



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:48 pm BST

PDB ID : 3SCX
Title : RB69 DNA Polymerase Triple Mutant(L561A/S565G/Y567A) Ternary Complex with dUpNpp and a Deoxy-terminated Primer in the Presence of Ca²⁺
Authors : Wang, M.; Wang, J.; Konigsberg, W.H.
Deposited on : 2011-06-08
Resolution : 2.35 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

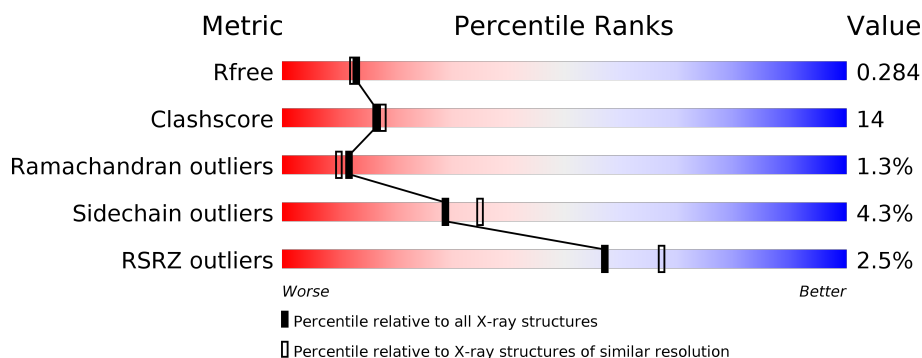
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	T	18	<div> <div>6%</div> <div> <div></div> <div>56%</div> <div>39%</div> <div>6%</div> </div> </div>
2	P	13	<div> <div>15%</div> <div>77%</div> <div>8%</div> </div>
3	A	903	<div> <div>2%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8385 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 DNA chain called 5'-D(*TP*CP*AP*AP*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	18	Total	C	N	O	P	0	0	0
			367	175	71	104	17			

- Molecule 2 is a DNA chain called 5'-D(*GP*CP*GP*GP*AP*CP*TP*GP*CP*TP*TP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			

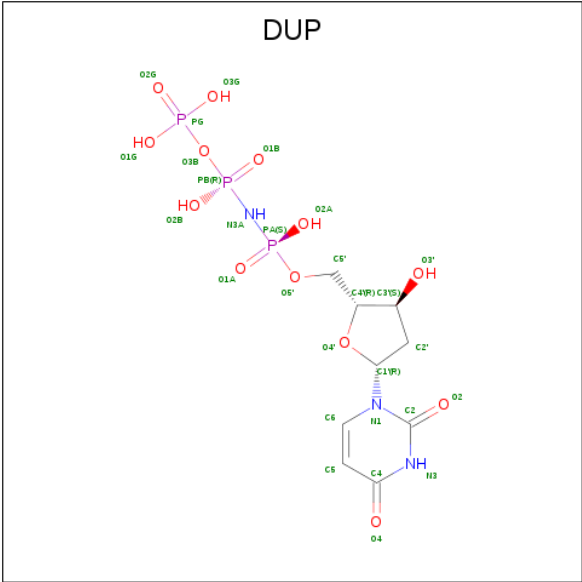
- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	903	Total	C	N	O	S	0	3	0
			7378	4740	1227	1378	33			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	327	ALA	ASP	ENGINEERED MUTATION	UNP Q38087
A	561	ALA	LEU	ENGINEERED MUTATION	UNP Q38087
A	565	GLY	SER	ENGINEERED MUTATION	UNP Q38087
A	567	ALA	TYR	ENGINEERED MUTATION	UNP Q38087
A	902	ALA	ASP	CONFLICT	UNP Q38087

- Molecule 4 is 2'-DEOXYURIDINE 5'-ALPHA,BETA-IMIDO-TRIPHOSPHATE (three-letter code: DUP) (formula: C₉H₁₆N₃O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Ca	0	0
			4	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	24	Total	O	0	0
			24	24		
6	P	12	Total	O	0	0
			12	12		
6	A	309	Total	O	0	0
			309	309		

● Molecule 1: 5'-D(*TP*CP*AP*AP*GP*TP*AP*AP*GP*CP*AP*GP*TP*CP*CP*GP*CP*G)-3'



