wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 08:04 AM EDT

PDB ID	:	1KNZ
Title	:	Recognition of the rotavirus mRNA 3' consensus by an asymmetric NSP3 homodimer
Authors	:	Deo, R.C.; Groft, C.M.; Rajashankar, K.R.; Burley, S.K.
Deposited on	:	2001-12-19
Resolution	:	2.45 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
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 (i)) were used in the production of this report:

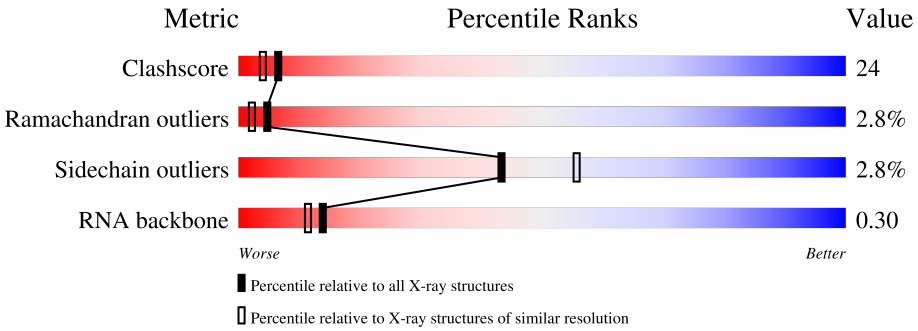
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.45 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))
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RNA backbone	3102	1001 (2.80-2.12)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	W	5	80% 20%
1	X	5	40% 40% 20%
1	Y	5	80% 20%
1	Z	5	20% 60% 20%
2	A	164	63% 29% • 6%
2	B	164	59% 23% • 16%

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Mol	Chain	Length	Quality of chain
2	C	164	
2	D	164	
2	I	164	
2	J	164	
2	M	164	
2	N	164	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9555 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 RNA chain called 5'-R(*UP*GP*AP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	W	5	Total	C	N	O	P	0	0	0
			102	47	18	33	4			
1	X	5	Total	C	N	O	P	0	0	0
			102	47	18	33	4			
1	Y	5	Total	C	N	O	P	0	0	0
			102	47	18	33	4			
1	Z	5	Total	C	N	O	P	0	0	0
			102	47	18	33	4			

- Molecule 2 is a protein called Nonstructural RNA-binding Protein 34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	154	Total	C	N	O	S	0	0	0
			1126	698	199	221	8			
2	B	138	Total	C	N	O	S	0	0	0
			1012	624	179	200	9			
2	C	154	Total	C	N	O	S	0	0	0
			1117	693	196	220	8			
2	D	138	Total	C	N	O	S	0	0	0
			1018	628	180	201	9			
2	I	154	Total	C	N	O	S	0	0	0
			1112	690	194	220	8			
2	J	138	Total	C	N	O	S	0	0	0
			1016	626	179	202	9			
2	M	154	Total	C	N	O	S	0	0	0
			1123	696	197	222	8			
2	N	138	Total	C	N	O	S	0	0	0
			1018	628	180	201	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	-	cloning artifact	UNP P03536

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	cloning artifact	UNP P03536
A	3	SER	-	cloning artifact	UNP P03536
B	1	LEU	-	cloning artifact	UNP P03536
B	2	GLY	-	cloning artifact	UNP P03536
B	3	SER	-	cloning artifact	UNP P03536
C	1	LEU	-	cloning artifact	UNP P03536
C	2	GLY	-	cloning artifact	UNP P03536
C	3	SER	-	cloning artifact	UNP P03536
D	1	LEU	-	cloning artifact	UNP P03536
D	2	GLY	-	cloning artifact	UNP P03536
D	3	SER	-	cloning artifact	UNP P03536
I	1	LEU	-	cloning artifact	UNP P03536
I	2	GLY	-	cloning artifact	UNP P03536
I	3	SER	-	cloning artifact	UNP P03536
J	1	LEU	-	cloning artifact	UNP P03536
J	2	GLY	-	cloning artifact	UNP P03536
J	3	SER	-	cloning artifact	UNP P03536
M	1	LEU	-	cloning artifact	UNP P03536
M	2	GLY	-	cloning artifact	UNP P03536
M	3	SER	-	cloning artifact	UNP P03536
N	1	LEU	-	cloning artifact	UNP P03536
N	2	GLY	-	cloning artifact	UNP P03536
N	3	SER	-	cloning artifact	UNP P03536

