



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:27 PM UTC

PDB ID : 5T3T / pdb_00005t3t
Title : Ebola virus VP30 CTD bound to nucleoprotein
Authors : Kirchdoerfer, R.N.; Moyer, C.L.; Abelson, D.M.; Saphire, E.O.
Deposited on : 2016-08-26
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 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:

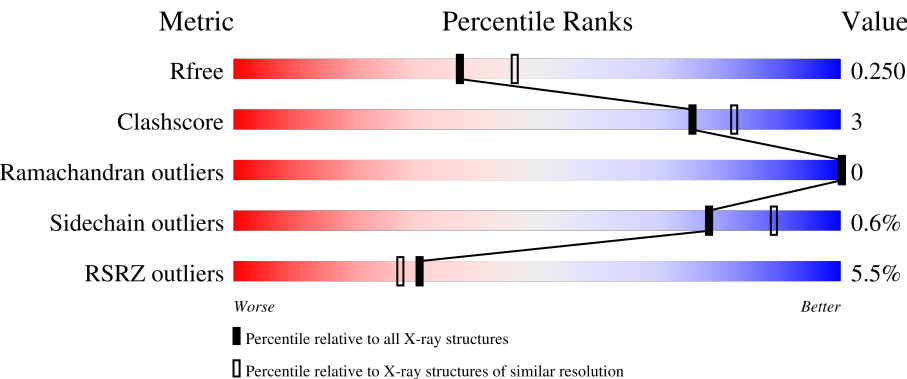
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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.



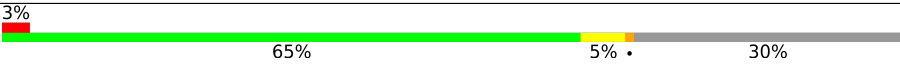
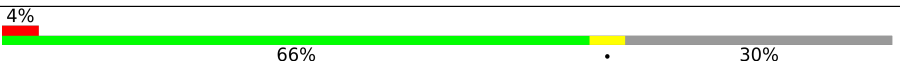
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 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	193	4% 65% 6% . 28%
1	B	193	3% 66% . 30%
1	C	193	2% 66% . 30%
1	D	193	4% 68% . 30%
1	E	193	6% 65% 6% . 29%

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Mol	Chain	Length	Quality of chain
1	F	193	 5% 67% 5% 30%
1	G	193	 3% 65% 5% 30%
1	H	193	 5% 65% 5% 30%
1	I	193	 3% 65% 5% 30%
1	J	193	 4% 66% 5% 30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11795 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 Fusion protein of Nucleoprotein and Minor nucleoprotein VP30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	0	0
			1103	703	196	199	5			
1	B	136	Total	C	N	O	S	0	0	0
			1078	688	191	194	5			
1	C	136	Total	C	N	O	S	0	0	0
			1078	688	191	194	5			
1	D	136	Total	C	N	O	S	0	0	0
			1078	688	191	194	5			
1	E	137	Total	C	N	O	S	0	0	0
			1085	693	192	195	5			
1	F	136	Total	C	N	O	S	0	0	0
			1078	688	191	194	5			
1	G	136	Total	C	N	O	S	0	0	0
			1078	688	191	194	5			
1	H	136	Total	C	N	O	S	0	0	0
			1078	688	191	194	5			
1	I	136	Total	C	N	O	S	0	0	0
			1078	688	191	194	5			
1	J	135	Total	C	N	O	S	0	0	0
			1071	683	190	193	5			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	MET	-	initiating methionine	UNP P18272
A	97	ALA	-	expression tag	UNP P18272
A	98	HIS	-	expression tag	UNP P18272
A	99	HIS	-	expression tag	UNP P18272
A	100	HIS	-	expression tag	UNP P18272
A	101	HIS	-	expression tag	UNP P18272
A	102	HIS	-	expression tag	UNP P18272
A	103	HIS	-	expression tag	UNP P18272
A	104	VAL	-	expression tag	UNP P18272

