



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:47 AM UTC

PDB ID : 5F7J / pdb_00005f7j
Title : Crystal structure of Mutant N87T of adenosine/Methylthioadenosine phosphorylase from Schistosoma mansoni in complex with Adenine
Authors : Torini, J.R.; Brandao-Neto, J.; DeMarco, R.; Pereira, H.M.
Deposited on : 2015-12-08
Resolution : 1.66 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

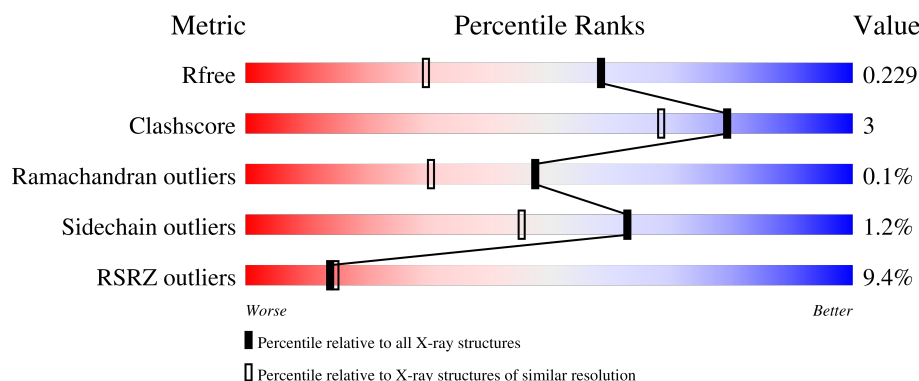
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	320	5% 81% 7% 12%
1	B	320	10% 82% 9% 9%
1	C	320	6% 83% 6% 10%
1	D	320	8% 85% 11%
1	E	320	15% 83% 8% 9%

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Mol	Chain	Length	Quality of chain
1	F	320	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14870 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 Methylthioadenosine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	1	0
			2171	1374	378	402	17			
1	B	291	Total	C	N	O	S	0	2	0
			2228	1413	386	412	17			
1	C	287	Total	C	N	O	S	0	1	0
			2192	1384	382	410	16			
1	D	286	Total	C	N	O	S	0	1	0
			2178	1377	380	404	17			
1	E	291	Total	C	N	O	S	0	2	0
			2235	1416	390	412	17			
1	F	273	Total	C	N	O	S	0	0	0
			2078	1318	359	385	16			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP I0B503
A	-19	GLY	-	expression tag	UNP I0B503
A	-18	SER	-	expression tag	UNP I0B503
A	-17	SER	-	expression tag	UNP I0B503
A	-16	HIS	-	expression tag	UNP I0B503
A	-15	HIS	-	expression tag	UNP I0B503
A	-14	HIS	-	expression tag	UNP I0B503
A	-13	HIS	-	expression tag	UNP I0B503
A	-12	HIS	-	expression tag	UNP I0B503
A	-11	HIS	-	expression tag	UNP I0B503
A	-10	SER	-	expression tag	UNP I0B503
A	-9	SER	-	expression tag	UNP I0B503
A	-8	GLY	-	expression tag	UNP I0B503
A	-7	LEU	-	expression tag	UNP I0B503
A	-6	VAL	-	expression tag	UNP I0B503
A	-5	PRO	-	expression tag	UNP I0B503
A	-4	ARG	-	expression tag	UNP I0B503

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP I0B503
A	-2	SER	-	expression tag	UNP I0B503
A	-1	HIS	-	expression tag	UNP I0B503
A	0	MET	-	expression tag	UNP I0B503
A	87	THR	ASN	engineered mutation	UNP I0B503
B	-20	MET	-	initiating methionine	UNP I0B503
B	-19	GLY	-	expression tag	UNP I0B503
B	-18	SER	-	expression tag	UNP I0B503
B	-17	SER	-	expression tag	UNP I0B503
B	-16	HIS	-	expression tag	UNP I0B503
B	-15	HIS	-	expression tag	UNP I0B503
B	-14	HIS	-	expression tag	UNP I0B503
B	-13	HIS	-	expression tag	UNP I0B503
B	-12	HIS	-	expression tag	UNP I0B503
B	-11	HIS	-	expression tag	UNP I0B503
B	-10	SER	-	expression tag	UNP I0B503
B	-9	SER	-	expression tag	UNP I0B503
B	-8	GLY	-	expression tag	UNP I0B503
B	-7	LEU	-	expression tag	UNP I0B503
B	-6	VAL	-	expression tag	UNP I0B503
B	-5	PRO	-	expression tag	UNP I0B503
B	-4	ARG	-	expression tag	UNP I0B503
B	-3	GLY	-	expression tag	UNP I0B503
B	-2	SER	-	expression tag	UNP I0B503
B	-1	HIS	-	expression tag	UNP I0B503
B	0	MET	-	expression tag	UNP I0B503
B	87	THR	ASN	engineered mutation	UNP I0B503
C	-20	MET	-	initiating methionine	UNP I0B503
C	-19	GLY	-	expression tag	UNP I0B503
C	-18	SER	-	expression tag	UNP I0B503
C	-17	SER	-	expression tag	UNP I0B503
C	-16	HIS	-	expression tag	UNP I0B503
C	-15	HIS	-	expression tag	UNP I0B503
C	-14	HIS	-	expression tag	UNP I0B503
C	-13	HIS	-	expression tag	UNP I0B503
C	-12	HIS	-	expression tag	UNP I0B503
C	-11	HIS	-	expression tag	UNP I0B503
C	-10	SER	-	expression tag	UNP I0B503
C	-9	SER	-	expression tag	UNP I0B503
C	-8	GLY	-	expression tag	UNP I0B503
C	-7	LEU	-	expression tag	UNP I0B503
C	-6	VAL	-	expression tag	UNP I0B503

