



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:07 AM GMT

PDB ID : 3H1C
Title : Crystal structure of Polynucleotide Phosphorylase (PNPase) core bound to RNase E and Tungstate
Authors : Nurmohamed, S.
Deposited on : 2009-04-11
Resolution : 3.57 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

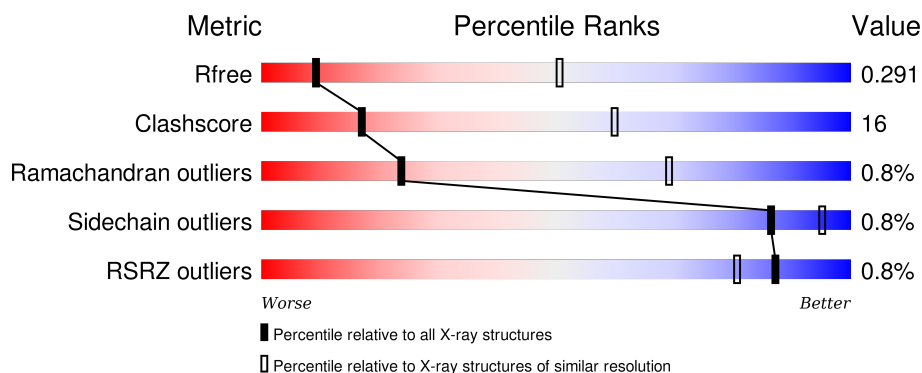
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 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.





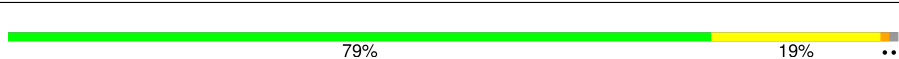
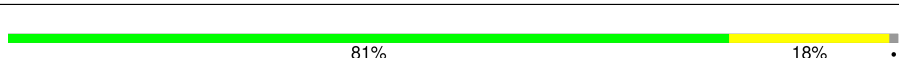
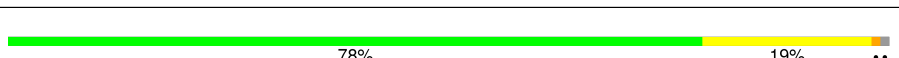
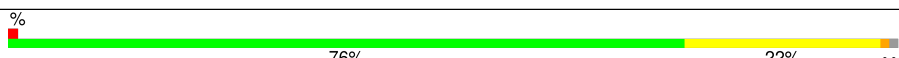
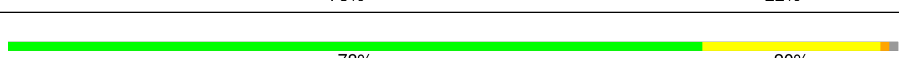
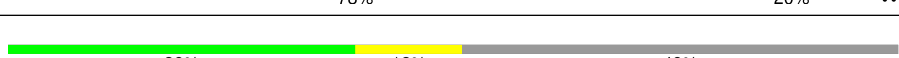
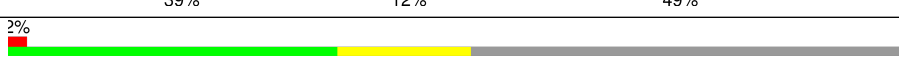
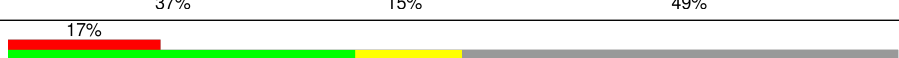
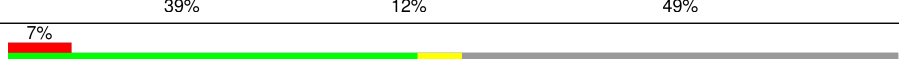
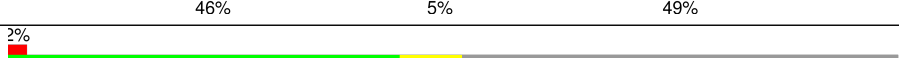
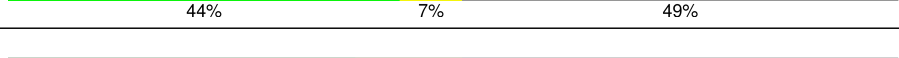
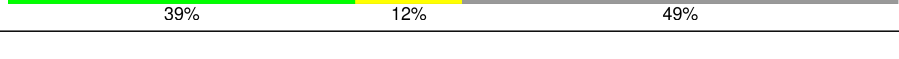



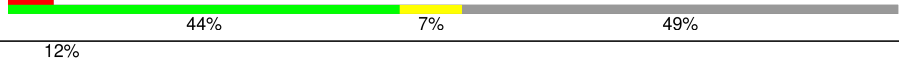

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1261 (3.76-3.40)
Clashscore	102246	1026 (3.72-3.44)
Ramachandran outliers	100387	1028 (3.74-3.42)
Sidechain outliers	100360	1028 (3.74-3.42)
RSRZ outliers	91569	1268 (3.76-3.40)

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. 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	549	<div> <div></div> <div>77%22%..</div> </div>
1	B	549	<div> <div></div> <div>76%23%..</div> </div>
1	C	549	<div> <div></div> <div>75%23%..</div> </div>
1	G	549	<div> <div>%</div> <div>77%21%..</div> </div>
1	I	549	<div> <div>%</div> <div>77%21%..</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	549	
1	M	549	
1	O	549	
1	R	549	
1	T	549	
1	V	549	
1	X	549	
2	D	41	
2	E	41	
2	F	41	
2	H	41	
2	J	41	
2	L	41	
2	N	41	
2	P	41	
2	S	41	
2	U	41	
2	W	41	
2	Y	41	

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
3	WO4	A	551	-	-	-	X
3	WO4	K	551	-	-	-	X
3	WO4	M	551	-	-	-	X
3	WO4	X	551	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51109 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 Polyribonucleotide nucleotidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			4075	2559	704	792	20			
1	B	544	Total	C	N	O	S	0	0	0
			4107	2575	717	797	18			
1	C	544	Total	C	N	O	S	0	0	0
			4121	2583	720	798	20			
1	G	543	Total	C	N	O	S	0	0	0
			4095	2571	715	789	20			
1	I	543	Total	C	N	O	S	0	0	0
			4109	2576	716	797	20			
1	K	544	Total	C	N	O	S	0	0	0
			4127	2588	721	798	20			
1	M	544	Total	C	N	O	S	0	0	0
			4116	2581	718	797	20			
1	O	544	Total	C	N	O	S	0	0	0
			4124	2584	723	798	19			
1	R	544	Total	C	N	O	S	0	0	0
			4134	2590	724	800	20			
1	T	543	Total	C	N	O	S	0	0	0
			4116	2582	720	795	19			
1	V	544	Total	C	N	O	S	0	0	0
			4118	2580	719	799	20			
1	X	544	Total	C	N	O	S	0	0	0
			4113	2581	717	795	20			

- Molecule 2 is a protein called Ribonuclease E.

