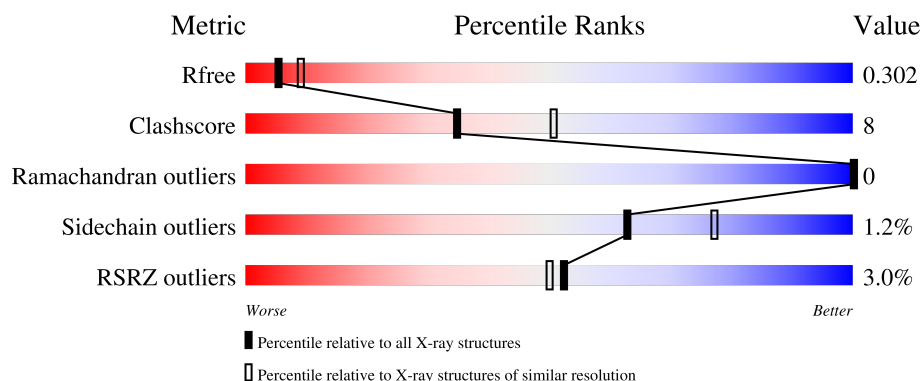
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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 ≥ 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	760	3% 78% 20% .
2	T	15	80% 20%
3	P	12	8% 67% 33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6778 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 10-92, TNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	748	Total	C	N	O	S	0	0	0
			6135	3952	1042	1127	14			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	ARG	LYS	engineered mutation	UNP D0VWU9
A	102	ALA	GLU	engineered mutation	UNP D0VWU9
A	107	VAL	ILE	engineered mutation	UNP D0VWU9
A	127	ILE	VAL	engineered mutation	UNP D0VWU9
A	136	THR	LYS	engineered mutation	UNP D0VWU9
A	141	ALA	ASP	engineered mutation	UNP D0VWU9
A	143	ALA	GLU	engineered mutation	UNP D0VWU9
A	147	HIS	GLU	engineered mutation	UNP D0VWU9
A	285	LYS	GLN	engineered mutation	UNP D0VWU9
A	296	ALA	THR	engineered mutation	UNP D0VWU9
A	297	GLN	THR	engineered mutation	UNP D0VWU9
A	304	GLY	ASN	engineered mutation	UNP D0VWU9
A	337	VAL	ILE	engineered mutation	UNP D0VWU9
A	339	HIS	GLN	engineered mutation	UNP D0VWU9
A	340	PRO	SER	engineered mutation	UNP D0VWU9
A	356	TYR	PHE	engineered mutation	UNP D0VWU9
A	375	ARG	LYS	engineered mutation	UNP D0VWU9
A	377	TYR	LEU	engineered mutation	UNP D0VWU9
A	378	GLU	ALA	engineered mutation	UNP D0VWU9
A	381	LEU	-	insertion	UNP D0VWU9
A	383	GLU	GLN	engineered mutation	UNP D0VWU9
A	386	ALA	GLU	engineered mutation	UNP D0VWU9
A	395	LYS	ARG	engineered mutation	UNP D0VWU9
A	466	ARG	LYS	engineered mutation	UNP D0VWU9
A	472	VAL	ILE	engineered mutation	UNP D0VWU9
A	474	LEU	PRO	engineered mutation	UNP D0VWU9
A	475	LEU	ILE	engineered mutation	UNP D0VWU9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	477	LYS	ARG	engineered mutation	UNP D0VWU9
A	486	ARG	ALA	engineered mutation	UNP D0VWU9
A	492	SER	ASN	engineered mutation	UNP D0VWU9
A	493	GLY	SER	engineered mutation	UNP D0VWU9
A	520	GLN	GLU	engineered mutation	UNP D0VWU9
A	523	GLU	THR	engineered mutation	UNP D0VWU9
A	524	THR	MET	engineered mutation	UNP D0VWU9
A	527	ARG	LYS	engineered mutation	UNP D0VWU9
A	533	PHE	TYR	engineered mutation	UNP D0VWU9
A	538	LEU	ILE	engineered mutation	UNP D0VWU9
A	540	ALA	SER	engineered mutation	UNP D0VWU9
A	548	PRO	THR	engineered mutation	UNP D0VWU9
A	550	HIS	PRO	engineered mutation	UNP D0VWU9
A	562	LYS	MET	engineered mutation	UNP D0VWU9
A	566	ASP	LYS	engineered mutation	UNP D0VWU9
A	575	LEU	ALA	engineered mutation	UNP D0VWU9
A	585	LYS	GLU	engineered mutation	UNP D0VWU9
A	602	ASP	GLY	engineered mutation	UNP D0VWU9
A	607	GLY	ARG	engineered mutation	UNP D0VWU9
A	615	GLY	ASP	engineered mutation	UNP D0VWU9
A	672	ARG	LYS	engineered mutation	UNP D0VWU9
A	717	SER	PRO	engineered mutation	UNP D0VWU9
A	724	ALA	THR	engineered mutation	UNP D0VWU9
A	741	PRO	ALA	engineered mutation	UNP D0VWU9
A	749	CYS	PHE	engineered mutation	UNP D0VWU9

