



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:03 pm BST

PDB ID : 5YJJ
Title : Crystal structure of PNPase from Staphylococcus epidermidis
Authors : Raj, R.; Gopal, B.
Deposited on : 2017-10-10
Resolution : 2.20 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
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

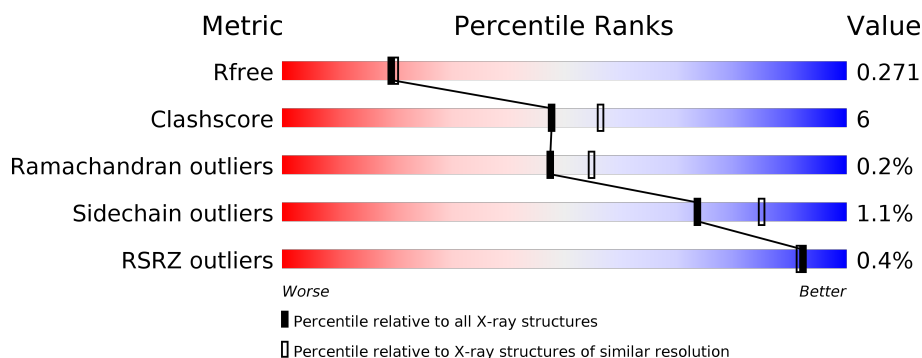
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	713	<div> <div>53%</div> <div>9%</div> <div>38%</div> </div>
1	B	713	<div> <div>53%</div> <div>8%</div> <div>38%</div> </div>
1	C	713	<div> <div>54%</div> <div>7%</div> <div>38%</div> </div>
1	D	713	<div> <div>55%</div> <div>6%</div> <div>38%</div> </div>
1	E	713	<div> <div>55%</div> <div>6%</div> <div>38%</div> </div>
1	F	713	<div> <div>54%</div> <div>8%</div> <div>38%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	801	-	-	X	-
2	PO4	B	801	-	-	X	-
2	PO4	C	801	-	-	X	-
2	PO4	D	801	-	-	X	-
2	PO4	E	801	-	-	X	-
2	PO4	F	801	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21469 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	442	Total	C	N	O	S	0	0	0
			3313	2090	569	637	17			
1	B	442	Total	C	N	O	S	0	0	0
			3313	2089	571	636	17			
1	C	442	Total	C	N	O	S	0	0	0
			3322	2097	574	634	17			
1	D	442	Total	C	N	O	S	0	0	0
			3311	2087	578	630	16			
1	E	441	Total	C	N	O	S	0	0	0
			3284	2073	565	629	17			
1	F	442	Total	C	N	O	S	0	0	0
			3271	2062	566	627	16			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q8CST1
A	-10	GLY	-	expression tag	UNP Q8CST1
A	-9	SER	-	expression tag	UNP Q8CST1
A	-8	SER	-	expression tag	UNP Q8CST1
A	-7	HIS	-	expression tag	UNP Q8CST1
A	-6	HIS	-	expression tag	UNP Q8CST1
A	-5	HIS	-	expression tag	UNP Q8CST1
A	-4	HIS	-	expression tag	UNP Q8CST1
A	-3	HIS	-	expression tag	UNP Q8CST1
A	-2	HIS	-	expression tag	UNP Q8CST1
A	-1	SER	-	expression tag	UNP Q8CST1
A	0	ASN	-	expression tag	UNP Q8CST1
B	-11	MET	-	expression tag	UNP Q8CST1
B	-10	GLY	-	expression tag	UNP Q8CST1
B	-9	SER	-	expression tag	UNP Q8CST1
B	-8	SER	-	expression tag	UNP Q8CST1
B	-7	HIS	-	expression tag	UNP Q8CST1

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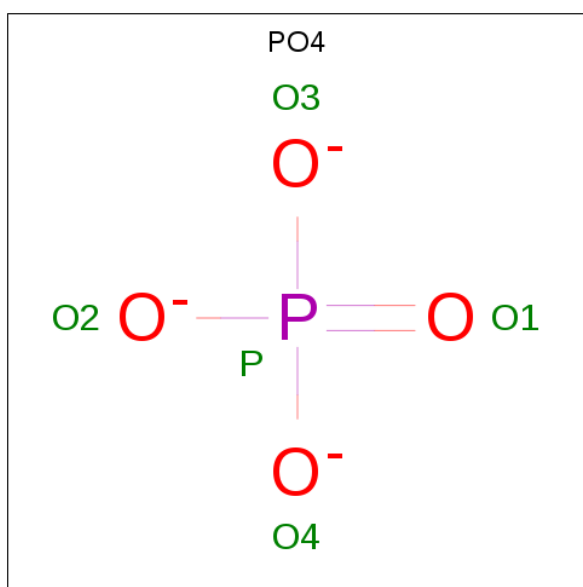
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q8CST1
B	-5	HIS	-	expression tag	UNP Q8CST1
B	-4	HIS	-	expression tag	UNP Q8CST1
B	-3	HIS	-	expression tag	UNP Q8CST1
B	-2	HIS	-	expression tag	UNP Q8CST1
B	-1	SER	-	expression tag	UNP Q8CST1
B	0	ASN	-	expression tag	UNP Q8CST1
C	-11	MET	-	expression tag	UNP Q8CST1
C	-10	GLY	-	expression tag	UNP Q8CST1
C	-9	SER	-	expression tag	UNP Q8CST1
C	-8	SER	-	expression tag	UNP Q8CST1
C	-7	HIS	-	expression tag	UNP Q8CST1
C	-6	HIS	-	expression tag	UNP Q8CST1
C	-5	HIS	-	expression tag	UNP Q8CST1
C	-4	HIS	-	expression tag	UNP Q8CST1
C	-3	HIS	-	expression tag	UNP Q8CST1
C	-2	HIS	-	expression tag	UNP Q8CST1
C	-1	SER	-	expression tag	UNP Q8CST1
C	0	ASN	-	expression tag	UNP Q8CST1
D	-11	MET	-	expression tag	UNP Q8CST1
D	-10	GLY	-	expression tag	UNP Q8CST1
D	-9	SER	-	expression tag	UNP Q8CST1
D	-8	SER	-	expression tag	UNP Q8CST1
D	-7	HIS	-	expression tag	UNP Q8CST1
D	-6	HIS	-	expression tag	UNP Q8CST1
D	-5	HIS	-	expression tag	UNP Q8CST1
D	-4	HIS	-	expression tag	UNP Q8CST1
D	-3	HIS	-	expression tag	UNP Q8CST1
D	-2	HIS	-	expression tag	UNP Q8CST1
D	-1	SER	-	expression tag	UNP Q8CST1
D	0	ASN	-	expression tag	UNP Q8CST1
E	-11	MET	-	expression tag	UNP Q8CST1
E	-10	GLY	-	expression tag	UNP Q8CST1
E	-9	SER	-	expression tag	UNP Q8CST1
E	-8	SER	-	expression tag	UNP Q8CST1
E	-7	HIS	-	expression tag	UNP Q8CST1
E	-6	HIS	-	expression tag	UNP Q8CST1
E	-5	HIS	-	expression tag	UNP Q8CST1
E	-4	HIS	-	expression tag	UNP Q8CST1
E	-3	HIS	-	expression tag	UNP Q8CST1
E	-2	HIS	-	expression tag	UNP Q8CST1
E	-1	SER	-	expression tag	UNP Q8CST1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	ASN	-	expression tag	UNP Q8CST1
F	-11	MET	-	expression tag	UNP Q8CST1
F	-10	GLY	-	expression tag	UNP Q8CST1
F	-9	SER	-	expression tag	UNP Q8CST1
F	-8	SER	-	expression tag	UNP Q8CST1
F	-7	HIS	-	expression tag	UNP Q8CST1
F	-6	HIS	-	expression tag	UNP Q8CST1
F	-5	HIS	-	expression tag	UNP Q8CST1
F	-4	HIS	-	expression tag	UNP Q8CST1
F	-3	HIS	-	expression tag	UNP Q8CST1
F	-2	HIS	-	expression tag	UNP Q8CST1
F	-1	SER	-	expression tag	UNP Q8CST1
F	0	ASN	-	expression tag	UNP Q8CST1