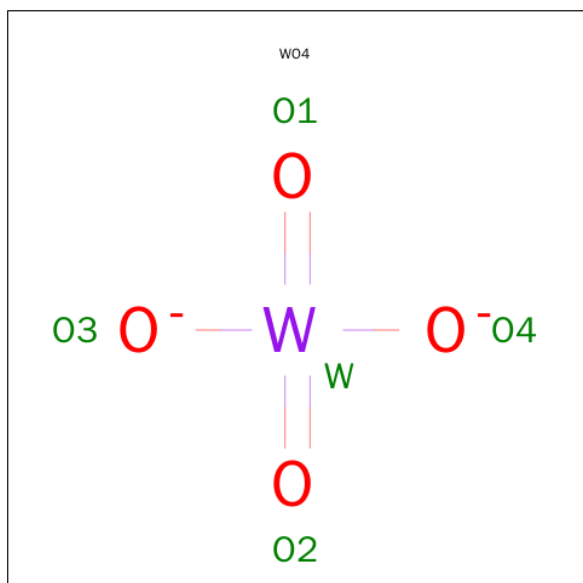
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	21	Total	C	N	O	0	0	0
			138	82	31	25			
2	E	21	Total	C	N	O	0	0	0
			138	82	31	25			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	21	Total	C	N	O	0	0	0
			138	82	31	25			
2	H	21	Total	C	N	O	0	0	0
			138	82	31	25			
2	J	21	Total	C	N	O	0	0	0
			138	82	31	25			
2	L	21	Total	C	N	O	0	0	0
			138	82	31	25			
2	N	21	Total	C	N	O	0	0	0
			138	82	31	25			
2	P	21	Total	C	N	O	0	0	0
			138	82	31	25			
2	S	21	Total	C	N	O	0	0	0
			138	82	31	25			
2	U	21	Total	C	N	O	0	0	0
			138	82	31	25			
2	W	21	Total	C	N	O	0	0	0
			131	78	29	24			
2	Y	21	Total	C	N	O	0	0	0
			138	82	31	25			

- Molecule 3 is TUNGSTATE(VI)ION (three-letter code: WO4) (formula: O₄W).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O W	0	0
			5 4 1			

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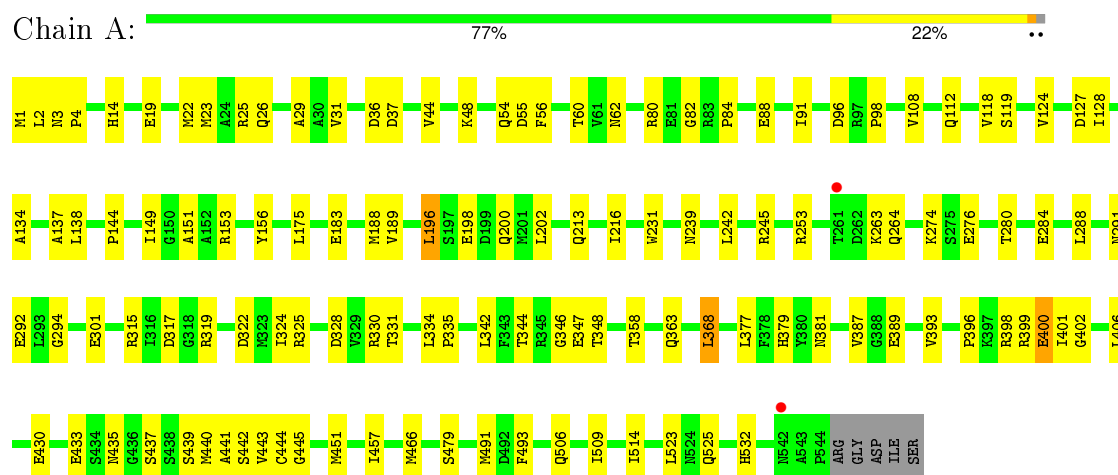
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	W 1	0	0
3	B	1	Total 5	O 4	W 1	0	0
3	B	1	Total 5	O 4	W 1	0	0
3	C	1	Total 5	O 4	W 1	0	0
3	G	1	Total 5	O 4	W 1	0	0
3	I	1	Total 5	O 4	W 1	0	0
3	K	1	Total 5	O 4	W 1	0	0
3	K	1	Total 5	O 4	W 1	0	0
3	M	1	Total 5	O 4	W 1	0	0
3	M	1	Total 5	O 4	W 1	0	0
3	O	1	Total 5	O 4	W 1	0	0
3	O	1	Total 5	O 4	W 1	0	0
3	R	1	Total 5	O 4	W 1	0	0
3	R	1	Total 5	O 4	W 1	0	0
3	T	1	Total 5	O 4	W 1	0	0
3	T	1	Total 5	O 4	W 1	0	0
3	V	1	Total 5	O 4	W 1	0	0
3	V	1	Total 5	O 4	W 1	0	0
3	X	1	Total 5	O 4	W 1	0	0
3	X	1	Total 5	O 4	W 1	0	0

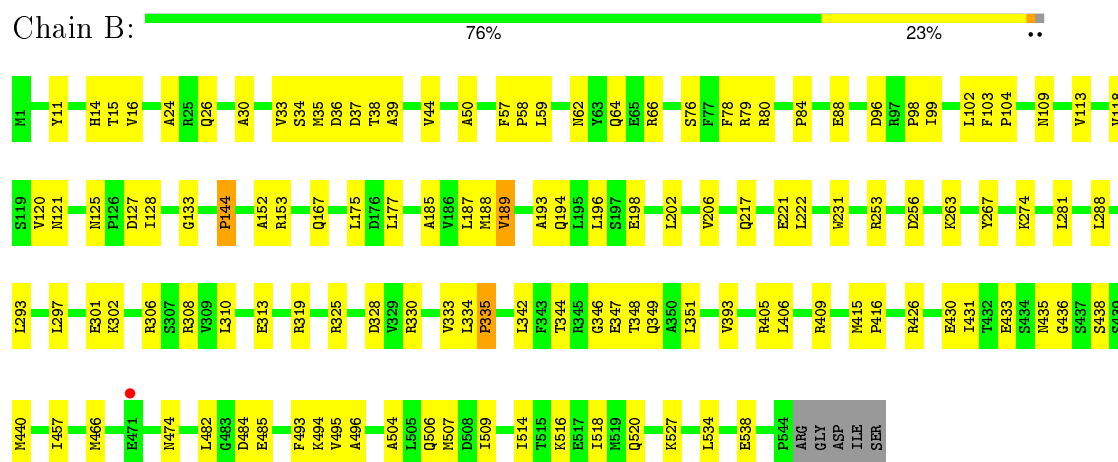
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