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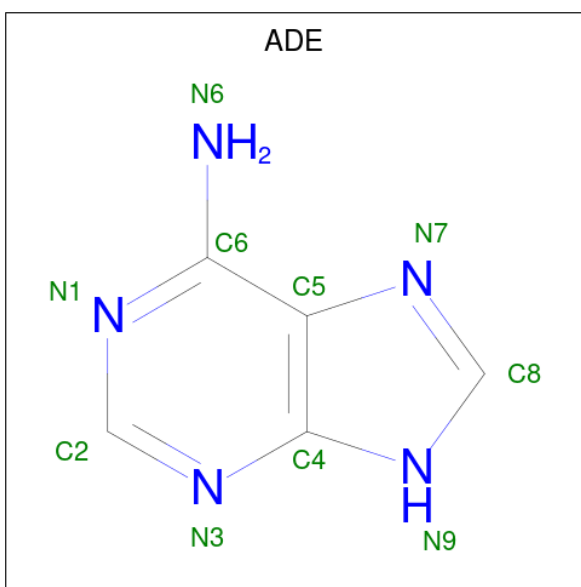
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C	-5	PRO	-	expression tag	UNP I0B503
C	-4	ARG	-	expression tag	UNP I0B503
C	-3	GLY	-	expression tag	UNP I0B503
C	-2	SER	-	expression tag	UNP I0B503
C	-1	HIS	-	expression tag	UNP I0B503
C	0	MET	-	expression tag	UNP I0B503
C	87	THR	ASN	engineered mutation	UNP I0B503
D	-20	MET	-	initiating methionine	UNP I0B503
D	-19	GLY	-	expression tag	UNP I0B503
D	-18	SER	-	expression tag	UNP I0B503
D	-17	SER	-	expression tag	UNP I0B503
D	-16	HIS	-	expression tag	UNP I0B503
D	-15	HIS	-	expression tag	UNP I0B503
D	-14	HIS	-	expression tag	UNP I0B503
D	-13	HIS	-	expression tag	UNP I0B503
D	-12	HIS	-	expression tag	UNP I0B503
D	-11	HIS	-	expression tag	UNP I0B503
D	-10	SER	-	expression tag	UNP I0B503
D	-9	SER	-	expression tag	UNP I0B503
D	-8	GLY	-	expression tag	UNP I0B503
D	-7	LEU	-	expression tag	UNP I0B503
D	-6	VAL	-	expression tag	UNP I0B503
D	-5	PRO	-	expression tag	UNP I0B503
D	-4	ARG	-	expression tag	UNP I0B503
D	-3	GLY	-	expression tag	UNP I0B503
D	-2	SER	-	expression tag	UNP I0B503
D	-1	HIS	-	expression tag	UNP I0B503
D	0	MET	-	expression tag	UNP I0B503
D	87	THR	ASN	engineered mutation	UNP I0B503
E	-20	MET	-	initiating methionine	UNP I0B503
E	-19	GLY	-	expression tag	UNP I0B503
E	-18	SER	-	expression tag	UNP I0B503
E	-17	SER	-	expression tag	UNP I0B503
E	-16	HIS	-	expression tag	UNP I0B503
E	-15	HIS	-	expression tag	UNP I0B503
E	-14	HIS	-	expression tag	UNP I0B503
E	-13	HIS	-	expression tag	UNP I0B503
E	-12	HIS	-	expression tag	UNP I0B503
E	-11	HIS	-	expression tag	UNP I0B503
E	-10	SER	-	expression tag	UNP I0B503
E	-9	SER	-	expression tag	UNP I0B503
E	-8	GLY	-	expression tag	UNP I0B503

