



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:44 AM GMT

PDB ID : 2O1J  
Title : Structure of the extended diarrhea-inducing domain of rotavirus enterotoxigenic protein NSP4  
Authors : Suguna, K.; Durga Rao, C.; Deepa, R.  
Deposited on : 2006-11-29  
Resolution : 2.70 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

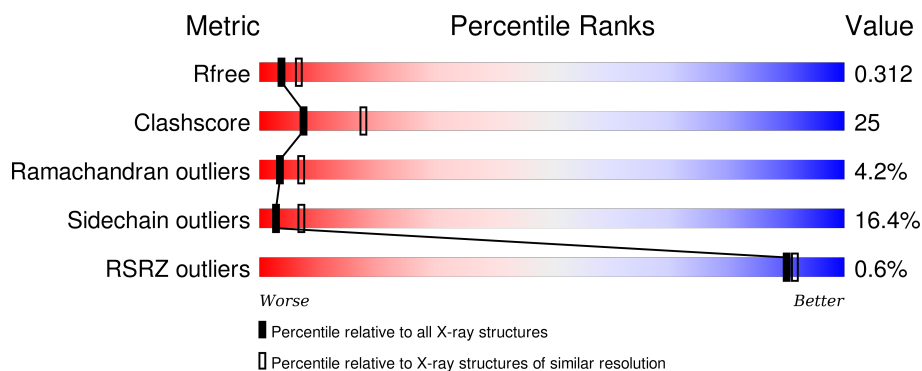
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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	52	
1	B	52	
1	C	52	
1	D	52	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1340 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 Nonstructural protein NSP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	44	Total	C	N	O	S	0	0	0
			335	211	55	66	3			
1	B	43	Total	C	N	O	S	0	0	0
			334	210	60	61	3			
1	C	44	Total	C	N	O	S	0	0	0
			327	207	55	62	3			
1	D	43	Total	C	N	O	S	0	0	0
			332	209	57	63	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	CYS	SEE REMARK 999	UNP Q9PYC1
A	135	THR	MET	SEE REMARK 999	UNP Q9PYC1
B	129	ARG	CYS	SEE REMARK 999	UNP Q9PYC1
B	135	THR	MET	SEE REMARK 999	UNP Q9PYC1
C	129	ARG	CYS	SEE REMARK 999	UNP Q9PYC1
C	135	THR	MET	SEE REMARK 999	UNP Q9PYC1
D	129	ARG	CYS	SEE REMARK 999	UNP Q9PYC1
D	135	THR	MET	SEE REMARK 999	UNP Q9PYC1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		

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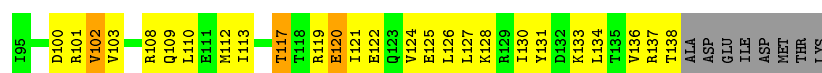
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	6	Total 6	O 6	0	0
3	C	1	Total 1	O 1	0	0
3	D	2	Total 2	O 2	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Nonstructural protein NSP4

Chain A: 



#### • Molecule 1: Nonstructural protein NSP4

Chain B: 



#### • Molecule 1: Nonstructural protein NSP4

Chain C: 



#### • Molecule 1: Nonstructural protein NSP4

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.61Å 180.43Å 48.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 14.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.5 (15.00-2.70) 94.5 (14.93-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0009	Depositor
R, $R_{free}$	0.248 , 0.314 0.242 , 0.312	Depositor DCC
$R_{free}$ test set	269 reflections (4.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 75.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	5 of 5814 reflections (0.086%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	1340	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.17 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.0536e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: CA

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	0.88	0/335	0.94	0/451
1	B	0.81	0/334	1.04	2/448 (0.4%)
1	C	0.81	0/327	0.96	0/441
1	D	0.84	0/332	1.01	0/446
All	All	0.84	0/1328	0.99	2/1786 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	LEU	CA-CB-CG	5.41	127.74	115.30
1	B	114	ASP	CB-CG-OD2	-5.07	113.73	118.30

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	335	0	323	27	0
1	B	334	0	335	20	0
1	C	327	0	315	18	0
1	D	332	0	328	25	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	6	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	1	0
All	All	1340	0	1301	67	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 25.