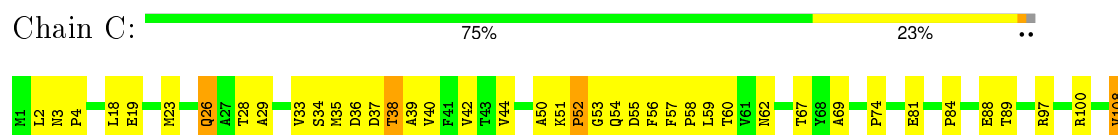
- Molecule 1: Polyrribonucleotide nucleotidyltransferase

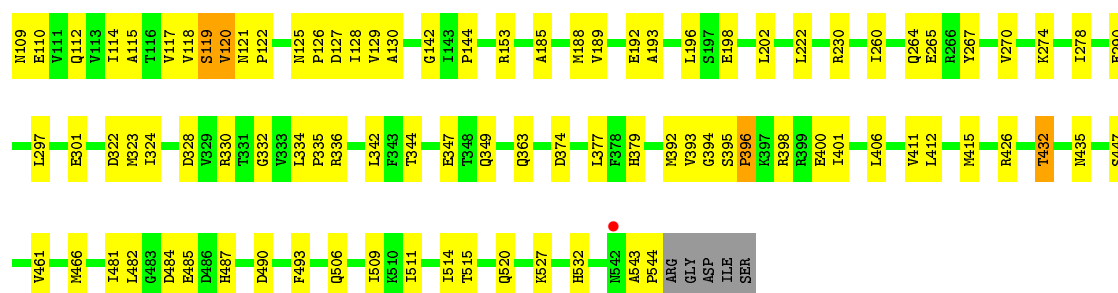


- Molecule 1: Polyrribonucleotide nucleotidyltransferase

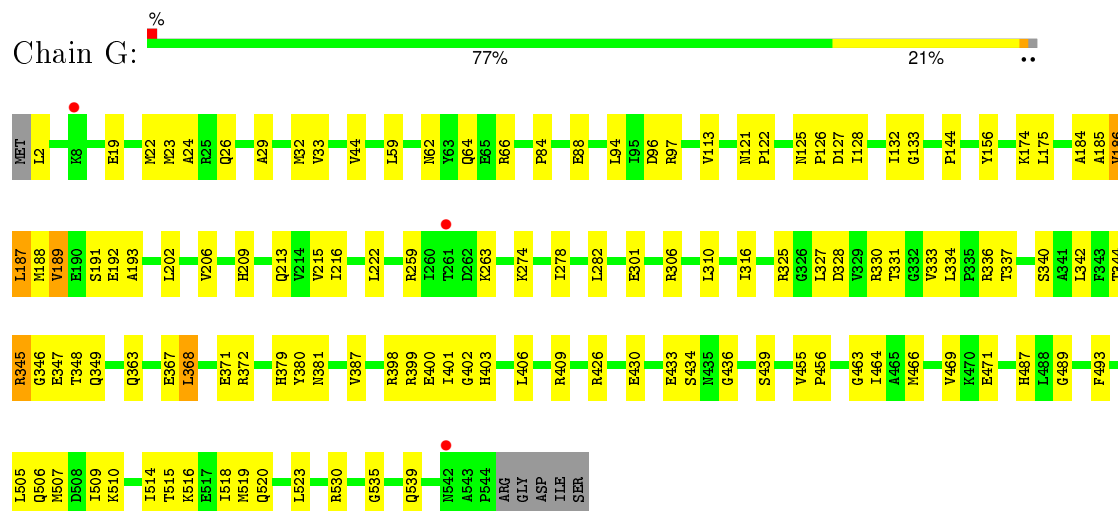


- Molecule 1: Polyrribonucleotide nucleotidyltransferase

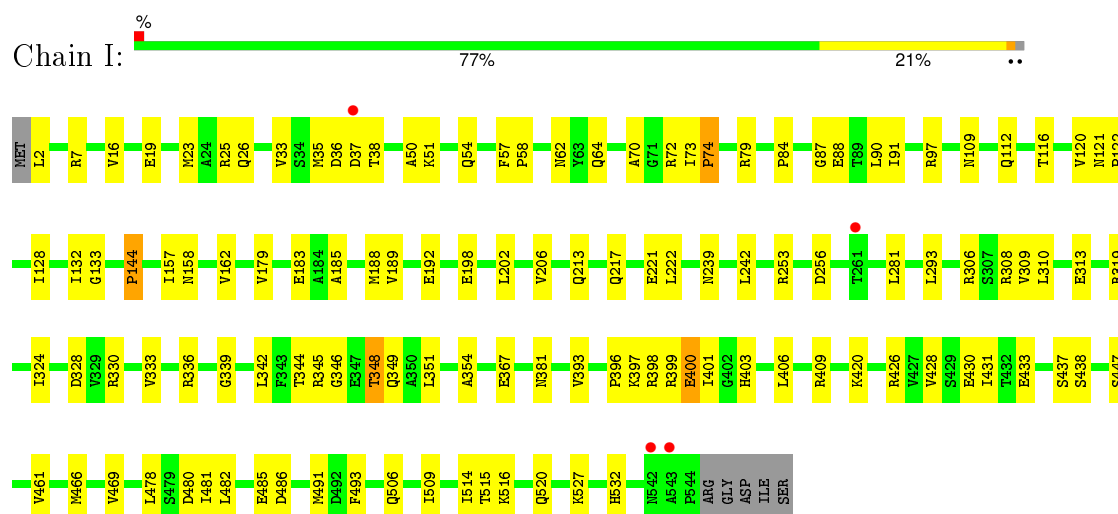




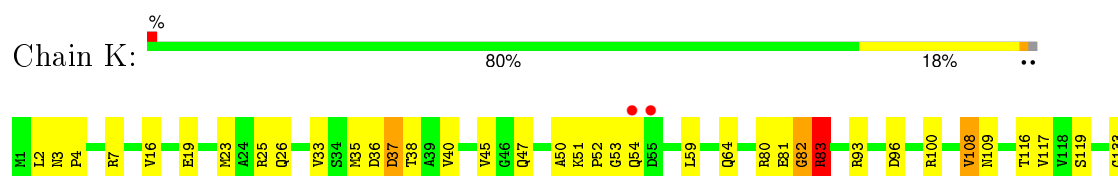
• Molecule 1: Polyribonucleotide nucleotidyltransferase