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

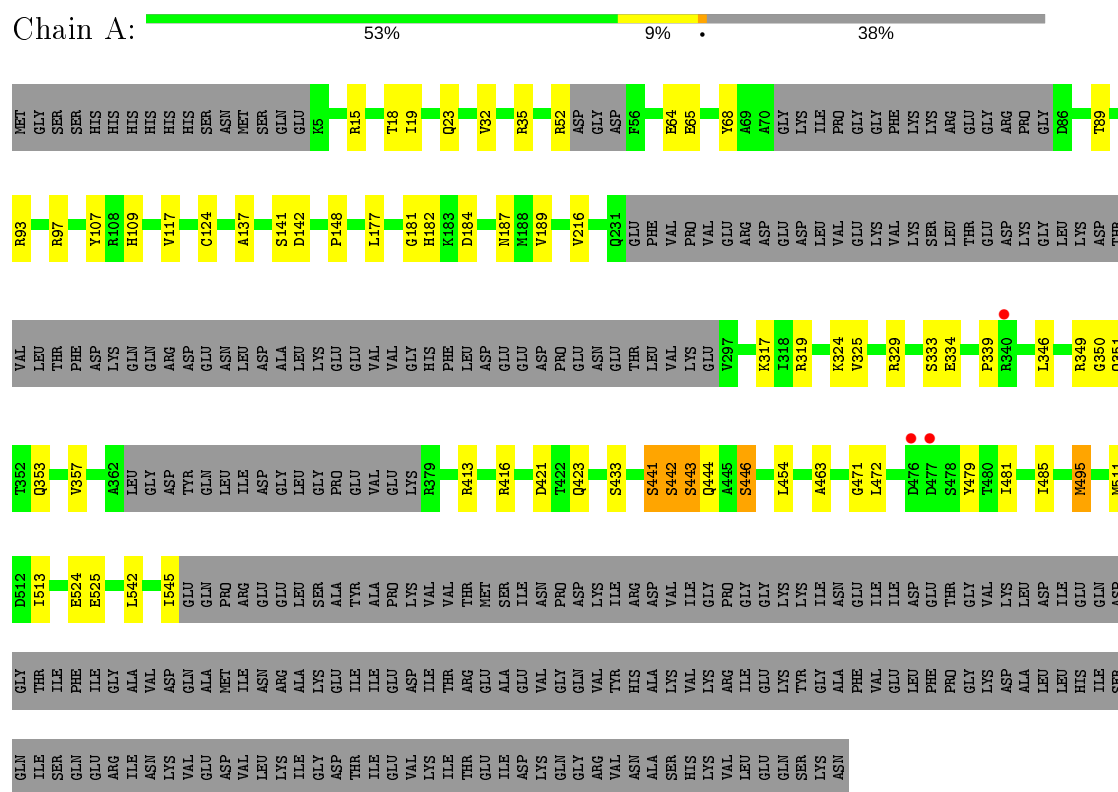
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	254	Total	O	0	0
			254	254		
4	B	269	Total	O	0	0
			269	269		
4	C	283	Total	O	0	0
			283	283		
4	D	266	Total	O	0	0
			266	266		
4	E	273	Total	O	0	0
			273	273		
4	F	274	Total	O	0	0
			274	274		