E892	E893	A894	A895	S896	L897	F898	D899	F900	F901	A902	F903
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.02Å 119.33Å 130.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.04 – 2.35 65.06 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.8 (88.04-2.35) 99.8 (65.06-2.35)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.259 0.243 , 0.284	Depositor DCC
R_{free} test set	2507 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	1.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8385	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: DUP, CA

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	T	0.67	0/412	1.28	2/634 (0.3%)
2	P	0.79	0/294	1.51	7/452 (1.5%)
3	A	0.38	0/7568	0.52	0/10227
All	All	0.42	0/8274	0.66	9/11313 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	108	DC	C1'-O4'-C4'	-7.07	103.03	110.10
1	T	8	DA	O4'-C1'-N9	6.95	112.87	108.00
2	P	108	DC	O4'-C4'-C3'	-6.44	101.92	104.50
2	P	103	DG	O4'-C1'-N9	6.41	112.49	108.00
2	P	115	DC	O4'-C4'-C3'	-6.08	102.07	104.50
1	T	18	DG	O4'-C1'-N9	5.52	111.87	108.00
2	P	111	DC	C1'-O4'-C4'	-5.49	104.61	110.10
2	P	108	DC	O4'-C1'-N1	5.44	111.81	108.00
2	P	115	DC	C1'-O4'-C4'	-5.15	104.95	110.10

There are no chirality outliers.

There are no planarity outliers.

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	T	367	0	203	11	0
2	P	263	0	148	4	0
3	A	7378	0	7274	214	0
4	A	28	0	12	1	0
5	A	4	0	0	0	0
6	A	309	0	0	14	0
6	P	12	0	0	0	0
6	T	24	0	0	2	0
All	All	8385	0	7637	222	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 14.