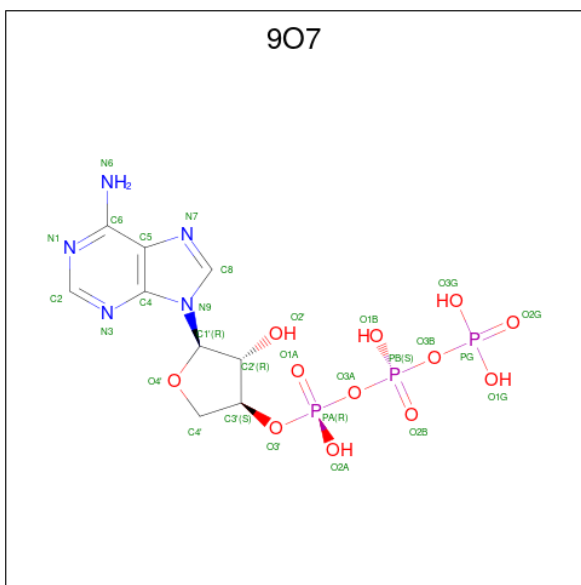
- Molecule 2 is a DNA chain called Template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	15	Total	C	N	O	P	0	0	0
			307	145	56	91	15			

- Molecule 3 is a DNA chain called Primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	12	Total	C	N	O	P	0	0	0
			244	115	46	71	12			

- Molecule 4 is [(3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-4-oxidanyl-oxolan-3-yl] [oxidanyl(phosphonooxy)phosphoryl] hydrogen phosphate (CCD ID: 9O7) (formula: C₉H₁₄N₅O₁₂P₃).

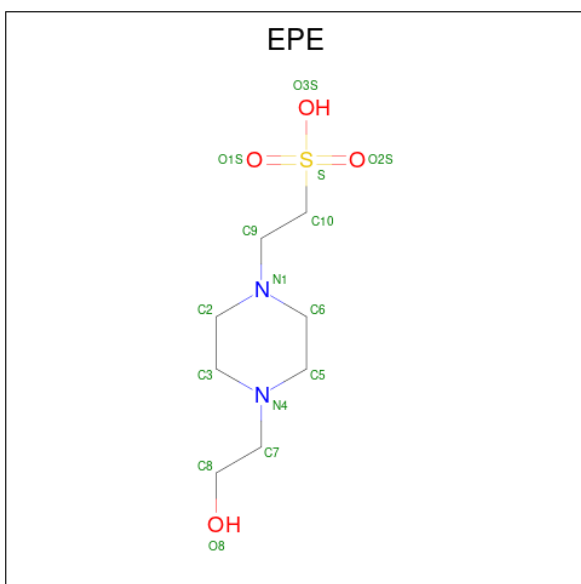


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			29	9	5	12	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

