



wwPDB X-ray Structure Validation Summary Report

Mar 5, 2026 – 06:26 PM UTC

PDB ID : 3ERC / pdb_00003erc
Title : Crystal structure of the heterodimeric vaccinia virus mRNA polyadenylate polymerase with three fragments of RNA and 3'-deoxy ATP
Authors : Li, C.; Li, H.; Zhou, S.; Poulos, T.L.; Gershon, P.D.
Deposited on : 2008-10-01
Resolution : 3.21 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (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

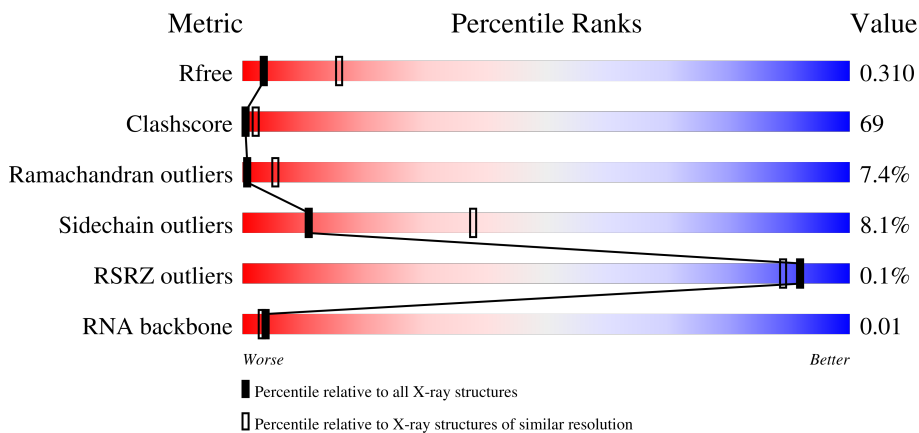
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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.





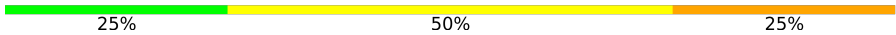
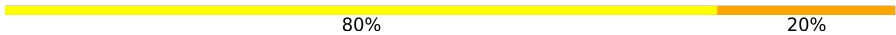
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)
RNA backbone	3983	1055 (3.50-2.94)

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	297	
1	B	297	
2	C	479	
2	D	479	

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Mol	Chain	Length	Quality of chain
3	E	5	 40% 40% 20%
3	F	5	 40% 60%
4	G	4	 25% 50% 25%
5	I	5	 80% 20%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12480 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 Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	Total	C	N	O	S	0	0	0
			2382	1552	394	424	12			
1	B	288	Total	C	N	O	S	0	0	0
			2382	1552	394	424	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	ALA	ARG	engineered mutation	UNP P07617
A	142	ALA	LYS	engineered mutation	UNP P07617
A	143	ALA	ARG	engineered mutation	UNP P07617
B	140	ALA	ARG	engineered mutation	UNP P07617
B	142	ALA	LYS	engineered mutation	UNP P07617
B	143	ALA	ARG	engineered mutation	UNP P07617

- Molecule 2 is a protein called Poly(A) polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	445	Total	C	N	O	S	0	0	0
			3627	2318	605	680	24			
2	D	445	Total	C	N	O	S	0	0	0
			3627	2318	605	680	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	36	SER	LEU	engineered mutation	UNP P23371
D	36	SER	LEU	engineered mutation	UNP P23371

- Molecule 3 is a RNA chain called RNA/DNA chimera (5'-D(CP*)R(UP*UP*)D(CP*C)-3').

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	E	5	Total	C	N	O	P	0	0	0
			94	45	13	32	4			
3	F	5	Total	C	N	O	P	0	0	0
			94	45	13	32	4			

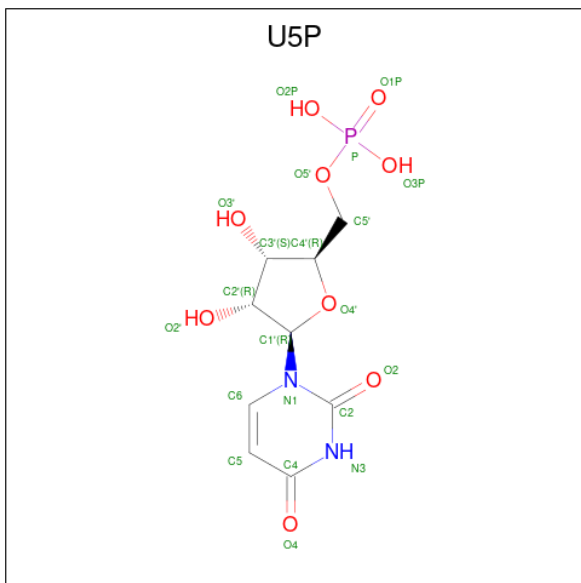
- Molecule 4 is a RNA chain called RNA/DNA chimera (5'-D(CP*)R(UP*UP*)-D(C)-3').

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	G	4	Total	C	N	O	P	0	0	0
			75	36	10	26	3			

- Molecule 5 is a RNA chain called RNA/DNA chimera (5'-D(CP*CP*)R(UP*UP*)D(C)-3').