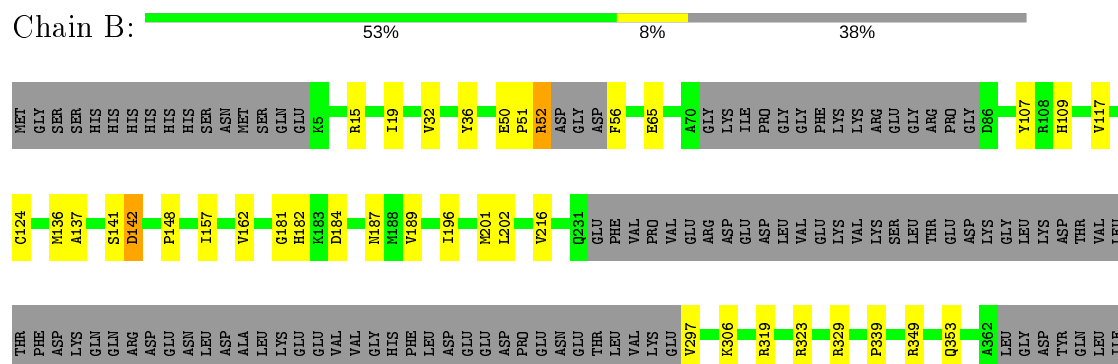
3 Residue-property plots

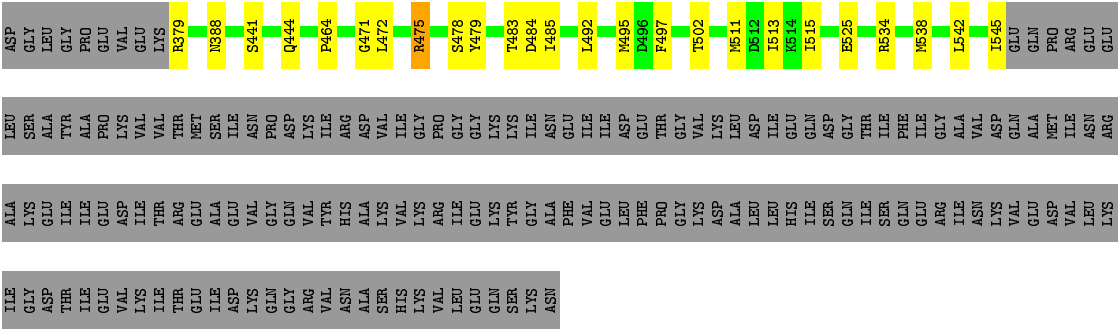
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Polyrribonucleotide nucleotidyltransferase