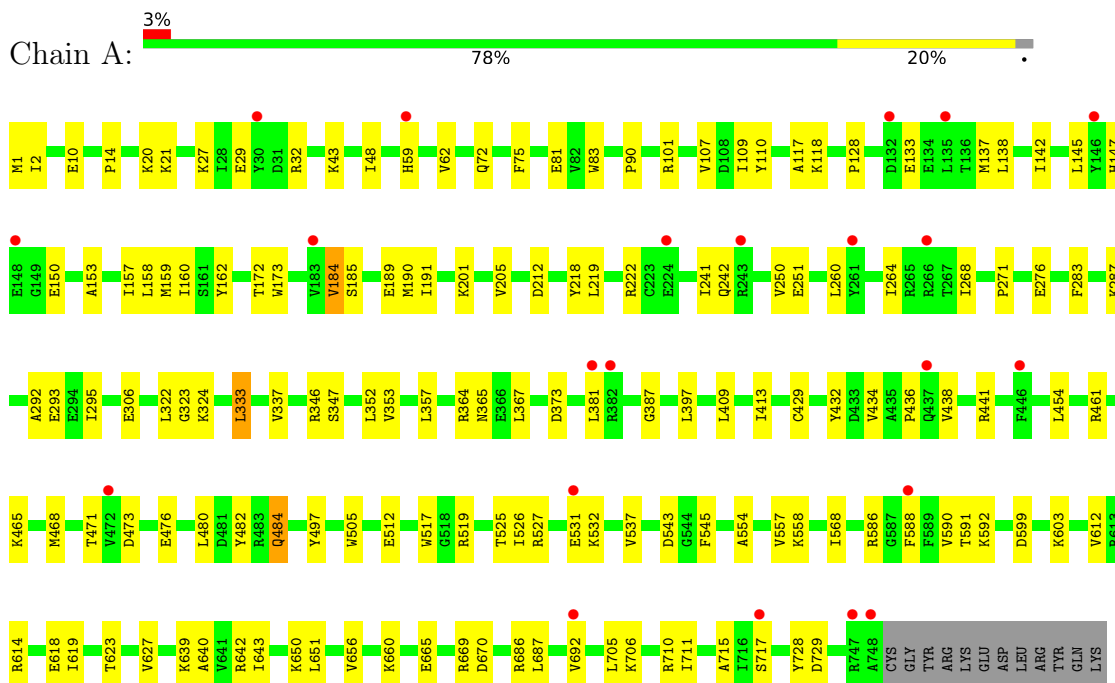
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	41	Total	O	0	0
			41	41		
7	T	2	Total	O	0	0
			2	2		
7	P	4	Total	O	0	0
			4	4		

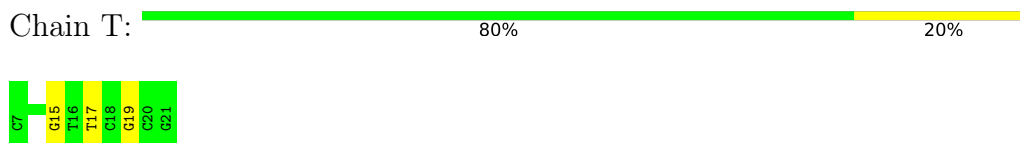
3 Residue-property plots [i](#)

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.