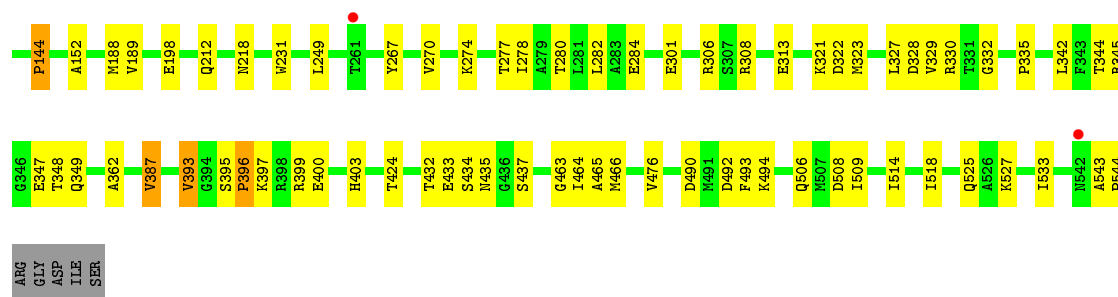


• Molecule 1: Polyribonucleotide nucleotidyltransferase

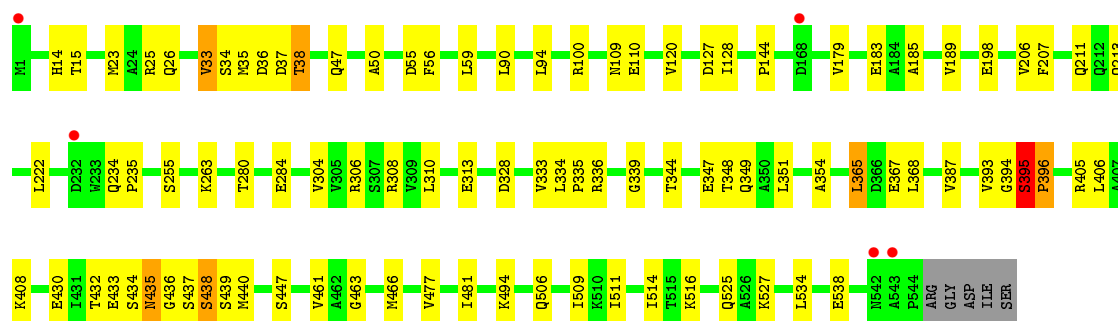
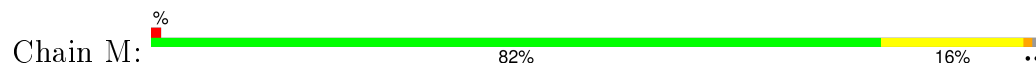


• Molecule 1: Polyribonucleotide nucleotidyltransferase

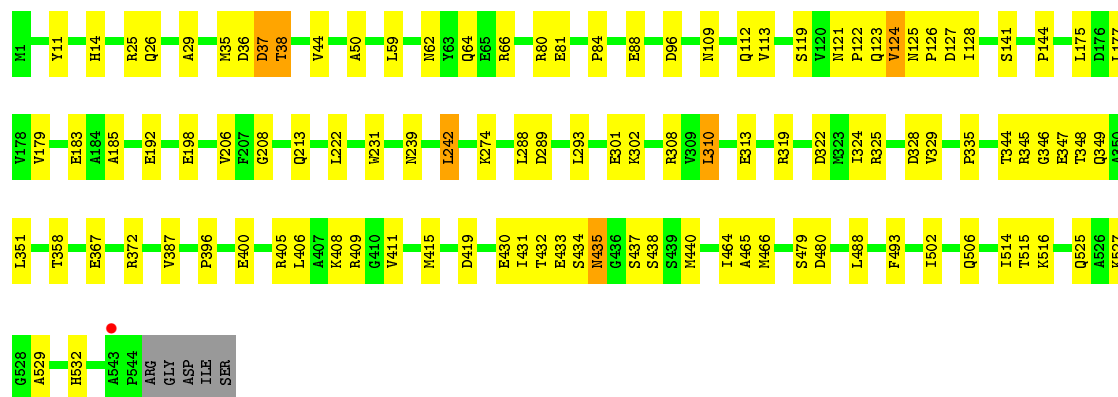
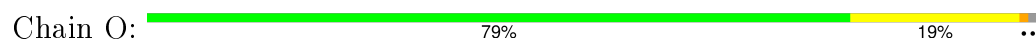




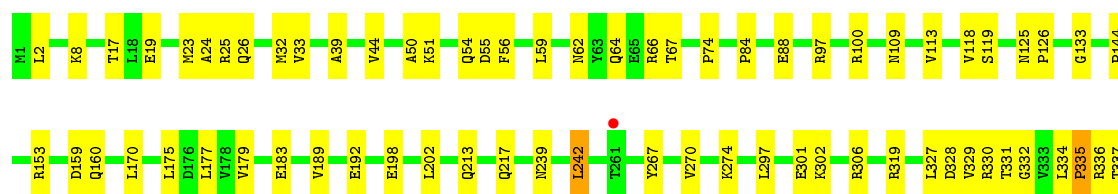
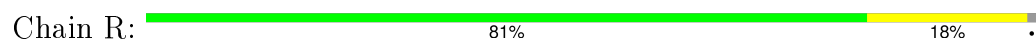
• Molecule 1: Polyribonucleotide nucleotidyltransferase