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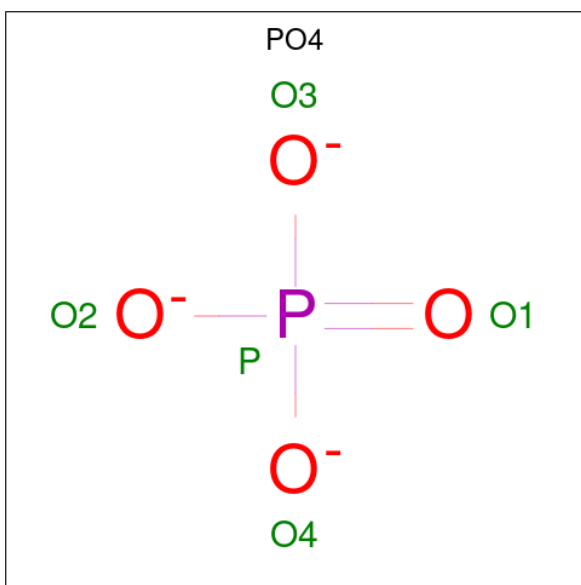
Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	LEU	-	expression tag	UNP I0B503
E	-6	VAL	-	expression tag	UNP I0B503
E	-5	PRO	-	expression tag	UNP I0B503
E	-4	ARG	-	expression tag	UNP I0B503
E	-3	GLY	-	expression tag	UNP I0B503
E	-2	SER	-	expression tag	UNP I0B503
E	-1	HIS	-	expression tag	UNP I0B503
E	0	MET	-	expression tag	UNP I0B503
E	87	THR	ASN	engineered mutation	UNP I0B503
F	-20	MET	-	initiating methionine	UNP I0B503
F	-19	GLY	-	expression tag	UNP I0B503
F	-18	SER	-	expression tag	UNP I0B503
F	-17	SER	-	expression tag	UNP I0B503
F	-16	HIS	-	expression tag	UNP I0B503
F	-15	HIS	-	expression tag	UNP I0B503
F	-14	HIS	-	expression tag	UNP I0B503
F	-13	HIS	-	expression tag	UNP I0B503
F	-12	HIS	-	expression tag	UNP I0B503
F	-11	HIS	-	expression tag	UNP I0B503
F	-10	SER	-	expression tag	UNP I0B503
F	-9	SER	-	expression tag	UNP I0B503
F	-8	GLY	-	expression tag	UNP I0B503
F	-7	LEU	-	expression tag	UNP I0B503
F	-6	VAL	-	expression tag	UNP I0B503
F	-5	PRO	-	expression tag	UNP I0B503
F	-4	ARG	-	expression tag	UNP I0B503
F	-3	GLY	-	expression tag	UNP I0B503
F	-2	SER	-	expression tag	UNP I0B503
F	-1	HIS	-	expression tag	UNP I0B503
F	0	MET	-	expression tag	UNP I0B503
F	87	THR	ASN	engineered mutation	UNP I0B503

- Molecule 2 is ADENINE (CCD ID: ADE) (formula: $C_5H_5N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			10	5	5		
2	B	1	Total	C	N	0	0
			10	5	5		
2	D	1	Total	C	N	0	0
			10	5	5		
2	E	1	Total	C	N	0	0
			10	5	5		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	E	1	Total O P 5 4 1	0	0
3	F	1	Total O P 5 4 1	0	0

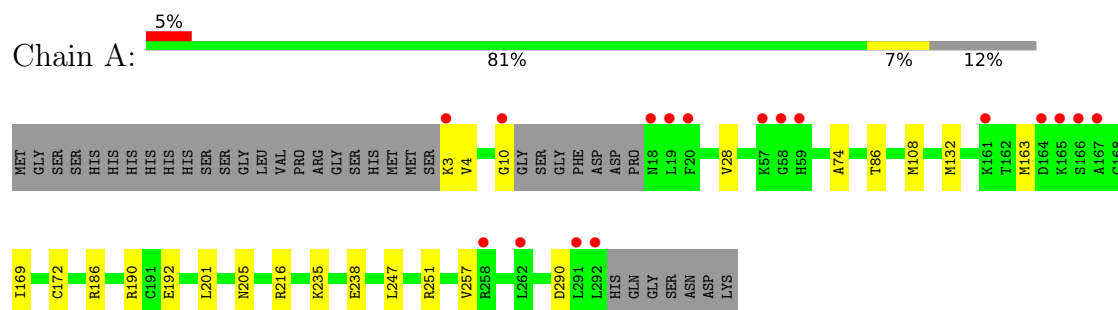
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	292	Total O 292 292	0	0
4	B	307	Total O 307 307	0	0
4	C	367	Total O 367 367	0	0
4	D	264	Total O 264 264	0	0
4	E	237	Total O 237 237	0	0
4	F	261	Total O 261 261	0	0