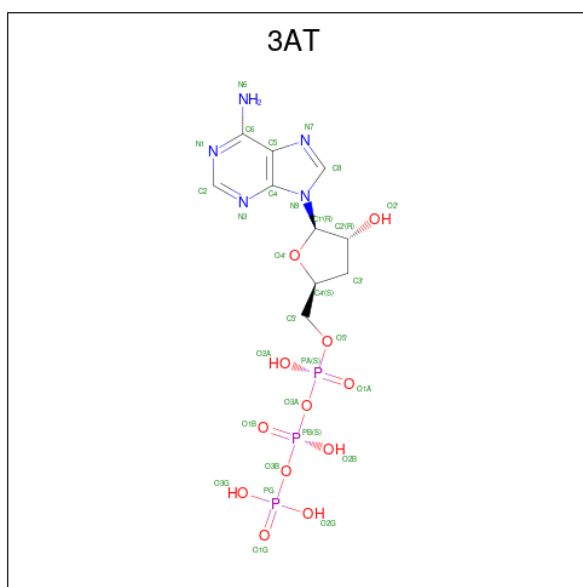
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
5	I	5	Total	C	N	O	P	0	0	0
			94	45	13	32	4			

- Molecule 6 is URIDINE-5'-MONOPHOSPHATE (CCD ID: U5P) (formula: C₉H₁₃N₂O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
6	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 7 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (CCD ID: 3AT) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
7	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	2	Total	Ca	0	0
			2	2		
8	D	2	Total	Ca	0	0
			2	2		

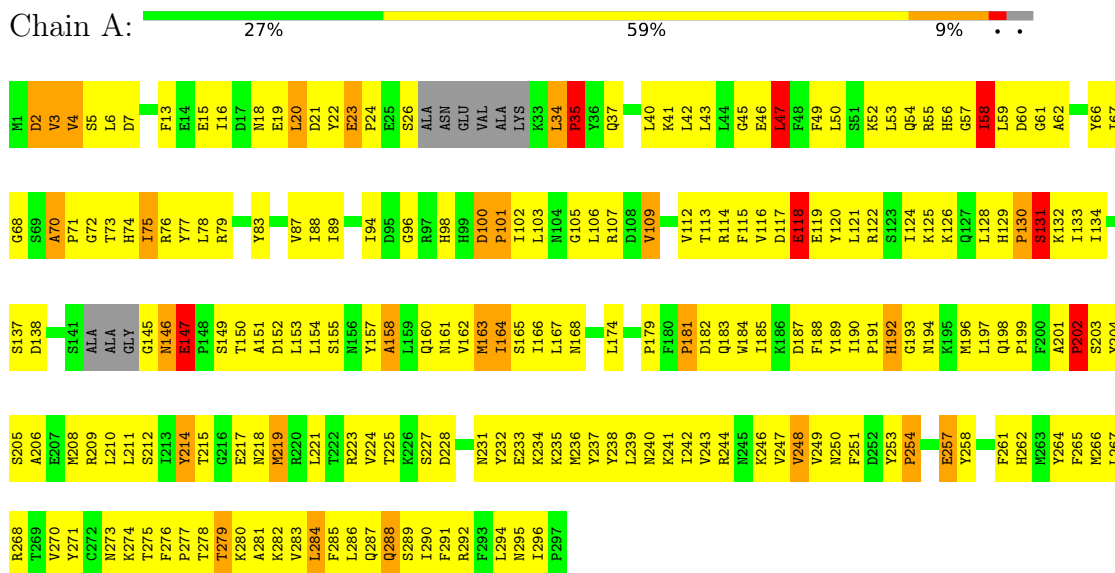
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	O	0	0
			1	1		

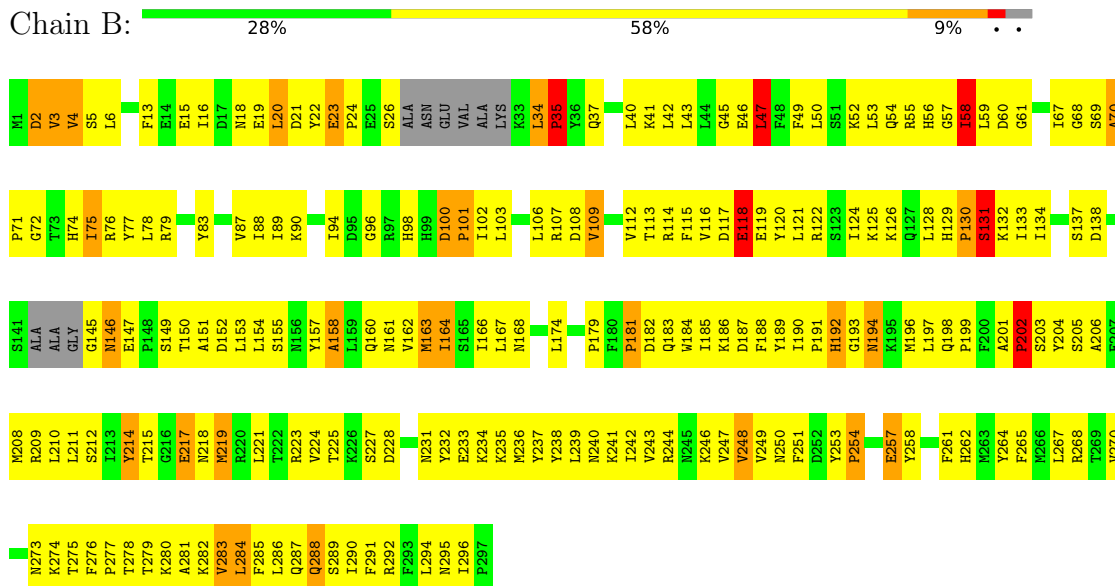
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase