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Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ASP	-	expression tag	UNP P18272
A	106	ASP	-	expression tag	UNP P18272
A	107	ASP	-	expression tag	UNP P18272
A	108	ASP	-	expression tag	UNP P18272
A	109	LYS	-	expression tag	UNP P18272
A	110	MET	-	expression tag	UNP P18272
B	96	MET	-	initiating methionine	UNP P18272
B	97	ALA	-	expression tag	UNP P18272
B	98	HIS	-	expression tag	UNP P18272
B	99	HIS	-	expression tag	UNP P18272
B	100	HIS	-	expression tag	UNP P18272
B	101	HIS	-	expression tag	UNP P18272
B	102	HIS	-	expression tag	UNP P18272
B	103	HIS	-	expression tag	UNP P18272
B	104	VAL	-	expression tag	UNP P18272
B	105	ASP	-	expression tag	UNP P18272
B	106	ASP	-	expression tag	UNP P18272
B	107	ASP	-	expression tag	UNP P18272
B	108	ASP	-	expression tag	UNP P18272
B	109	LYS	-	expression tag	UNP P18272
B	110	MET	-	expression tag	UNP P18272
C	96	MET	-	initiating methionine	UNP P18272
C	97	ALA	-	expression tag	UNP P18272
C	98	HIS	-	expression tag	UNP P18272
C	99	HIS	-	expression tag	UNP P18272
C	100	HIS	-	expression tag	UNP P18272
C	101	HIS	-	expression tag	UNP P18272
C	102	HIS	-	expression tag	UNP P18272
C	103	HIS	-	expression tag	UNP P18272
C	104	VAL	-	expression tag	UNP P18272
C	105	ASP	-	expression tag	UNP P18272
C	106	ASP	-	expression tag	UNP P18272
C	107	ASP	-	expression tag	UNP P18272
C	108	ASP	-	expression tag	UNP P18272
C	109	LYS	-	expression tag	UNP P18272
C	110	MET	-	expression tag	UNP P18272
D	96	MET	-	initiating methionine	UNP P18272
D	97	ALA	-	expression tag	UNP P18272
D	98	HIS	-	expression tag	UNP P18272
D	99	HIS	-	expression tag	UNP P18272
D	100	HIS	-	expression tag	UNP P18272
D	101	HIS	-	expression tag	UNP P18272

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Chain	Residue	Modelled	Actual	Comment	Reference
D	102	HIS	-	expression tag	UNP P18272
D	103	HIS	-	expression tag	UNP P18272
D	104	VAL	-	expression tag	UNP P18272
D	105	ASP	-	expression tag	UNP P18272
D	106	ASP	-	expression tag	UNP P18272
D	107	ASP	-	expression tag	UNP P18272
D	108	ASP	-	expression tag	UNP P18272
D	109	LYS	-	expression tag	UNP P18272
D	110	MET	-	expression tag	UNP P18272
E	96	MET	-	initiating methionine	UNP P18272
E	97	ALA	-	expression tag	UNP P18272
E	98	HIS	-	expression tag	UNP P18272
E	99	HIS	-	expression tag	UNP P18272
E	100	HIS	-	expression tag	UNP P18272
E	101	HIS	-	expression tag	UNP P18272
E	102	HIS	-	expression tag	UNP P18272
E	103	HIS	-	expression tag	UNP P18272
E	104	VAL	-	expression tag	UNP P18272
E	105	ASP	-	expression tag	UNP P18272
E	106	ASP	-	expression tag	UNP P18272
E	107	ASP	-	expression tag	UNP P18272
E	108	ASP	-	expression tag	UNP P18272
E	109	LYS	-	expression tag	UNP P18272
E	110	MET	-	expression tag	UNP P18272
F	96	MET	-	initiating methionine	UNP P18272
F	97	ALA	-	expression tag	UNP P18272
F	98	HIS	-	expression tag	UNP P18272
F	99	HIS	-	expression tag	UNP P18272
F	100	HIS	-	expression tag	UNP P18272
F	101	HIS	-	expression tag	UNP P18272
F	102	HIS	-	expression tag	UNP P18272
F	103	HIS	-	expression tag	UNP P18272
F	104	VAL	-	expression tag	UNP P18272
F	105	ASP	-	expression tag	UNP P18272
F	106	ASP	-	expression tag	UNP P18272
F	107	ASP	-	expression tag	UNP P18272
F	108	ASP	-	expression tag	UNP P18272
F	109	LYS	-	expression tag	UNP P18272
F	110	MET	-	expression tag	UNP P18272
G	96	MET	-	initiating methionine	UNP P18272
G	97	ALA	-	expression tag	UNP P18272
G	98	HIS	-	expression tag	UNP P18272