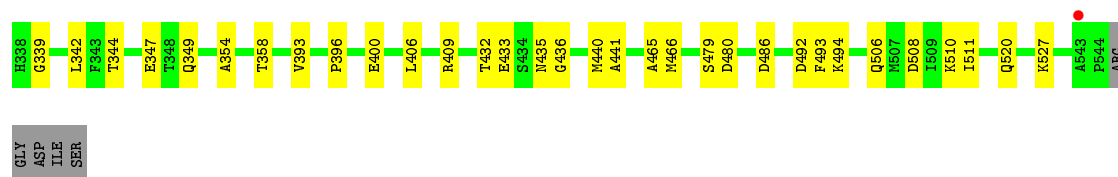


• Molecule 1: Polyribonucleotide nucleotidyltransferase

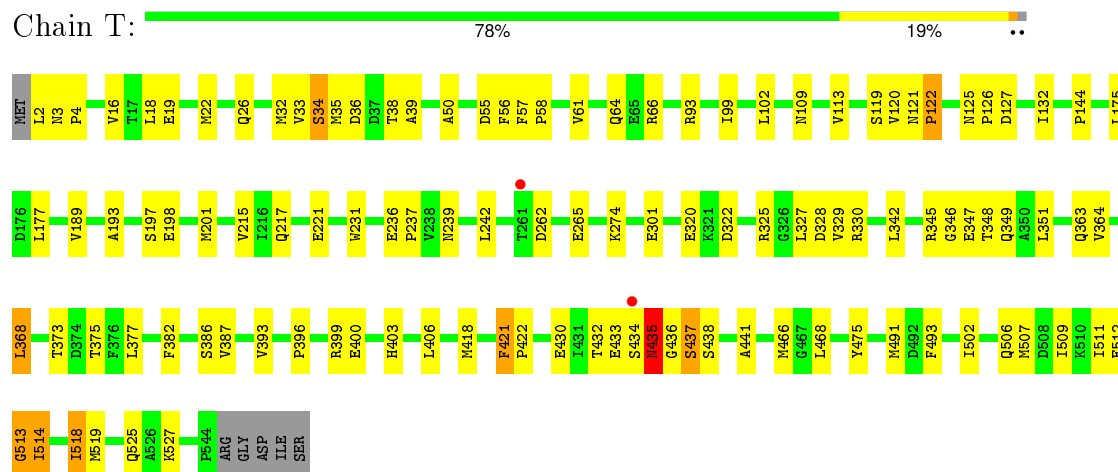


• Molecule 1: Polyribonucleotide nucleotidyltransferase

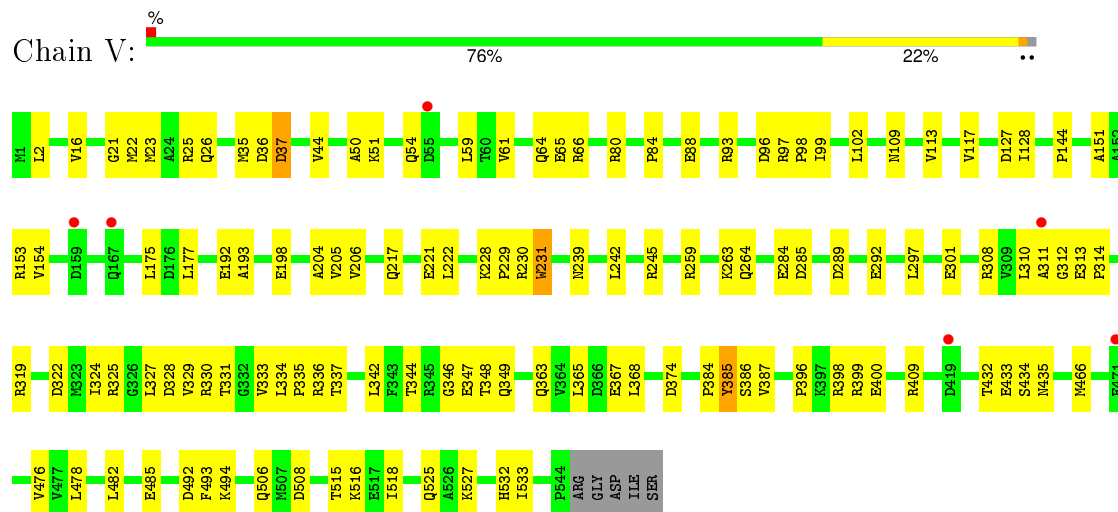




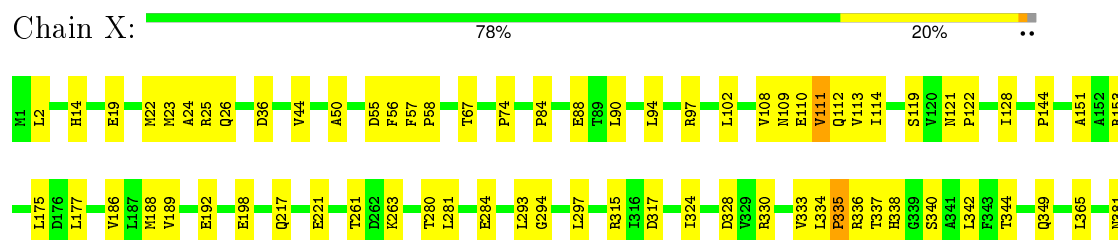
- Molecule 1: Polyribonucleotide nucleotidyltransferase

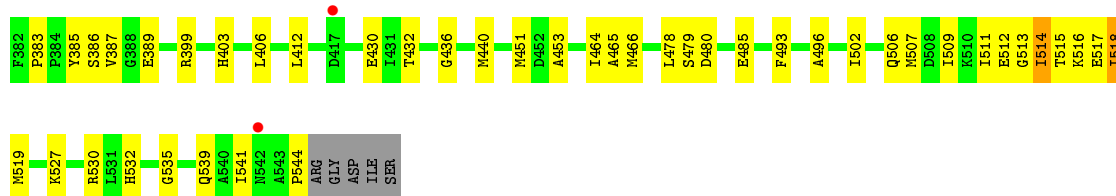


- Molecule 1: Polyribonucleotide nucleotidyltransferase



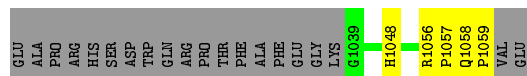
- Molecule 1: Polyribonucleotide nucleotidyltransferase