All (222) 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)
3:A:252:VAL:CG2	3:A:253:ILE:HB	1.10	1.56
3:A:252:VAL:CG2	3:A:253:ILE:CB	1.97	1.40
3:A:256:MET:N	3:A:257:TYR:HB2	1.29	1.40
3:A:255:ASN:CB	3:A:256:MET:HA	1.17	1.38
3:A:893:LYS:HA	3:A:894:LYS:CB	1.56	1.35
3:A:255:ASN:CB	3:A:256:MET:CA	2.07	1.31
3:A:252:VAL:HG22	3:A:253:ILE:CB	1.53	1.30
3:A:256:MET:H	3:A:257:TYR:CB	1.58	1.16
3:A:253:ILE:O	3:A:254:GLU:HG3	1.46	1.12
3:A:256:MET:N	3:A:257:TYR:CB	2.13	1.12
3:A:255:ASN:HB2	3:A:256:MET:CA	1.78	1.10
3:A:255:ASN:HB2	3:A:256:MET:HA	1.26	1.09
3:A:896:SER:HB2	3:A:897:LEU:HA	1.11	1.08
3:A:253:ILE:HG23	3:A:254:GLU:N	1.54	1.07
3:A:253:ILE:HG23	3:A:254:GLU:H	0.93	1.07
3:A:252:VAL:HG22	3:A:253:ILE:CG2	1.85	1.05
3:A:252:VAL:HG23	3:A:253:ILE:CB	1.72	1.05
3:A:893:LYS:HA	3:A:894:LYS:HB3	1.04	1.04
3:A:896:SER:HB2	3:A:898:PHE:O	1.56	1.03
3:A:256:MET:CA	3:A:257:TYR:HB2	1.89	1.02
3:A:893:LYS:CA	3:A:894:LYS:HB3	1.88	1.02
3:A:896:SER:CB	3:A:897:LEU:HA	1.89	0.99
3:A:893:LYS:CA	3:A:894:LYS:CB	2.42	0.98
3:A:253:ILE:CG2	3:A:254:GLU:H	1.70	0.97
3:A:255:ASN:HB3	3:A:256:MET:CA	1.80	0.96
3:A:252:VAL:HG22	3:A:253:ILE:HB	1.13	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:896:SER:HB2	3:A:897:LEU:CA	1.96	0.95
3:A:897:LEU:HA	3:A:898:PHE:O	1.66	0.94
3:A:893:LYS:HA	3:A:894:LYS:HB2	1.52	0.91
3:A:255:ASN:HB3	3:A:256:MET:HA	0.90	0.90
3:A:900:MET:HG2	3:A:901:PHE:N	1.88	0.88
3:A:260:ARG:HD2	6:A:1136:HOH:O	1.73	0.87
3:A:900:MET:HG2	3:A:901:PHE:H	1.39	0.86
3:A:256:MET:HG2	3:A:257:TYR:CD2	2.12	0.85
3:A:597:ILE:O	3:A:601:VAL:HG23	1.77	0.85
3:A:881:GLU:HG2	3:A:891:TYR:CE1	2.12	0.85
3:A:192:ASP:HB3	6:A:1143:HOH:O	1.80	0.82
3:A:253:ILE:CG2	3:A:254:GLU:N	2.29	0.81
3:A:253:ILE:HD12	3:A:253:ILE:C	2.00	0.81
3:A:793:VAL:HG23	3:A:794:GLY:N	1.96	0.80
3:A:252:VAL:HG22	3:A:253:ILE:HG22	1.62	0.80
3:A:252:VAL:CG2	3:A:260:ARG:O	2.30	0.79
3:A:40:HIS:HD2	6:A:1117:HOH:O	1.66	0.79
3:A:252:VAL:HG22	3:A:253:ILE:CA	2.13	0.78
3:A:202:LEU:O	3:A:206:GLN:HG2	1.82	0.78
3:A:642:ARG:HG3	3:A:646:HIS:ND1	1.98	0.78
3:A:252:VAL:HG23	3:A:253:ILE:HB	0.79	0.78
3:A:252:VAL:HG23	3:A:260:ARG:O	1.83	0.78
3:A:256:MET:H	3:A:257:TYR:HB2	0.83	0.76
3:A:256:MET:HG2	3:A:257:TYR:CG	2.21	0.75
3:A:255:ASN:HB2	3:A:256:MET:CB	2.17	0.74
3:A:253:ILE:O	3:A:254:GLU:CG	2.30	0.74
3:A:896:SER:CB	3:A:898:PHE:O	2.34	0.73
3:A:878:LYS:HB3	3:A:879:PRO:HD3	1.71	0.73
3:A:794:GLY:HA3	3:A:796:PHE:N	2.03	0.73
3:A:303:LEU:H	3:A:303:LEU:HD22	1.54	0.72
3:A:611:THR:HG21	3:A:614:GLU:HG3	1.72	0.72
3:A:794:GLY:HA3	3:A:796:PHE:H	1.55	0.72
1:T:13:DT:H2'	6:T:151:HOH:O	1.88	0.71
3:A:794:GLY:CA	3:A:796:PHE:H	2.05	0.69
3:A:892:GLU:O	3:A:894:LYS:HB2	1.93	0.69
3:A:252:VAL:CG2	3:A:253:ILE:CG2	2.56	0.69
3:A:894:LYS:O	3:A:895:ALA:O	2.10	0.69
3:A:514:LEU:HD13	3:A:533:LEU:HD11	1.73	0.69
3:A:41:CYS:HB2	3:A:45:GLN:NE2	2.08	0.68
3:A:143:ASP:OD2	3:A:208:LYS:NZ	2.26	0.68
3:A:252:VAL:HG22	3:A:253:ILE:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:639:SER:O	3:A:641:PHE:N	2.28	0.66
3:A:794:GLY:N	3:A:796:PHE:H	1.93	0.66
3:A:251:LYS:HG3	6:A:1115:HOH:O	1.95	0.65
3:A:475:ILE:HD12	3:A:566:LEU:HD23	1.77	0.65
1:T:2:DC:H4'	3:A:254:GLU:HB2	1.78	0.65
3:A:659:MET:O	3:A:663:ILE:HG13	1.97	0.65
3:A:249:ARG:HG3	3:A:250:VAL:O	1.97	0.64
3:A:255:ASN:OD1	3:A:255:ASN:N	2.30	0.64
3:A:793:VAL:CG2	3:A:794:GLY:N	2.60	0.64