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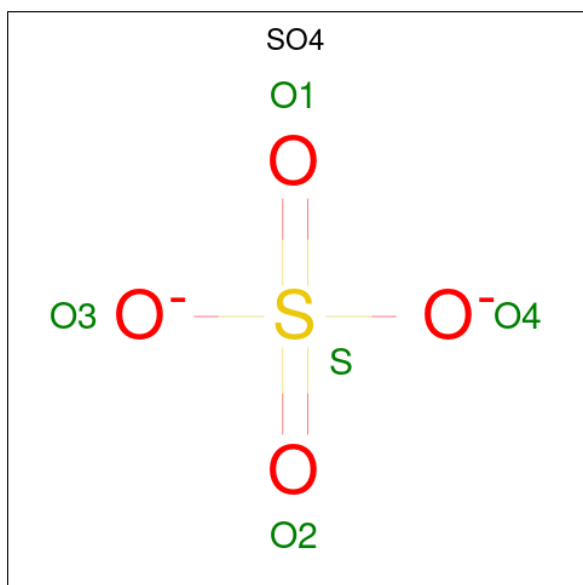
Chain	Residue	Modelled	Actual	Comment	Reference
G	99	HIS	-	expression tag	UNP P18272
G	100	HIS	-	expression tag	UNP P18272
G	101	HIS	-	expression tag	UNP P18272
G	102	HIS	-	expression tag	UNP P18272
G	103	HIS	-	expression tag	UNP P18272
G	104	VAL	-	expression tag	UNP P18272
G	105	ASP	-	expression tag	UNP P18272
G	106	ASP	-	expression tag	UNP P18272
G	107	ASP	-	expression tag	UNP P18272
G	108	ASP	-	expression tag	UNP P18272
G	109	LYS	-	expression tag	UNP P18272
G	110	MET	-	expression tag	UNP P18272
H	96	MET	-	initiating methionine	UNP P18272
H	97	ALA	-	expression tag	UNP P18272
H	98	HIS	-	expression tag	UNP P18272
H	99	HIS	-	expression tag	UNP P18272
H	100	HIS	-	expression tag	UNP P18272
H	101	HIS	-	expression tag	UNP P18272
H	102	HIS	-	expression tag	UNP P18272
H	103	HIS	-	expression tag	UNP P18272
H	104	VAL	-	expression tag	UNP P18272
H	105	ASP	-	expression tag	UNP P18272
H	106	ASP	-	expression tag	UNP P18272
H	107	ASP	-	expression tag	UNP P18272
H	108	ASP	-	expression tag	UNP P18272
H	109	LYS	-	expression tag	UNP P18272
H	110	MET	-	expression tag	UNP P18272
I	96	MET	-	initiating methionine	UNP P18272
I	97	ALA	-	expression tag	UNP P18272
I	98	HIS	-	expression tag	UNP P18272
I	99	HIS	-	expression tag	UNP P18272
I	100	HIS	-	expression tag	UNP P18272
I	101	HIS	-	expression tag	UNP P18272
I	102	HIS	-	expression tag	UNP P18272
I	103	HIS	-	expression tag	UNP P18272
I	104	VAL	-	expression tag	UNP P18272
I	105	ASP	-	expression tag	UNP P18272
I	106	ASP	-	expression tag	UNP P18272
I	107	ASP	-	expression tag	UNP P18272
I	108	ASP	-	expression tag	UNP P18272
I	109	LYS	-	expression tag	UNP P18272
I	110	MET	-	expression tag	UNP P18272

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Chain	Residue	Modelled	Actual	Comment	Reference
J	96	MET	-	initiating methionine	UNP P18272
J	97	ALA	-	expression tag	UNP P18272
J	98	HIS	-	expression tag	UNP P18272
J	99	HIS	-	expression tag	UNP P18272
J	100	HIS	-	expression tag	UNP P18272
J	101	HIS	-	expression tag	UNP P18272
J	102	HIS	-	expression tag	UNP P18272
J	103	HIS	-	expression tag	UNP P18272
J	104	VAL	-	expression tag	UNP P18272
J	105	ASP	-	expression tag	UNP P18272
J	106	ASP	-	expression tag	UNP P18272
J	107	ASP	-	expression tag	UNP P18272
J	108	ASP	-	expression tag	UNP P18272
J	109	LYS	-	expression tag	UNP P18272
J	110	MET	-	expression tag	UNP P18272

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

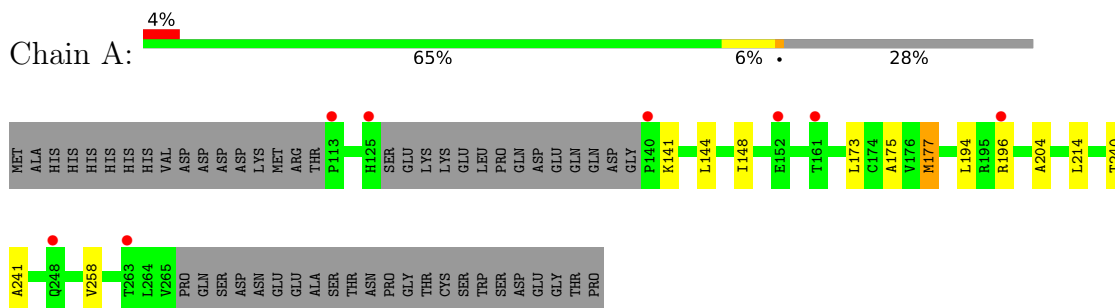
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total	O	0	0
			84	84		
3	B	87	Total	O	0	0
			87	87		
3	C	84	Total	O	0	0
			84	84		
3	D	86	Total	O	0	0
			86	86		
3	E	69	Total	O	0	0
			69	69		
3	F	72	Total	O	0	0
			72	72		
3	G	92	Total	O	0	0
			92	92		
3	H	97	Total	O	0	0
			97	97		
3	I	85	Total	O	0	0
			85	85		
3	J	99	Total	O	0	0
			99	99		