All (67) 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:C:109:GLN:HG2	1:D:110:LEU:HD21	1.25	1.13
1:A:109:GLN:HG2	1:B:110:LEU:CD2	1.80	1.10
1:A:109:GLN:HG2	1:B:110:LEU:HD22	1.34	1.07
1:A:109:GLN:CG	1:B:110:LEU:CD2	2.50	0.90
1:A:100:ASP:C	1:A:102:VAL:H	1.80	0.84
1:C:100:ASP:C	1:C:102:VAL:H	1.81	0.81
1:B:111:GLU:OE1	1:B:111:GLU:HA	1.85	0.75
1:C:109:GLN:HG2	1:D:110:LEU:CD2	2.14	0.74
1:A:109:GLN:CG	1:B:110:LEU:HD21	2.19	0.73
1:B:123:GLN:NE2	1:C:123:GLN:HB3	2.05	0.71
1:D:109:GLN:O	1:D:113:ILE:HG13	1.92	0.70
1:C:123:GLN:HE22	1:D:120:GLU:HB3	1.57	0.69
1:A:136:VAL:C	1:A:138:THR:H	1.96	0.69
1:A:121:ILE:O	1:A:124:VAL:HG12	1.93	0.68
1:D:134:LEU:O	1:D:136:VAL:N	2.27	0.68
1:C:100:ASP:C	1:C:102:VAL:N	2.44	0.67
1:D:129:ARG:HH21	1:D:133:LYS:NZ	1.95	0.64
1:A:134:LEU:HD11	1:D:130:ILE:HG23	1.79	0.63
1:A:109:GLN:HG3	1:B:110:LEU:HD21	1.80	0.63
1:B:120:GLU:O	1:B:124:VAL:HG23	1.99	0.63
1:A:100:ASP:C	1:A:102:VAL:N	2.47	0.63
1:A:113:ILE:O	1:A:117:THR:OG1	2.17	0.62
1:A:130:ILE:HG23	1:B:134:LEU:HD11	1.81	0.62
1:C:136:VAL:C	1:C:138:THR:H	2.04	0.61
1:D:129:ARG:HH21	1:D:133:LYS:HZ1	1.49	0.60
1:D:134:LEU:C	1:D:136:VAL:H	2.07	0.58
1:C:118:THR:HA	1:C:121:ILE:HD12	1.85	0.58
1:B:117:THR:O	1:B:121:ILE:HD12	2.04	0.57
1:C:102:VAL:HG23	1:D:103:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:O	1:A:138:THR:N	2.35	0.57
1:A:120:GLU:OE1	1:D:119:ARG:HD3	2.06	0.55
1:D:108:ARG:NH2	3:D:3:HOH:O	2.41	0.54
1:A:131:TYR:CE1	1:D:129:ARG:HG3	2.42	0.54
1:A:119:ARG:O	1:A:122:GLU:N	2.41	0.53
1:D:134:LEU:C	1:D:136:VAL:N	2.62	0.52
1:D:99:MET:O	1:D:103:VAL:HG23	2.10	0.52
1:D:135:THR:CG2	1:D:135:THR:O	2.58	0.50
1:D:116:LEU:O	1:D:119:ARG:N	2.40	0.50
1:A:119:ARG:O	1:A:120:GLU:C	2.50	0.49
1:C:121:ILE:O	1:C:122:GLU:C	2.50	0.49
1:B:113:ILE:CG2	1:B:113:ILE:O	2.60	0.49
1:B:111:GLU:OE1	1:B:111:GLU:CA	2.56	0.48
1:A:131:TYR:OH	1:D:133:LYS:HE2	2.12	0.48
1:D:135:THR:HG23	1:D:135:THR:O	2.14	0.48
1:C:130:ILE:O	1:C:130:ILE:CG2	2.61	0.47
1:A:131:TYR:HD1	1:D:130:ILE:HG13	1.78	0.47
1:B:110:LEU:O	1:B:111:GLU:C	2.53	0.46
1:B:123:GLN:HE22	1:C:123:GLN:HB3	1.75	0.46
1:B:129:ARG:HD2	1:C:131:TYR:CE1	2.52	0.45
1:A:100:ASP:O	1:A:102:VAL:N	2.44	0.45
1:A:130:ILE:HG23	1:B:134:LEU:CD1	2.46	0.45
1:A:108:ARG:O	1:A:112:MET:HG3	2.17	0.44
1:A:102:VAL:HG12	1:A:103:VAL:N	2.33	0.44
1:B:124:VAL:HG12	1:B:124:VAL:O	2.18	0.44
1:C:124:VAL:O	1:C:127:LEU:N	2.49	0.44
1:D:129:ARG:O	1:D:133:LYS:HG3	2.19	0.43
1:B:133:LYS:HE3	1:C:131:TYR:CE1	2.54	0.42
1:A:136:VAL:C	1:A:138:THR:N	2.65	0.42
1:A:127:LEU:HD12	1:D:123:GLN:HG2	2.01	0.42
1:B:103:VAL:O	1:B:104:LYS:C	2.58	0.41
1:C:100:ASP:O	1:C:102:VAL:N	2.53	0.41
1:D:136:VAL:O	1:D:137:ARG:O	2.39	0.41
1:A:134:LEU:CD1	1:D:130:ILE:HG23	2.50	0.41
1:D:101:ARG:O	1:D:102:VAL:C	2.59	0.41
1:C:99:MET:HE3	1:C:99:MET:HB3	1.97	0.41
1:A:133:LYS:O	1:A:136:VAL:N	2.54	0.40
1:B:126:LEU:HD22	1:C:127:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	42/52 (81%)	35 (83%)	5 (12%)	2 (5%)	3	5
1	B	41/52 (79%)	35 (85%)	6 (15%)	0	100	100
1	C	42/52 (81%)	35 (83%)	4 (10%)	3 (7%)	1	2
1	D	41/52 (79%)	35 (85%)	4 (10%)	2 (5%)	3	5
All	All	166/208 (80%)	140 (84%)	19 (11%)	7 (4%)	3	7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ARG
1	A	101	ARG
1	C	101	ARG
1	D	135	THR
1	C	137	ARG
1	C	126	LEU
1	D	102	VAL

