

# Full wwPDB X-ray Structure Validation Report (i)

### Feb 12, 2024 – 01:25 AM EST

PDB ID	:	3CW1
Title	:	Crystal Structure of Human Spliceosomal U1 snRNP
Authors	:	Pomeranz Krummel, D.A.; Oubridge, C.; Leung, A.K.; Li, J.; Nagai, K.
Deposited on	:	2008-04-21
Resolution	:	5.49  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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 5.49 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	e Percentile Ranks	Value
Clashscore		0
RNA backbone		0.00
	Worse	Better
	Percentile relative to all X-ray structures	
	Percentile relative to X-ray structures of similar resolution	
	Whole prohive	Similar resolution

Motrio	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
Clashscore	141614	$1010 \ (7.10-3.90)$
RNA backbone	3102	1074 (7.80-3.00)

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 <=5%

Mol	Chain	Length	Quality of ch	ain
1	V	138	100%	
1	V	138	99%	
1	W	138	100%	
1	х	138	100%	
2	D	126	60%	40%
2	S	126	60%	40%
2	Т	126	60%	40%
2	U	126	60%	40%
3	А	174	37%	63%
3	Н	174	37%	63%



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Mol	Chain	Length	Quality of chain			
3	Ι	174	36%	64%		
3	J	174	36%	64%		
4	В	119	65%	35%		
4	М	119	65%	35%		
4	Ν	119	64%	36%		
4	Ο	119	65%	35%		
5	С	118	75%	25%		
5	Р	118	73%	27%		
5	Q	118	75%	25%		
5	R	118	72%	28%		
6	1	86	87%	13%		
6	2	86	88%	12%		
6	F	86	88%	12%		
6	Z	86	81%	19%		
7	Е	92	82%	18%		
7	W	92	82%	18%		
7	Х	92	82%	18%		
7	Y	92	82%	18%		
8	3	76	96%	•		
8	4	76	96%	•		
8	5	76	96%	·		
8	G	76	96%	•		
9	6	216	56%	44%		
9	7	216	56%	44%		
9	8	216	56%	44%		



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Mol	Chain	Length	Quality of chain		
9	K	216	55%	44%	
10	0	77	70%	30%	
10	9	77	75%	25%	
10	L	77	74%	26%	
10	1	77	75%	25%	



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## 2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 3365 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.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	V	138	Total P 138 138	0	0	138
1	V	138	Total P 138 138	0	0	138
1	W	138	Total P 138 138	0	0	138
1	х	138	Total P 138 138	0	0	138

• Molecule 1 is a RNA chain called U1 snRNA.

• Molecule 2 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	D	76	Total C 76 76	0	0	76
2	S	76	Total         C           76         76	0	0	76
2	Т	76	Total         C           76         76	0	0	76
2	U	76	Total         C           76         76	0	0	76

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	66	CYS	SER	conflict	UNP P62318
S	266	CYS	SER	conflict	UNP P62318
Т	466	CYS	SER	conflict	UNP P62318
U	666	CYS	SER	conflict	UNP P62318

• Molecule 3 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	А	64	$\begin{array}{cc} \text{Total} & \text{C} \\ 64 & 64 \end{array}$	0	0	64
3	Н	64	Total         C           64         64	0	0	64
3	Ι	63	Total         C           63         63	0	0	63
3	J	63	Total C 63 63	0	0	63

• Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	В	77	Total C 77 77	0	0	77
4	М	77	$\begin{array}{cc} \text{Total} & \text{C} \\ 77 & 77 \end{array}$	0	0	77
4	Ν	76	Total C 76 76	0	0	76
4	О	77	Total C 77 77	0	0	77

• Molecule 5 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	С	88	Total         C           88         88	0	0	88
5	Р	86	Total         C           86         86	0	0	86
5	Q	89	Total C 89 89	0	0	89
5	R	85	Total C 85 85	0	0	85