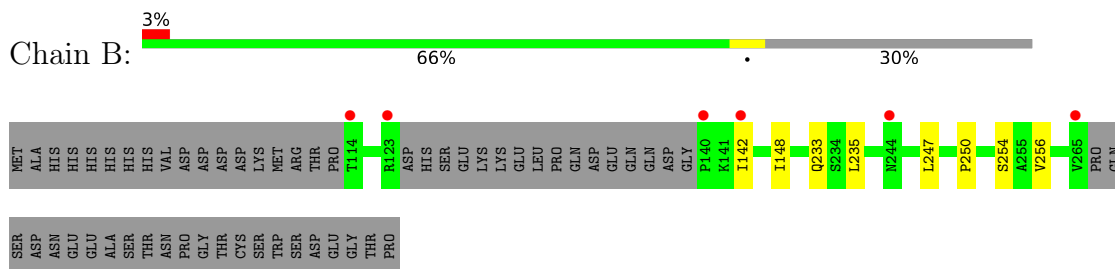
3 Residue-property plots

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

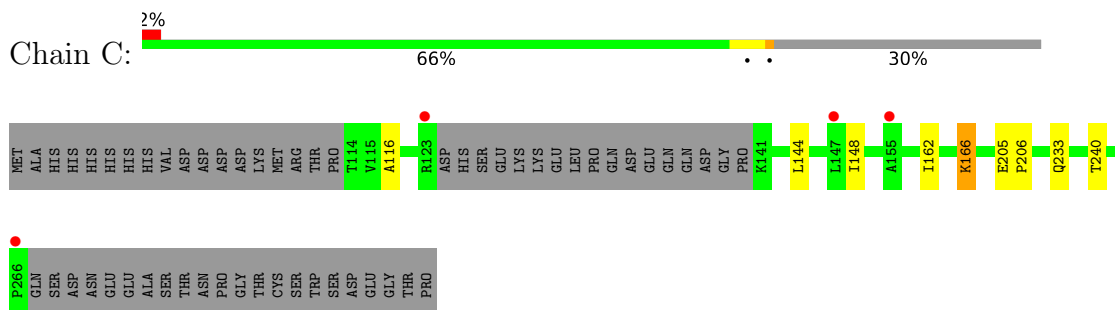
- Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30



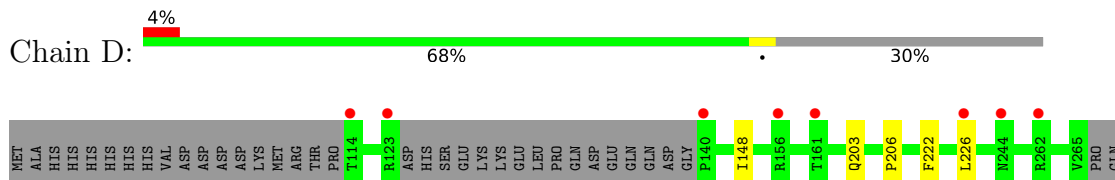
- Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30