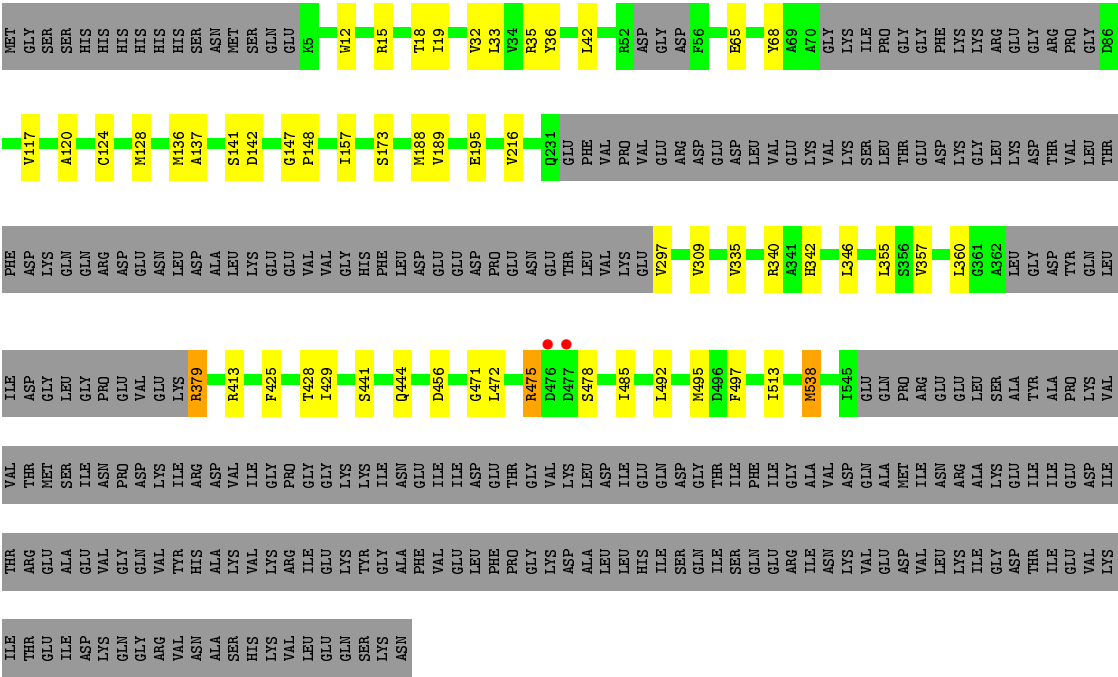


- Molecule 1: Polyrribonucleotide nucleotidyltransferase

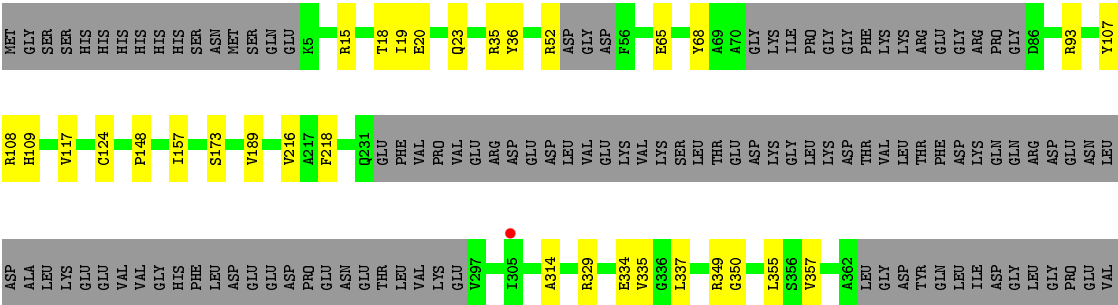


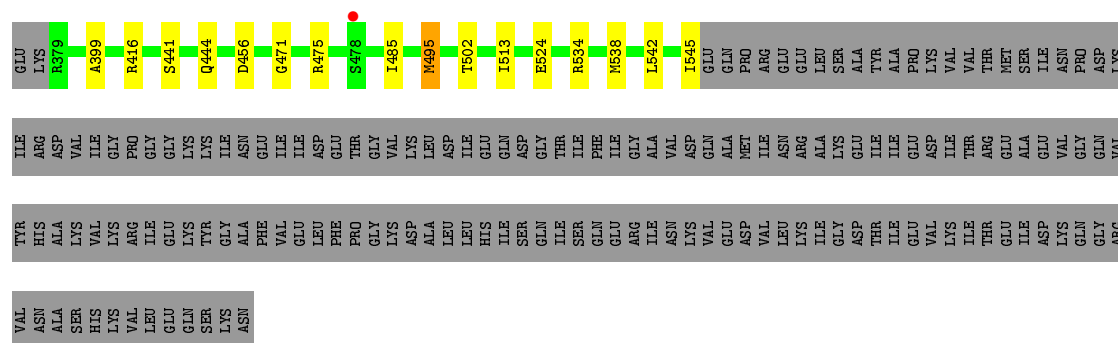


● Molecule 1: Polyribonucleotide nucleotidyltransferase

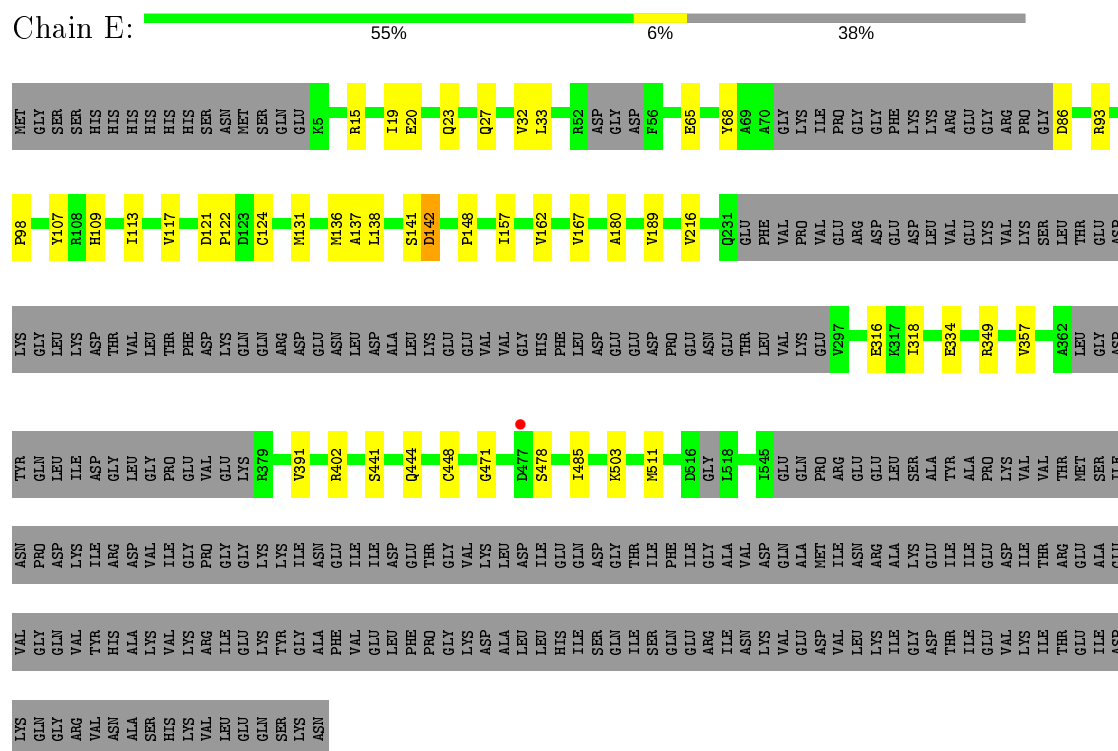


● Molecule 1: Polyribonucleotide nucleotidyltransferase

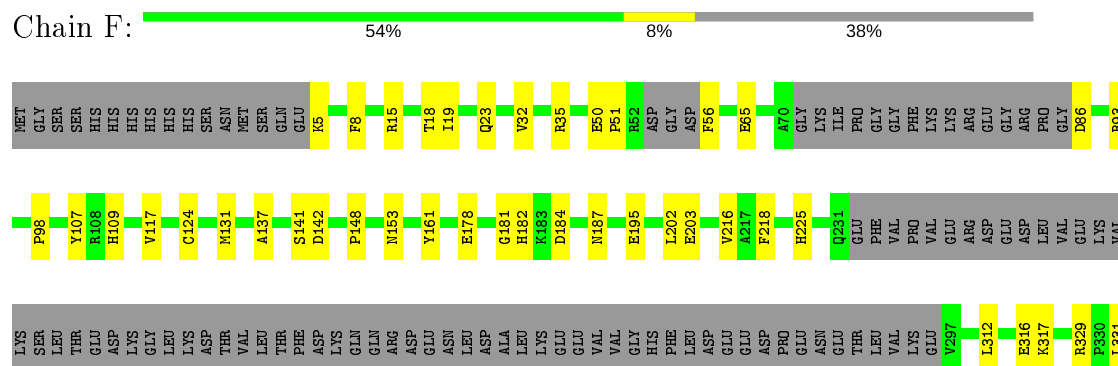


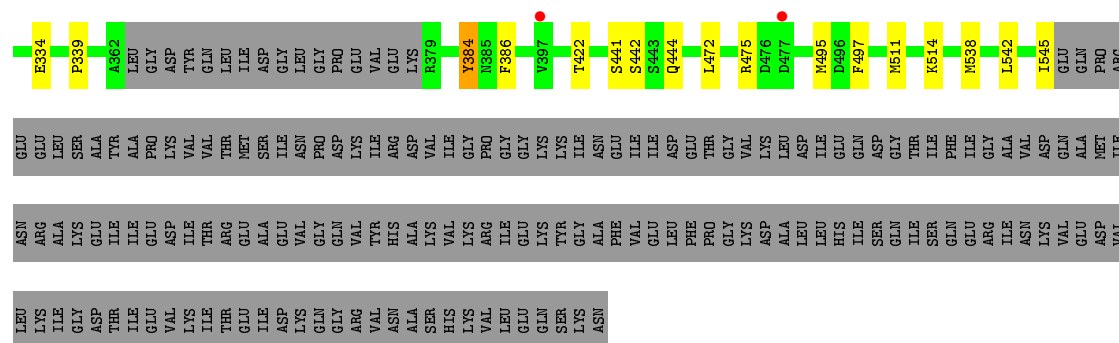


- Molecule 1: Polyrribonucleotide nucleotidyltransferase



- Molecule 1: Polyribonucleotide nucleotidyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.19Å 93.16Å 143.15Å 73.54° 87.61° 60.07°	Depositor
Resolution (Å)	73.04 – 2.20 73.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.6 (73.04-2.20) 97.5 (73.04-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.237 , 0.259 0.250 , 0.271	Depositor DCC
R_{free} test set	9795 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	1.719	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.058 for h,h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21469	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.37% 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: PO4, MG

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	0.42	0/3365	0.56	0/4554
1	B	0.32	0/3365	0.52	0/4558
1	C	0.32	0/3373	0.52	0/4564
1	D	0.39	0/3363	0.58	0/4553
1	E	0.35	0/3334	0.55	0/4511
1	F	0.39	1/3323 (0.0%)	0.55	0/4500
All	All	0.37	1/20123 (0.0%)	0.55	0/27240