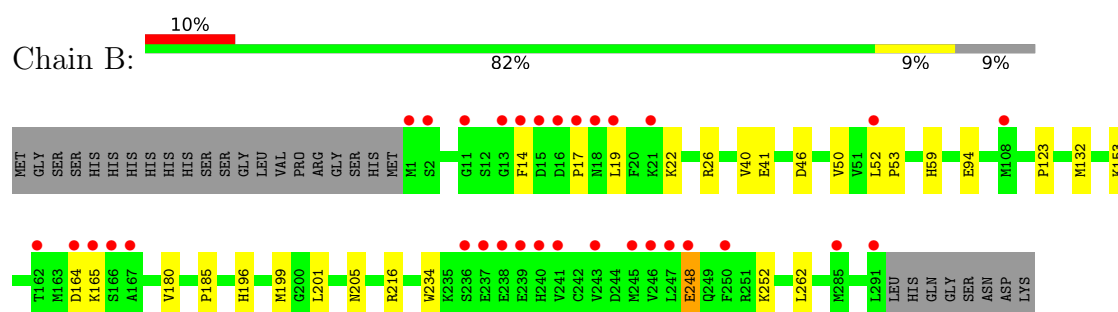
3 Residue-property plots [i](#)

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

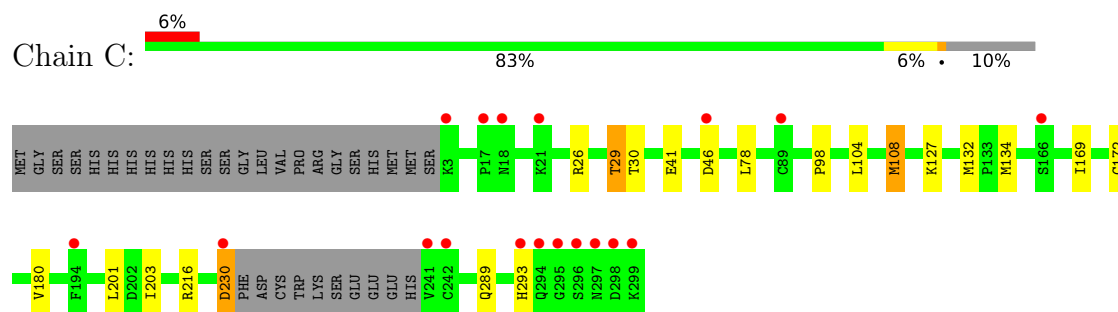
- Molecule 1: Methylthioadenosine phosphorylase



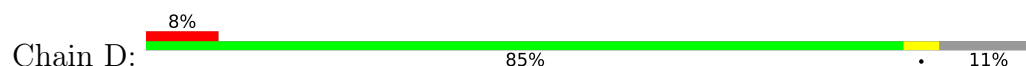
- Molecule 1: Methylthioadenosine phosphorylase

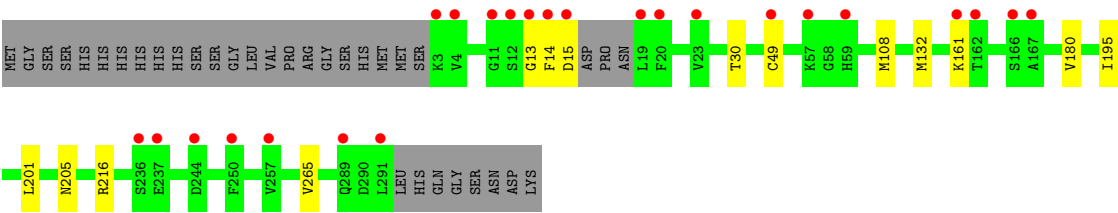


- Molecule 1: Methylthioadenosine phosphorylase

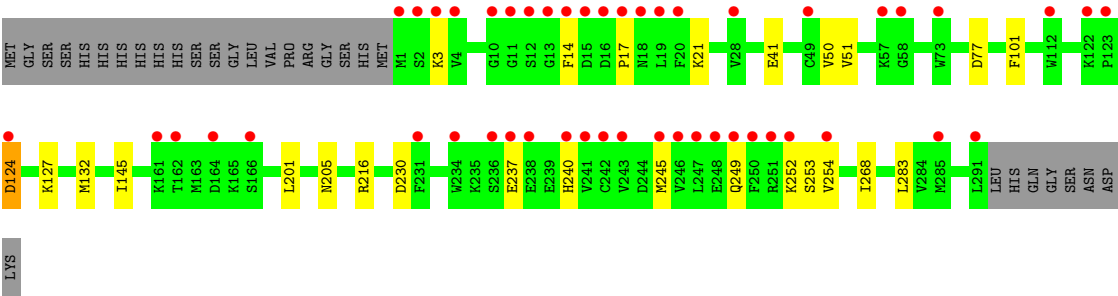
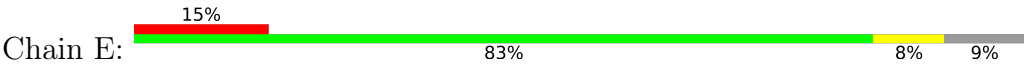