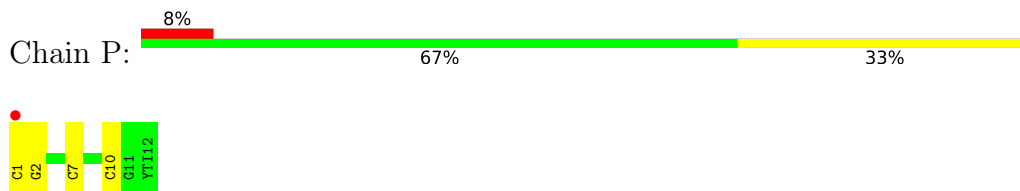
- Molecule 1: 10-92, TNA polymerase



- Molecule 2: Template



- Molecule 3: Primer



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.87Å 99.53Å 110.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.39 – 2.73 45.39 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.39-2.73) 99.0 (45.39-2.73)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.242 , 0.301 0.243 , 0.302	Depositor DCC
R_{free} test set	2000 reflections (8.62%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 17.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6778	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9O7, MG, YTI, EPE

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	0.09	0/6275	0.24	0/8470
2	T	0.17	0/343	0.31	0/527
3	P	0.19	0/253	0.34	0/388
All	All	0.10	0/6871	0.25	0/9385

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6135	0	6165	96	0
2	T	307	0	169	4	0
3	P	244	0	122	3	0
4	A	29	0	0	1	0
5	A	1	0	0	0	0
6	A	15	0	17	3	0
7	A	41	0	0	1	0
7	P	4	0	0	0	0
7	T	2	0	0	0	0
All	All	6778	0	6473	99	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 8.