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	384	TYR	CE1-CZ	-5.39	1.31	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3313	0	3265	53	0
1	B	3313	0	3261	51	0
1	C	3322	0	3288	41	0
1	D	3311	0	3257	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3284	0	3209	30	0
1	F	3271	0	3179	45	0
2	A	5	0	0	3	0
2	B	5	0	0	2	0
2	C	5	0	0	2	0
2	D	5	0	0	2	0
2	E	5	0	0	2	0
2	F	5	0	0	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	254	0	0	6	0
4	B	269	0	0	9	0
4	C	283	0	0	4	0
4	D	266	0	0	2	0
4	E	273	0	0	5	0
4	F	274	0	0	5	0
All	All	21469	0	19459	239	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (239) 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:E:121:ASP:OD2	1:E:122:PRO:HD2	1.64	0.96
1:A:524:GLU:HG3	1:B:202:LEU:HD21	1.52	0.92
1:B:306:LYS:HA	1:B:492:LEU:HD23	1.55	0.89
1:F:312:LEU:O	1:F:316:GLU:CB	2.23	0.87
1:A:524:GLU:HG3	1:B:202:LEU:CD2	2.05	0.87
1:F:181:GLY:HA2	1:F:187:ASN:HB2	1.65	0.78
1:E:148:PRO:HG2	1:E:216:VAL:HG13	1.66	0.77
1:B:181:GLY:HA2	1:B:187:ASN:HB2	1.68	0.73
1:B:349:ARG:NH2	4:B:902:HOH:O	2.21	0.73
1:C:120:ALA:O	1:C:340:ARG:NH1	2.22	0.73
1:D:495:MET:HB3	1:D:513:ILE:HG22	1.70	0.73
1:D:148:PRO:HG2	1:D:216:VAL:HG13	1.72	0.72
1:A:317:LYS:HZ2	1:A:325:VAL:H	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ARG:NH2	4:C:902:HOH:O	2.24	0.71
1:D:441:SER:HA	2:D:801:PO4:O1	1.92	0.69
1:E:316:GLU:HB2	1:E:318:ILE:HG22	1.74	0.69
1:C:19:ILE:HG23	1:C:32:VAL:CG1	2.22	0.69
1:B:196:ILE:HD11	1:B:201:MET:CE	2.23	0.68
1:C:148:PRO:HG2	1:C:216:VAL:HG13	1.75	0.68
1:E:15:ARG:HD3	1:E:124:CYS:SG	2.34	0.67
1:A:181:GLY:HA2	1:A:187:ASN:HB2	1.77	0.67
1:B:319:ARG:NH2	1:B:483:THR:O	2.21	0.67
1:F:441:SER:HA	2:F:801:PO4:P	2.34	0.67
1:C:441:SER:HA	2:C:801:PO4:P	2.36	0.66
1:A:441:SER:OG	1:A:444:GLN:HG2	1.94	0.66
1:C:379:ARG:NH2	1:C:425:PHE:O	2.29	0.66
1:B:297:VAL:N	4:B:910:HOH:O	2.29	0.66
1:D:65:GLU:HA	1:D:117:VAL:HB	1.78	0.65
1:A:141:SER:O	1:A:142:ASP:HB3	1.96	0.65
1:F:8:PHE:HE2	1:F:225:HIS:HD2	1.45	0.65
1:C:19:ILE:HG23	1:C:32:VAL:HG13	1.77	0.65
1:C:441:SER:HA	2:C:801:PO4:O4	1.97	0.65
1:F:312:LEU:O	1:F:317:LYS:N	2.30	0.65
1:A:317:LYS:O	1:A:317:LYS:HD3	1.98	0.64
1:A:317:LYS:NZ	1:A:325:VAL:H	1.96	0.63
1:E:86:ASP:N	4:E:906:HOH:O	2.31	0.63
1:D:52:ARG:O	1:D:52:ARG:HG2	1.99	0.62
1:E:349:ARG:NH2	4:E:901:HOH:O	2.25	0.62
1:C:425:PHE:HE2	1:C:429:ILE:HD11	1.62	0.62
1:A:441:SER:HA	2:A:801:PO4:P	2.40	0.61
1:E:441:SER:HA	2:E:801:PO4:O1	2.00	0.61
1:B:196:ILE:HD11	1:B:201:MET:HE3	1.83	0.61
1:D:524:GLU:HG3	1:F:202:LEU:HD11	1.82	0.61
1:F:312:LEU:HA	1:F:316:GLU:CB	2.30	0.61
1:F:5:LYS:N	4:F:909:HOH:O	2.34	0.61
1:F:329:ARG:O	1:F:331:LEU:HD12	2.01	0.60
1:F:93:ARG:NH2	4:F:910:HOH:O	2.35	0.60
1:C:538:MET:SD	4:C:964:HOH:O	2.56	0.60
1:F:50:GLU:HG3	1:F:51:PRO:HD2	1.83	0.60
1:A:433:SER:CB	1:A:446:SER:HB3	2.32	0.60
1:B:441:SER:HA	2:B:801:PO4:P	2.42	0.60
1:B:534:ARG:O	1:B:538:MET:HG3	2.02	0.60
1:A:65:GLU:HA	1:A:117:VAL:HB	1.83	0.60
1:D:15:ARG:HD2	1:D:36:TYR:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:472:LEU:HB2	1:F:495:MET:SD	2.41	0.60
1:C:425:PHE:CE2	1:C:429:ILE:HD11	2.36	0.59
1:B:52:ARG:HH11	1:B:52:ARG:HG2	1.67	0.59
1:E:441:SER:HA	2:E:801:PO4:P	2.42	0.59
1:C:15:ARG:NH1	1:C:36:TYR:OH	2.34	0.59
1:D:15:ARG:HD2	1:D:36:TYR:CZ	2.38	0.59
1:B:50:GLU:HG3	1:B:51:PRO:HD2	1.84	0.59
1:B:15:ARG:HD3	1:B:124:CYS:SG	2.42	0.58
1:F:86:ASP:N	4:F:914:HOH:O	2.37	0.58
1:A:317:LYS:HZ2	1:A:325:VAL:HG13	1.68	0.58
1:A:441:SER:HB2	4:A:912:HOH:O	2.02	0.58
1:B:441:SER:HA	2:B:801:PO4:O4	2.04	0.58
1:D:534:ARG:NH1	4:D:902:HOH:O	2.22	0.57
1:F:441:SER:OG	1:F:444:GLN:HG2	2.04	0.57
1:E:93:ARG:NH2	4:E:909:HOH:O	2.38	0.56
1:B:441:SER:OG	1:B:444:GLN:HG2	2.04	0.56
1:F:514:LYS:NZ	4:F:917:HOH:O	2.39	0.56
1:A:324:LYS:NZ	4:A:914:HOH:O	2.37	0.55
1:F:148:PRO:HG2	1:F:216:VAL:HG13	1.88	0.55
1:F:441:SER:HA	2:F:801:PO4:O4	2.05	0.55