- Molecule 1: Methylthioadenosine phosphorylase

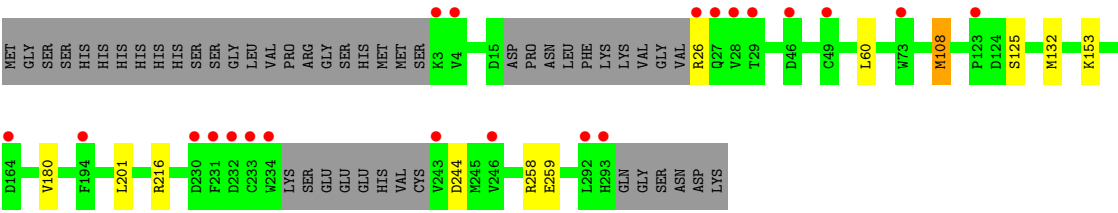
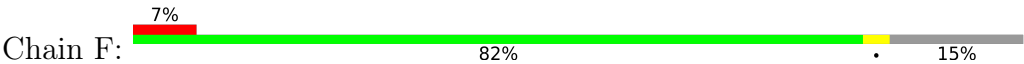




● Molecule 1: Methylthioadenosine phosphorylase



● Molecule 1: Methylthioadenosine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.49Å 82.11Å 150.27Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	73.73 – 1.66 73.73 – 1.66	Depositor EDS
% Data completeness (in resolution range)	95.3 (73.73-1.66) 95.8 (73.73-1.66)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.66Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.195 , 0.226 0.199 , 0.229	Depositor DCC
R_{free} test set	10852 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtrriage
Anisotropy	0.164	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14870	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1894e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, ADE

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	0.37	0/2216	0.54	0/3005
1	B	0.35	0/2279	0.52	0/3090
1	C	0.42	0/2235	0.58	0/3028
1	D	0.35	0/2223	0.52	0/3015
1	E	0.33	0/2286	0.50	0/3099
1	F	0.35	0/2118	0.53	0/2871
All	All	0.36	0/13357	0.53	0/18108

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2171	0	2162	15	0
1	B	2228	0	2231	18	0
1	C	2192	0	2196	14	0
1	D	2178	0	2160	7	0
1	E	2235	0	2237	14	0
1	F	2078	0	2071	8	0
2	A	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	292	0	0	3	0
4	B	307	0	0	4	1
4	C	367	0	0	1	0
4	D	264	0	0	0	0
4	E	237	0	0	1	0
4	F	261	0	0	1	1
All	All	14870	0	13073	71	1

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 3.