• Molecule 6 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	76	Total C 76 76	0	0	76
6	Z	70	Total         C           70         70	0	0	70
6	1	75	Total         C           75         75	0	0	75



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	2	76	Total C 76 76	0	0	76

• Molecule 7 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	Е	75	Total         C           75         75	0	0	75
7	W	75	Total         C           75         75	0	0	75
7	Х	75	Total         C           75         75	0	0	75
7	Y	75	Total C 75 75	0	0	75

• Molecule 8 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	G	73	Total         C           73         73	0	0	73
8	3	73	Total         C           73         73	0	0	73
8	4	73	Total         C           73         73	0	0	73
8	5	73	Total         C           73         73	0	0	73

• Molecule 9 is a protein called U1 small nuclear ribonucleoprotein 70 kDa.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	K	120	Total C 120 120	0	0	120
9	6	120	Total         C           120         120	0	0	120
9	7	120	Total         C           120         120	0	0	120
9	8	120	Total         C           120         120	0	0	120

• Molecule 10 is a protein called U1 small nuclear ribonucleoprotein C.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	L	57	$\begin{array}{cc} {\rm Total} & {\rm C} \\ 57 & 57 \end{array}$	0	0	57
10	9	58	Total         C           58         58	0	0	58
10	0	54	$\begin{array}{cc} \text{Total} & \text{C} \\ 54 & 54 \end{array}$	0	0	54
10	1	58	$\begin{array}{cc} \text{Total} & \text{C} \\ 58 & 58 \end{array}$	0	0	58

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	39	CYS	GLN	conflict	UNP P09234
9	239	CYS	GLN	conflict	UNP P09234
0	439	CYS	GLN	conflict	UNP P09234
l	639	CYS	GLN	conflict	UNP P09234

• Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total Zn 1 1	0	0
11	9	1	Total Zn 1 1	0	0
11	0	1	Total Zn 1 1	0	0
11	1	1	Total Zn 1 1	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. 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. 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.

 $\bullet$  Molecule 1: U1 snRNA

Chain V:	100%
There are no	outlier residues recorded for this chain.
• Molecule 1:	U1 snRNA
Chain v:	99%
A201 A214 G364	
• Molecule 1:	U1 snRNA
Chain w:	100%
There are no	outlier residues recorded for this chain.
• Molecule 1:	U1 snRNA
Chain x:	100%
There are no	outlier residues recorded for this chain.
• Molecule 2:	Small nuclear ribonucleoprotein Sm D3
Chain D:	60% 40%
MET SER ILE GLY VAL VAL P6 P6 MET MET LEU	SER NET LYS ANN CYS ANN CLYS CLY CLY CLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A
• Molecule 2:	Small nuclear ribonucleoprotein Sm D3
Chain S:	60% 40%
MET SER ILE GLY VAL P206 P206 MET MET LEU	ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA
• Molecule 2:	Small nuclear ribonucleoprotein Sm D3