1:A:351:GLN:NE2	4:A:906:HOH:O	2.32	0.55
1:B:513:ILE:HD12	1:B:515:ILE:HD12	1.88	0.55
1:E:448:CYS:SG	4:E:901:HOH:O	2.36	0.55
1:A:349:ARG:HH21	1:A:349:ARG:HG2	1.70	0.55
1:C:342:HIS:HB3	1:C:360:LEU:HD13	1.88	0.55
1:A:317:LYS:HE3	1:A:324:LYS:HG2	1.89	0.55
1:E:107:TYR:CZ	1:E:109:HIS:HB2	2.42	0.55
1:D:441:SER:OG	1:D:444:GLN:HG2	2.07	0.54
1:F:15:ARG:HD3	1:F:124:CYS:SG	2.47	0.54
1:F:23:GLN:NE2	1:F:334:GLU:OE2	2.40	0.54
1:A:23:GLN:NE2	1:A:334:GLU:OE2	2.36	0.54
1:D:335:VAL:HG23	1:D:456:ASP:HB2	1.90	0.54
1:D:23:GLN:NE2	1:D:334:GLU:OE2	2.36	0.54
1:B:148:PRO:HG2	1:B:216:VAL:HG13	1.89	0.53
1:C:297:VAL:N	4:C:919:HOH:O	2.39	0.53
1:C:335:VAL:HG23	1:C:456:ASP:HB2	1.91	0.53
1:A:542:LEU:HA	1:A:545:ILE:HG22	1.90	0.53
1:B:65:GLU:HA	1:B:117:VAL:HB	1.90	0.53
1:D:329:ARG:HD2	1:D:350:GLY:HA3	1.91	0.53
1:E:23:GLN:NE2	1:E:334:GLU:OE2	2.39	0.53
1:B:141:SER:O	1:B:142:ASP:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:TYR:CZ	1:B:109:HIS:HB2	2.44	0.53
1:A:137:ALA:O	1:A:141:SER:HB3	2.08	0.53
1:A:421:ASP:HB3	1:A:423:GLN:OE1	2.09	0.52
1:D:524:GLU:HG3	1:F:202:LEU:CD1	2.39	0.52
1:B:19:ILE:HG23	1:B:32:VAL:HG13	1.92	0.52
1:C:32:VAL:HG21	1:C:136:MET:HB3	1.92	0.52
1:E:189:VAL:HB	1:F:511:MET:HE3	1.90	0.52
1:F:442:SER:N	2:F:801:PO4:O2	2.35	0.52
1:A:524:GLU:HG3	1:B:202:LEU:HD22	1.88	0.51
1:D:441:SER:HA	2:D:801:PO4:P	2.50	0.51
1:C:15:ARG:HD3	1:C:124:CYS:SG	2.50	0.51
1:B:306:LYS:NZ	4:B:905:HOH:O	2.26	0.51
1:A:353:GLN:NE2	4:A:918:HOH:O	2.44	0.51
1:C:475:ARG:O	1:C:478:SER:N	2.43	0.51
1:B:472:LEU:HB2	1:B:495:MET:SD	2.51	0.51
1:E:65:GLU:HA	1:E:117:VAL:HB	1.92	0.51
1:F:8:PHE:CE2	1:F:225:HIS:HD2	2.27	0.51
1:C:472:LEU:HB2	1:C:495:MET:SD	2.51	0.50
1:A:524:GLU:CG	1:B:202:LEU:CD2	2.86	0.50
1:C:471:GLY:HA3	1:C:485:ILE:HG21	1.93	0.50
1:C:65:GLU:HA	1:C:117:VAL:HB	1.93	0.50
1:F:86:ASP:N	4:F:920:HOH:O	2.45	0.50
1:B:52:ARG:NH1	1:B:52:ARG:HG2	2.27	0.50
1:D:19:ILE:HD13	1:D:218:PHE:HE2	1.75	0.50
1:F:137:ALA:O	1:F:141:SER:HB3	2.12	0.50
1:C:342:HIS:CB	1:C:360:LEU:HD13	2.42	0.50
1:F:312:LEU:O	1:F:316:GLU:CA	2.59	0.50
1:F:65:GLU:HA	1:F:117:VAL:HB	1.93	0.49
1:F:441:SER:N	2:F:801:PO4:O4	2.43	0.49
1:C:33:LEU:HD13	1:C:42:LEU:HD23	1.95	0.49
1:A:495:MET:HB3	1:A:513:ILE:HG22	1.94	0.49
1:E:441:SER:OG	1:E:444:GLN:HG2	2.13	0.49
1:B:379:ARG:N	4:B:921:HOH:O	2.46	0.48
1:D:107:TYR:CZ	1:D:109:HIS:HB2	2.48	0.48
1:D:18:THR:HB	1:D:35:ARG:HB2	1.95	0.48
1:B:542:LEU:HA	1:B:545:ILE:HG22	1.96	0.48
1:B:349:ARG:HD3	1:B:484:ASP:OD1	2.13	0.48
1:F:153:ASN:HD22	1:F:178:GLU:HG3	1.79	0.48
1:A:15:ARG:HD3	1:A:124:CYS:SG	2.53	0.48
1:A:19:ILE:HG23	1:A:32:VAL:HG13	1.94	0.48
1:A:472:LEU:HD11	1:A:479:TYR:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:SER:OG	2:A:801:PO4:O4	2.29	0.48
1:B:141:SER:O	1:B:142:ASP:CB	2.62	0.48
1:B:137:ALA:O	1:B:141:SER:HB3	2.14	0.47
1:C:495:MET:HE2	1:C:497:PHE:HB2	1.96	0.47
1:B:475:ARG:NH2	4:B:920:HOH:O	2.46	0.47
1:A:107:TYR:CZ	1:A:109:HIS:HB2	2.50	0.47
1:A:463:ALA:HB1	4:A:1027:HOH:O	2.14	0.47
1:E:19:ILE:HG23	1:E:32:VAL:HG13	1.96	0.47
1:A:187:ASN:OD1	1:C:513:ILE:HD11	2.15	0.47
1:C:428:THR:C	1:C:429:ILE:HD12	2.36	0.47
1:B:15:ARG:NH1	1:B:36:TYR:OH	2.44	0.47
1:A:511:MET:HE3	1:B:189:VAL:HB	1.96	0.47
1:E:19:ILE:HD13	1:E:136:MET:HG3	1.96	0.47
1:B:502:THR:OG1	1:C:195:GLU:OE1	2.24	0.46
1:C:441:SER:OG	1:C:444:GLN:HG2	2.14	0.46
1:A:148:PRO:HG2	1:A:216:VAL:HG13	1.97	0.46
1:B:353:GLN:NE2	4:B:909:HOH:O	2.48	0.46
1:C:157:ILE:HG13	1:C:173:SER:HA	1.98	0.46
1:B:19:ILE:HD13	1:B:136:MET:HG3	1.98	0.46
1:D:20:GLU:OE2	1:D:35:ARG:HD2	2.16	0.46
1:E:157:ILE:HD12	1:E:162:VAL:HG21	1.96	0.46
1:C:346:LEU:HB2	1:C:355:LEU:HD23	1.98	0.46
1:F:107:TYR:CZ	1:F:109:HIS:HB2	2.51	0.46
1:A:93:ARG:O	1:A:97:ARG:HG3	2.16	0.46
1:F:98:PRO:HG3	1:F:131:MET:SD	2.56	0.46
1:A:182:HIS:CE1	1:A:184:ASP:HB2	2.51	0.46
1:A:64:GLU:OE1	4:A:901:HOH:O	2.21	0.46