All (71) 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:B:248:GLU:OE1	1:B:252:LYS:NZ	2.17	0.75
1:C:98:PRO:HG3	1:C:230[A]:ASP:HA	1.70	0.73
1:A:163:MET:SD	4:A:552:HOH:O	2.50	0.68
1:B:123:PRO:O	4:B:401:HOH:O	2.12	0.67
1:D:132:MET:HE2	1:D:216:ARG:HG2	1.76	0.65
1:F:26:ARG:O	4:F:401:HOH:O	2.13	0.65
1:E:132:MET:HE2	1:E:216:ARG:HG2	1.78	0.64
1:B:180:VAL:HB	1:B:201:LEU:HD13	1.80	0.63
1:B:132:MET:HE2	1:B:216:ARG:HG2	1.80	0.63
1:A:132:MET:HE2	1:A:216:ARG:HG2	1.81	0.62
1:F:132:MET:HE2	1:F:216:ARG:HG2	1.80	0.62
1:C:26:ARG:HD2	1:C:78:LEU:HD21	1.84	0.59
1:C:132:MET:HE2	1:C:216:ARG:HG2	1.85	0.59
1:B:41:GLU:HG2	1:B:50:VAL:HG22	1.84	0.58
1:C:29:THR:HG22	1:C:30:THR:H	1.69	0.56
1:E:21:LYS:O	4:E:401:HOH:O	2.18	0.56
1:B:94:GLU:HG2	1:B:234:TRP:HH2	1.70	0.56
1:E:249:GLN:HA	1:E:252:LYS:HE2	1.88	0.55
1:C:104:LEU:HD21	1:C:203:ILE:HD11	1.89	0.55
1:C:46:ASP:OD1	4:C:401:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:485:HOH:O	1:B:59:HIS:HE1	1.91	0.53
1:B:14:PHE:HD1	1:B:17:PRO:HB3	1.75	0.51
1:E:41:GLU:HG2	1:E:50:VAL:HG22	1.93	0.51
1:D:49:CYS:SG	1:D:265:VAL:HG11	2.51	0.51
1:C:98:PRO:HG3	1:C:230[B]:ASP:HA	1.92	0.50
1:B:46:ASP:OD2	4:B:402:HOH:O	2.19	0.49
1:E:127:LYS:HD2	1:F:60:LEU:HD22	1.95	0.49
1:A:238:GLU:H	1:A:238:GLU:CD	2.21	0.49
1:D:108:MET:HE3	1:D:201:LEU:HD11	1.94	0.49
1:A:3:LYS:HE2	1:A:4:VAL:HG22	1.95	0.48
1:C:180:VAL:HB	1:C:201:LEU:HD13	1.95	0.48
1:D:13:GLY:C	1:D:15:ASP:H	2.21	0.48
1:E:17:PRO:HB3	1:E:51:VAL:HG11	1.96	0.48
1:F:244:ASP:N	1:F:244:ASP:OD1	2.44	0.47
1:D:180:VAL:HB	1:D:201:LEU:HD13	1.96	0.47
1:D:195:ILE:CD1	1:F:108:MET:HG3	2.44	0.47
1:B:52:LEU:HD12	1:B:53:PRO:HD2	1.96	0.47
1:A:169:ILE:O	1:A:172:CYS:HB3	2.13	0.47
1:A:192:GLU:HG2	1:C:108:MET:HG2	1.96	0.47
1:E:230:ASP:HA	1:E:245:MET:HE2	1.98	0.45
1:B:19:LEU:HB3	1:B:262:LEU:HD21	1.98	0.45
1:B:196:HIS:HA	1:B:199:MET:CE	2.46	0.45
1:A:3:LYS:HA	1:A:3:LYS:HD2	1.72	0.44
1:A:28:VAL:HG21	1:A:74:ALA:HB1	1.99	0.44
1:A:290:ASP:O	4:A:401:HOH:O	2.21	0.43
1:E:145:ILE:HG21	1:E:268:ILE:HG13	2.00	0.43
1:E:124:ASP:OD1	1:E:124:ASP:N	2.35	0.43
1:E:132:MET:HE1	1:E:283:LEU:HG	2.00	0.43
1:C:169:ILE:O	1:C:172:CYS:HB3	2.19	0.43
1:C:289:GLN:OE1	1:C:293:HIS:NE2	2.51	0.43
1:C:26:ARG:NH1	1:C:41:GLU:OE2	2.53	0.42
1:D:195:ILE:HD13	1:F:108:MET:HG3	2.02	0.42
1:F:153:LYS:HE2	1:F:259:GLU:HB3	2.02	0.42
1:B:185:PRO:HD2	4:B:591:HOH:O	2.20	0.41
1:A:108:MET:HE3	1:A:201:LEU:HD11	2.02	0.41
1:B:153:LYS:HE3	4:B:509:HOH:O	2.21	0.41
1:E:237:GLU:HA	1:E:240:HIS:CE1	2.56	0.41
1:A:247:LEU:O	1:A:251:ARG:HG3	2.20	0.41
1:E:3:LYS:HD2	1:E:3:LYS:HA	1.85	0.41
1:B:26:ARG:NE	1:B:41:GLU:OE1	2.46	0.41
1:B:164:ASP:OD1	1:B:165:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:180:VAL:HB	1:F:201:LEU:HD13	2.02	0.41
1:A:190:ARG:NH2	1:A:235:LYS:O	2.52	0.40
1:A:10:GLY:HA2	1:A:86:THR:HG22	2.02	0.40
1:B:22:LYS:HG2	1:B:40:VAL:HG11	2.02	0.40
1:C:127:LYS:N	1:C:127:LYS:HD2	2.35	0.40
1:A:186:ARG:HD2	1:C:134:MET:HG3	2.02	0.40
1:E:14:PHE:CE2	1:E:254:VAL:HG23	2.57	0.40
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.89	0.40
1:B:14:PHE:CD1	1:B:17:PRO:HB3	2.55	0.40
1:E:101:PHE:HE1	1:E:253:SER:HB3	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:402:HOH:O	4:F:609:HOH:O[2_645]	2.14	0.06