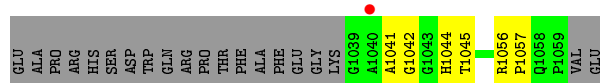
- Molecule 2: Ribonuclease E

Chain D: 39% 12% 49%



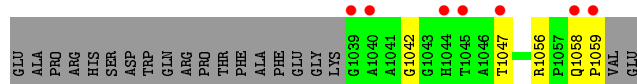
- Molecule 2: Ribonuclease E

Chain E: 2% 37% 15% 49%



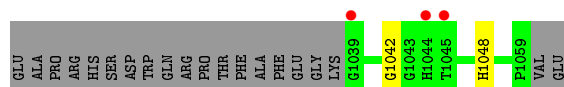
- Molecule 2: Ribonuclease E

Chain F: 17% 39% 12% 49%



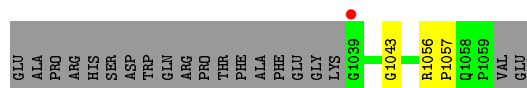
- Molecule 2: Ribonuclease E

Chain H: 7% 46% 5% 49%



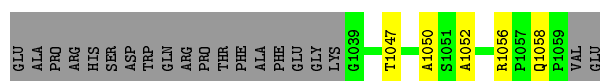
- Molecule 2: Ribonuclease E

Chain J: 2% 44% 7% 49%



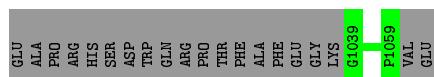
- Molecule 2: Ribonuclease E

Chain L: 39% 12% 49%



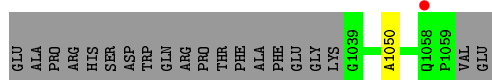
- Molecule 2: Ribonuclease E

Chain N:  51% 49%




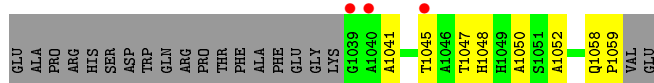
• Molecule 2: Ribonuclease E

Chain P:  2% 49% 49%

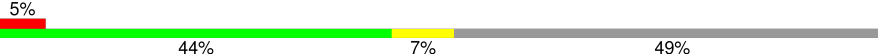


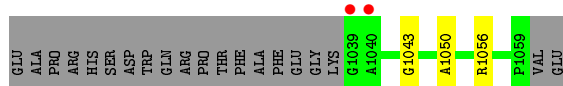
• Molecule 2: Ribonuclease E

Chain S:  7% 32% 20% 49%




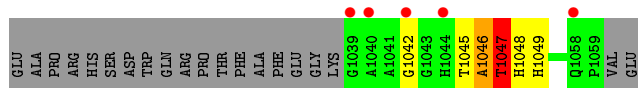
• Molecule 2: Ribonuclease E

Chain U:  5% 44% 7% 49%



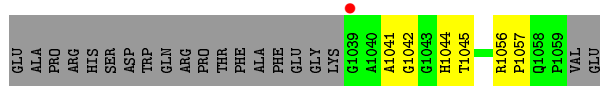
• Molecule 2: Ribonuclease E

Chain W:  12% 37% 10% 49%



• Molecule 2: Ribonuclease E

Chain Y:  2% 37% 15% 49%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	167.74Å 262.89Å 264.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.57 20.15 – 3.57	Depositor EDS
% Data completeness (in resolution range)	94.2 (25.00-3.57) 94.2 (20.15-3.57)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.62Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.270 , 0.304 0.267 , 0.291	Depositor DCC
R_{free} test set	6514 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 26.7	EDS
Estimated twinning fraction	0.038 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 129939 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	51109	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: WO4

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	0.35	0/4138	0.47	0/5621
1	B	0.30	0/4170	0.46	0/5660
1	C	0.37	0/4184	0.47	1/5675 (0.0%)
1	G	0.41	0/4158	0.51	2/5643 (0.0%)
1	I	0.38	0/4172	0.50	2/5660 (0.0%)
1	K	0.37	0/4190	0.54	4/5681 (0.1%)
1	M	0.33	0/4179	0.58	9/5668 (0.2%)
1	O	0.34	0/4187	0.47	2/5679 (0.0%)
1	R	0.30	0/4197	0.46	0/5690
1	T	0.32	0/4179	0.48	1/5667 (0.0%)
1	V	0.36	0/4180	0.47	1/5671 (0.0%)
1	X	0.30	0/4175	0.48	2/5661 (0.0%)
2	D	0.34	0/143	0.47	0/196
2	E	0.31	0/143	0.38	0/196
2	F	0.32	0/143	0.49	0/196
2	H	0.32	0/143	0.39	0/196
2	J	0.33	0/143	0.48	0/196
2	L	0.36	0/143	0.47	0/196
2	N	0.33	0/143	0.38	0/196
2	P	0.33	0/143	0.39	0/196
2	S	0.32	0/143	0.38	0/196
2	U	0.32	0/143	0.40	0/196
2	W	0.49	0/135	0.68	0/185
2	Y	0.32	0/143	0.41	0/196
All	All	0.35	0/51817	0.49	24/70317 (0.0%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	438	SER	CB-CA-C	13.85	136.42	110.10
1	M	434	SER	CB-CA-C	-13.49	84.47	110.10
1	K	37	ASP	CB-CA-C	-13.04	84.33	110.40
1	M	435	ASN	N-CA-CB	-10.55	91.60	110.60
1	M	394	GLY	N-CA-C	8.54	134.46	113.10

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	A	4075	0	4044	154	0
1	B	4107	0	4096	134	0
1	C	4121	0	4126	186	0
1	G	4095	0	4087	168	0
1	I	4109	0	4108	138	0
1	K	4127	0	4141	148	0
1	M	4116	0	4116	98	0
1	O	4124	0	4130	119	0
1	R	4134	0	4150	101	0
1	T	4116	0	4127	160	0
1	V	4118	0	4115	173	0
1	X	4113	0	4117	176	0
2	D	138	0	125	5	0
2	E	138	0	125	8	0
2	F	138	0	125	16	0
2	H	138	0	125	2	0
2	J	138	0	125	2	0
2	L	138	0	125	8	0
2	N	138	0	125	0	0
2	P	138	0	125	1	0
2	S	138	0	125	9	0
2	U	138	0	125	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	131	0	115	21	0
2	Y	138	0	125	5	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	G	5	0	0	1	0
3	I	5	0	0	0	0
3	K	10	0	0	0	0
3	M	10	0	0	0	0
3	O	10	0	0	0	0
3	R	10	0	0	0	0
3	T	10	0	0	0	0
3	V	10	0	0	0	0
3	X	10	0	0	1	0
All	All	51109	0	50847	1659	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 16.