3:A:881:GLU:HG2	3:A:891:TYR:HE1	1.63	0.64
3:A:252:VAL:CG2	3:A:253:ILE:CA	2.73	0.63
3:A:171:GLN:OE1	3:A:304:LYS:HE2	1.98	0.63
3:A:11:ILE:HD12	3:A:16:PHE:CD2	2.33	0.62
3:A:639:SER:OG	3:A:640:LYS:N	2.30	0.62
3:A:253:ILE:HG12	3:A:260:ARG:HG3	1.80	0.62
3:A:794:GLY:H	3:A:796:PHE:H	1.47	0.62
3:A:752:MET:HG3	3:A:760:LEU:HD23	1.82	0.61
3:A:816:LYS:HD3	3:A:817:GLY:N	2.14	0.61
3:A:253:ILE:C	3:A:253:ILE:CD1	2.69	0.61
3:A:816:LYS:HD3	3:A:817:GLY:H	1.65	0.61
3:A:254:GLU:C	3:A:255:ASN:OD1	2.40	0.61
1:T:1:DT:H3	3:A:786:ASN:HD21	1.50	0.60
1:T:8:DA:H5''	3:A:705:LYS:HD3	1.83	0.60
2:P:113:DT:H2''	2:P:114:DA:H5'	1.84	0.59
3:A:300:VAL:O	3:A:300:VAL:HG23	2.04	0.58
3:A:599:ARG:O	3:A:603:GLU:HG3	2.03	0.57
3:A:739:LYS:HE3	3:A:742:GLN:OE1	2.04	0.57
3:A:415:LEU:HD22	3:A:623:ASP:HB3	1.87	0.57
3:A:10:GLN:HG3	3:A:65:MET:CE	2.36	0.56
3:A:773:GLN:HG3	6:A:1035:HOH:O	2.05	0.56
3:A:897:LEU:CA	3:A:898:PHE:O	2.48	0.56
3:A:889:LEU:HD12	3:A:889:LEU:C	2.26	0.56
3:A:899:ASP:OD1	3:A:902:ALA:HB3	2.06	0.56
3:A:256:MET:CA	3:A:257:TYR:CB	2.76	0.56
1:T:2:DC:C4'	3:A:254:GLU:HB2	2.35	0.55
3:A:794:GLY:CA	3:A:796:PHE:N	2.68	0.55
3:A:423:VAL:HB	3:A:425:ILE:HG13	1.88	0.55
3:A:873:GLU:HA	3:A:877:ILE:HB	1.89	0.55
3:A:389:GLN:HB3	6:A:1174:HOH:O	2.05	0.55
3:A:760:LEU:HD13	3:A:760:LEU:C	2.27	0.55
3:A:793:VAL:CG2	3:A:794:GLY:H	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:896:SER:CB	3:A:897:LEU:CA	2.65	0.54
3:A:900:MET:CG	3:A:901:PHE:H	2.16	0.53
3:A:899:ASP:OD1	3:A:900:MET:CE	2.56	0.53
3:A:216:TRP:O	3:A:217:ASN:HB2	2.08	0.53
3:A:319:ARG:CG	3:A:323[A]:TYR:CE1	2.91	0.53
3:A:894:LYS:O	3:A:895:ALA:C	2.48	0.53
3:A:637:GLY:O	3:A:638:GLU:CB	2.57	0.52
3:A:396:VAL:O	3:A:705:LYS:HE2	2.09	0.52
3:A:897:LEU:HA	3:A:898:PHE:C	2.29	0.52
3:A:402:ASN:HA	3:A:886:ALA:O	2.09	0.52
3:A:793:VAL:HG23	3:A:794:GLY:H	1.70	0.52
3:A:637:GLY:O	3:A:638:GLU:HB2	2.10	0.52
3:A:471:VAL:HG13	3:A:566:LEU:HD21	1.93	0.51
3:A:621:ASP:O	3:A:622:THR:HB	2.11	0.51
3:A:897:LEU:HD12	3:A:898:PHE:O	2.10	0.51
3:A:679:HIS:HD2	6:A:916:HOH:O	1.94	0.51
3:A:896:SER:HB3	3:A:898:PHE:CB	2.40	0.51
3:A:319:ARG:HD3	3:A:323[A]:TYR:CE1	2.46	0.51
3:A:402:ASN:OD1	3:A:403:ARG:N	2.40	0.51
3:A:899:ASP:OD1	3:A:900:MET:HE2	2.11	0.51
3:A:606:ASN:OD1	3:A:611:THR:HG23	2.12	0.50
3:A:414:SER:HA	4:A:904:DUP:O3B	2.12	0.50
3:A:811:TYR:CE2	3:A:815:ILE:HD13	2.47	0.50
3:A:875:THR:O	3:A:879:PRO:HG2	2.12	0.50
3:A:291:ASP:OD2	3:A:302:LYS:HB2	2.12	0.50
3:A:891:TYR:CE1	6:A:1199:HOH:O	2.54	0.49
3:A:702:TRP:CD1	3:A:708:TYR:HB3	2.47	0.49
3:A:900:MET:CG	3:A:901:PHE:N	2.67	0.49
3:A:854:ILE:HD11	3:A:858:ILE:HD11	1.93	0.49
3:A:207:GLN:HG2	3:A:208:LYS:HG3	1.95	0.48
3:A:605:LEU:HA	3:A:608:VAL:HG22	1.95	0.48
3:A:614:GLU:HB2	3:A:616:PHE:CE2	2.48	0.48
3:A:839:ASN:OD1	3:A:841:PHE:HB2	2.13	0.48
3:A:900:MET:CE	3:A:901:PHE:H	2.27	0.48
3:A:150:ASP:OD2	3:A:317:HIS:CE1	2.67	0.47
3:A:353:ILE:HG13	3:A:354:GLN:O	2.14	0.47
3:A:396:VAL:HG12	3:A:705:LYS:HG2	1.96	0.47
3:A:794:GLY:HA3	3:A:796:PHE:HD2	1.79	0.47
3:A:611:THR:CG2	3:A:614:GLU:HG3	2.44	0.47
3:A:792:ASP:OD2	3:A:795:GLY:HA2	2.14	0.47
2:P:104:DC:H2"	2:P:105:DG:OP2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:330:ARG:HA	3:A:333:GLN:HE21	1.79	0.46
3:A:426:SER:OG	3:A:427:PRO:HD2	2.15	0.46
3:A:839:ASN:HB2	3:A:840:PRO:HD2	1.98	0.46
3:A:896:SER:HB2	3:A:897:LEU:HD12	1.97	0.46