Chain T:	60%	40%
MET SER SER ILE GLY VAL P406 P406 MET MET LEU	LYS NET MET LYS LYS LYS ASN ASN ASN ASN ASN ALA ALA ALA ALA ALA ALA ALA ALA ALA	VAL VAL ALA ALA ARG GLY ARG GLY ARG GLY ARG GLY TILE PHE PHE CISN ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG
• Molecule 2:	Small nuclear ribonucleoprotein	n Sm D3
Chain U:	60%	40%
MET SER ILE GLY VAL P606 P606 MET MET	LYS SER NET NET NET NET ASN ASN ASN CLN CLN CLN CLN CLN ALA ALA ALA ALA ALA ALA ALA CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	VAL ALA ALA ALA ALA ALA ALA ALA ALA ALA
• Molecule 3:	Small nuclear ribonucleoprotein	n-associated proteins B and B'
Chain A:	37%	63%
MET THR VAL GLY CVS SER SER SFR SFR SFR SFR SFR	ARG LYS LYS LYS PRO PRO ARO ALA ALA ALA ALA GLU GLU GLU GLV CYS ASP CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	TLE ARG ARG ARG ARG PRO ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
PRO MET PRO GLN ALA ALA GLY LEU ALA	GLY VAL VAL ARG GLY VAL GLY FRO GLN VAL MET THR FRO GLN GLN GLN ARG GLY ALA	ALA ALA ALA ALA ALA ALA ALA ALA ALA CLA C
• Molecule 3:	Small nuclear ribonucleoprotei	n-associated proteins B and B'
Chain H:	37%	63%
MET THR VAL GLY LYS SER SER SER SER SER SPHE	ARG LLYS LLYS LLYS PPAO LLYS ASN ASN ASN ALA ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	TILE ALA ARG VAL ARG CALY ALA ARA ALA ALA ALA ALA ALA ALA ALA ALA
PRO MET PRO GLN ALA PRO ALA GLY LEU	GLY VAL ARG ARG ARG ARG CLY CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	ALA ALA ALA ALA ALA ALA ALA ALA ALA CLY PRO FRO FRO FRO FRO GLY GLY GLY GLY
• Molecule 3:	Small nuclear ribonucleoprotei	n-associated proteins B and B'
Chain I:	36%	64%
MET THR VAL GLY LYS SER SER SER SER SER SER SER	PHE ARG LYS LYS LYS PRO FYS ARG CLN GLN GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU	GLY TLE ARG ARG PRO PRO PRO GLY GLY GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A
VAL PRO MET PRO GLN ALA PRO GLY LEU	ALA ALA PRO VAL VAL VAL VAL CLY FRO FRO FRO FRO FRO FRO FRO FRO FRO FRO	ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA
• Molecule 3:	Small nuclear ribonucleoprotein	n-associated proteins B and B'
Chain J:	36%	64%
MET THR VAL GLY LYS SER SER SER E647 PHE	ARG LYS LYS LYS LYS PRO PRO LYS ALA ALA ALA ALA ALU GLU GLU GLU GLU GLU CLU CLU CLU ARF ARF ARF ARF ARF ARF ARF ARF ARF ARF	GLY ILE ARG PRO PRO PRO PRO ALA ALA ALA ALA GLY GLY GLY GLY GLY ARG GLY ALA GLY ALA GLY ALA GLY ALA GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A
VAL PRO MET PRO GLN GLN ALA ALA GLY LEU	ALA ALA PRO PRO ARG CLY VAL CLN CLN CLN CLN CLN CLN CLN CLN CLN CL	ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA



• Molecule 4:	Small nuclear ribonucleoprotein Sm D1	
Chain B:	65%	35%
MET K2 K2 LEU LEU VAL ASP VAL GLU	PR0 LYS VML LYS SER LYS LYS LYS ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG	
• Molecule 4:	Small nuclear ribonucleoprotein Sm D1	
Chain M:	65%	35%
MET K202 T278 LEU LEU VAL ASP VAL GLU	PR0 LYS VAL LYS FER LYS CYS ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG	
• Molecule 4:	Small nuclear ribonucleoprotein Sm D1	
Chain N:	64%	36%
MET K402 D477 THR LEU LEU VAL ASP VAL	CLU LYS LYS SER LYS SER LYS LYS CLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	ARG
• Molecule 4:	Small nuclear ribonucleoprotein Sm D1	
Chain O:	65%	35%
MET K602 T678 LEU LEU VAL ASP VAL CLU GLU	PRO LVS LVS LVS LVS LVS LVS LVS ARC ARC ARC ARC ARC ARC ARC ARC ARC ARC	
• Molecule 5:	Small nuclear ribonucleoprotein Sm D2	
Chain C:	75%	25%
MET SER SER LEU LEU LEU ASN PXS PXS SER SER	M11 T75 CLU CLU CLU CLU CLY CLYS CLYS CLYS CLYS CLYS CLYS CLYS	
• Molecule 5:	Small nuclear ribonucleoprotein Sm D2	
Chain P:	73%	27%
MET SER LEU LEU LEU ASN LYS PRO LYS SER SER	M211 T275 GLU GLU GLU CLY CLYS CLYS CLYS CLYS CLYS CLYS CLYS	
• Molecule 5:	Small nuclear ribonucleoprotein Sm D2	
Chain Q:	75%	25%
MET SER LEU LEU LEU ASN ASN PRO LYS SER GLU	M411 E476 VAL PRO PRO FRO FRO LYS C492 LYS C492 LYS PRO LYS C492 LYS A1A A1A C514 LS14 LYS C114 LS14 LYS C114 C514 C514 C514 C514 C514 C514 C514	
• Molecule 5:	Small nuclear ribonucleoprotein Sm D2	

