



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:34 PM GMT

PDB ID : 4U01
Title : HCV NS3/4A serine protease in complex with 6570
Authors : Parsy, C.C.; Alexandre, F.-R.; Brandt, G.; Caillet, C.; Chaves, D.; Derock, M.; Gloux, D.; Griffon, Y.; Lallo, L.B.; Leroy, F.; Liuzzi, M.; Loi, A.-G.; Mayes, B.; Moulat, L.; Moussa, A.; Chiara, M.; Roques, V.; Rosinovsky, E.; Seifer, M.; Stewart, A.; Wang, J.; Standring, D.; Surleraux, D.
Deposited on : 2014-07-11
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

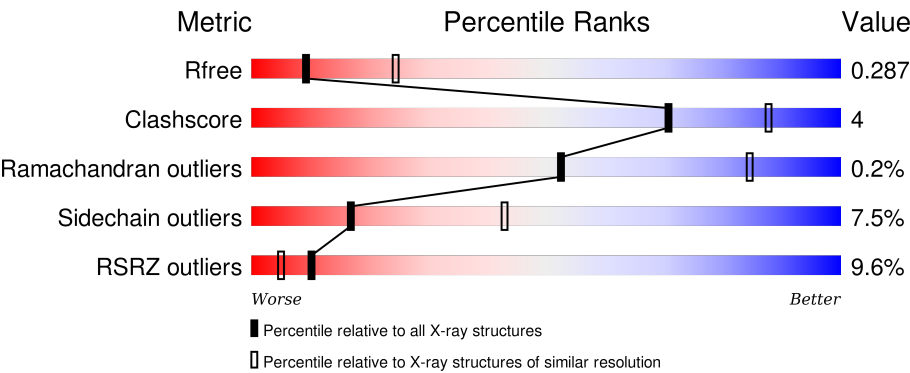
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	203	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>75%13%•10%</div></div>
1	B	203	<div><div>8%</div><div></div><div></div><div></div><div></div></div> <div>76%12%•10%</div>

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Mol	Chain	Length	Quality of chain
1	F	203	
1	G	203	
1	H	203	
1	J	203	
2	K	16	
2	L	16	
2	M	16	
2	N	16	
2	O	16	
2	P	16	
2	Q	16	
2	T	16	
2	U	16	