3:A:147:TYR:CE2	3:A:187:ILE:HD12	2.51	0.46
3:A:415:LEU:HD22	3:A:623:ASP:CB	2.45	0.46
3:A:330:ARG:HH11	3:A:333:GLN:HE22	1.64	0.46
3:A:450:PRO:HD2	6:A:968:HOH:O	2.16	0.46
3:A:825:VAL:HG12	3:A:828:GLU:HG3	1.97	0.46
3:A:893:LYS:CA	3:A:894:LYS:HB2	2.31	0.46
3:A:436:VAL:HG12	3:A:437:ALA:O	2.15	0.45
3:A:44:SER:O	3:A:46:ALA:N	2.49	0.45
3:A:351:ALA:O	3:A:352:LYS:HB2	2.16	0.45
3:A:797:PRO:HG2	3:A:806:ARG:NH1	2.32	0.45
3:A:605:LEU:HA	3:A:608:VAL:CG2	2.48	0.44
3:A:876:PHE:O	3:A:879:PRO:HD2	2.17	0.44
3:A:3:GLU:HG2	3:A:22:SER:N	2.31	0.44
3:A:130:LYS:HE3	3:A:131:HIS:CE1	2.52	0.44
3:A:183:ILE:HD13	3:A:183:ILE:HA	1.78	0.44
3:A:250:VAL:CG1	3:A:251:LYS:N	2.80	0.44
1:T:12:DG:OP1	3:A:874:LYS:HE3	2.17	0.44
3:A:899:ASP:N	3:A:899:ASP:OD2	2.47	0.44
2:P:106:DG:H2''	2:P:107:DA:C8	2.52	0.44
3:A:882:GLY:HA3	6:A:1037:HOH:O	2.17	0.44
3:A:303:LEU:CD2	6:A:951:HOH:O	2.65	0.43
3:A:640:LYS:O	3:A:640:LYS:CG	2.66	0.43
3:A:731:GLU:HA	3:A:734:LYS:HD3	2.00	0.43
1:T:13:DT:H6	6:T:151:HOH:O	2.01	0.43
3:A:255:ASN:CB	3:A:256:MET:CB	2.85	0.43
3:A:253:ILE:HG21	3:A:259:SER:HA	2.00	0.43
3:A:530:ILE:HA	3:A:533:LEU:HD12	1.99	0.43
3:A:206:GLN:NE2	3:A:241:ARG:HE	2.16	0.43
3:A:131:HIS:HA	3:A:132:PRO:HD3	1.89	0.43
1:T:1:DT:H4'	1:T:2:DC:O5'	2.19	0.43
1:T:9:DG:H2'	1:T:10:DC:C6	2.53	0.43
3:A:580:LEU:HA	3:A:580:LEU:HD12	1.84	0.43
3:A:772:ARG:NE	6:A:986:HOH:O	2.35	0.43
3:A:143:ASP:O	3:A:144:ASP:HB3	2.18	0.42
3:A:749:ILE:O	3:A:753:LEU:HG	2.19	0.42
3:A:761:GLN:HE22	3:A:893:LYS:HB2	1.83	0.42
1:T:12:DG:OP1	3:A:874:LYS:CE	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:413:THR:O	3:A:414:SER:C	2.56	0.42
3:A:41:CYS:HB2	3:A:42:PRO:CD	2.49	0.42
3:A:364:THR:O	3:A:368:ILE:HG13	2.19	0.42
3:A:899:ASP:CG	3:A:902:ALA:HB3	2.40	0.42
3:A:43:GLU:O	3:A:44:SER:C	2.58	0.42
3:A:253:ILE:CG1	3:A:254:GLU:N	2.82	0.42
3:A:40:HIS:CE1	3:A:55:LYS:HE2	2.54	0.42
3:A:540:GLU:O	3:A:543:PHE:HB3	2.20	0.42
3:A:738:PRO:HB3	3:A:779:ILE:HA	2.00	0.42
3:A:254:GLU:CA	3:A:255:ASN:OD1	2.68	0.41
3:A:660:GLU:N	3:A:661:PRO:CD	2.83	0.41
1:T:1:DT:H3	3:A:786:ASN:ND2	2.16	0.41
3:A:862:VAL:O	3:A:866:MET:HG3	2.20	0.41
3:A:878:LYS:N	3:A:879:PRO:CD	2.82	0.41
3:A:41:CYS:HB2	3:A:42:PRO:HD2	2.02	0.41
3:A:821:ALA:HA	3:A:822:PRO:HD3	1.93	0.41
3:A:825:VAL:CG1	3:A:828:GLU:HG3	2.50	0.41
3:A:303:LEU:HD21	6:A:951:HOH:O	2.19	0.41
3:A:771:PHE:CD2	3:A:872:LEU:HD13	2.56	0.41
2:P:108:DC:H2'	2:P:109:DT:H72	2.01	0.41
3:A:787:ASN:HB2	6:A:1144:HOH:O	2.20	0.41
3:A:207:GLN:HG2	3:A:208:LYS:CG	2.50	0.41
3:A:604:TYR:O	3:A:608:VAL:HG22	2.19	0.41
3:A:408:MET:HA	3:A:687:ALA:O	2.21	0.41
3:A:899:ASP:OD1	3:A:900:MET:HE1	2.20	0.41
3:A:441:ASP:HB3	3:A:447:ALA:HB2	2.03	0.41
3:A:651:LEU:HA	3:A:651:LEU:HD23	1.95	0.41
3:A:796:PHE:HB3	3:A:797:PRO:CD	2.50	0.41
3:A:884:THR:HG21	3:A:891:TYR:HB3	2.03	0.41
3:A:896:SER:HB3	3:A:898:PHE:HB3	2.03	0.41
3:A:150:ASP:OD2	3:A:317:HIS:HE1	2.03	0.40
3:A:254:GLU:HA	3:A:255:ASN:OD1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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
3	A	904/903 (100%)	859 (95%)	33 (4%)	12 (1%)	12 10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	253	ILE
3	A	254	GLU
3	A	639	SER
3	A	640	LYS
3	A	894	LYS
3	A	895	ALA
3	A	45	GLN
3	A	257	TYR
3	A	638	GLU
3	A	898	PHE
3	A	896	SER
3	A	795	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
3	A	799/796 (100%)	765 (96%)	34 (4%)	29 35