All (99) 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:627:VAL:HG13	1:A:640:ALA:HB1	1.75	0.69
1:A:293:GLU:N	1:A:293:GLU:OE1	2.25	0.69
1:A:242:GLN:NE2	1:A:251:GLU:OE1	2.25	0.69
1:A:434:VAL:HG22	1:A:441:ARG:HG2	1.77	0.67
1:A:43:LYS:HD3	1:A:107:VAL:HG22	1.77	0.65
1:A:531:GLU:OE1	1:A:532:LYS:NZ	2.30	0.64
1:A:612:VAL:HG12	3:P:10:DC:H5''	1.79	0.64
1:A:138:LEU:HD11	1:A:162:TYR:HB2	1.80	0.64
1:A:159:MET:HG2	1:A:172:THR:HB	1.79	0.63
1:A:465:LYS:HG3	1:A:484:GLN:HG3	1.79	0.62
1:A:201:LYS:NZ	7:A:901:HOH:O	2.32	0.62
1:A:686:ARG:NH2	1:A:715:ALA:O	2.30	0.60
6:A:803:EPE:H21	2:T:15:DG:H21	1.66	0.60
1:A:364:ARG:HG2	1:A:364:ARG:HH11	1.67	0.60
1:A:137:MET:HG2	1:A:205:VAL:HB	1.85	0.58
1:A:461:ARG:HH21	1:A:484:GLN:HE21	1.52	0.58
1:A:157:ILE:HG13	1:A:222:ARG:HG3	1.87	0.56
1:A:137:MET:HE1	1:A:324:LYS:HA	1.88	0.56
6:A:803:EPE:H21	2:T:15:DG:N2	2.21	0.55
1:A:264:ILE:HG23	1:A:268:ILE:HD12	1.88	0.54
1:A:429:CYS:HB2	1:A:432:TYR:CZ	2.43	0.54
1:A:184:VAL:HG13	1:A:189:GLU:HG2	1.90	0.53
1:A:20:LYS:HD3	1:A:29:GLU:HG3	1.89	0.53
1:A:413:ILE:HD13	1:A:517:TRP:HB3	1.89	0.53
1:A:145:LEU:HB2	1:A:158:LEU:HD21	1.91	0.53
1:A:59:HIS:O	1:A:59:HIS:ND1	2.40	0.52
1:A:438:VAL:HG11	1:A:512:GLU:HB3	1.90	0.52
1:A:373:ASP:OD1	1:A:373:ASP:N	2.43	0.52
1:A:72:GLN:NE2	1:A:81:GLU:OE2	2.36	0.52
1:A:711:ILE:HD12	2:T:17:DT:H3'	1.92	0.51
1:A:527:ARG:O	1:A:531:GLU:HG3	2.10	0.51
1:A:10:GLU:CD	1:A:32:ARG:HH21	2.18	0.50
1:A:599:ASP:OD1	1:A:603:LYS:N	2.43	0.50
1:A:669:ARG:HH12	3:P:7:DC:P	2.35	0.50
1:A:153:ALA:HA	1:A:218:TYR:CZ	2.46	0.50
1:A:397:LEU:HD11	1:A:586:ARG:HB3	1.94	0.50
1:A:497:TYR:HE2	1:A:505:TRP:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:PHE:HE1	1:A:322:LEU:HG	1.76	0.49
1:A:1:MET:HE3	1:A:133:GLU:HB2	1.94	0.49
1:A:142:ILE:HG22	1:A:160:ILE:HG12	1.95	0.48
1:A:590:VAL:HG12	1:A:591:THR:HG22	1.94	0.48
1:A:72:GLN:O	1:A:365:ASN:ND2	2.45	0.47
1:A:409:LEU:HD22	1:A:543:ASP:HB3	1.96	0.47
1:A:651:LEU:HD12	1:A:656:VAL:HG21	1.97	0.47
1:A:48:ILE:HG12	1:A:83:TRP:CZ3	2.49	0.47
1:A:705:LEU:HA	1:A:728:TYR:HA	1.97	0.47
1:A:436:PRO:O	1:A:438:VAL:N	2.43	0.47
1:A:639:LYS:O	1:A:643:ILE:HG13	2.15	0.47
1:A:623:THR:O	1:A:627:VAL:HG23	2.16	0.46
1:A:639:LYS:HA	1:A:642:ARG:HB2	1.97	0.46
1:A:241:ILE:HG12	1:A:250:VAL:HG22	1.97	0.46
1:A:271:PRO:HA	1:A:614:ARG:HD3	1.98	0.46
1:A:687:LEU:HB3	1:A:692:VAL:HB	1.97	0.46
1:A:706:LYS:HE2	1:A:729:ASP:HA	1.98	0.46
1:A:276:GLU:HG3	1:A:287:LYS:HD3	1.98	0.46
1:A:353:VAL:O	1:A:357:LEU:HG	2.15	0.46
1:A:268:ILE:HG12	1:A:482:TYR:CZ	2.50	0.46
1:A:260:LEU:HD21	1:A:323:GLY:HA2	1.98	0.45
1:A:160:ILE:HD11	1:A:219:LEU:HD21	1.99	0.45
1:A:185:SER:OG	1:A:189:GLU:OE1	2.30	0.45
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.82	0.45
1:A:101:ARG:HG3	1:A:109:ILE:HG12	1.99	0.45
1:A:619:ILE:HG12	1:A:651:LEU:HD11	1.99	0.45
1:A:337:VAL:HG21	1:A:352:LEU:HD22	1.99	0.44
1:A:147:HIS:HB2	1:A:150:GLU:CD	2.42	0.44
3:P:1:DC:H2'	3:P:2:DG:C8	2.53	0.44
1:A:190:MET:HE2	1:A:190:MET:HB3	1.83	0.44
1:A:387:GLY:O	1:A:519:ARG:NH1	2.41	0.44
1:A:397:LEU:HB2	1:A:588:PHE:HE1	1.83	0.44
1:A:292:ALA:HA	1:A:295:ILE:HG12	1.99	0.43
1:A:531:GLU:HB2	1:A:532:LYS:HD2	2.00	0.43
1:A:618:GLU:HB3	1:A:660:LYS:HA	1.99	0.43
1:A:665:GLU:OE1	6:A:803:EPE:H32	2.19	0.43
1:A:21:LYS:O	1:A:133:GLU:HG3	2.20	0.42
1:A:173:TRP:CD1	1:A:173:TRP:H	2.36	0.42
1:A:473:ASP:HB3	1:A:476:GLU:OE1	2.18	0.42
1:A:2:ILE:HB	1:A:128:PRO:HA	2.01	0.42
1:A:110:TYR:HB2	1:A:367:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ALA:O	1:A:558:LYS:HG3	2.20	0.42
1:A:669:ARG:HG3	1:A:670:ASP:O	2.19	0.42
1:A:468:MET:HG3	1:A:480:LEU:HB2	2.02	0.42
1:A:471:THR:HG21	1:A:476:GLU:HB2	2.02	0.42
1:A:14:PRO:HG3	1:A:90:PRO:HD3	2.01	0.42
1:A:27:LYS:HE3	1:A:27:LYS:HB2	1.93	0.42
1:A:222:ARG:HD2	1:A:222:ARG:HA	1.83	0.42
1:A:306:GLU:H	1:A:306:GLU:CD	2.27	0.41
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.93	0.41
1:A:212:ASP:OD2	1:A:346:ARG:NE	2.35	0.41
1:A:526:ILE:HG23	1:A:537:VAL:HG21	2.02	0.41
1:A:75:PHE:CD1	1:A:367:LEU:HD23	2.56	0.41
1:A:461:ARG:HH12	4:A:801:9O7:PG	2.43	0.41
1:A:591:THR:OG1	1:A:592:LYS:N	2.53	0.41
1:A:710:ARG:HD3	2:T:19:DG:P	2.61	0.40
1:A:190:MET:HE3	1:A:191:ILE:HG13	2.04	0.40
1:A:525:THR:HG23	1:A:568:ILE:HG12	2.03	0.40
1:A:650:LYS:NZ	1:A:650:LYS:HB2	2.36	0.40
1:A:117:ALA:HB3	1:A:118:LYS:HZ2	1.87	0.40
1:A:283:PHE:CE1	1:A:322:LEU:HG	2.56	0.40
1:A:537:VAL:HG13	1:A:545:PHE:HB2	2.02	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	746/760 (98%)	723 (97%)	23 (3%)	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	646/657 (98%)	638 (99%)	8 (1%)	63 77