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
4	ZN	G	302	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13360 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 Non-structural 3 protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1337	829	244	254	10			
1	B	182	Total	C	N	O	S	0	0	0
			1337	829	244	254	10			
1	C	182	Total	C	N	O	S	0	0	0
			1337	829	244	254	10			
1	D	182	Total	C	N	O	S	0	0	0
			1337	829	244	254	10			
1	E	182	Total	C	N	O	S	0	0	0
			1337	829	244	254	10			
1	F	182	Total	C	N	O	S	0	0	0
			1337	829	244	254	10			
1	G	182	Total	C	N	O	S	0	0	0
			1337	829	244	254	10			
1	H	182	Total	C	N	O	S	0	0	0
			1337	829	244	254	10			
1	J	182	Total	C	N	O	S	0	0	0
			1337	829	244	254	10			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A6N4J4
A	26	ARG	LYS	conflict	UNP A6N4J4
A	181	ALA	-	expression tag	UNP A6N4J4
A	182	SER	-	expression tag	UNP A6N4J4
A	183	LYS	-	expression tag	UNP A6N4J4
A	184	LYS	-	expression tag	UNP A6N4J4
A	185	LYS	-	expression tag	UNP A6N4J4
A	186	LYS	-	expression tag	UNP A6N4J4
A	187	LYS	-	expression tag	UNP A6N4J4
A	188	GLY	-	expression tag	UNP A6N4J4
A	189	SER	-	expression tag	UNP A6N4J4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	190	VAL	-	expression tag	UNP A6N4J4
A	191	VAL	-	expression tag	UNP A6N4J4
A	192	ILE	-	expression tag	UNP A6N4J4
A	193	VAL	-	expression tag	UNP A6N4J4
A	194	GLY	-	expression tag	UNP A6N4J4
A	195	ARG	-	expression tag	UNP A6N4J4
A	196	ILE	-	expression tag	UNP A6N4J4
A	197	ILE	-	expression tag	UNP A6N4J4
A	198	LEU	-	expression tag	UNP A6N4J4
A	199	SER	-	expression tag	UNP A6N4J4
A	200	GLY	-	expression tag	UNP A6N4J4
A	201	ARG	-	expression tag	UNP A6N4J4
A	202	LYS	-	expression tag	UNP A6N4J4
B	0	MET	-	initiating methionine	UNP A6N4J4
B	26	ARG	LYS	conflict	UNP A6N4J4
B	181	ALA	-	expression tag	UNP A6N4J4
B	182	SER	-	expression tag	UNP A6N4J4
B	183	LYS	-	expression tag	UNP A6N4J4
B	184	LYS	-	expression tag	UNP A6N4J4
B	185	LYS	-	expression tag	UNP A6N4J4
B	186	LYS	-	expression tag	UNP A6N4J4
B	187	LYS	-	expression tag	UNP A6N4J4
B	188	GLY	-	expression tag	UNP A6N4J4
B	189	SER	-	expression tag	UNP A6N4J4
B	190	VAL	-	expression tag	UNP A6N4J4
B	191	VAL	-	expression tag	UNP A6N4J4
B	192	ILE	-	expression tag	UNP A6N4J4
B	193	VAL	-	expression tag	UNP A6N4J4
B	194	GLY	-	expression tag	UNP A6N4J4
B	195	ARG	-	expression tag	UNP A6N4J4
B	196	ILE	-	expression tag	UNP A6N4J4
B	197	ILE	-	expression tag	UNP A6N4J4
B	198	LEU	-	expression tag	UNP A6N4J4
B	199	SER	-	expression tag	UNP A6N4J4
B	200	GLY	-	expression tag	UNP A6N4J4
B	201	ARG	-	expression tag	UNP A6N4J4
B	202	LYS	-	expression tag	UNP A6N4J4
C	0	MET	-	initiating methionine	UNP A6N4J4
C	26	ARG	LYS	conflict	UNP A6N4J4
C	181	ALA	-	expression tag	UNP A6N4J4
C	182	SER	-	expression tag	UNP A6N4J4
C	183	LYS	-	expression tag	UNP A6N4J4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	184	LYS	-	expression tag	UNP A6N4J4
C	185	LYS	-	expression tag	UNP A6N4J4
C	186	LYS	-	expression tag	UNP A6N4J4
C	187	LYS	-	expression tag	UNP A6N4J4
C	188	GLY	-	expression tag	UNP A6N4J4
C	189	SER	-	expression tag	UNP A6N4J4
C	190	VAL	-	expression tag	UNP A6N4J4
C	191	VAL	-	expression tag	UNP A6N4J4
C	192	ILE	-	expression tag	UNP A6N4J4
C	193	VAL	-	expression tag	UNP A6N4J4
C	194	GLY	-	expression tag	UNP A6N4J4
C	195	ARG	-	expression tag	UNP A6N4J4
C	196	ILE	-	expression tag	UNP A6N4J4
C	197	ILE	-	expression tag	UNP A6N4J4
C	198	LEU	-	expression tag	UNP A6N4J4
C	199	SER	-	expression tag	UNP A6N4J4
C	200	GLY	-	expression tag	UNP A6N4J4
C	201	ARG	-	expression tag	UNP A6N4J4
C	202	LYS	-	expression tag	UNP A6N4J4
D	0	MET	-	initiating methionine	UNP A6N4J4
D	26	ARG	LYS	conflict	UNP A6N4J4
D	181	ALA	-	expression tag	UNP A6N4J4
D	182	SER	-	expression tag	UNP A6N4J4
D	183	LYS	-	expression tag	UNP A6N4J4
D	184	LYS	-	expression tag	UNP A6N4J4
D	185	LYS	-	expression tag	UNP A6N4J4
D	186	LYS	-	expression tag	UNP A6N4J4
D	187	LYS	-	expression tag	UNP A6N4J4
D	188	GLY	-	expression tag	UNP A6N4J4
D	189	SER	-	expression tag	UNP A6N4J4
D	190	VAL	-	expression tag	UNP A6N4J4
D	191	VAL	-	expression tag	UNP A6N4J4
D	192	ILE	-	expression tag	UNP A6N4J4
D	193	VAL	-	expression tag	UNP A6N4J4
D	194	GLY	-	expression tag	UNP A6N4J4
D	195	ARG	-	expression tag	UNP A6N4J4
D	196	ILE	-	expression tag	UNP A6N4J4
D	197	ILE	-	expression tag	UNP A6N4J4
D	198	LEU	-	expression tag	UNP A6N4J4
D	199	SER	-	expression tag	UNP A6N4J4
D	200	GLY	-	expression tag	UNP A6N4J4
D	201	ARG	-	expression tag	UNP A6N4J4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	202	LYS	-	expression tag	UNP A6N4J4
E	0	MET	-	initiating methionine	UNP A6N4J4
E	26	ARG	LYS	conflict	UNP A6N4J4