- Molecule 1: Cap-specific mRNA (nucleoside-2'-O-)-methyltransferase



• Molecule 2: Poly(A) polymerase catalytic subunit

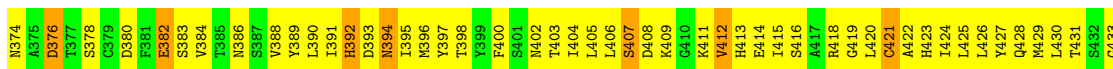
Chain C: 15% 62% 14% 7%

MET	ASN	ARG	ASN	ASP	GLN	ASN	THR	LEU	PRO	N12	I13	I14	L15	K16	I17	I18	E19	Z20	Y21	S27	V28	N29	E30	Y31	H32	M33	K34	K35	S36	Q37	A38	R39	N40	I41	Q42	K43	I44	T45	V46	F47	N48	K49	D50	I51	F52	V53	S54	S54	L55	V56	K57	K58	M59	K60							
K61	R62	F63	F64	V67	R68	T69	S70	E73	I74	K75	D76	R77	R78	L79	S80	Y81	F82	S83	K84	Q85	G22	R24	V25	P26	I91	G92	K93	L94	F95	T96	I97	I98	E99	L100	Q101	S102	V103	L104	V105	T106	T107	Y108	T109	D110	I111	L112	G113	V114	F115	T116	R117	L118	L119	LYS	ALA	PRO	ASN	VAL	I184	I184	ILE
SER	SER	LYS	ILE	TYR	M130	V131	M134	E135	E136	I137	A138	R139	D140	M141	L142	M143	S144	M145	R146	V147	A148	V149	ILE	ASP	L175	ALA	LYS	VAL	MET	GLY	ARG	HIS	ASN	V161	S162	S163	L164	V165	K166	N167	V168	M169	K170	L171	M172	E173	E174	Y175	L176	R177	R178	H179	S182	C183	T184	C185	C185				
Y186	G187	S188	Y189	S190	L191	Y192	L193	I194	M195	P196	E197	I198	R199	Y200	G201	D202	V203	D204	L205	L206	Q207	T208	N209	S210	R211	T212	F213	L214	T215	D216	L217	A218	F219	L220	L221	K222	F223	L224	T225	G226	N227	N228	L229	I230	L231	S232	K233	I234	P235	Y236	L237	R238	N239	Y240	M241	V242	K304	F305	L371	K372	A307
E246	N247	D248	H250	L251	L252	D253	T257	M258	M259	D260	T261	M262	M263	V264	V265	P266	K267	L268	F269	D271	L270	D271	R211	T212	T213	L214	T215	D216	L217	F280	Q281	L282	L283	M284	M285	L286	K287	M288	F289	S290	Q291	L292	D293	R294	L295	E296	D297	L298	S299	K300	R301	P302	E303	K304	F305	L371	D372	A307			
R308	R309	A310	R312	R313	E314	Y315	R317	H320	G321	I322	V323	F324	D325	G326	K327	R328	N329	N330	N331	L270	D271	K332	K333	K334	C335	I336	I337	D338	R341	R342	I343	V344	T345	T346	T347	T348	K349	D350	Y351	F352	K355	K356	C357	L358	V359	Y360	V365	L366	S367	D368	I370	L371	D372	A307							
L373	N374	D376	T377	S378	E314	Y315	F381	S383	V384	T385	N386	S387	V388	R389	L390	I391	H392	R393	N394	I395	N396	Y397	T398	Y399	F400	S401	N402	T403	L404	L406	S407	D408	K409	G410	K411	V412	H413	H414	E415	S416	R417	G418	G419	L420	C421	A422	H423	L424	L425	L426	Y427	O428	H429	L430	T431	S432	A307				
G433	E434	Y435	K436	Q437	C438	L439	S440	D441	L442	L443	M444	S445	M446	M447	M448	R449	D450	K451	L452	P453	L454	Y455	H457	T458	E459	K462	G465	R466	H467	L470	M471	L472	E473	K474	D475	L476	L477	V478	F479	K355	K356	C357	L358	V359	Y360	V365	L366	S367	D368	I370	L371	D372	A307								

• Molecule 2: Poly(A) polymerase catalytic subunit

Chain D: 15% 62% 14% 7%

MET	ASN	ARG	ASN	ASP	GLN	ASN	THR	LEU	PRO	N12	I13	I14	L15	K16	I17	I18	E19	Z20	Y21	S27	V28	N29	E30	Y31	H32	M33	K34	K35	S36	Q37	A38	R39	N40	I41	Q42	K43	I44	T45	V46	F47	N48	K49	D50	I51	F52	V53	S54	S54	L55	V56	K57	K58	M59	K60								
K61	R62	F63	F64	V67	R68	T69	S70	E73	I74	K75	D76	R77	R78	L79	S80	Y81	F82	S83	K84	Q85	G22	R24	V25	P26	I91	G92	K93	L94	F95	T96	I97	I98	E99	L100	Q101	S102	V103	L104	V105	T106	T107	Y108	T109	D110	I111	L112	G113	V114	F115	T116	R117	L118	L119	LYS	ALA	PRO	ASN	VAL	I184	I184	ILE	
SER	SER	LYS	ILE	TYR	M130	V131	I132	S133	E135	E136	L137	A138	R139	D140	M141	L142	M143	S144	M145	R146	V147	A148	V149	ILE	ASP	L175	ALA	LYS	VAL	MET	GLY	ARG	HIS	ASN	V161	S162	S163	L164	V165	K166	N167	V168	M169	K170	L171	M172	E173	E174	Y175	L176	R177	R178	H179	S182	C183	T184	C185	C185				
C185	Y186	G187	S188	Y189	S190	L191	Y192	L193	I194	M195	P196	E197	I198	R199	Y200	G201	D202	L203	D204	L205	L206	Q207	T208	N209	S210	R211	T212	F213	L214	T215	D216	L217	A218	F219	L220	L221	K222	F223	L224	T225	G226	N227	N228	L229	I230	L231	S232	K233	I234	P235	Y236	L237	R238	N239	Y240	M241	V242	K304	F305	L371	D372	A307
D246	N247	D248	H250	L251	L252	D253	T257	M258	M259	D260	T261	M262	M263	V264	V265	P266	K267	L268	F269	D271	L270	D271	R211	T212	T213	L214	T215	D216	L217	F280	Q281	L282	L283	M284	M285	L286	K287	M288	F289	S290	Q291	L292	D293	R294	L295	E296	D297	L298	S299	K300	R301	P302	E303	K304	F305	L371	D372	A307				
R308	R309	A310	R312	R313	E314	Y315	R317	H320	G321	I322	V323	F324	D325	G326	K327	R328	N329	N330	N331	L270	D271	K332	K333	K334	C335	I336	I337	D338	R341	R342	I343	V344	T345	T346	T347	T348	K349	D350	Y351	F352	K355	K356	C357	L358	V359	Y360	V365	L366	S367	D368	I370	L371	D372	A307								



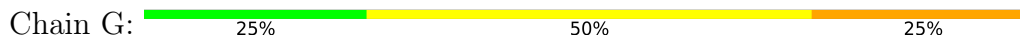
- Molecule 3: RNA/DNA chimera (5'-D(CP*)R(UP*UP*)D(CP*C)-3')