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	280/320 (88%)	276 (99%)	4 (1%)	0	100	100
1	B	291/320 (91%)	289 (99%)	2 (1%)	0	100	100
1	C	283/320 (88%)	280 (99%)	3 (1%)	0	100	100
1	D	283/320 (88%)	277 (98%)	5 (2%)	1 (0%)	30	15
1	E	291/320 (91%)	288 (99%)	3 (1%)	0	100	100
1	F	267/320 (83%)	267 (100%)	0	0	100	100
All	All	1695/1920 (88%)	1677 (99%)	17 (1%)	1 (0%)	48	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	14	PHE

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	237/274 (86%)	235 (99%)	2 (1%)	73	60
1	B	244/274 (89%)	242 (99%)	2 (1%)	73	60
1	C	242/274 (88%)	238 (98%)	4 (2%)	53	32
1	D	236/274 (86%)	233 (99%)	3 (1%)	61	42
1	E	244/274 (89%)	240 (98%)	4 (2%)	55	34
1	F	226/274 (82%)	223 (99%)	3 (1%)	61	42
All	All	1429/1644 (87%)	1411 (99%)	18 (1%)	63	42

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	257	VAL
1	B	205	ASN
1	B	248	GLU
1	C	29	THR
1	C	108	MET
1	C	230[A]	ASP
1	C	230[B]	ASP
1	D	30	THR
1	D	161	LYS
1	D	205	ASN
1	E	77	ASP
1	E	124	ASP
1	E	201	LEU
1	E	205	ASN
1	F	108	MET
1	F	125	SER
1	F	258	ARG

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

Mol	Chain	Res	Type
1	B	59	HIS
1	C	27	GLN
1	F	256	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	PO4	B	302	-	4,4,4	0.80	0	6,6,6	0.71	0
2	ADE	A	301	-	11,11,11	0.80	0	15,15,15	0.41	0
2	ADE	D	301	-	11,11,11	0.72	0	15,15,15	0.53	0
3	PO4	F	301	-	4,4,4	0.69	0	6,6,6	0.68	0
3	PO4	E	302	-	4,4,4	0.80	0	6,6,6	0.82	0
2	ADE	E	301	-	11,11,11	0.63	0	15,15,15	0.46	0
2	ADE	B	301	-	11,11,11	0.52	0	15,15,15	0.43	0
3	PO4	C	301	-	4,4,4	0.84	0	6,6,6	0.73	0

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
2	ADE	D	301	-	-	-	0/2/2/2
2	ADE	A	301	-	-	-	0/2/2/2
2	ADE	E	301	-	-	-	0/2/2/2
2	ADE	B	301	-	-	-	0/2/2/2

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.

No monomer is involved in short contacts.