E	181	ALA	-	expression tag	UNP A6N4J4
E	182	SER	-	expression tag	UNP A6N4J4
E	183	LYS	-	expression tag	UNP A6N4J4
E	184	LYS	-	expression tag	UNP A6N4J4
E	185	LYS	-	expression tag	UNP A6N4J4
E	186	LYS	-	expression tag	UNP A6N4J4
E	187	LYS	-	expression tag	UNP A6N4J4
E	188	GLY	-	expression tag	UNP A6N4J4
E	189	SER	-	expression tag	UNP A6N4J4
E	190	VAL	-	expression tag	UNP A6N4J4
E	191	VAL	-	expression tag	UNP A6N4J4
E	192	ILE	-	expression tag	UNP A6N4J4
E	193	VAL	-	expression tag	UNP A6N4J4
E	194	GLY	-	expression tag	UNP A6N4J4
E	195	ARG	-	expression tag	UNP A6N4J4
E	196	ILE	-	expression tag	UNP A6N4J4
E	197	ILE	-	expression tag	UNP A6N4J4
E	198	LEU	-	expression tag	UNP A6N4J4
E	199	SER	-	expression tag	UNP A6N4J4
E	200	GLY	-	expression tag	UNP A6N4J4
E	201	ARG	-	expression tag	UNP A6N4J4
E	202	LYS	-	expression tag	UNP A6N4J4
F	0	MET	-	initiating methionine	UNP A6N4J4
F	26	ARG	LYS	conflict	UNP A6N4J4
F	181	ALA	-	expression tag	UNP A6N4J4
F	182	SER	-	expression tag	UNP A6N4J4
F	183	LYS	-	expression tag	UNP A6N4J4
F	184	LYS	-	expression tag	UNP A6N4J4
F	185	LYS	-	expression tag	UNP A6N4J4
F	186	LYS	-	expression tag	UNP A6N4J4
F	187	LYS	-	expression tag	UNP A6N4J4
F	188	GLY	-	expression tag	UNP A6N4J4
F	189	SER	-	expression tag	UNP A6N4J4
F	190	VAL	-	expression tag	UNP A6N4J4
F	191	VAL	-	expression tag	UNP A6N4J4
F	192	ILE	-	expression tag	UNP A6N4J4
F	193	VAL	-	expression tag	UNP A6N4J4
F	194	GLY	-	expression tag	UNP A6N4J4
F	195	ARG	-	expression tag	UNP A6N4J4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	196	ILE	-	expression tag	UNP A6N4J4
F	197	ILE	-	expression tag	UNP A6N4J4
F	198	LEU	-	expression tag	UNP A6N4J4
F	199	SER	-	expression tag	UNP A6N4J4
F	200	GLY	-	expression tag	UNP A6N4J4
F	201	ARG	-	expression tag	UNP A6N4J4
F	202	LYS	-	expression tag	UNP A6N4J4
G	0	MET	-	initiating methionine	UNP A6N4J4
G	26	ARG	LYS	conflict	UNP A6N4J4
G	181	ALA	-	expression tag	UNP A6N4J4
G	182	SER	-	expression tag	UNP A6N4J4
G	183	LYS	-	expression tag	UNP A6N4J4
G	184	LYS	-	expression tag	UNP A6N4J4
G	185	LYS	-	expression tag	UNP A6N4J4
G	186	LYS	-	expression tag	UNP A6N4J4
G	187	LYS	-	expression tag	UNP A6N4J4
G	188	GLY	-	expression tag	UNP A6N4J4
G	189	SER	-	expression tag	UNP A6N4J4
G	190	VAL	-	expression tag	UNP A6N4J4
G	191	VAL	-	expression tag	UNP A6N4J4
G	192	ILE	-	expression tag	UNP A6N4J4
G	193	VAL	-	expression tag	UNP A6N4J4
G	194	GLY	-	expression tag	UNP A6N4J4
G	195	ARG	-	expression tag	UNP A6N4J4
G	196	ILE	-	expression tag	UNP A6N4J4
G	197	ILE	-	expression tag	UNP A6N4J4
G	198	LEU	-	expression tag	UNP A6N4J4
G	199	SER	-	expression tag	UNP A6N4J4
G	200	GLY	-	expression tag	UNP A6N4J4
G	201	ARG	-	expression tag	UNP A6N4J4
G	202	LYS	-	expression tag	UNP A6N4J4
H	0	MET	-	initiating methionine	UNP A6N4J4
H	26	ARG	LYS	conflict	UNP A6N4J4
H	181	ALA	-	expression tag	UNP A6N4J4
H	182	SER	-	expression tag	UNP A6N4J4
H	183	LYS	-	expression tag	UNP A6N4J4
H	184	LYS	-	expression tag	UNP A6N4J4
H	185	LYS	-	expression tag	UNP A6N4J4
H	186	LYS	-	expression tag	UNP A6N4J4
H	187	LYS	-	expression tag	UNP A6N4J4
H	188	GLY	-	expression tag	UNP A6N4J4
H	189	SER	-	expression tag	UNP A6N4J4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	190	VAL	-	expression tag	UNP A6N4J4
H	191	VAL	-	expression tag	UNP A6N4J4
H	192	ILE	-	expression tag	UNP A6N4J4
H	193	VAL	-	expression tag	UNP A6N4J4
H	194	GLY	-	expression tag	UNP A6N4J4
H	195	ARG	-	expression tag	UNP A6N4J4
H	196	ILE	-	expression tag	UNP A6N4J4
H	197	ILE	-	expression tag	UNP A6N4J4
H	198	LEU	-	expression tag	UNP A6N4J4
H	199	SER	-	expression tag	UNP A6N4J4
H	200	GLY	-	expression tag	UNP A6N4J4
H	201	ARG	-	expression tag	UNP A6N4J4
H	202	LYS	-	expression tag	UNP A6N4J4
J	0	MET	-	initiating methionine	UNP A6N4J4
J	26	ARG	LYS	conflict	UNP A6N4J4
J	181	ALA	-	expression tag	UNP A6N4J4
J	182	SER	-	expression tag	UNP A6N4J4
J	183	LYS	-	expression tag	UNP A6N4J4
J	184	LYS	-	expression tag	UNP A6N4J4
J	185	LYS	-	expression tag	UNP A6N4J4
J	186	LYS	-	expression tag	UNP A6N4J4
J	187	LYS	-	expression tag	UNP A6N4J4
J	188	GLY	-	expression tag	UNP A6N4J4
J	189	SER	-	expression tag	UNP A6N4J4
J	190	VAL	-	expression tag	UNP A6N4J4
J	191	VAL	-	expression tag	UNP A6N4J4
J	192	ILE	-	expression tag	UNP A6N4J4
J	193	VAL	-	expression tag	UNP A6N4J4
J	194	GLY	-	expression tag	UNP A6N4J4
J	195	ARG	-	expression tag	UNP A6N4J4
J	196	ILE	-	expression tag	UNP A6N4J4
J	197	ILE	-	expression tag	UNP A6N4J4
J	198	LEU	-	expression tag	UNP A6N4J4
J	199	SER	-	expression tag	UNP A6N4J4
J	200	GLY	-	expression tag	UNP A6N4J4
J	201	ARG	-	expression tag	UNP A6N4J4
J	202	LYS	-	expression tag	UNP A6N4J4