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	61	LEU
3	A	102	LYS
3	A	113	PHE
3	A	154	SER
3	A	183	ILE

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Mol	Chain	Res	Type
3	A	207	GLN
3	A	249	ARG
3	A	251	LYS
3	A	253	ILE
3	A	255	ASN
3	A	259	SER
3	A	287	SER
3	A	291	ASP
3	A	295	GLU
3	A	302	LYS
3	A	303	LEU
3	A	309	ILE
3	A	314	GLU
3	A	332	LEU
3	A	440	HIS
3	A	452	ASP
3	A	580	LEU
3	A	640	LYS
3	A	693	LEU
3	A	739	LYS
3	A	790	LYS
3	A	816	LYS
3	A	835	LEU
3	A	837	GLU
3	A	855	THR
3	A	873	GLU
3	A	899	ASP
3	A	900	MET
3	A	903	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	40	HIS
3	A	45	GLN
3	A	105	HIS
3	A	112	ASN
3	A	131	HIS
3	A	203	ASN
3	A	206	GLN
3	A	299	ASN
3	A	333	GLN

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Mol	Chain	Res	Type
3	A	339	GLN
3	A	386	HIS
3	A	546	GLN
3	A	564	ASN
3	A	679	HIS
3	A	761	GLN
3	A	773	GLN
3	A	786	ASN
3	A	787	ASN
3	A	823	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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$
4	DUP	A	904	5	28,29,29	2.96	7 (25%)	37,45,45	2.33	9 (24%)