### 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	34/51 (67%)	27 (79%)	7 (21%)	1	4
1	B	34/51 (67%)	29 (85%)	5 (15%)	4	9
1	C	32/51 (63%)	24 (75%)	8 (25%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	34/51 (67%)	32 (94%)	2 (6%)	24	51
All	All	134/204 (66%)	112 (84%)	22 (16%)	3	7

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	VAL
1	A	110	LEU
1	A	117	THR
1	A	120	GLU
1	A	125	GLU
1	A	126	LEU
1	A	128	LYS
1	B	106	MET
1	B	111	GLU
1	B	113	ILE
1	B	118	THR
1	B	126	LEU
1	C	110	LEU
1	C	113	ILE
1	C	117	THR
1	C	119	ARG
1	C	123	GLN
1	C	124	VAL
1	C	133	LYS
1	C	135	THR
1	D	112	MET
1	D	135	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	123	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	44/52 (84%)	-0.41	0 <b>100</b> <b>100</b>	3, 16, 40, 42	0
1	B	43/52 (82%)	-0.60	1 (2%) 64 64	3, 21, 38, 41	0
1	C	44/52 (84%)	-0.44	0 <b>100</b> <b>100</b>	4, 19, 41, 41	0
1	D	43/52 (82%)	-0.33	0 <b>100</b> <b>100</b>	3, 19, 39, 42	0
All	All	174/208 (83%)	-0.45	1 (0%) <b>90</b> <b>91</b>	3, 19, 41, 42	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	ARG	2.1

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CA	B	501	1/1	0.98	0.11	-0.46	2,2,2,2	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.