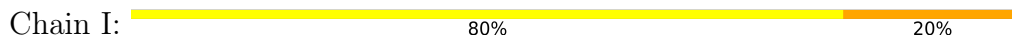
- Molecule 3: RNA/DNA chimera (5'-D(CP*)R(UP*UP*)D(CP*C)-3')



- Molecule 4: RNA/DNA chimera (5'-D(CP*)R(UP*UP*)-D(C)-3')



- Molecule 5: RNA/DNA chimera (5'-D(CP*CP*)R(UP*UP*)D(C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.92Å 77.15Å 108.03Å 89.52° 73.45° 63.76°	Depositor
Resolution (Å)	38.55 – 3.21 38.55 – 3.21	Depositor EDS
% Data completeness (in resolution range)	93.8 (38.55-3.21) 93.8 (38.55-3.21)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.18Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.245 , 0.309 0.247 , 0.310	Depositor DCC
R_{free} test set	1453 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	78.7	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.056 for h,h-k,h-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12480	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% 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: U5P, 3AT, 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	A	0.61	0/2444	1.05	23/3308 (0.7%)
1	B	0.63	0/2444	1.05	20/3308 (0.6%)
2	C	0.55	1/3686 (0.0%)	1.07	26/4972 (0.5%)
2	D	0.55	0/3686	1.07	26/4972 (0.5%)
3	E	0.62	0/103	0.80	0/156
3	F	0.50	0/103	0.80	0/156
4	G	0.52	0/82	0.57	0/124
5	I	0.50	0/103	0.58	0/156
All	All	0.58	1/12651 (0.0%)	1.05	95/17152 (0.6%)

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
2	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	323	VAL	CA-CB	5.04	1.61	1.54

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	226	GLY	N-CA-C	-9.85	101.55	115.43
2	D	226	GLY	N-CA-C	-9.79	101.63	115.43
2	C	164	LEU	N-CA-C	-9.73	100.51	112.38
2	D	164	LEU	N-CA-C	-9.55	100.73	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	296	GLU	N-CA-C	-9.07	102.14	113.02

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	455	TYR	Sidechain

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	2382	0	2389	243	0
1	B	2382	0	2389	251	0
2	C	3627	0	3689	618	0
2	D	3627	0	3689	630	0
3	E	94	0	55	7	0
3	F	94	0	55	14	0
4	G	75	0	44	5	0
5	I	94	0	55	11	0
6	C	20	0	11	3	0
6	D	20	0	11	3	0
7	C	30	0	12	3	0
7	D	30	0	12	4	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
9	C	1	0	0	2	0
All	All	12480	0	12411	1716	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 69.

The worst 5 of 1716 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)
2:C:168:VAL:HA	2:C:171:LEU:HD12	1.23	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:168:VAL:HA	2:D:171:LEU:HD12	1.22	1.10
2:D:333:MET:HE3	2:D:348:THR:HA	1.33	1.09
2:C:333:MET:HE3	2:C:348:THR:HA	1.34	1.09
2:C:86:THR:HB	2:C:87:GLN:HE22	1.20	1.06

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	282/297 (95%)	207 (73%)	57 (20%)	18 (6%)	1	7
1	B	282/297 (95%)	203 (72%)	61 (22%)	18 (6%)	1	7
2	C	439/479 (92%)	293 (67%)	110 (25%)	36 (8%)	0	4
2	D	439/479 (92%)	295 (67%)	109 (25%)	35 (8%)	1	4
All	All	1442/1552 (93%)	998 (69%)	337 (23%)	107 (7%)	1	5

5 of 107 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	146	ASN
1	A	147	GLU
1	A	277	PRO
1	B	2	ASP

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	266/270 (98%)	247 (93%)	19 (7%)	13	43
1	B	266/270 (98%)	247 (93%)	19 (7%)	13	43
2	C	422/453 (93%)	386 (92%)	36 (8%)	10	35
2	D	422/453 (93%)	385 (91%)	37 (9%)	9	34
All	All	1376/1446 (95%)	1265 (92%)	111 (8%)	11	38

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	264	VAL
2	D	471	ASN
2	C	448	ASN
2	D	462	LYS
2	D	328	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	101	GLN
2	D	341	ASN
2	C	329	ASN
2	D	330	ASN
2	D	428	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	1/5 (20%)	1 (100%)	0
3	F	1/5 (20%)	0	0
4	G	1/4 (25%)	1 (100%)	0
5	I	1/5 (20%)	1 (100%)	0
All	All	4/19 (21%)	3 (75%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	603	U

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Mol	Chain	Res	Type
4	G	502	U
5	I	703	U

There are no RNA pucker outliers to report.

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 [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	U5P	C	600	-	18,21,22	0.48	0	25,30,33	0.64	1 (4%)
6	U5P	D	602	-	18,21,22	0.44	0	25,30,33	0.56	1 (4%)
7	3AT	C	801	8	30,32,32	2.65	7 (23%)	42,50,50	2.07	9 (21%)
7	3AT	D	800	8	30,32,32	2.69	8 (26%)	42,50,50	1.95	7 (16%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	U5P	C	600	-	-	1/7/25/26	0/2/2/2
6	U5P	D	602	-	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	3AT	C	801	8	-	7/22/34/34	0/3/3/3
7	3AT	D	800	8	-	7/22/34/34	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	800	3AT	PB-O3B	8.63	1.68	1.59
7	C	801	3AT	PA-O3A	7.10	1.67	1.59
7	C	801	3AT	PB-O3A	6.96	1.67	1.59
7	C	801	3AT	PB-O3B	6.79	1.66	1.59
7	D	800	3AT	PB-O3A	5.77	1.65	1.59

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	800	3AT	N3-C2-N1	-6.50	118.75	128.58
7	C	801	3AT	N3-C2-N1	-6.45	118.82	128.58
7	C	801	3AT	C5-C4-N3	-4.72	120.22	126.72
7	C	801	3AT	N3-C4-N9	4.66	135.09	127.17
7	D	800	3AT	N3-C4-N9	4.42	134.68	127.17