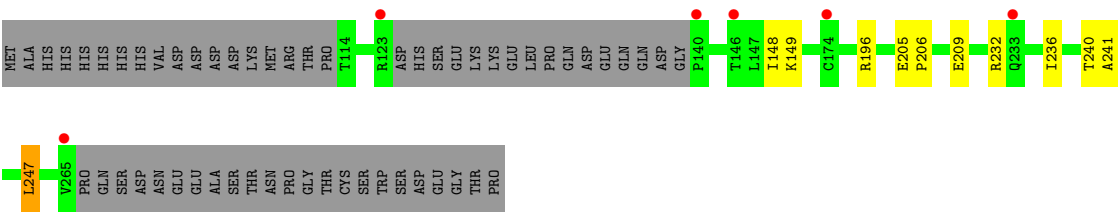


- Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30

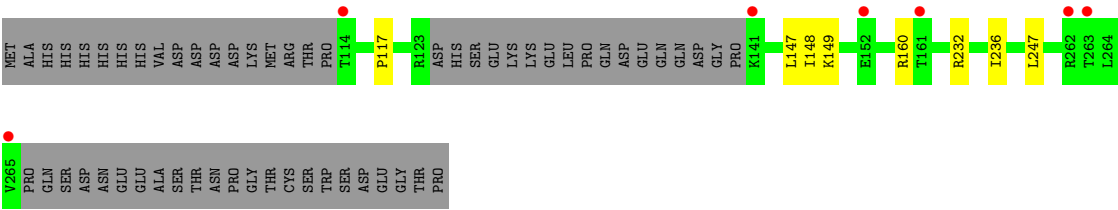


- Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30





● Molecule 1: Fusion protein of Nucleoprotein and Minor nucleoprotein VP30



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.88Å 116.78Å 95.04Å 90.00° 108.52° 90.00°	Depositor
Resolution (Å)	90.12 – 2.20 90.12 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (90.12-2.20) 98.7 (90.12-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.214 , 0.249 0.212 , 0.250	Depositor DCC
R_{free} test set	4477 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11795	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.83	0/1124	1.27	0/1523
1	B	0.83	0/1097	1.28	0/1486
1	C	0.77	0/1097	1.21	0/1487
1	D	0.85	0/1097	1.25	0/1486
1	E	0.81	1/1105 (0.1%)	1.25	0/1498
1	F	0.86	0/1097	1.25	0/1487
1	G	0.87	0/1097	1.30	0/1486
1	H	0.85	0/1097	1.28	0/1487
1	I	0.81	0/1097	1.26	0/1486
1	J	0.87	0/1089	1.25	0/1475
All	All	0.84	1/10997 (0.0%)	1.26	0/14901

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	265	VAL	CA-C	5.04	1.58	1.52

There are no bond angle outliers.