1:C:137:ALA:O	1:C:141:SER:HB3	2.16	0.46
1:B:56:PHE:N	4:B:923:HOH:O	2.48	0.46
1:D:471:GLY:HA3	1:D:485:ILE:HG21	1.97	0.45
1:D:349:ARG:NH2	1:D:441:SER:O	2.49	0.45
1:E:27:GLN:NE2	1:E:391:VAL:HA	2.31	0.45
1:A:433:SER:HB3	1:A:446:SER:HB3	1.97	0.45
1:D:314:ALA:HB3	1:D:475:ARG:HD2	1.98	0.45
1:A:441:SER:C	1:A:443:SER:N	2.65	0.45
1:F:542:LEU:HA	1:F:545:ILE:HG22	1.99	0.45
1:C:136:MET:HA	1:C:136:MET:CE	2.46	0.45
1:A:441:SER:HA	2:A:801:PO4:O1	2.17	0.44
1:A:18:THR:HB	1:A:35:ARG:HB2	2.00	0.44
1:C:19:ILE:HD13	1:C:136:MET:HG3	1.98	0.44
1:D:93:ARG:HD2	1:E:402:ARG:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:386:PHE:CD2	1:F:386:PHE:O	2.71	0.44
1:F:441:SER:CA	2:F:801:PO4:O4	2.65	0.44
1:B:196:ILE:HD11	1:B:201:MET:HE2	1.99	0.44
1:D:399:ALA:O	4:D:901:HOH:O	2.21	0.44
1:E:471:GLY:HA3	1:E:485:ILE:HG21	1.99	0.44
1:D:337:LEU:HD13	1:D:355:LEU:HD21	1.99	0.44
1:F:312:LEU:CA	1:F:316:GLU:CB	2.96	0.44
1:C:68:TYR:CD1	1:C:357:VAL:HG11	2.53	0.43
1:A:319:ARG:HD2	1:A:325:VAL:HA	1.99	0.43
1:B:464:PRO:HB2	1:B:538:MET:HE1	2.00	0.43
1:E:137:ALA:O	1:E:141:SER:HB3	2.17	0.43
1:A:471:GLY:HA3	1:A:485:ILE:HG21	1.99	0.43
1:C:335:VAL:O	4:C:901:HOH:O	2.21	0.43
1:A:413:ARG:HG3	1:A:416:ARG:HH21	1.82	0.43
1:C:335:VAL:CG2	1:C:456:ASP:HB2	2.48	0.43
1:E:122:PRO:HB2	1:E:167:VAL:HG21	2.01	0.43
1:F:18:THR:HB	1:F:35:ARG:HB2	2.00	0.43
1:A:177:LEU:HD11	1:A:189:VAL:HG13	2.01	0.42
1:A:68:TYR:CD1	1:A:357:VAL:HG11	2.55	0.42
1:D:502:THR:OG1	1:F:195:GLU:OE1	2.25	0.42
1:A:329:ARG:HD2	1:A:350:GLY:HA3	2.02	0.42
1:B:182:HIS:CE1	1:B:184:ASP:HB2	2.54	0.42
1:B:56:PHE:N	4:B:928:HOH:O	2.51	0.42
1:A:317:LYS:NZ	1:A:325:VAL:HG13	2.35	0.42
1:B:495:MET:HE3	1:B:497:PHE:CD2	2.55	0.42
1:E:503:LYS:HG2	4:E:967:HOH:O	2.19	0.42
1:D:189:VAL:HB	1:E:511:MET:HE3	2.02	0.42
1:F:495:MET:HE2	1:F:497:PHE:HB2	2.01	0.42
1:B:19:ILE:HG23	1:B:32:VAL:CG1	2.50	0.41
1:B:323:ARG:CZ	1:B:329:ARG:HG3	2.50	0.41
1:B:388:ASN:ND2	4:B:922:HOH:O	2.53	0.41
1:A:141:SER:O	1:A:142:ASP:CB	2.66	0.41
1:A:89:THR:O	1:A:93:ARG:HG3	2.20	0.41
1:C:18:THR:HB	1:C:35:ARG:HB2	2.01	0.41
1:F:161:TYR:OH	1:F:203:GLU:HB2	2.20	0.41
1:C:12:TRP:HH2	1:C:128:MET:HB3	1.85	0.41
1:F:19:ILE:HD12	1:F:218:PHE:CE2	2.56	0.41
1:D:157:ILE:HG13	1:D:173:SER:HA	2.02	0.41
1:E:131:MET:HE3	1:E:180:ALA:HB2	2.02	0.41
1:E:98:PRO:HG3	1:E:131:MET:SD	2.60	0.41
1:D:542:LEU:HA	1:D:545:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:TYR:CD1	1:E:357:VAL:HG11	2.56	0.41
1:A:333:SER:HA	1:A:346:LEU:O	2.21	0.41
1:F:19:ILE:HG23	1:F:32:VAL:HG13	2.03	0.41
1:F:497:PHE:CE2	1:F:511:MET:HE2	2.55	0.41
1:A:481:ILE:HG13	1:A:525:GLU:HG3	2.03	0.41
1:D:538:MET:HB2	1:D:538:MET:HE2	1.86	0.41
1:C:147:GLY:HA3	1:C:148:PRO:HA	1.94	0.41
1:D:68:TYR:CD1	1:D:357:VAL:HG11	2.56	0.41
1:F:182:HIS:CE1	1:F:184:ASP:HB2	2.56	0.41
1:F:538:MET:HE2	1:F:538:MET:HB2	1.86	0.41
1:B:471:GLY:HA3	1:B:485:ILE:HG21	2.02	0.40
1:B:478:SER:OG	1:B:479:TYR:N	2.55	0.40
1:C:309:VAL:HG11	1:C:492:LEU:CD1	2.51	0.40
1:D:15:ARG:HD3	1:D:124:CYS:SG	2.60	0.40
1:B:511:MET:HE3	1:C:189:VAL:HB	2.03	0.40
1:E:20:GLU:HB2	1:E:33:LEU:HB3	2.02	0.40
1:A:441:SER:O	1:A:442:SER:C	2.58	0.40
1:B:157:ILE:HD12	1:B:162:VAL:HG21	2.04	0.40
1:D:108:ARG:HH11	1:D:108:ARG:HD2	1.68	0.40
1:E:113:ILE:HD11	1:E:138:LEU:HD11	2.03	0.40
1:F:384:TYR:OH	1:F:442:SER:OG	2.20	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	
1	A	432/713 (61%)	419 (97%)	13 (3%)	0	100	100
1	B	432/713 (61%)	418 (97%)	13 (3%)	1 (0%)	47	55
1	C	432/713 (61%)	419 (97%)	12 (3%)	1 (0%)	47	55
1	D	432/713 (61%)	422 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	429/713 (60%)	417 (97%)	11 (3%)	1 (0%)	47	55
1	F	432/713 (61%)	421 (98%)	9 (2%)	2 (0%)	29	31
All	All	2589/4278 (60%)	2516 (97%)	68 (3%)	5 (0%)	47	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	422	THR
1	B	142	ASP
1	E	142	ASP
1	F	142	ASP
1	C	142	ASP