- Molecule 2 is a protein called NS4A protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	13	Total	C	N	O	0	0	0
			93	61	17	15			

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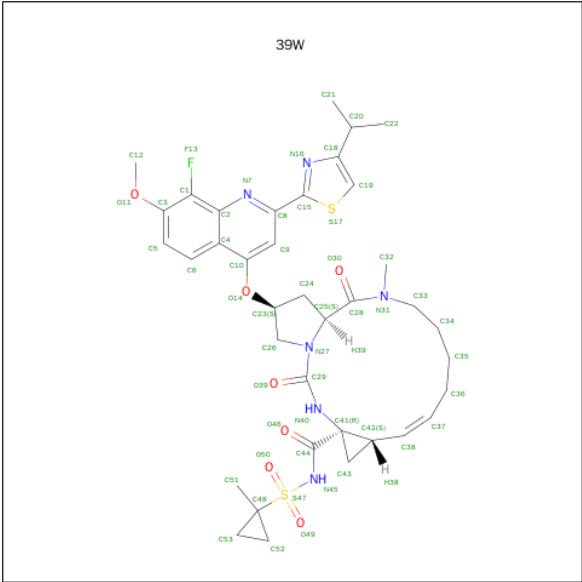
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	L	13	Total	C	N	O	0	0	0
			93	61	17	15			
2	M	13	Total	C	N	O	0	0	0
			93	61	17	15			
2	N	13	Total	C	N	O	0	0	0
			93	61	17	15			
2	O	13	Total	C	N	O	0	0	0
			93	61	17	15			
2	P	13	Total	C	N	O	0	0	0
			93	61	17	15			
2	Q	13	Total	C	N	O	0	0	0
			93	61	17	15			
2	T	13	Total	C	N	O	0	0	0
			93	61	17	15			
2	U	13	Total	C	N	O	0	0	0
			93	61	17	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	220	LYS	-	expression tag	UNP F0UY39
K	235	LYS	-	expression tag	UNP F0UY39
L	220	LYS	-	expression tag	UNP F0UY39
L	235	LYS	-	expression tag	UNP F0UY39
M	220	LYS	-	expression tag	UNP F0UY39
M	235	LYS	-	expression tag	UNP F0UY39
N	220	LYS	-	expression tag	UNP F0UY39
N	235	LYS	-	expression tag	UNP F0UY39
O	220	LYS	-	expression tag	UNP F0UY39
O	235	LYS	-	expression tag	UNP F0UY39
P	220	LYS	-	expression tag	UNP F0UY39
P	235	LYS	-	expression tag	UNP F0UY39
Q	220	LYS	-	expression tag	UNP F0UY39
Q	235	LYS	-	expression tag	UNP F0UY39
T	220	LYS	-	expression tag	UNP F0UY39
T	235	LYS	-	expression tag	UNP F0UY39
U	220	LYS	-	expression tag	UNP F0UY39
U	235	LYS	-	expression tag	UNP F0UY39