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	1103	0	1136	12	0
1	B	1078	0	1117	9	0
1	C	1078	0	1116	10	0
1	D	1078	0	1117	7	0
1	E	1085	0	1124	9	0
1	F	1078	0	1116	4	0
1	G	1078	0	1117	5	1
1	H	1078	0	1116	8	0
1	I	1078	0	1117	11	0
1	J	1071	0	1109	8	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	15	0	0	0	0
2	F	20	0	0	0	0
2	G	15	0	0	0	0
2	H	15	0	0	0	0
2	I	15	0	0	0	0
2	J	15	0	0	0	0
3	A	84	0	0	0	0
3	B	87	0	0	0	0
3	C	84	0	0	1	0
3	D	86	0	0	0	0
3	E	69	0	0	1	0
3	F	72	0	0	0	0
3	G	92	0	0	0	0
3	H	97	0	0	0	0
3	I	85	0	0	1	0
3	J	99	0	0	2	1
All	All	11795	0	11185	66	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 (66) 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:205:GLU:HB3	1:E:206:PRO:HD3	1.59	0.84
1:C:162:ILE:HD12	1:C:166:LYS:HB3	1.59	0.82
1:C:205:GLU:HB3	1:C:206:PRO:HD3	1.64	0.80
1:I:205:GLU:HB3	1:I:206:PRO:HD3	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:222:PHE:CE2	1:H:226:LEU:HD11	2.20	0.77
1:A:173:LEU:O	1:A:177:MET:HG3	1.88	0.73
1:I:236:ILE:O	1:I:240:THR:HG22	1.94	0.68
1:H:231:ASP:OD1	1:H:234:SER:HB2	1.93	0.68
1:A:194:LEU:HD21	1:A:204:ALA:HB2	1.78	0.66
1:E:196:ARG:HB2	3:E:456:HOH:O	1.95	0.66
1:H:222:PHE:CZ	1:H:226:LEU:HD21	2.32	0.65
1:J:149:LYS:NZ	3:J:401:HOH:O	2.30	0.63
1:I:209:GLU:HB3	1:J:117:PRO:HG3	1.79	0.63
1:D:222:PHE:CE2	1:D:226:LEU:HD11	2.37	0.60
1:G:159:ILE:O	1:G:162:ILE:HG12	2.02	0.59
1:G:254:SER:OG	1:G:256:VAL:HG22	2.02	0.58
1:I:148:ILE:HG23	1:I:247:LEU:HD22	1.87	0.57
1:B:254:SER:OG	1:B:256:VAL:HG22	2.04	0.56
1:J:148:ILE:HG23	1:J:247:LEU:CD2	2.35	0.56
1:H:231:ASP:OD1	1:H:234:SER:CB	2.54	0.55
1:I:148:ILE:HG23	1:I:247:LEU:CD2	2.38	0.54
1:J:232:ARG:HE	1:J:236:ILE:HD11	1.74	0.53
1:A:148:ILE:HD12	1:B:148:ILE:HD12	1.91	0.53
1:C:144:LEU:HB3	1:D:148:ILE:HD11	1.91	0.53
1:E:233:GLN:HG3	1:E:237:MET:HE2	1.91	0.52
1:G:160:ARG:HG2	1:G:236:ILE:HG21	1.92	0.52
1:E:262:ARG:O	1:E:265:VAL:HG22	2.11	0.51
1:A:196:ARG:HE	1:A:241:ALA:HA	1.75	0.51
1:A:173:LEU:O	1:A:177:MET:CG	2.59	0.50
1:I:196:ARG:HE	1:I:241:ALA:HA	1.76	0.50
1:B:142:ILE:HG22	1:B:142:ILE:O	2.12	0.49
1:J:148:ILE:HG23	1:J:247:LEU:HD22	1.94	0.49
1:J:160:ARG:HA	1:J:236:ILE:HD13	1.95	0.49
1:H:151:ALA:HB2	1:H:177:MET:SD	2.53	0.49
1:C:148:ILE:HD12	1:D:148:ILE:HD12	1.95	0.48
1:D:203:GLN:O	1:D:206:PRO:HD2	2.12	0.48
1:H:196:ARG:HE	1:H:241:ALA:HA	1.78	0.48
1:E:148:ILE:HD11	1:F:144:LEU:CB	2.43	0.48
1:A:144:LEU:HB3	1:B:148:ILE:HD11	1.95	0.48
1:E:148:ILE:HD11	1:F:144:LEU:HB2	1.96	0.47
1:A:148:ILE:CD1	1:B:148:ILE:HD12	2.44	0.46
1:F:203:GLN:O	1:F:206:PRO:HD2	2.16	0.46
1:E:205:GLU:HB3	1:E:206:PRO:CD	2.38	0.46
1:I:149:LYS:HE2	3:I:482:HOH:O	2.16	0.45
1:J:149:LYS:HD2	3:J:401:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:HD12	1:B:148:ILE:CD1	2.47	0.45
1:C:148:ILE:HD12	1:D:148:ILE:CD1	2.46	0.45
1:C:116:ALA:HB1	1:D:226:LEU:HD23	1.97	0.45
1:E:159:ILE:O	1:E:162:ILE:HG12	2.17	0.45
1:J:147:LEU:HD23	1:J:147:LEU:HA	1.86	0.45
1:C:148:ILE:CD1	1:D:148:ILE:HD12	2.48	0.43
1:A:175:ALA:HB2	1:A:214:LEU:HD22	1.99	0.43
1:C:240:THR:HG22	3:C:431:HOH:O	2.18	0.43
1:A:141:LYS:HB3	1:B:250:PRO:HG3	2.00	0.43
1:I:205:GLU:N	1:I:206:PRO:CD	2.82	0.43
1:H:160:ARG:HD2	1:I:232:ARG:HD3	2.01	0.42
1:C:205:GLU:N	1:C:206:PRO:CD	2.83	0.42
1:A:196:ARG:HH21	1:A:240:THR:HG22	1.85	0.41
1:E:151:ALA:HB2	1:E:177:MET:SD	2.60	0.41
1:G:144:LEU:HB3	1:H:148:ILE:HD11	2.03	0.41
1:B:233:GLN:HG3	1:C:233:GLN:HG3	2.01	0.41
1:A:258:VAL:HG22	1:B:142:ILE:HD12	2.01	0.41
1:I:205:GLU:HB3	1:I:206:PRO:CD	2.43	0.41
1:F:151:ALA:HB2	1:F:177:MET:SD	2.61	0.41
1:G:173:LEU:O	1:G:177:MET:HG3	2.22	0.40
1:I:205:GLU:CB	1:I:206:PRO:HD3	2.42	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)
1:G:161:THR:CG2	3:J:424:HOH:O[1_565]	1.93	0.27