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

Mol	Chain	Res	Type
1	A	62	VAL
1	A	184	VAL
1	A	333	LEU
1	A	347	SER
1	A	381	LEU
1	A	484	GLN
1	A	557	VAL
1	A	717	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	A	418	ASN
1	A	484	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
6	EPE	A	803	-	15,15,15	1.01	0	19,20,20	0.97	0
4	9O7	A	801	5	30,31,31	4.55	12 (40%)	41,49,49	2.11	14 (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
6	EPE	A	803	-	-	3/9/19/19	0/1/1/1
4	9O7	A	801	5	-	8/21/34/34	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	9O7	PB-O3A	19.63	1.80	1.59
4	A	801	9O7	PA-O3'	9.06	1.86	1.59
4	A	801	9O7	O3'-C3'	-5.89	1.33	1.46
4	A	801	9O7	PA-O3A	-4.60	1.54	1.59
4	A	801	9O7	PB-O3B	-4.17	1.55	1.59
4	A	801	9O7	C4-N3	3.79	1.41	1.34
4	A	801	9O7	C2-N1	3.40	1.40	1.33
4	A	801	9O7	C4'-C3'	3.05	1.58	1.52
4	A	801	9O7	C6-N6	2.77	1.41	1.34
4	A	801	9O7	C5-C4	2.62	1.43	1.39
4	A	801	9O7	C8-N9	2.52	1.41	1.37
4	A	801	9O7	C8-N7	2.34	1.36	1.31