- Molecule 3 is (2S,3aS,10Z,11aS,12aR)-2-({8-fluoro-7-methoxy-2-[4-(propan-2-yl)-1,3-thiazol-2-yl]quinolin-4-yl}oxy)-5-methyl-N-[(1-methylcyclopropyl)sulfonyl]-4,14-dioxo-1,2,3,3a,4,5,6,7,8,9,11a,12,13,14-tetradecahydro-12aH-cyclopropa[m]pyrrolo[1,2-c][1,3,6]triazacyclotetradecine-12a-carboxamide (three-letter code: 39W) (formula: C₃₇H₄₅FN₆O₇S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	B	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	C	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	D	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	E	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	F	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	G	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	H	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0
3	J	1	Total 53	C 37	F 1	N 6	O 7	S 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

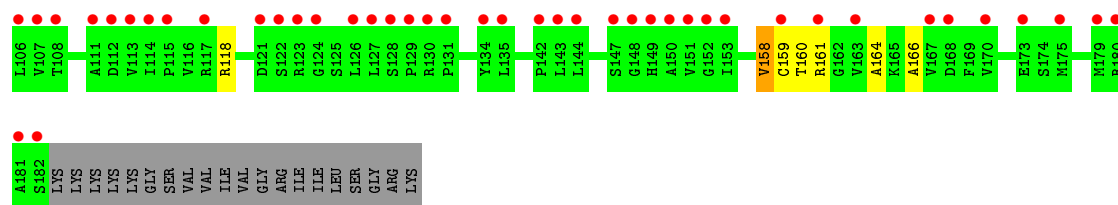
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Zn 1	0	0
4	H	1	Total 1	Zn 1	0	0
4	B	1	Total 1	Zn 1	0	0
4	C	1	Total 1	Zn 1	0	0
4	A	1	Total 1	Zn 1	0	0
4	F	1	Total 1	Zn 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0
5	D	1	Total 1	Cl 1	0	0
5	E	1	Total 1	Cl 1	0	0