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	W	7	Total O 7 7	0	0
3	X	13	Total O 13 13	0	0
3	Y	5	Total O 5 5	0	0
3	Z	7	Total O 7 7	0	0
3	A	84	Total O 84 84	0	0
3	B	64	Total O 64 64	0	0
3	C	79	Total O 79 79	0	0
3	D	61	Total O 61 61	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	85	Total O 85 85	0	0
3	J	63	Total O 63 63	0	0
3	M	76	Total O 76 76	0	0
3	N	61	Total O 61 61	0	0

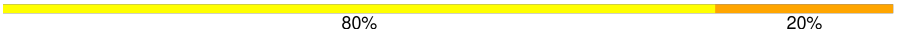
3 Residue-property plots (i)

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.

Note EDS was not executed.

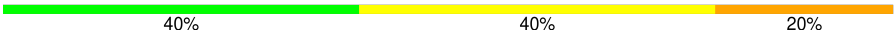
• Molecule 1: 5'-R(*UP*GP*AP*CP*C)-3'

Chain W:



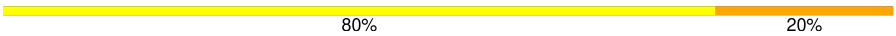
• Molecule 1: 5'-R(*UP*GP*AP*CP*C)-3'

Chain X:



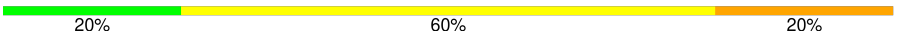
• Molecule 1: 5'-R(*UP*GP*AP*CP*C)-3'

Chain Y:



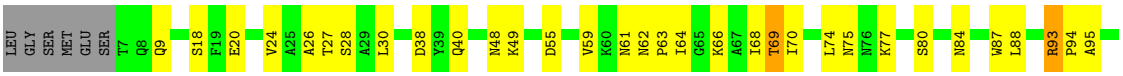
• Molecule 1: 5'-R(*UP*GP*AP*CP*C)-3'

Chain Z:



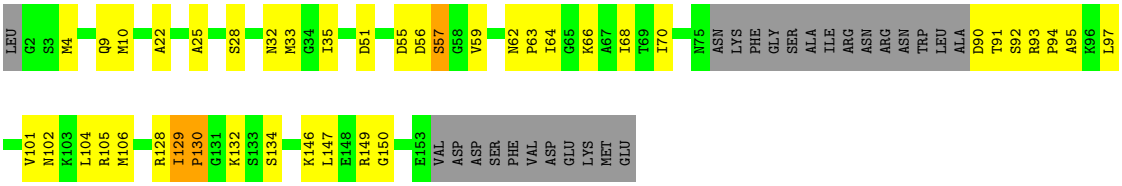
• Molecule 2: Nonstructural RNA-binding Protein 34

Chain A:



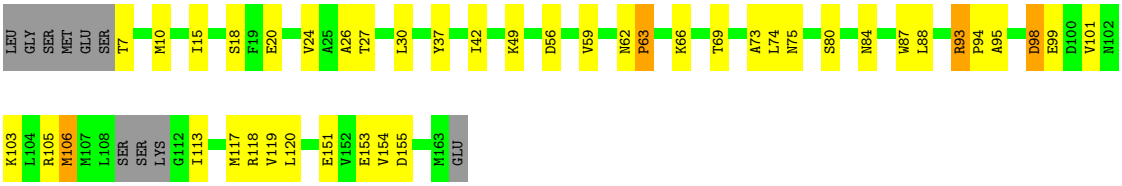
• Molecule 2: Nonstructural RNA-binding Protein 34

Chain B:



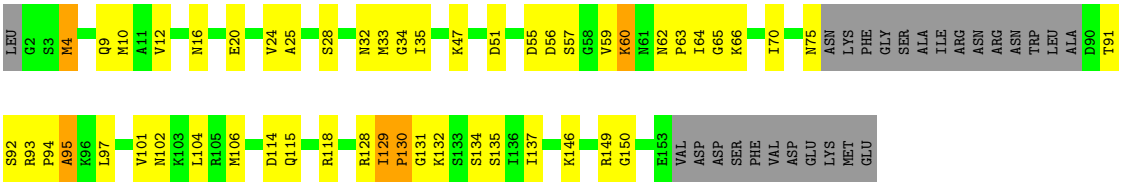
• Molecule 2: Nonstructural RNA-binding Protein 34

Chain C:



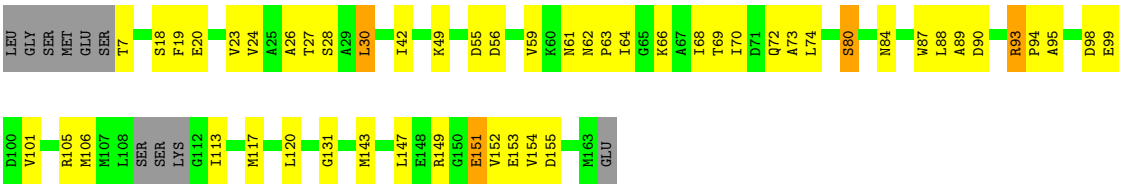
• Molecule 2: Nonstructural RNA-binding Protein 34

Chain D:



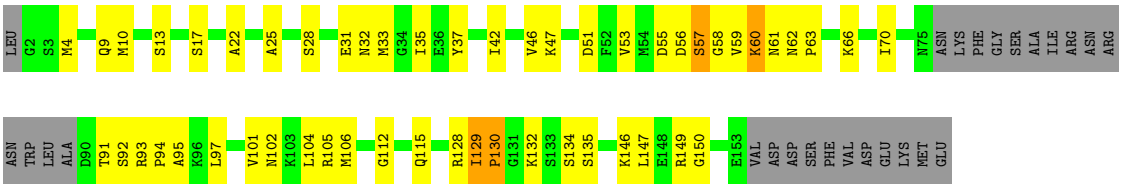
• Molecule 2: Nonstructural RNA-binding Protein 34

Chain I:



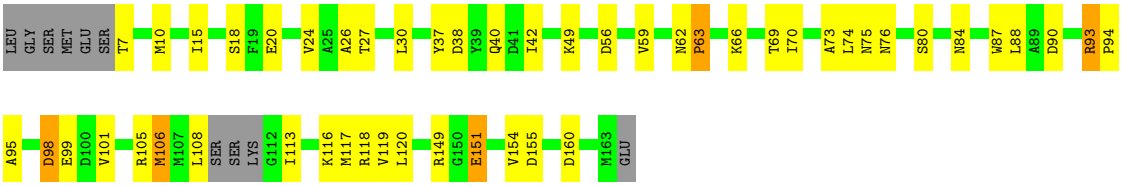
• Molecule 2: Nonstructural RNA-binding Protein 34

Chain J:



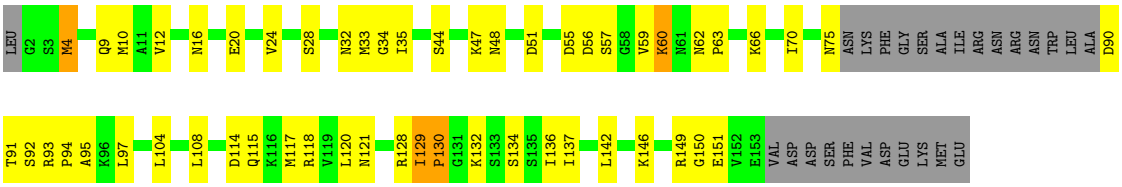
• Molecule 2: Nonstructural RNA-binding Protein 34

Chain M:



• Molecule 2: Nonstructural RNA-binding Protein 34

Chain N:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	40.27Å 85.36Å 96.05Å 89.99° 90.00° 90.05°	Depositor
Resolution (Å)	22.00 – 2.45	Depositor
% Data completeness (in resolution range)	(Not available) (22.00-2.45)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9555	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	W	0.48	0/113	1.05	0/174
1	X	0.45	0/113	0.93	0/174
1	Y	0.49	0/113	1.04	0/174
1	Z	0.43	0/113	1.02	0/174
2	A	0.41	0/1137	0.59	0/1536
2	B	0.37	0/1020	0.61	0/1371
2	C	0.35	0/1128	0.53	0/1526
2	D	0.37	0/1026	0.62	0/1379
2	I	0.36	0/1123	0.54	0/1520
2	J	0.36	0/1024	0.61	0/1376
2	M	0.35	0/1134	0.54	0/1533
2	N	0.37	0/1026	0.62	0/1379
All	All	0.37	0/9070	0.61	0/12316