The worst 5 of 1659 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:I:310:LEU:HD21	1:I:469:VAL:CG1	1.47	1.44
1:G:26:GLN:NE2	1:K:387:VAL:HA	1.36	1.40
1:R:51:LYS:HB3	1:R:54:GLN:CG	1.52	1.36
1:O:239:ASN:ND2	1:O:242:LEU:HB2	1.40	1.35
1:V:342:LEU:HD11	1:V:349:GLN:NE2	1.40	1.32

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	542/549 (99%)	496 (92%)	40 (7%)	6 (1%)	17	64
1	B	542/549 (99%)	508 (94%)	30 (6%)	4 (1%)	26	72
1	C	542/549 (99%)	497 (92%)	39 (7%)	6 (1%)	17	64
1	G	541/549 (98%)	500 (92%)	38 (7%)	3 (1%)	30	74
1	I	541/549 (98%)	502 (93%)	36 (7%)	3 (1%)	30	74
1	K	542/549 (99%)	502 (93%)	34 (6%)	6 (1%)	17	64
1	M	542/549 (99%)	501 (92%)	37 (7%)	4 (1%)	26	72
1	O	542/549 (99%)	507 (94%)	32 (6%)	3 (1%)	30	74
1	R	542/549 (99%)	505 (93%)	33 (6%)	4 (1%)	26	72
1	T	541/549 (98%)	499 (92%)	36 (7%)	6 (1%)	17	64
1	V	542/549 (99%)	506 (93%)	33 (6%)	3 (1%)	30	74
1	X	542/549 (99%)	510 (94%)	29 (5%)	3 (1%)	30	74
2	D	19/41 (46%)	19 (100%)	0	0	100	100
2	E	19/41 (46%)	19 (100%)	0	0	100	100
2	F	19/41 (46%)	17 (90%)	2 (10%)	0	100	100
2	H	19/41 (46%)	19 (100%)	0	0	100	100
2	J	19/41 (46%)	18 (95%)	1 (5%)	0	100	100
2	L	19/41 (46%)	19 (100%)	0	0	100	100
2	N	19/41 (46%)	17 (90%)	2 (10%)	0	100	100
2	P	19/41 (46%)	18 (95%)	1 (5%)	0	100	100
2	S	19/41 (46%)	19 (100%)	0	0	100	100
2	U	19/41 (46%)	18 (95%)	1 (5%)	0	100	100
2	W	19/41 (46%)	13 (68%)	4 (21%)	2 (10%)	1	10
2	Y	19/41 (46%)	19 (100%)	0	0	100	100
All	All	6729/7080 (95%)	6248 (93%)	428 (6%)	53 (1%)	24	69

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	38	THR
1	G	187	LEU
1	G	189	VAL
1	O	37	ASP
1	O	38	THR

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	
1	A	426/446 (96%)	422 (99%)	4 (1%)	84	94
1	B	432/446 (97%)	430 (100%)	2 (0%)	92	97
1	C	436/446 (98%)	429 (98%)	7 (2%)	70	90
1	G	429/446 (96%)	426 (99%)	3 (1%)	88	96
1	I	435/446 (98%)	432 (99%)	3 (1%)	88	96
1	K	437/446 (98%)	433 (99%)	4 (1%)	84	94
1	M	434/446 (97%)	429 (99%)	5 (1%)	78	92
1	O	436/446 (98%)	430 (99%)	6 (1%)	74	91
1	R	439/446 (98%)	437 (100%)	2 (0%)	92	97
1	T	435/446 (98%)	432 (99%)	3 (1%)	88	96
1	V	435/446 (98%)	434 (100%)	1 (0%)	95	99
1	X	433/446 (97%)	430 (99%)	3 (1%)	88	96
2	D	11/28 (39%)	11 (100%)	0	100	100
2	E	11/28 (39%)	11 (100%)	0	100	100
2	F	11/28 (39%)	11 (100%)	0	100	100
2	H	11/28 (39%)	11 (100%)	0	100	100
2	J	11/28 (39%)	11 (100%)	0	100	100
2	L	11/28 (39%)	11 (100%)	0	100	100
2	N	11/28 (39%)	11 (100%)	0	100	100
2	P	11/28 (39%)	11 (100%)	0	100	100
2	S	11/28 (39%)	11 (100%)	0	100	100
2	U	11/28 (39%)	11 (100%)	0	100	100
2	W	9/28 (32%)	8 (89%)	1 (11%)	8	38
2	Y	11/28 (39%)	11 (100%)	0	100	100
All	All	5337/5688 (94%)	5293 (99%)	44 (1%)	86	95

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	26	GLN
1	M	33	VAL
2	W	1047	THR
1	K	80	ARG
1	K	108	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	349	GLN
1	O	123	GLN
1	V	349	GLN
1	K	532	HIS
1	M	403	HIS

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](#)

21 ligands are modelled in this entry.

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
3	WO4	A	550	-	2,4,4	11.39	2 (100%)	0,6,6	0.00	-
3	WO4	A	551	-	2,4,4	11.38	2 (100%)	0,6,6	0.00	-
3	WO4	B	550	-	2,4,4	11.40	2 (100%)	0,6,6	0.00	-
3	WO4	B	551	-	2,4,4	11.38	2 (100%)	0,6,6	0.00	-
3	WO4	C	550	-	2,4,4	11.37	2 (100%)	0,6,6	0.00	-
3	WO4	G	550	-	2,4,4	11.37	2 (100%)	0,6,6	0.00	-
3	WO4	I	550	-	2,4,4	11.36	2 (100%)	0,6,6	0.00	-
3	WO4	K	550	-	2,4,4	11.36	2 (100%)	0,6,6	0.00	-
3	WO4	K	551	-	2,4,4	11.37	2 (100%)	0,6,6	0.00	-
3	WO4	M	550	-	2,4,4	10.45	2 (100%)	0,6,6	0.00	-
3	WO4	M	551	-	2,4,4	11.38	2 (100%)	0,6,6	0.00	-
3	WO4	O	550	-	2,4,4	11.40	2 (100%)	0,6,6	0.00	-
3	WO4	O	551	-	2,4,4	11.39	2 (100%)	0,6,6	0.00	-
3	WO4	R	550	-	2,4,4	11.38	2 (100%)	0,6,6	0.00	-
3	WO4	R	551	-	2,4,4	11.39	2 (100%)	0,6,6	0.00	-
3	WO4	T	550	-	2,4,4	11.37	2 (100%)	0,6,6	0.00	-
3	WO4	T	551	-	2,4,4	11.40	2 (100%)	0,6,6	0.00	-
3	WO4	V	550	-	2,4,4	11.39	2 (100%)	0,6,6	0.00	-
3	WO4	V	551	-	2,4,4	11.37	2 (100%)	0,6,6	0.00	-
3	WO4	X	550	-	2,4,4	11.37	2 (100%)	0,6,6	0.00	-
3	WO4	X	551	-	2,4,4	11.40	2 (100%)	0,6,6	0.00	-