- Molecule 2: NS4A protein

Chain K: 56% 25% 19%



- Molecule 2: NS4A protein

Chain L: 69% 13% 19%



- Molecule 2: NS4A protein

Chain M: 44% 31% 6% 19%



- Molecule 2: NS4A protein

Chain N: 6% 69% 13% 19%



- Molecule 2: NS4A protein

Chain O: 6% 63% 19% 19%

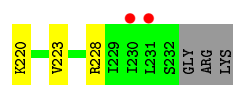


- Molecule 2: NS4A protein

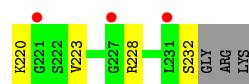
Chain P: 6% 56% 25% 19%



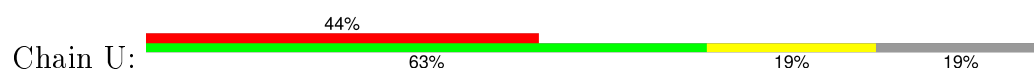
- Molecule 2: NS4A protein



- Molecule 2: NS4A protein



- Molecule 2: NS4A protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	150.03Å 174.36Å 133.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.23 – 2.80 43.22 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.23-2.80) 97.0 (43.22-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.233 , 0.290 0.234 , 0.287	Depositor DCC
R_{free} test set	2088 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	72.3	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 41817 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13360	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 39W, CL

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	0.47	0/1363	0.63	0/1857
1	B	0.38	0/1363	0.58	0/1857
1	C	0.42	0/1363	0.59	0/1857
1	D	0.42	0/1363	0.61	0/1857
1	E	0.40	0/1363	0.57	0/1857
1	F	0.41	0/1363	0.56	0/1857
1	G	0.40	0/1363	0.58	0/1857
1	H	0.37	0/1363	0.54	0/1857
1	J	0.35	0/1363	0.50	0/1857
2	K	0.40	0/92	0.72	0/122
2	L	0.52	0/92	0.66	0/122
2	M	0.45	0/92	0.71	0/122
2	N	0.57	0/92	0.71	0/122
2	O	0.46	0/92	0.67	0/122
2	P	0.41	0/92	0.64	0/122
2	Q	0.45	0/92	0.57	0/122
2	T	0.43	0/92	0.75	0/122
2	U	0.39	0/92	0.65	0/122
All	All	0.41	0/13095	0.58	0/17811

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	1337	0	1344	14	0
1	B	1337	0	1345	13	0
1	C	1337	0	1344	13	0
1	D	1337	0	1344	12	0
1	E	1337	0	1344	11	0
1	F	1337	0	1345	14	0
1	G	1337	0	1346	15	0
1	H	1337	0	1344	12	0
1	J	1337	0	1344	6	0
2	K	93	0	112	3	0
2	L	93	0	112	1	0
2	M	93	0	112	5	0
2	N	93	0	112	2	0
2	O	93	0	112	2	0
2	P	93	0	112	2	0
2	Q	93	0	112	4	0
2	T	93	0	112	4	0
2	U	93	0	112	4	0
3	A	53	0	44	4	0
3	B	53	0	44	0	0
3	C	53	0	44	2	0
3	D	53	0	44	6	0
3	E	53	0	44	3	0
3	F	53	0	44	1	0
3	G	53	0	44	0	0
3	H	53	0	44	3	0
3	J	53	0	44	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	2	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
All	All	13360	0	13504	119	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 4.

The worst 5 of 119 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:G:97:CYS:SG	4:G:302:ZN:ZN	1.57	0.92
1:A:159:CYS:HB3	1:A:164:ALA:HA	1.57	0.86
1:D:36:VAL:HG13	2:N:223:VAL:CG1	2.20	0.71
1:H:159:CYS:HB3	1:H:164:ALA:HA	1.76	0.68
1:D:159:CYS:HB3	1:D:164:ALA:HA	1.76	0.68

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	180/203 (89%)	174 (97%)	5 (3%)	1 (1%)	30	65
1	B	180/203 (89%)	172 (96%)	8 (4%)	0	100	100
1	C	180/203 (89%)	170 (94%)	10 (6%)	0	100	100
1	D	180/203 (89%)	171 (95%)	8 (4%)	1 (1%)	30	65
1	E	180/203 (89%)	173 (96%)	7 (4%)	0	100	100
1	F	180/203 (89%)	170 (94%)	10 (6%)	0	100	100
1	G	180/203 (89%)	174 (97%)	6 (3%)	0	100	100
1	H	180/203 (89%)	170 (94%)	10 (6%)	0	100	100
1	J	180/203 (89%)	173 (96%)	6 (3%)	1 (1%)	30	65
2	K	11/16 (69%)	11 (100%)	0	0	100	100
2	L	11/16 (69%)	11 (100%)	0	0	100	100
2	M	11/16 (69%)	11 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	11/16 (69%)	11 (100%)	0	0	100	100
2	O	11/16 (69%)	11 (100%)	0	0	100	100
2	P	11/16 (69%)	11 (100%)	0	0	100	100
2	Q	11/16 (69%)	11 (100%)	0	0	100	100
2	T	11/16 (69%)	11 (100%)	0	0	100	100
2	U	11/16 (69%)	11 (100%)	0	0	100	100
All	All	1719/1971 (87%)	1646 (96%)	70 (4%)	3 (0%)	52	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLY
1	D	109	ARG
1	J	161	ARG