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
4	DUP	A	904	5	-	3/19/34/34	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904	DUP	C6-N1	-7.31	1.34	1.47
4	A	904	DUP	O2-C2	6.84	1.35	1.23
4	A	904	DUP	O4-C4	6.41	1.36	1.23
4	A	904	DUP	C6-C5	-4.91	1.39	1.52
4	A	904	DUP	C5-C4	-4.85	1.38	1.50
4	A	904	DUP	PB-O1B	4.37	1.53	1.46
4	A	904	DUP	PA-O1A	3.60	1.51	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904	DUP	C2'-C1'-N1	-7.19	106.82	115.61
4	A	904	DUP	C4-N3-C2	-6.30	120.57	125.79
4	A	904	DUP	N3-C2-N1	4.51	121.42	116.65
4	A	904	DUP	O2A-PA-O1A	4.06	118.42	109.92
4	A	904	DUP	O2B-PB-O1B	4.04	118.39	109.92
4	A	904	DUP	PG-O3B-PB	-3.16	121.49	132.62
4	A	904	DUP	C5-C6-N1	2.63	120.30	111.61
4	A	904	DUP	O2-C2-N1	-2.56	119.89	123.11
4	A	904	DUP	C5-C4-N3	2.25	119.17	116.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

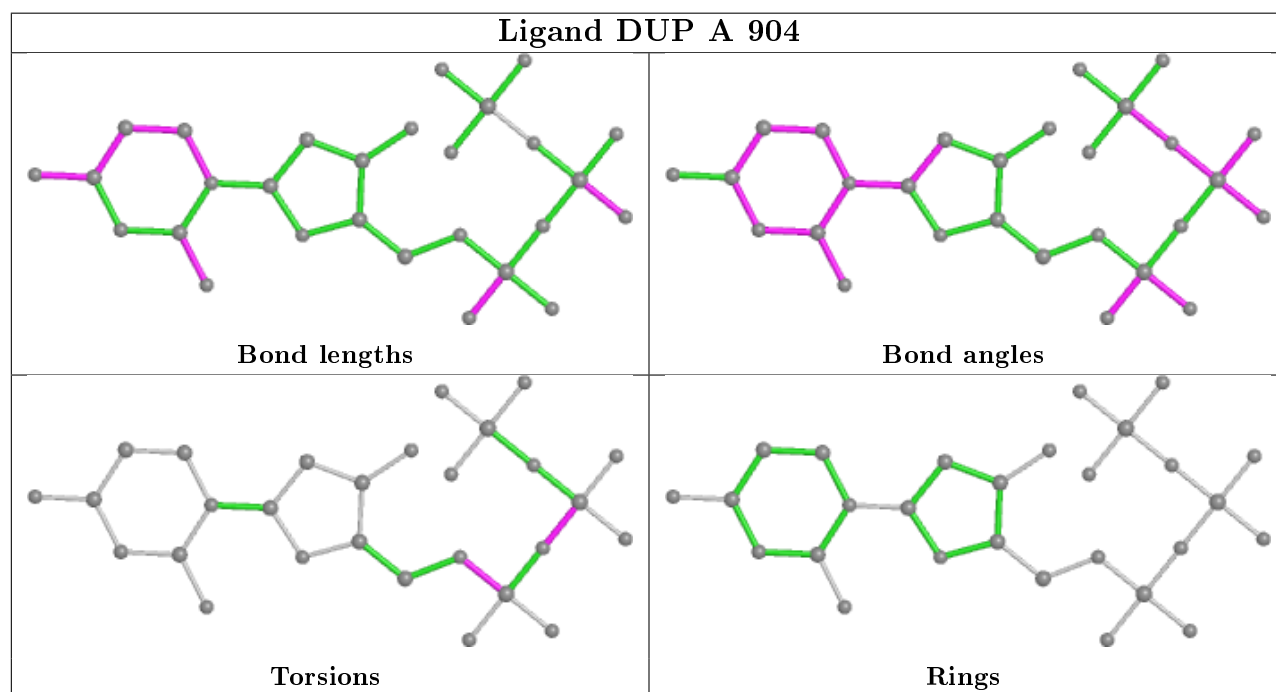
Mol	Chain	Res	Type	Atoms
4	A	904	DUP	C5'-O5'-PA-O2A
4	A	904	DUP	PA-N3A-PB-O1B
4	A	904	DUP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	904	DUP	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	T	18/18 (100%)	0.12	1 (5%) 24 35	41, 47, 75, 95	0
2	P	13/13 (100%)	-0.13	0 100 100	40, 46, 63, 64	0
3	A	903/903 (100%)	0.25	22 (2%) 59 68	30, 40, 70, 183	0
All	All	934/934 (100%)	0.25	23 (2%) 57 67	30, 41, 71, 183	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	253	ILE	10.7
3	A	903	PHE	9.9
3	A	257	TYR	7.7
3	A	255	ASN	7.5
3	A	901	PHE	7.1
1	T	1	DT	4.2
3	A	256	MET	4.1
3	A	254	GLU	3.8
3	A	259	SER	3.6
3	A	902	ALA	3.4
3	A	45	GLN	3.3
3	A	514	LEU	2.9
3	A	252	VAL	2.8
3	A	871	LEU	2.6
3	A	899	ASP	2.5
3	A	44	SER	2.5
3	A	323[A]	TYR	2.5
3	A	647	TRP	2.4
3	A	258	GLY	2.3
3	A	43	GLU	2.1
3	A	303	LEU	2.1
3	A	407	VAL	2.1
3	A	900	MET	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](#)