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	600	U5P	C4'-C5'-O5'-P
6	D	602	U5P	C2'-C1'-N1-C2
6	D	602	U5P	C2'-C1'-N1-C6
7	C	801	3AT	PB-O3B-PG-O3G
7	C	801	3AT	C3'-C4'-C5'-O5'

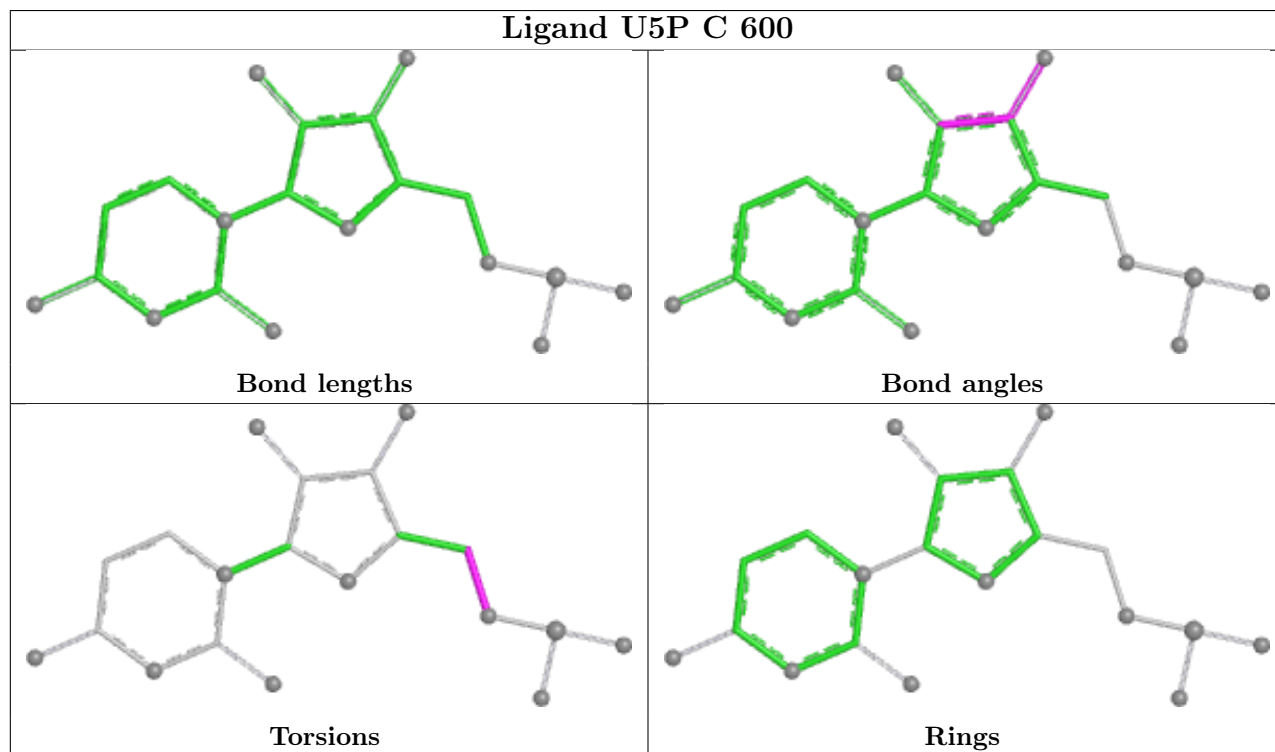
There are no ring outliers.