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	147/165 (89%)	135 (92%)	12 (8%)	14	38
1	B	147/165 (89%)	140 (95%)	7 (5%)	31	66
1	C	147/165 (89%)	141 (96%)	6 (4%)	37	72
1	D	147/165 (89%)	134 (91%)	13 (9%)	12	35
1	E	147/165 (89%)	134 (91%)	13 (9%)	12	35
1	F	147/165 (89%)	134 (91%)	13 (9%)	12	35
1	G	147/165 (89%)	138 (94%)	9 (6%)	23	55
1	H	147/165 (89%)	140 (95%)	7 (5%)	31	66
1	J	147/165 (89%)	138 (94%)	9 (6%)	23	55
2	K	11/13 (85%)	9 (82%)	2 (18%)	2	6
2	L	11/13 (85%)	10 (91%)	1 (9%)	12	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	11/13 (85%)	7 (64%)	4 (36%)	0	0
2	N	11/13 (85%)	10 (91%)	1 (9%)	12	33
2	O	11/13 (85%)	9 (82%)	2 (18%)	2	6
2	P	11/13 (85%)	8 (73%)	3 (27%)	0	1
2	Q	11/13 (85%)	10 (91%)	1 (9%)	12	33
2	T	11/13 (85%)	9 (82%)	2 (18%)	2	6
2	U	11/13 (85%)	10 (91%)	1 (9%)	12	33
All	All	1422/1602 (89%)	1316 (92%)	106 (8%)	17	43

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	119	ARG
1	F	118	ARG
2	O	228	ARG
1	E	158	VAL
1	F	40	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	77	ASN
1	E	34	GLN
1	J	8	GLN
1	E	8	GLN
1	E	73	GLN

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 22 ligands modelled in this entry, 13 are monoatomic - leaving 9 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$
3	39W	A	301	-	54,59,59	2.16	8 (14%)	68,91,91	2.12	17 (25%)
3	39W	B	301	-	54,59,59	2.17	8 (14%)	68,91,91	2.11	19 (27%)
3	39W	C	301	-	54,59,59	1.97	8 (14%)	68,91,91	2.17	17 (25%)
3	39W	D	301	-	54,59,59	2.21	7 (12%)	68,91,91	2.28	20 (29%)
3	39W	E	301	-	54,59,59	2.04	8 (14%)	68,91,91	2.08	19 (27%)
3	39W	F	301	-	54,59,59	2.10	8 (14%)	68,91,91	1.96	19 (27%)
3	39W	G	301	-	54,59,59	2.02	8 (14%)	68,91,91	2.11	18 (26%)
3	39W	H	301	-	54,59,59	2.11	8 (14%)	68,91,91	2.15	18 (26%)
3	39W	J	301	-	54,59,59	2.09	8 (14%)	68,91,91	1.93	17 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	39W	A	301	-	-	0/48/84/84	0/4/7/7
3	39W	B	301	-	-	0/48/84/84	0/4/7/7
3	39W	C	301	-	-	0/48/84/84	0/4/7/7
3	39W	D	301	-	-	0/48/84/84	0/4/7/7
3	39W	E	301	-	-	0/48/84/84	0/4/7/7
3	39W	F	301	-	-	0/48/84/84	0/4/7/7
3	39W	G	301	-	-	0/48/84/84	0/4/7/7
3	39W	H	301	-	-	0/48/84/84	0/4/7/7
3	39W	J	301	-	-	0/48/84/84	0/4/7/7

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	39W	C15-S17	-10.88	1.58	1.73
3	D	301	39W	C15-S17	-10.67	1.58	1.73
3	A	301	39W	C15-S17	-10.50	1.59	1.73
3	F	301	39W	C15-S17	-10.17	1.59	1.73
3	H	301	39W	C15-S17	-10.08	1.59	1.73