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	135/193 (70%)	133 (98%)	2 (2%)	0	100	100
1	B	132/193 (68%)	130 (98%)	2 (2%)	0	100	100
1	C	132/193 (68%)	130 (98%)	2 (2%)	0	100	100
1	D	132/193 (68%)	130 (98%)	2 (2%)	0	100	100
1	E	133/193 (69%)	131 (98%)	2 (2%)	0	100	100
1	F	132/193 (68%)	130 (98%)	2 (2%)	0	100	100
1	G	132/193 (68%)	129 (98%)	3 (2%)	0	100	100
1	H	132/193 (68%)	130 (98%)	2 (2%)	0	100	100
1	I	132/193 (68%)	130 (98%)	2 (2%)	0	100	100
1	J	131/193 (68%)	128 (98%)	3 (2%)	0	100	100
All	All	1323/1930 (68%)	1301 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	122/171 (71%)	121 (99%)	1 (1%)	73	85
1	B	119/171 (70%)	117 (98%)	2 (2%)	53	69
1	C	119/171 (70%)	118 (99%)	1 (1%)	73	85
1	D	119/171 (70%)	119 (100%)	0	100	100
1	E	120/171 (70%)	120 (100%)	0	100	100
1	F	119/171 (70%)	117 (98%)	2 (2%)	53	69
1	G	119/171 (70%)	119 (100%)	0	100	100
1	H	119/171 (70%)	119 (100%)	0	100	100
1	I	119/171 (70%)	118 (99%)	1 (1%)	73	85
1	J	118/171 (69%)	118 (100%)	0	100	100
All	All	1193/1710 (70%)	1186 (99%)	7 (1%)	78	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	MET
1	B	235	LEU
1	B	247	LEU
1	C	166	LYS
1	F	163	GLU
1	F	248	GLN
1	I	247	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	C	201	GLN
1	E	201	GLN
1	E	244	ASN
1	H	201	GLN
1	I	244	ASN
1	J	244	ASN

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](#)

27 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	$\# Z > 2$
2	SO4	I	303	-	4,4,4	0.27	0	6,6,6	0.13	0
2	SO4	D	302	-	4,4,4	0.39	0	6,6,6	0.08	0
2	SO4	I	302	-	4,4,4	0.29	0	6,6,6	0.17	0
2	SO4	G	302	-	4,4,4	0.37	0	6,6,6	0.17	0
2	SO4	H	303	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	F	303	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	C	302	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	I	301	-	4,4,4	0.29	0	6,6,6	0.22	0
2	SO4	J	302	-	4,4,4	0.41	0	6,6,6	0.12	0
2	SO4	A	301	-	4,4,4	0.21	0	6,6,6	0.23	0
2	SO4	E	303	-	4,4,4	0.24	0	6,6,6	0.18	0
2	SO4	J	303	-	4,4,4	0.30	0	6,6,6	0.17	0
2	SO4	F	301	-	4,4,4	0.27	0	6,6,6	0.21	0
2	SO4	G	301	-	4,4,4	0.21	0	6,6,6	0.19	0
2	SO4	F	304	-	4,4,4	0.25	0	6,6,6	0.19	0
2	SO4	C	301	-	4,4,4	0.36	0	6,6,6	0.36	0
2	SO4	B	302	-	4,4,4	0.38	0	6,6,6	0.43	0
2	SO4	E	302	-	4,4,4	0.40	0	6,6,6	0.18	0
2	SO4	A	302	-	4,4,4	0.38	0	6,6,6	0.12	0
2	SO4	H	302	-	4,4,4	0.32	0	6,6,6	0.14	0
2	SO4	F	302	-	4,4,4	0.36	0	6,6,6	0.10	0
2	SO4	G	303	-	4,4,4	0.30	0	6,6,6	0.18	0
2	SO4	B	301	-	4,4,4	0.41	0	6,6,6	0.13	0
2	SO4	H	301	-	4,4,4	0.36	0	6,6,6	0.32	0
2	SO4	J	301	-	4,4,4	0.25	0	6,6,6	0.36	0
2	SO4	D	301	-	4,4,4	0.17	0	6,6,6	0.21	0
2	SO4	E	301	-	4,4,4	0.27	0	6,6,6	0.31	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.