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	9O7	O3A-PB-O2B	-6.36	91.58	110.70
4	A	801	9O7	O2A-PA-O3A	4.28	118.84	107.27
4	A	801	9O7	O3'-PA-O1A	-4.21	96.35	109.81
4	A	801	9O7	O2A-PA-O3'	-3.95	90.62	106.70
4	A	801	9O7	C1'-N9-C8	-3.39	119.57	127.09
4	A	801	9O7	O1B-PB-O3B	2.89	115.09	107.27
4	A	801	9O7	O1B-PB-O3A	-2.67	100.06	107.27
4	A	801	9O7	N3-C4-N9	2.49	131.41	127.17
4	A	801	9O7	C4-N9-C1'	2.47	132.40	126.63
4	A	801	9O7	C5-C4-N3	-2.44	123.36	126.72
4	A	801	9O7	N9-C8-N7	-2.37	110.57	113.94
4	A	801	9O7	O3B-PB-O2B	2.25	117.49	110.70
4	A	801	9O7	O3G-PG-O3B	2.24	112.16	104.64
4	A	801	9O7	C4-N9-C8	2.18	108.02	105.74

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	9O7	C3'-O3'-PA-O3A
6	A	803	EPE	C8-C7-N4-C3
6	A	803	EPE	N4-C7-C8-O8
4	A	801	9O7	PG-O3B-PB-O3A
6	A	803	EPE	S-C10-C9-N1
4	A	801	9O7	PA-O3A-PB-O1B
4	A	801	9O7	PB-O3A-PA-O2A
4	A	801	9O7	C3'-O3'-PA-O1A
4	A	801	9O7	C3'-O3'-PA-O2A
4	A	801	9O7	PA-O3A-PB-O2B
4	A	801	9O7	PG-O3B-PB-O1B

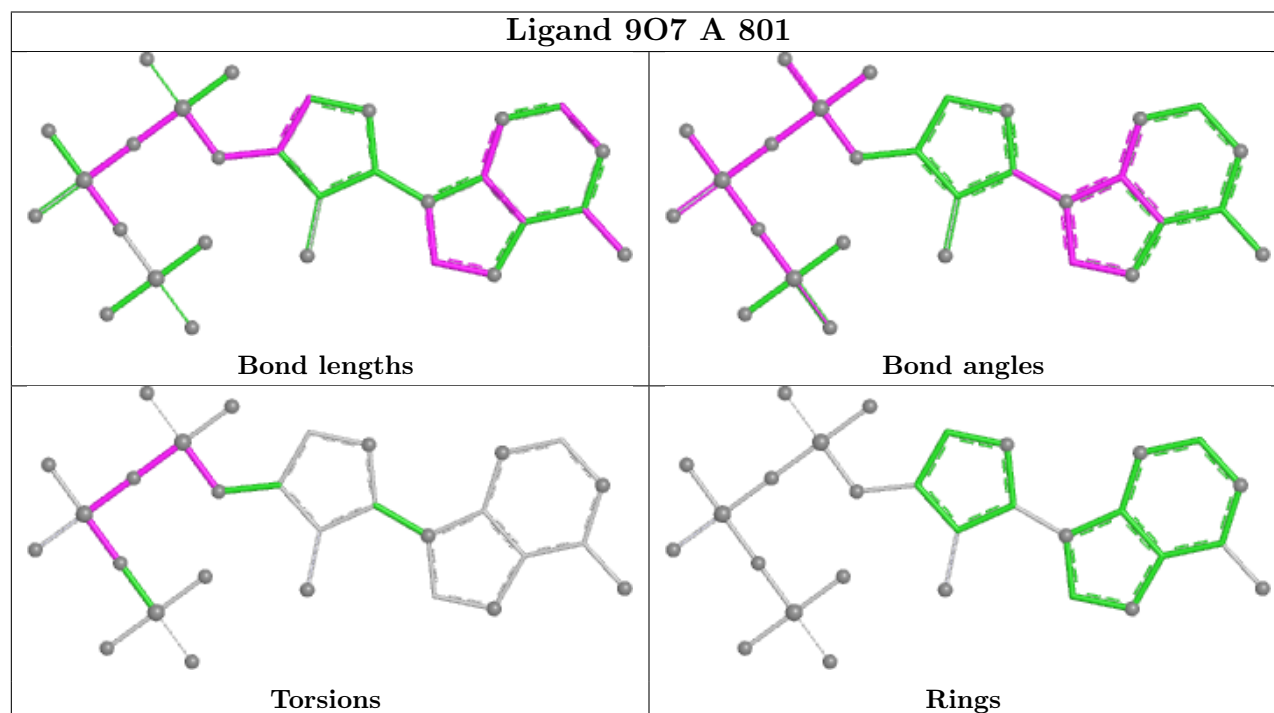
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	803	EPE	3	0
4	A	801	9O7	1	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	748/760 (98%)	0.53	22 (2%) 53 51	29, 41, 64, 90	0
2	T	15/15 (100%)	0.45	0 100 100	36, 43, 65, 71	0
3	P	11/12 (91%)	0.29	1 (9%) 15 14	44, 49, 61, 61	0
All	All	774/787 (98%)	0.53	23 (2%) 52 50	29, 41, 64, 90	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	5.8
1	A	588	PHE	5.2
1	A	437	GLN	3.0
1	A	148	GLU	2.9
1	A	382	ARG	2.8
1	A	747	ARG	2.7
1	A	59	HIS	2.7
1	A	692	VAL	2.5
1	A	243	ARG	2.4
1	A	224	GLU	2.3
3	P	1	DC	2.3
1	A	266	ARG	2.3
1	A	261	TYR	2.3
1	A	446	PHE	2.3
1	A	132	ASP	2.2
1	A	472	VAL	2.2
1	A	531	GLU	2.1
1	A	135	LEU	2.1
1	A	146	TYR	2.1
1	A	183	VAL	2.1
1	A	381	LEU	2.1
1	A	717	SER	2.0
1	A	30	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