R L D W I D E PDB TEIN DATA BANK

Chain R:	72%	28%
MET SER LEU LEU LEU ASN LYS PRO LYS SER GLU GLU	MG73 THR THR 7HR 7HR 7HR 7HL 7H 7H 7H 7H 7H 7H 7H 7H 7H 7H 7H 7H 7H	
• Molecule 6: S	Small nuclear ribonucleoprotein F	
Chain F:	88%	12%
MET SER LEU PRO LEU NG NG GLY GLY MET	ARG GLU	
• Molecule 6: S	Small nuclear ribonucleoprotein F	
Chain Z:	81%	19%
MET SER LEU PRO LLEU N206 N206 GLU GLU GLU	GLU ASP CLY CLY MRC GLU GLU GLU	
• Molecule 6: S	Small nuclear ribonucleoprotein F	
Chain 1:	87%	13%
MET SER LEU PRO LEU ASN ASN ASN ASN CLU GLU	MET ARG GLU	
• Molecule 6: S	Small nuclear ribonucleoprotein F	
Chain 2:	88%	12%
MET SER LEU PRO NGOG NGOG GLY GLY MET	GLU	
• Molecule 7: S	Small nuclear ribonucleoprotein E	
Chain E:	82%	18%
MET ALA TYR ARG GLY GLN GLN CLN CLN GLN GLN	LYS MALT VAL GLN PRO N92 N92	
• Molecule 7: S	Small nuclear ribonucleoprotein E	
Chain W:	82%	18%
MET ALA TYR ARG GLY GLN GLN CLY GLN GLN GLN	LYS VAL MET VAL CLN PLO I218 N292 N292	
• Molecule 7: S	Small nuclear ribonucleoprotein E	



Chain X:	82%	18%
MET ALA TYR TYR GLY GLN GLN GLN CLN CYS VAL	LYS VAL VAL VAL GLN 1418 1418 N492	
• Molecule 7:	Small nuclear ribonucleoprotein E	
Chain Y:	82%	18%
MET ALA TYR ARG GLY GLN GLN CLN CLN VAL	CLN NG2 B10 B10 CAL CAL CAL CAL	
• Molecule 8:	Small nuclear ribonucleoprotein G	
Chain G:	96%	·
MET SER LYS A4 V76		
• Molecule 8:	Small nuclear ribonucleoprotein G	
Chain 3:	96%	·
MET SER LYS A204 V276		
• Molecule 8:	Small nuclear ribonucleoprotein G	
Chain 4:	96%	·
MET SER LYS A404 V476		
• Molecule 8:	Small nuclear ribonucleoprotein G	
Chain 5:	96%	·
MET SER LYS A604 V676		
• Molecule 9:	U1 small nuclear ribonucle oprotein 70 kDa	
Chain K:	55% 44%	
MET THR GLN GLN LEU PRO ASN ASN ASN	P23 P23 CUU CUU CUU CUU CUU CUU CUU CUU CUU CU	THR R63 ASP ASP ASP ASN ASN PRO ASN ASN
ALA ALA GLN GLY ASP ALA PHE FHE FHE H153	AND THE THE ANG ANG ANG ANG ANG ANG ANG ANG	
	PROTEIN DATA BANK	

• Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa Chain 6: 56% 44% AET ALN CHE CEU LEU LYS LEU PRO NSN VSN ALA GLN GLY ASP ASP ALA ALA PHE • Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa Chain 7: 56% 44% MET THR GLN GLN PHE PHE PRO PRO HIS ASN ASP PRO ALA GLN GLY ASP ALA ALA ALA • Molecule 9: U1 small nuclear ribonucleoprotein 70 kDa Chain 8: 56% 44% MET THR 3LN 3LN 7LEU PHE PRO PRO The second secon ALA GLN GLY ASP ALA ARG THR VAL LYS CLYS • Molecule 10: U1 small nuclear ribonucleoprotein C Chain L: 74% 26% MET PRO LYS • Molecule 10: U1 small nuclear ribonucleoprotein C Chain 9: 75% 25% ALAALAALA ER LA • Molecule 10: U1 small nuclear ribonucleoprotein C Chain 0: 70% 30%



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• Molecule 10: U1 small nuclear ribonucleoprotein C





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	126.47Å 127.08Å 152.02Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$95.42^{\circ}$ $105.92^{\circ}$ $101.80^{\circ}$	Depositor
Bosolution(Å)	123.09 - 5.49	Depositor
Itesolution (A)	122.79 - 5.49	EDS
% Data completeness	(Not available) $(123.09-5.49)$	Depositor
(in resolution range)	99.0(122.79-5.49)	EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.99 (at 5.42 \text{\AA})$	Xtriage
Refinement program		Depositor
B B.	(Not available) , (Not available)	Depositor
It, Itfree	0.469 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	251.7	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.59 , -6.2	EDS
L-test for $twinning^2$	$<  L  > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.72	EDS
Total number of atoms	3365	wwPDB-VP
Average B, all atoms $(Å^2)$	231.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: ZN

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	V	138	0	0	0	0
1	V	138	0	0	0	1
1	W	138	0	0	0	0
1	Х	138	0	0	0	0
2	D	76	0	0	0	0
2	S	76	0	0	0	0
2	Т	76	0	0	0	0
2	U	76	0	0	0	0
3	А	64	0	0	0	0
3	Н	64	0	0	0	0
3	Ι	63	0	0	0	0
3	J	63	0	0	0	0
4	В	77	0	0	0	0
4	М	77	0	0	0	0
4	N	76	0	0	0	0
4	Ō	77	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	С	88	0	0	0	0
5	Р	86	0	0	0	0
5	Q	89	0	0	0	0
5	R	85	0	0	0	0
6	1	75	0	0	0	0
6	2	76	0	0	0	0
6	F	76	0	0	0	0
6	Ζ	70	0	0	0	0
7	Е	75	0	0	0	0
7	W	75	0	0	0	0
7	Х	75	0	0	0	0
7	Y	75	0	0	0	0
8	3	73	0	0	0	0
8	4	73	0	0	0	0
8	5	73	0	0	0	0
8	G	73	0	0	0	0
9	6	120	0	0	0	0
9	7	120	0	0	0	0
9	8	120	0	0	0	0
9	K	120	0	0	0	1
10	0	54	0	0	0	0
10	9	58	0	0	0	0
10	L	57	0	0	0	0
10	1	58	0	0	0	0
11	0	1	0	0	0	0
11	9	1	0	0	0	0
11	L	1	0	0	0	0
11	1	1	0	0	0	0
All	All	3365	0	0	0	1

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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 0.

There are no clashes within the asymmetric unit.

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:v:214:A:P	9:K:153:HIS:CA[1_545]	2.05	0.15



### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

#### 5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	V	0/138	-	-
1	V	0/138	-	-
1	W	0/138	-	-
1	Х	0/138	-	-
All	All	0/552	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 (i)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