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

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	W	102	0	56	8	0
1	X	102	0	56	6	0
1	Y	102	0	56	7	0
1	Z	102	0	56	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1126	0	1066	56	0
2	B	1012	0	980	54	0
2	C	1117	0	1048	62	0
2	D	1018	0	993	70	0
2	I	1112	0	1038	64	0
2	J	1016	0	984	69	0
2	M	1123	0	1059	68	0
2	N	1018	0	993	73	0
3	A	84	0	0	7	0
3	B	64	0	0	5	0
3	C	79	0	0	6	0
3	D	61	0	0	7	0
3	I	85	0	0	7	0
3	J	63	0	0	9	0
3	M	76	0	0	7	0
3	N	61	0	0	12	0
3	W	7	0	0	1	0
3	X	13	0	0	2	0
3	Y	5	0	0	1	0
3	Z	7	0	0	2	0
All	All	9555	0	8385	413	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 24.

The worst 5 of 413 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)
2:C:59:VAL:O	2:C:63:PRO:HD2	1.56	1.03
2:M:62:ASN:HB3	2:M:63:PRO:HD3	1.37	1.03
2:I:62:ASN:HB3	2:I:63:PRO:HD3	1.41	1.00
2:A:62:ASN:HB3	2:A:63:PRO:HD3	1.46	0.96
2:M:59:VAL:O	2:M:63:PRO:HD2	1.65	0.96

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
2	A	150/164 (92%)	145 (97%)	4 (3%)	1 (1%)	22 25
2	B	134/164 (82%)	119 (89%)	9 (7%)	6 (4%)	2 1
2	C	150/164 (92%)	143 (95%)	6 (4%)	1 (1%)	22 25
2	D	134/164 (82%)	120 (90%)	7 (5%)	7 (5%)	2 0
2	I	150/164 (92%)	141 (94%)	8 (5%)	1 (1%)	22 25
2	J	134/164 (82%)	117 (87%)	10 (8%)	7 (5%)	2 0
2	M	150/164 (92%)	142 (95%)	6 (4%)	2 (1%)	12 11
2	N	134/164 (82%)	119 (89%)	8 (6%)	7 (5%)	2 0
All	All	1136/1312 (87%)	1046 (92%)	58 (5%)	32 (3%)	5 2

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	113	ILE
2	B	56	ASP
2	B	95	ALA
2	B	130	PRO
2	C	113	ILE

5.3.2 Protein sidechains (i)

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
2	A	114/144 (79%)	110 (96%)	4 (4%)	36 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	106/144 (74%)	104 (98%)	2 (2%)	57 69
2	C	112/144 (78%)	107 (96%)	5 (4%)	27 36
2	D	108/144 (75%)	107 (99%)	1 (1%)	78 86
2	I	111/144 (77%)	105 (95%)	6 (5%)	22 28
2	J	107/144 (74%)	106 (99%)	1 (1%)	78 86
2	M	114/144 (79%)	109 (96%)	5 (4%)	28 37
2	N	108/144 (75%)	107 (99%)	1 (1%)	78 86
All	All	880/1152 (76%)	855 (97%)	25 (3%)	43 56

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	93	ARG
2	I	151	GLU
2	N	130	PRO
2	I	106	MET
2	J	130	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	75	ASN
2	N	115	GLN
2	N	121	ASN
2	N	32	ASN
2	D	61	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	W	4/5 (80%)	1 (25%)	0
1	X	4/5 (80%)	1 (25%)	0
1	Y	4/5 (80%)	1 (25%)	0
1	Z	4/5 (80%)	1 (25%)	0
All	All	16/20 (80%)	4 (25%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	W	5	C
1	X	5	C
1	Y	5	C
1	Z	5	C

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)

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.