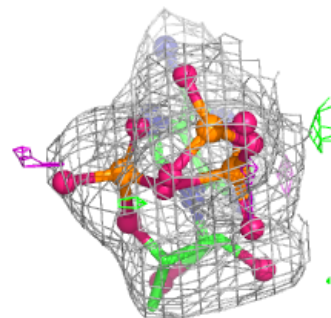
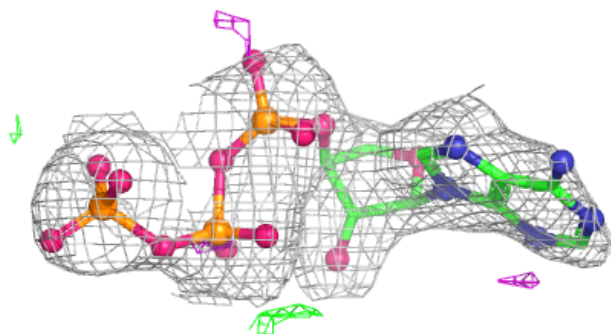
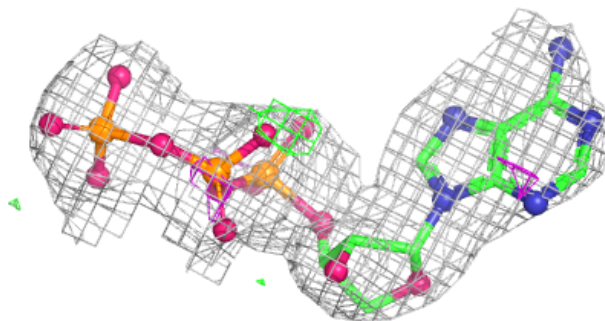
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EPE	A	803	15/15	0.85	0.14	42,44,47,47	0
4	9O7	A	801	29/29	0.91	0.10	39,41,42,43	0
5	MG	A	802	1/1	0.96	0.08	38,38,38,38	0

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 9O7 A 801:

$2mF_o - DF_c$ (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.