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(Å²)	Q<0.9
1	A	139/193 (72%)	0.52	8 (5%)	29	25	30, 40, 60, 77	0
1	B	136/193 (70%)	0.45	6 (4%)	39	36	31, 41, 58, 67	0
1	C	136/193 (70%)	0.48	4 (2%)	53	50	29, 40, 56, 75	0
1	D	136/193 (70%)	0.48	8 (5%)	28	25	30, 40, 56, 80	0
1	E	137/193 (70%)	0.65	11 (8%)	18	16	31, 44, 63, 78	0
1	F	136/193 (70%)	0.65	9 (6%)	24	21	33, 44, 65, 81	0
1	G	136/193 (70%)	0.43	6 (4%)	39	36	31, 40, 57, 77	0
1	H	136/193 (70%)	0.47	10 (7%)	20	18	28, 41, 60, 70	0
1	I	136/193 (70%)	0.58	6 (4%)	39	36	32, 41, 57, 69	0
1	J	135/193 (69%)	0.43	7 (5%)	33	29	31, 41, 54, 87	0
All	All	1363/1930 (70%)	0.51	75 (5%)	30	27	28, 41, 59, 87	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	PRO	5.6
1	I	140	PRO	5.1
1	G	113	PRO	4.9
1	E	140	PRO	4.0
1	B	140	PRO	3.8
1	C	123	ARG	3.5
1	C	266	PRO	3.5
1	H	226	LEU	3.3
1	G	162	ILE	3.2
1	I	265	VAL	3.0
1	G	161	THR	3.0
1	J	161	THR	3.0
1	H	233	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	266	PRO	2.9
1	I	233	GLN	2.9
1	A	125	HIS	2.9
1	G	152	GLU	2.8
1	D	123	ARG	2.8
1	H	114	THR	2.7
1	E	266	PRO	2.7
1	A	248	GLN	2.7
1	D	114	THR	2.7
1	A	140	PRO	2.7
1	F	123	ARG	2.7
1	I	123	ARG	2.6
1	J	152	GLU	2.6
1	A	263	THR	2.5
1	D	161	THR	2.5
1	E	248	GLN	2.5
1	J	262	ARG	2.4
1	A	161	THR	2.4
1	J	141	LYS	2.4
1	D	156	ARG	2.4
1	G	123	ARG	2.4
1	F	202	ASP	2.4
1	G	202	ASP	2.3
1	H	266	PRO	2.3
1	I	146	THR	2.3
1	E	177	MET	2.3
1	B	244	ASN	2.3
1	F	263	THR	2.3
1	H	156	ARG	2.3
1	F	156	ARG	2.3
1	B	114	THR	2.2
1	D	262	ARG	2.2
1	E	114	THR	2.2
1	J	114	THR	2.2
1	C	147	LEU	2.2
1	A	152	GLU	2.2
1	B	142	ILE	2.2
1	H	247	LEU	2.2
1	D	244	ASN	2.2
1	J	265	VAL	2.2
1	H	115	VAL	2.1
1	E	152	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	174	CYS	2.1
1	B	123	ARG	2.1
1	H	245	ILE	2.1
1	F	163	GLU	2.1
1	E	262	ARG	2.1
1	E	263	THR	2.1
1	F	161	THR	2.1
1	C	155	ALA	2.1
1	D	226	LEU	2.1
1	F	158	ASP	2.1
1	E	123	ARG	2.1
1	J	263	THR	2.1
1	B	265	VAL	2.1
1	E	121	VAL	2.1
1	H	262	ARG	2.1
1	D	140	PRO	2.0
1	A	196	ARG	2.0
1	E	156	ARG	2.0
1	H	195	ARG	2.0
1	F	146	THR	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(Å ²)	Q<0.9
2	SO4	F	303	5/5	0.67	0.15	65,65,74,79	0
2	SO4	H	303	5/5	0.68	0.16	60,62,74,78	0
2	SO4	G	303	5/5	0.73	0.11	70,76,80,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	F	304	5/5	0.74	0.14	58,63,75,85	0
2	SO4	E	303	5/5	0.75	0.13	66,67,79,81	0
2	SO4	J	303	5/5	0.76	0.13	58,61,71,79	0
2	SO4	I	303	5/5	0.85	0.11	62,64,79,81	0
2	SO4	G	302	5/5	0.85	0.17	53,58,65,69	0
2	SO4	F	302	5/5	0.88	0.22	54,58,64,68	0
2	SO4	A	302	5/5	0.88	0.18	52,55,62,67	0
2	SO4	E	302	5/5	0.89	0.24	55,58,65,68	0
2	SO4	D	302	5/5	0.91	0.17	51,53,60,67	0
2	SO4	B	301	5/5	0.91	0.17	55,58,65,67	0
2	SO4	H	302	5/5	0.91	0.16	53,55,60,61	0
2	SO4	J	302	5/5	0.93	0.16	47,54,62,63	0
2	SO4	I	302	5/5	0.93	0.16	54,58,65,66	0
2	SO4	C	302	5/5	0.95	0.16	48,56,60,61	0
2	SO4	E	301	5/5	0.95	0.07	44,46,52,52	0
2	SO4	D	301	5/5	0.95	0.09	41,43,48,49	0
2	SO4	I	301	5/5	0.96	0.09	42,46,51,53	0
2	SO4	F	301	5/5	0.96	0.08	44,49,52,52	0
2	SO4	A	301	5/5	0.96	0.10	45,49,53,55	0
2	SO4	J	301	5/5	0.96	0.11	44,48,49,51	0
2	SO4	B	302	5/5	0.96	0.08	42,46,49,52	0
2	SO4	C	301	5/5	0.96	0.08	44,46,54,55	0
2	SO4	G	301	5/5	0.97	0.06	43,45,47,53	0
2	SO4	H	301	5/5	0.97	0.07	44,44,48,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.