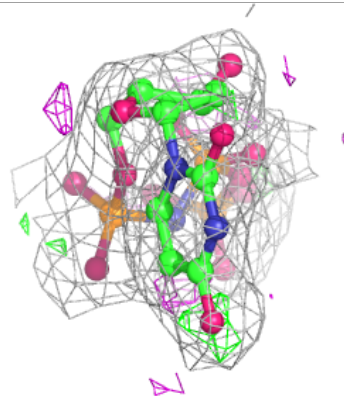
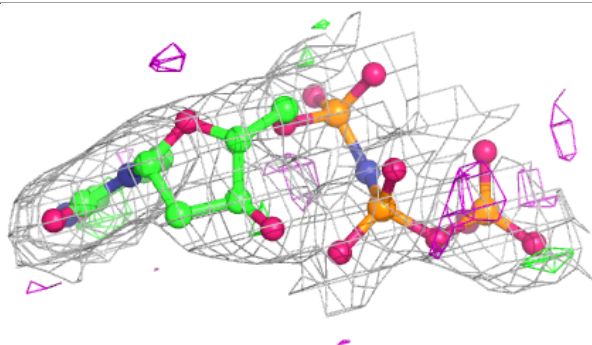
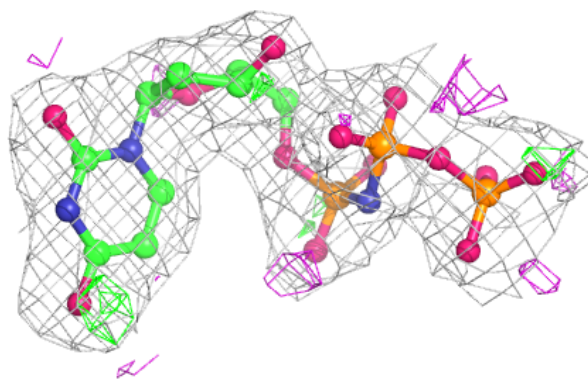
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CA	A	907	1/1	0.83	0.07	85,85,85,85	0
5	CA	A	908	1/1	0.84	0.21	47,47,47,47	0
5	CA	A	906	1/1	0.86	0.04	50,50,50,50	0
5	CA	A	905	1/1	0.90	0.11	68,68,68,68	0
4	DUP	A	904	28/28	0.92	0.14	38,39,44,46	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 DUP A 904:

$2mF_o - DF_c$ (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.