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	343/601 (57%)	335 (98%)	8 (2%)	50	63
1	B	340/601 (57%)	336 (99%)	4 (1%)	71	83
1	C	345/601 (57%)	341 (99%)	4 (1%)	71	83
1	D	336/601 (56%)	334 (99%)	2 (1%)	86	93
1	E	336/601 (56%)	334 (99%)	2 (1%)	86	93
1	F	330/601 (55%)	327 (99%)	3 (1%)	78	88
All	All	2030/3606 (56%)	2007 (99%)	23 (1%)	73	85

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	339	PRO
1	A	441	SER
1	A	442	SER
1	A	443	SER

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Mol	Chain	Res	Type
1	A	446	SER
1	A	454	LEU
1	A	495	MET
1	B	52	ARG
1	B	339	PRO
1	B	475	ARG
1	B	525	GLU
1	C	188	MET
1	C	379	ARG
1	C	475	ARG
1	C	538	MET
1	D	416	ARG
1	D	495	MET
1	E	142	ASP
1	E	478	SER
1	F	56	PHE
1	F	339	PRO
1	F	475	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	GLN
1	B	383	HIS
1	B	388	ASN
1	D	109	HIS
1	E	27	GLN
1	E	115	ASN
1	E	225	HIS
1	F	225	HIS
1	F	302	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	801	3	4,4,4	0.92	0	6,6,6	0.43	0
2	PO4	F	801	3	4,4,4	0.92	0	6,6,6	0.43	0
2	PO4	D	801	3	4,4,4	0.92	0	6,6,6	0.43	0
2	PO4	B	801	3	4,4,4	0.92	0	6,6,6	0.44	0
2	PO4	C	801	3	4,4,4	0.92	0	6,6,6	0.43	0
2	PO4	E	801	-	4,4,4	0.92	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PO4	3	0
2	F	801	PO4	5	0
2	D	801	PO4	2	0
2	B	801	PO4	2	0
2	C	801	PO4	2	0
2	E	801	PO4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	442/713 (61%)	-0.22	3 (0%) 87 86	9, 20, 37, 53	0
1	B	442/713 (61%)	-0.23	0 100 100	10, 20, 37, 45	0
1	C	442/713 (61%)	-0.23	2 (0%) 91 90	8, 20, 38, 48	0
1	D	442/713 (61%)	-0.23	2 (0%) 91 90	8, 21, 39, 48	0
1	E	441/713 (61%)	-0.26	1 (0%) 95 94	9, 20, 38, 50	0
1	F	442/713 (61%)	-0.24	2 (0%) 91 90	10, 20, 37, 50	0
All	All	2651/4278 (61%)	-0.24	10 (0%) 92 91	8, 20, 38, 53	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	478	SER	4.2
1	F	477	ASP	3.1
1	A	477	ASP	3.0
1	E	477	ASP	2.8
1	C	477	ASP	2.8
1	D	305	ILE	2.4
1	F	397	VAL	2.3
1	A	476	ASP	2.3
1	C	476	ASP	2.2
1	A	340	ARG	2.0

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 [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(Å ²)	Q<0.9
3	MG	D	802	1/1	0.93	0.14	28,28,28,28	0
3	MG	F	802	1/1	0.97	0.26	26,26,26,26	0
2	PO4	F	801	5/5	0.97	0.12	8,12,25,29	0
3	MG	C	802	1/1	0.97	0.15	27,27,27,27	0
3	MG	E	802	1/1	0.97	0.27	27,27,27,27	0
3	MG	B	802	1/1	0.98	0.24	28,28,28,28	0
3	MG	A	802	1/1	0.98	0.34	27,27,27,27	0
2	PO4	D	801	5/5	0.98	0.10	13,14,22,23	0
2	PO4	A	801	5/5	0.99	0.11	7,13,23,28	0
2	PO4	C	801	5/5	0.99	0.10	9,15,20,20	0
2	PO4	E	801	5/5	0.99	0.12	10,12,18,30	0
2	PO4	B	801	5/5	0.99	0.09	8,13,17,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.