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
3	WO4	A	550	-	-	0/0/0/0	0/0/0/0
3	WO4	A	551	-	-	0/0/0/0	0/0/0/0
3	WO4	B	550	-	-	0/0/0/0	0/0/0/0
3	WO4	B	551	-	-	0/0/0/0	0/0/0/0
3	WO4	C	550	-	-	0/0/0/0	0/0/0/0
3	WO4	G	550	-	-	0/0/0/0	0/0/0/0
3	WO4	I	550	-	-	0/0/0/0	0/0/0/0
3	WO4	K	550	-	-	0/0/0/0	0/0/0/0
3	WO4	K	551	-	-	0/0/0/0	0/0/0/0
3	WO4	M	550	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	WO4	M	551	-	-	0/0/0/0	0/0/0/0
3	WO4	O	550	-	-	0/0/0/0	0/0/0/0
3	WO4	O	551	-	-	0/0/0/0	0/0/0/0
3	WO4	R	550	-	-	0/0/0/0	0/0/0/0
3	WO4	R	551	-	-	0/0/0/0	0/0/0/0
3	WO4	T	550	-	-	0/0/0/0	0/0/0/0
3	WO4	T	551	-	-	0/0/0/0	0/0/0/0
3	WO4	V	550	-	-	0/0/0/0	0/0/0/0
3	WO4	V	551	-	-	0/0/0/0	0/0/0/0
3	WO4	X	550	-	-	0/0/0/0	0/0/0/0
3	WO4	X	551	-	-	0/0/0/0	0/0/0/0

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	550	WO4	W-O1	10.45	2.02	1.74
3	M	550	WO4	W-O2	10.45	2.02	1.74
3	K	550	WO4	W-O2	11.34	2.04	1.74
3	I	550	WO4	W-O2	11.34	2.04	1.74
3	R	550	WO4	W-O2	11.36	2.04	1.74

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	550	WO4	1	0
3	X	550	WO4	1	0

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	544/549 (99%)	-0.25	2 (0%) 93 90	15, 50, 83, 103	1 (0%)
1	B	544/549 (99%)	-0.32	1 (0%) 95 93	9, 39, 76, 101	1 (0%)
1	C	544/549 (99%)	-0.27	1 (0%) 95 93	14, 48, 83, 106	1 (0%)
1	G	543/549 (98%)	-0.26	3 (0%) 90 85	20, 51, 83, 111	1 (0%)
1	I	543/549 (98%)	-0.30	4 (0%) 89 83	14, 40, 76, 98	1 (0%)
1	K	544/549 (99%)	-0.30	4 (0%) 89 83	13, 43, 82, 115	1 (0%)
1	M	544/549 (99%)	-0.18	5 (0%) 85 79	20, 54, 89, 110	1 (0%)
1	O	544/549 (99%)	-0.30	1 (0%) 95 93	8, 41, 79, 97	1 (0%)
1	R	544/549 (99%)	-0.24	2 (0%) 93 90	13, 46, 83, 101	1 (0%)
1	T	543/549 (98%)	-0.25	2 (0%) 93 90	20, 53, 84, 108	1 (0%)
1	V	544/549 (99%)	-0.17	6 (1%) 82 74	19, 62, 92, 105	1 (0%)
1	X	544/549 (99%)	-0.19	2 (0%) 93 90	20, 52, 85, 100	1 (0%)
2	D	21/41 (51%)	0.56	0 100 100	44, 80, 95, 96	0
2	E	21/41 (51%)	0.52	1 (4%) 34 27	34, 69, 98, 104	0
2	F	21/41 (51%)	1.19	7 (33%) 0 1	70, 92, 111, 117	0
2	H	21/41 (51%)	0.65	3 (14%) 4 3	62, 95, 107, 109	0
2	J	21/41 (51%)	0.33	1 (4%) 34 27	43, 70, 85, 91	0
2	L	21/41 (51%)	0.32	0 100 100	49, 78, 103, 107	0
2	N	21/41 (51%)	0.34	0 100 100	64, 84, 97, 97	0
2	P	21/41 (51%)	0.28	1 (4%) 34 27	33, 73, 93, 98	0
2	S	21/41 (51%)	0.82	3 (14%) 4 3	64, 96, 117, 121	0
2	U	21/41 (51%)	0.64	2 (9%) 10 9	49, 91, 107, 111	0
2	W	21/41 (51%)	1.42	5 (23%) 1 1	78, 111, 130, 134	0
2	Y	21/41 (51%)	0.41	1 (4%) 34 27	62, 90, 101, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	6777/7080 (95%)	-0.22	57 (0%) 87 81	8, 49, 88, 134	12 (0%)

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	1044	HIS	4.6
1	C	542	ASN	4.0
2	U	1039	GLY	3.6
2	H	1045	THR	3.5
2	W	1039	GLY	3.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	WO4	M	551	5/5	0.74	0.52	4.40	131,133,133,137	5
3	WO4	X	551	5/5	0.94	0.43	3.77	88,90,91,93	5
3	WO4	A	551	5/5	0.87	0.36	2.29	103,105,108,113	5
3	WO4	K	551	5/5	0.89	0.32	2.07	96,97,101,108	5
3	WO4	B	551	5/5	0.92	0.32	1.80	88,89,93,97	5
3	WO4	M	550	5/5	0.78	0.38	1.79	112,113,118,118	5
3	WO4	V	550	5/5	0.79	0.36	1.77	107,108,112,113	5
3	WO4	K	550	5/5	0.84	0.33	1.58	78,79,82,88	5
3	WO4	T	550	5/5	0.90	0.37	1.54	103,104,113,115	5
3	WO4	R	551	5/5	0.92	0.34	1.40	86,88,95,98	5
3	WO4	V	551	5/5	0.91	0.33	1.37	102,102,105,109	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	WO4	O	550	5/5	0.91	0.25	0.76	100,100,105,109	5
3	WO4	G	550	5/5	0.87	0.30	0.75	79,79,88,93	5
3	WO4	T	551	5/5	0.81	0.35	0.50	113,114,117,119	5
3	WO4	C	550	5/5	0.89	0.28	0.32	80,84,89,90	5
3	WO4	O	551	5/5	0.93	0.25	0.20	71,75,80,87	5
3	WO4	X	550	5/5	0.92	0.24	0.07	94,99,99,100	5
3	WO4	R	550	5/5	0.93	0.26	-0.10	106,107,111,116	5
3	WO4	B	550	5/5	0.91	0.23	-0.15	72,73,77,82	5
3	WO4	A	550	5/5	0.93	0.23	-0.36	84,86,88,93	5
3	WO4	I	550	5/5	0.95	0.22	-0.71	89,90,91,91	5

6.5 Other polymers

There are no such residues in this entry.