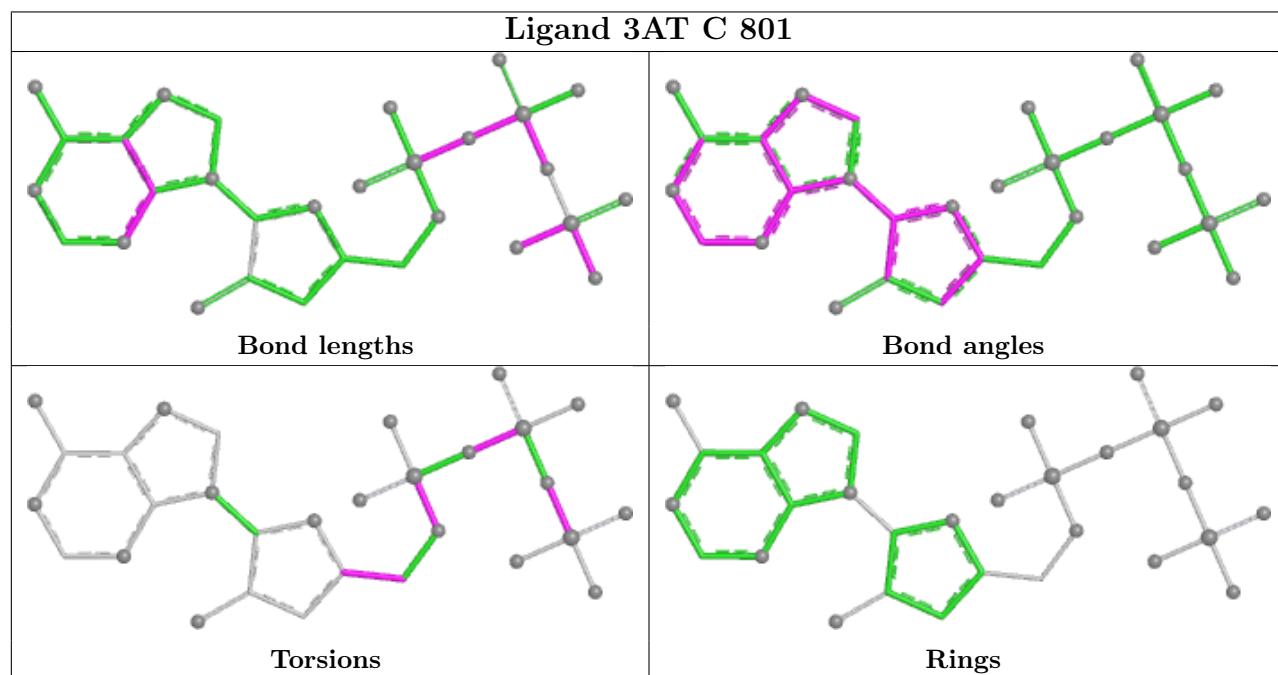
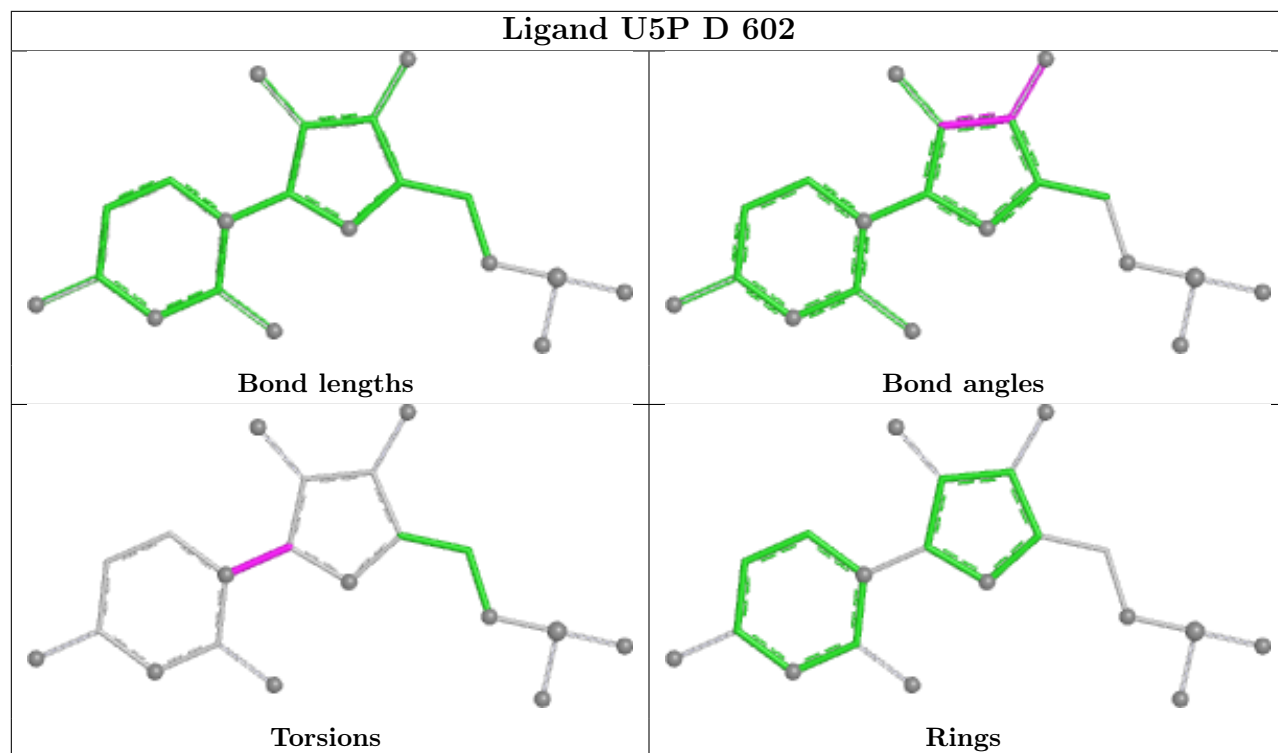
4 monomers are involved in 13 short contacts:

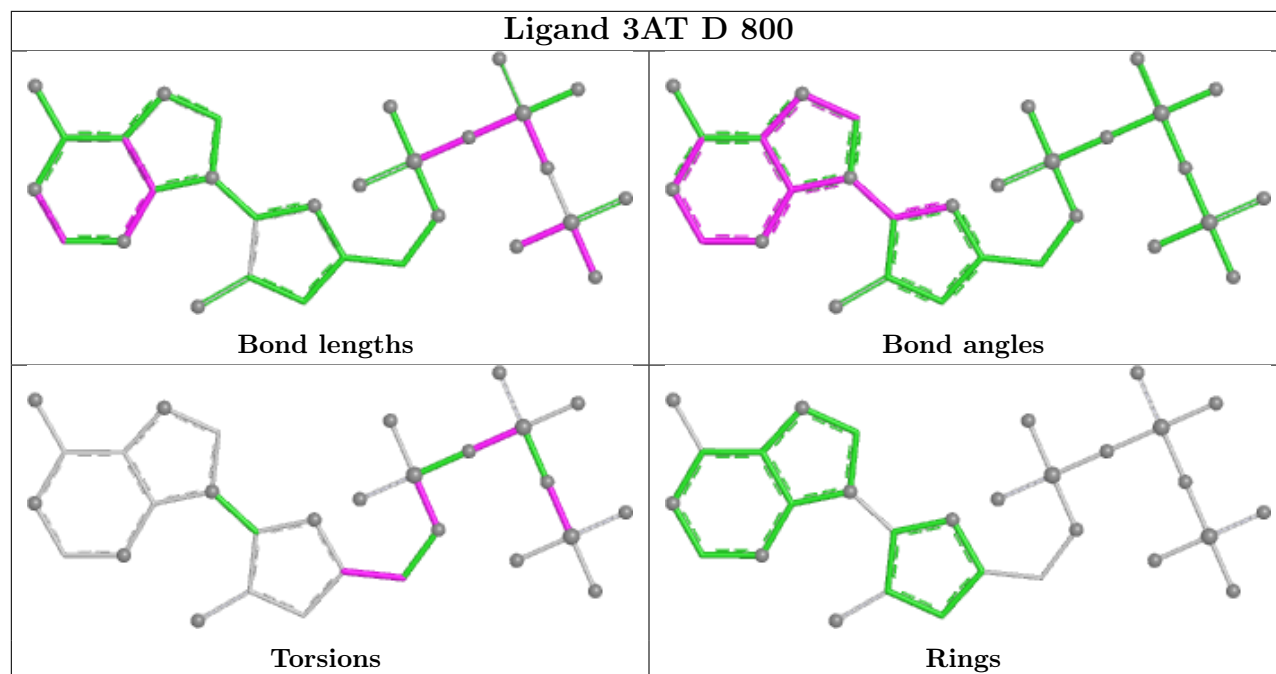
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	600	U5P	3	0
6	D	602	U5P	3	0
7	C	801	3AT	3	0
7	D	800	3AT	4	0