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	39W	O49-S47-O50	-6.38	107.36	120.29
3	H	301	39W	C52-C53-C48	-5.75	56.97	60.19
3	D	301	39W	C52-C53-C48	-5.65	57.03	60.19
3	G	301	39W	O49-S47-O50	-5.60	108.94	120.29
3	B	301	39W	C52-C53-C48	-5.57	57.07	60.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	39W	4	0
3	C	301	39W	2	0
3	D	301	39W	6	0
3	E	301	39W	3	0
3	F	301	39W	1	0
3	H	301	39W	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	182/203 (89%)	0.13	3 (1%) 74 66	40, 63, 100, 127	1 (0%)
1	B	182/203 (89%)	0.42	17 (9%) 11 5	52, 89, 137, 173	0
1	C	182/203 (89%)	0.33	6 (3%) 50 38	51, 88, 123, 176	0
1	D	182/203 (89%)	0.16	6 (3%) 50 38	42, 76, 110, 155	1 (0%)
1	E	182/203 (89%)	0.21	8 (4%) 38 26	52, 81, 125, 147	0
1	F	182/203 (89%)	0.33	6 (3%) 50 38	47, 85, 125, 167	0
1	G	182/203 (89%)	0.16	6 (3%) 50 38	51, 84, 131, 173	0
1	H	182/203 (89%)	0.81	26 (14%) 4 2	70, 106, 146, 187	0
1	J	182/203 (89%)	1.91	75 (41%) 0 0	69, 143, 185, 215	0
2	K	13/16 (81%)	-0.01	0 100 100	45, 59, 79, 95	0
2	L	13/16 (81%)	0.34	0 100 100	50, 68, 99, 118	0
2	M	13/16 (81%)	0.17	0 100 100	57, 64, 104, 126	0
2	N	13/16 (81%)	0.30	1 (7%) 16 8	51, 61, 93, 103	0
2	O	13/16 (81%)	0.27	1 (7%) 16 8	57, 69, 98, 112	0
2	P	13/16 (81%)	0.81	1 (7%) 16 8	78, 95, 115, 118	0
2	Q	13/16 (81%)	0.55	2 (15%) 3 1	57, 67, 98, 121	0
2	T	13/16 (81%)	1.44	3 (23%) 1 1	98, 112, 139, 158	0
2	U	13/16 (81%)	2.41	7 (53%) 0 0	104, 110, 173, 195	0
All	All	1755/1971 (89%)	0.51	168 (9%) 10 5	40, 87, 153, 215	2 (0%)

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	152	GLY	13.6
1	J	124	GLY	10.9
1	J	113	VAL	10.4

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Mol	Chain	Res	Type	RSRZ
1	A	1	ALA	9.5
2	U	231	LEU	8.2

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	39W	A	301	53/53	0.96	0.21	0.57	47,54,63,64	0
3	39W	G	301	53/53	0.95	0.20	0.49	57,62,66,70	0
4	ZN	A	302	1/1	0.96	0.18	0.37	89,89,89,89	0
3	39W	D	301	53/53	0.98	0.20	0.35	47,55,62,65	0
3	39W	E	301	53/53	0.96	0.20	0.10	48,63,65,67	0
4	ZN	C	302	1/1	0.82	0.16	0.07	127,127,127,127	0
3	39W	F	301	53/53	0.96	0.20	0.04	54,59,64,66	0
3	39W	H	301	53/53	0.96	0.20	-0.04	55,62,67,70	0
4	ZN	F	302	1/1	0.97	0.18	-0.20	93,93,93,93	0
3	39W	B	301	53/53	0.96	0.17	-0.53	56,62,65,68	0
3	39W	J	301	53/53	0.91	0.20	-0.58	67,74,77,79	0
4	ZN	H	302	1/1	0.87	0.14	-0.60	114,114,114,114	0
3	39W	C	301	53/53	0.97	0.18	-0.63	53,60,63,66	0
4	ZN	G	302	1/1	0.97	0.16	-0.77	115,115,115,115	0
4	ZN	E	302	1/1	0.93	0.10	-1.16	141,141,141,141	0
4	ZN	J	302	1/1	0.67	0.07	-1.17	314,314,314,314	0
4	ZN	D	302	1/1	0.86	0.14	-1.18	87,87,87,87	0
4	ZN	B	302	1/1	0.89	0.13	-1.50	117,117,117,117	0
5	CL	D	303	1/1	0.42	0.27	-	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CL	E	303	1/1	0.92	0.25	-	91,91,91,91	0
5	CL	G	303	1/1	0.82	0.27	-	81,81,81,81	0
5	CL	B	303	1/1	0.85	0.17	-	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.