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	283/320 (88%)	0.30	17 (6%)	27	31	13, 26, 49, 73	1 (0%)
1	B	291/320 (90%)	0.47	32 (10%)	10	11	15, 26, 60, 95	2 (0%)
1	C	287/320 (89%)	0.07	18 (6%)	26	29	13, 21, 47, 79	1 (0%)
1	D	286/320 (89%)	0.46	24 (8%)	17	19	15, 28, 55, 75	1 (0%)
1	E	291/320 (90%)	0.77	48 (16%)	4	4	18, 30, 66, 100	2 (0%)
1	F	273/320 (85%)	0.49	21 (7%)	19	22	16, 28, 55, 75	0
All	All	1711/1920 (89%)	0.43	160 (9%)	14	15	13, 27, 58, 100	7 (0%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	14	PHE	8.4
1	F	233	CYS	8.3
1	E	250	PHE	7.2
1	D	14	PHE	7.0
1	E	13	GLY	6.9
1	B	250	PHE	6.7
1	F	231	PHE	6.5
1	F	234	TRP	6.1
1	D	19	LEU	5.8
1	A	19	LEU	5.7
1	E	17	PRO	5.7
1	E	291	LEU	5.7
1	A	18	ASN	5.4
1	E	11	GLY	5.4
1	F	243	VAL	5.2
1	C	241	VAL	5.1
1	F	292	LEU	5.0
1	B	19	LEU	5.0
1	B	14	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	17	PRO	4.8
1	A	292	LEU	4.8
1	E	247	LEU	4.7
1	B	1	MET	4.7
1	E	1	MET	4.4
1	E	243	VAL	4.3
1	C	230[A]	ASP	4.3
1	F	232	ASP	4.1
1	B	247	LEU	4.1
1	B	13	GLY	4.1
1	C	89	CYS	4.1
1	B	291	LEU	4.0
1	D	13	GLY	4.0
1	E	18	ASN	3.9
1	C	299	LYS	3.9
1	C	296	SER	3.9
1	D	162	THR	3.8
1	B	16	ASP	3.8
1	B	2	SER	3.8
1	E	246	VAL	3.7
1	F	293	HIS	3.6
1	C	295	GLY	3.6
1	F	49	CYS	3.6
1	C	17	PRO	3.6
1	A	165	LYS	3.6
1	B	15	ASP	3.6
1	F	27	GLN	3.6
1	D	166	SER	3.5
1	C	242	CYS	3.5
1	B	18	ASN	3.5
1	E	236	SER	3.5
1	F	28	VAL	3.5
1	D	15	ASP	3.4
1	E	19	LEU	3.4
1	B	246	VAL	3.4
1	C	297	ASN	3.4
1	E	12	SER	3.4
1	D	3	LYS	3.3
1	D	11	GLY	3.3
1	B	108	MET	3.3
1	B	236	SER	3.3
1	C	298	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	57	LYS	3.2
1	A	166	SER	3.2
1	D	12	SER	3.1
1	C	293	HIS	3.1
1	A	59	HIS	3.1
1	D	49	CYS	3.1
1	F	26	ARG	3.1
1	F	230	ASP	3.0
1	E	252	LYS	3.0
1	F	3	LYS	3.0
1	F	73	TRP	3.0
1	E	15	ASP	3.0
1	F	123	PRO	3.0
1	D	23	VAL	3.0
1	D	167	ALA	3.0
1	F	246	VAL	2.9
1	A	291	LEU	2.9
1	E	248	GLU	2.9
1	A	3	LYS	2.9
1	E	16	ASP	2.8
1	B	237	GLU	2.8
1	B	165	LYS	2.8
1	E	73	TRP	2.7
1	F	194	PHE	2.7
1	B	243	VAL	2.7
1	D	291	LEU	2.7
1	B	166	SER	2.7
1	E	240	HIS	2.7
1	E	251	ARG	2.7
1	A	167	ALA	2.7
1	A	164	ASP	2.7
1	D	236	SER	2.7
1	D	59	HIS	2.6
1	E	2	SER	2.6
1	C	18	ASN	2.6
1	D	57	LYS	2.6
1	E	245	MET	2.6
1	B	248	GLU	2.6
1	E	49	CYS	2.6
1	B	167	ALA	2.6
1	A	10	GLY	2.5
1	E	249	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	161	LYS	2.5
1	E	241	VAL	2.5
1	F	46	ASP	2.5
1	E	162	THR	2.5
1	E	234	TRP	2.5
1	F	29	THR	2.5
1	E	161	LYS	2.5
1	E	242	CYS	2.5
1	B	162	THR	2.5
1	E	237	GLU	2.5
1	D	4	VAL	2.5
1	B	239	GLU	2.5
1	D	244	ASP	2.4
1	E	123	PRO	2.4
1	E	166	SER	2.4
1	B	52	LEU	2.4
1	E	112	TRP	2.4
1	D	257	VAL	2.4
1	B	240	HIS	2.4
1	B	285	MET	2.4
1	D	289	GLN	2.3
1	E	4	VAL	2.3
1	D	250	PHE	2.3
1	E	254	VAL	2.3
1	E	164	ASP	2.3
1	A	57	LYS	2.3
1	A	161	LYS	2.3
1	E	3	LYS	2.3
1	E	122	LYS	2.3
1	B	241	VAL	2.3
1	E	124	ASP	2.2
1	C	294	GLN	2.2
1	B	21	LYS	2.2
1	A	58	GLY	2.2
1	E	20	PHE	2.2
1	C	21	LYS	2.2
1	C	166	SER	2.2
1	B	245	MET	2.2
1	E	285	MET	2.1
1	D	237	GLU	2.1
1	E	10	GLY	2.1
1	B	164	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	231	PHE	2.1
1	F	164	ASP	2.1
1	A	258	ARG	2.1
1	E	28	VAL	2.1
1	F	4	VAL	2.1
1	A	262	LEU	2.1
1	C	194	PHE	2.1
1	B	11	GLY	2.1
1	E	58	GLY	2.1
1	D	20	PHE	2.1
1	E	238	GLU	2.0
1	B	238	GLU	2.0
1	A	20	PHE	2.0
1	C	46	ASP	2.0
1	C	3	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADE	B	301	10/10	0.92	0.09	33,35,38,40	0
2	ADE	E	301	10/10	0.93	0.09	34,36,38,38	0
3	PO4	B	302	5/5	0.96	0.15	27,27,29,30	0
3	PO4	E	302	5/5	0.96	0.11	29,31,32,33	0
2	ADE	D	301	10/10	0.97	0.05	20,22,25,26	0
2	ADE	A	301	10/10	0.97	0.05	17,18,20,21	0
3	PO4	F	301	5/5	0.98	0.05	20,21,22,25	0
3	PO4	C	301	5/5	0.99	0.03	16,16,17,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.