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	288/297 (96%)	-0.35	0 100 100	41, 68, 94, 133	0
1	B	288/297 (96%)	-0.31	0 100 100	41, 66, 93, 124	0
2	C	445/479 (92%)	-0.15	1 (0%) 91 85	47, 90, 123, 156	0
2	D	445/479 (92%)	-0.05	0 100 100	41, 94, 130, 162	0
3	E	5/5 (100%)	-0.10	0 100 100	101, 102, 150, 157	0
3	F	5/5 (100%)	-0.21	0 100 100	97, 100, 138, 157	0
4	G	4/4 (100%)	0.13	0 100 100	81, 97, 119, 122	0
5	I	5/5 (100%)	-0.06	0 100 100	95, 101, 116, 116	0
All	All	1485/1571 (94%)	-0.19	1 (0%) 92 89	41, 82, 122, 162	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	91	ILE	2.1

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,

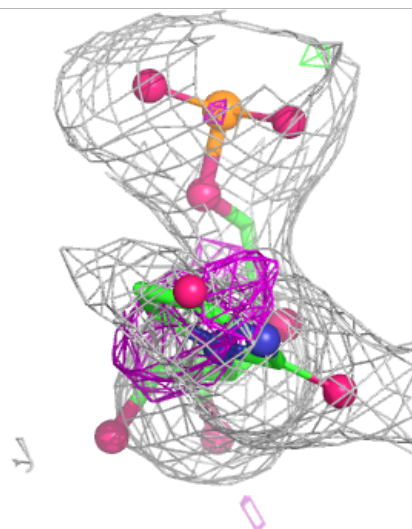
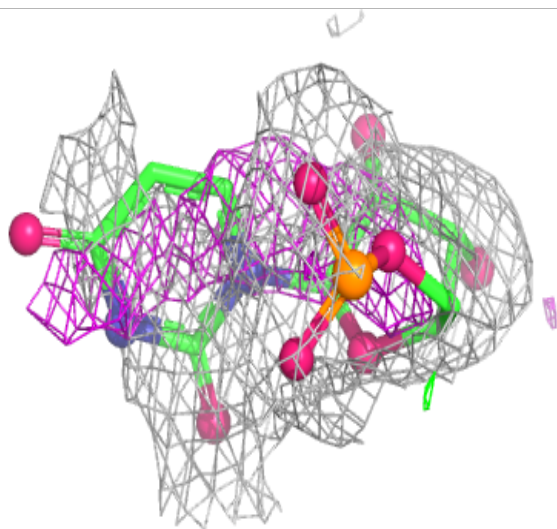
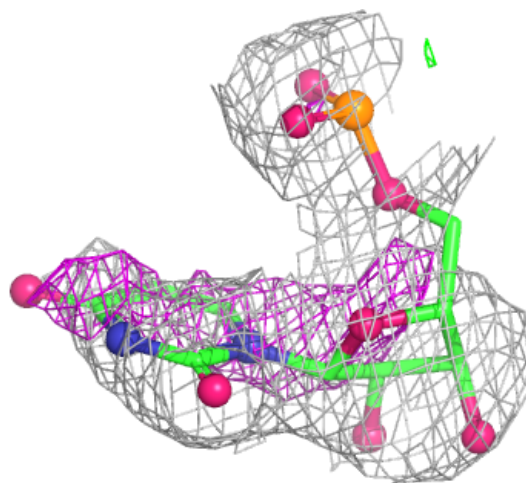
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	U5P	D	602	20/21	0.76	0.12	79,79,79,79	0
6	U5P	C	600	20/21	0.77	0.11	79,79,79,79	0
8	CA	C	901	1/1	0.87	0.07	79,79,79,79	0
7	3AT	D	800	30/30	0.93	0.09	79,108,108,108	0
7	3AT	C	801	30/30	0.94	0.08	79,93,97,97	0
8	CA	C	902	1/1	0.94	0.05	79,79,79,79	0
8	CA	D	903	1/1	0.95	0.05	79,79,79,79	0
8	CA	D	904	1/1	0.98	0.04	79,79,79,79	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.

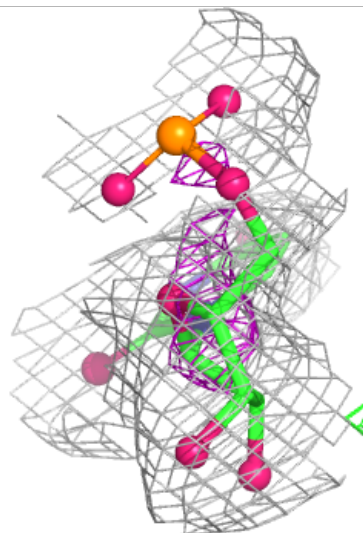
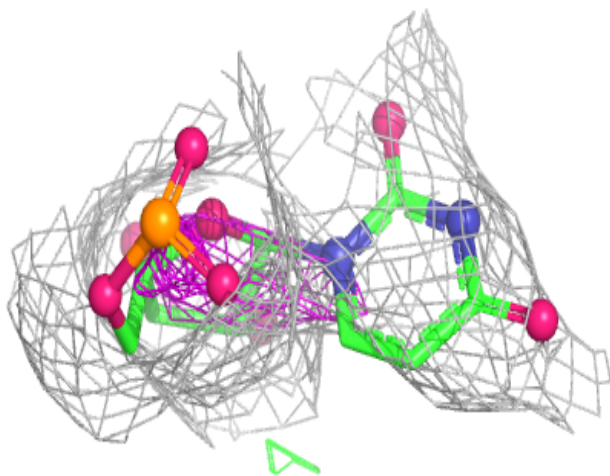
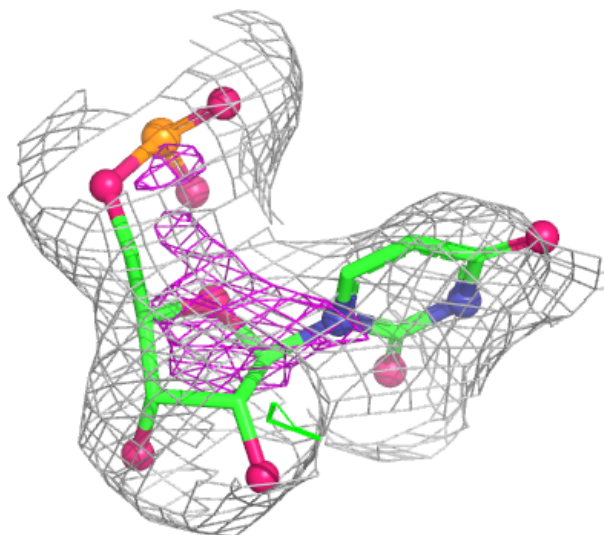
Electron density around U5P D 602:

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



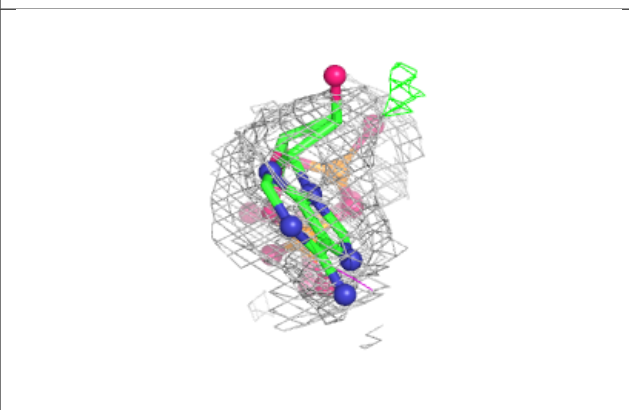
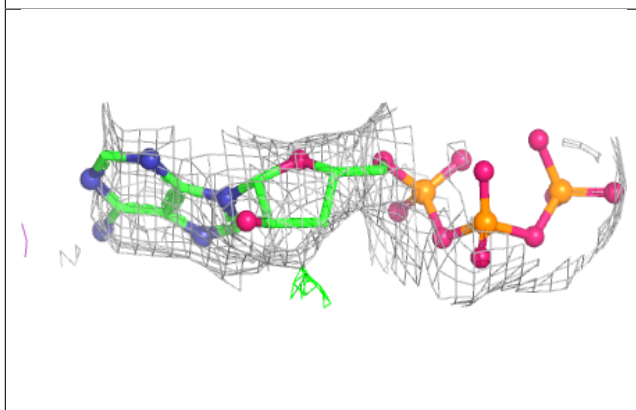
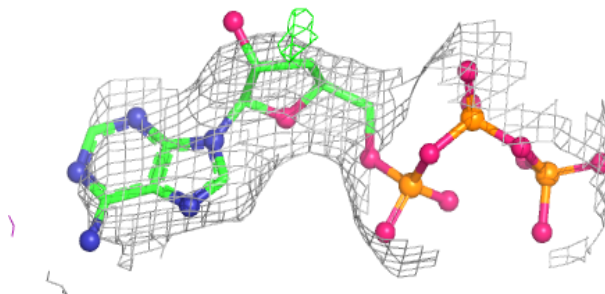
Electron density around U5P C 600:

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

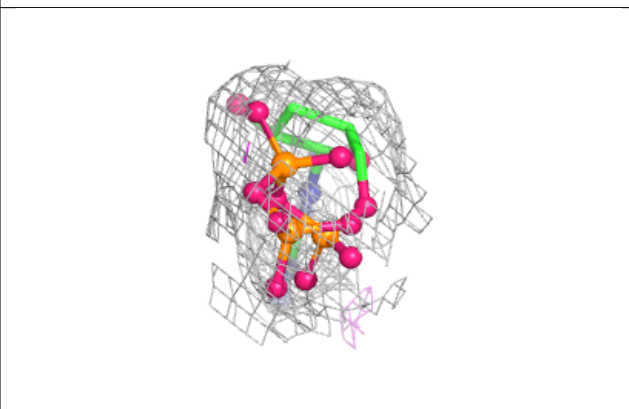
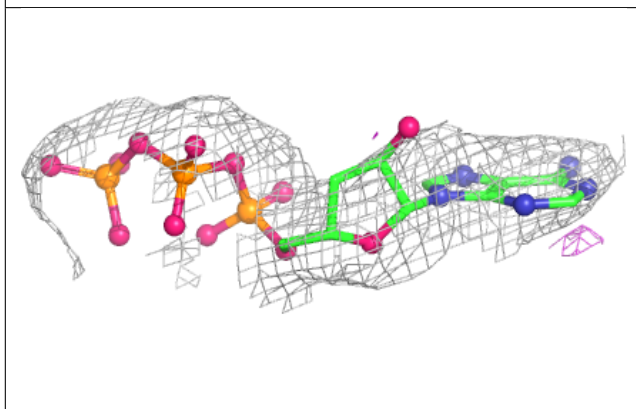
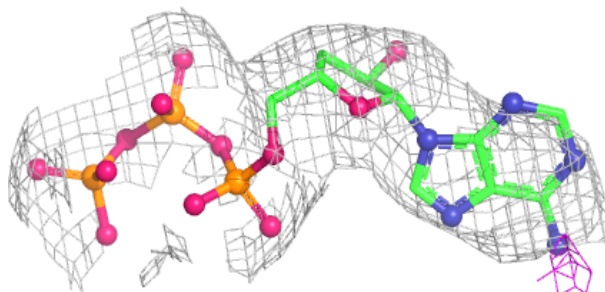


Electron density around 3AT D 800:

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

**Electron density around 3AT C 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.