



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2018 – 03:42 PM EDT

PDB ID : 6E8R  
Title : Structure of the SNX32 PX domain in complex with Chlamydial protein IncE  
in space group I121  
Authors : Paul, B.; Collins, B.  
Deposited on : 2018-07-31  
Resolution : 2.27 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : rb-20031172  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

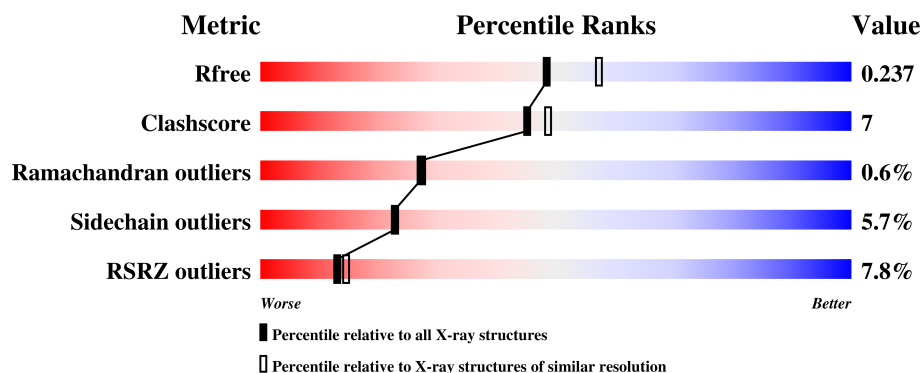
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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))
$R_{free}$	111664	1178 (2.26-2.26)
Clashscore	122126	1286 (2.26-2.26)
Ramachandran outliers	120053	1253 (2.26-2.26)
Sidechain outliers	120020	1254 (2.26-2.26)
RSRZ outliers	108989	1158 (2.26-2.26)

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	150	<div> <div>3%</div> <div>83%</div> <div>8%</div> <div>5%</div> </div>
1	B	150	<div> <div>12%</div> <div>77%</div> <div>14%</div> <div>6%</div> </div>
2	C	25	<div> <div>4%</div> <div>60%</div> <div>20%</div> <div>20%</div> </div>
2	D	25	<div> <div>4%</div> <div>44%</div> <div>32%</div> <div>24%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5390 atoms, of which 2542 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 Sorting nexin-32.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	142	Total	C	H	N	O	S	0	0	0
			2291	746	1125	198	219	3			
1	B	141	Total	C	H	N	O	S	0	0	0
			2278	741	1121	196	217	3			

- Molecule 2 is a protein called IncE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	H	N	O	0	0	0
			295	95	149	25	26			
2	D	19	Total	C	H	N	O	0	0	0
			289	93	147	24	25			


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	135	Total	O	0	0
			135	135		
3	B	89	Total	O	0	0
			89	89		
3	C	10	Total	O	0	0
			10	10		
3	D	3	Total	O	0	0
			3	3		

### 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 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: Sorting nexin-32

Chain A: 



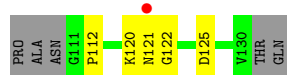
#### • Molecule 1: Sorting nexin-32

Chain B: 




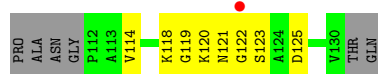
#### • Molecule 2: IncE

Chain C: 



#### • Molecule 2: IncE

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.88Å 46.00Å 134.21Å 90.00° 105.59° 90.00°	Depositor
Resolution (Å)	43.77 – 2.27 43.77 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.77-2.27) 94.5 (43.77-2.27)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.186 , 0.239 0.187 , 0.237	Depositor DCC
$R_{free}$ test set	1280 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	A	0.91	2/1195 (0.2%)	0.75	1/1614 (0.1%)
1	B	0.63	1/1186 (0.1%)	0.65	0/1602
2	C	0.80	0/148	0.84	2/198 (1.0%)
2	D	0.84	0/144	1.14	1/192 (0.5%)
All	All	0.79	3/2673 (0.1%)	0.74	4/3606 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
2	D	0	1
All	All	1	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	LYS	CE-NZ	17.27	1.92	1.49
1	A	65	GLU	CB-CG	-6.51	1.39	1.52
1	B	65	GLU	CB-CG	-6.06	1.40	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	125	ASP	CB-CG-OD2	-5.55	113.30	118.30
2	C	125	ASP	CB-CG-OD1	5.42	123.18	118.30
2	D	122	GLY	C-N-CA	5.27	134.87	121.70
1	A	118	LYS	CD-CE-NZ	5.04	123.30	111.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	108	ASP	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ASP	Peptide
2	D	121	ASN	Peptide

## 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	1166	1125	1131	9	7
1	B	1157	1121	1123	23	0
2	C	146	149	149	4	0
2	D	142	147	147	3	7
3	A	135	0	0	3	1
3	B	89	0	0	1	1
3	C	10	0	0	0	0
3	D	3	0	0	0	0
All	All	2848	2542	2550	36	9

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 7.

All (36) 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:A:118:LYS:NZ	1:A:118:LYS:CE	1.92	1.32
1:A:39:LYS:NZ	3:A:201:HOH:O	1.73	1.18
1:A:107:GLY:O	1:A:109:SER:N	1.87	1.06
1:B:112:THR:HG23	1:B:115:GLU:HB3	1.55	0.89
1:B:108:ASP:HA	1:B:111:VAL:HG12	1.70	0.73
1:B:108:ASP:HA	1:B:111:VAL:CG1	2.21	0.70
1:B:116:PHE:HA	1:B:119:MET:SD	2.38	0.64
1:A:37:ARG:HD2	2:C:112:PRO:HD2	1.83	0.60
1:B:65:GLU:HG3	3:B:220:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PHE:O	1:A:98:ARG:HG3	2.03	0.58
1:B:107:GLY:O	1:B:108:ASP:CB	2.53	0.56
1:B:112:THR:HG23	1:B:115:GLU:CB	2.32	0.52
1:A:98:ARG:NH1	3:A:207:HOH:O	2.44	0.50
1:B:36:GLU:OE2	1:B:41:LYS:CE	2.60	0.50
1:B:132:LYS:HE3	2:D:125:ASP:OD2	2.11	0.50
1:B:113:ARG:HB2	1:B:113:ARG:HH11	1.78	0.49
1:B:108:ASP:OD2	1:B:108:ASP:O	2.30	0.48
1:B:38:ASP:OD1	1:B:98:ARG:NH1	2.46	0.48
1:B:108:ASP:CG	1:B:108:ASP:O	2.53	0.47
2:C:120:LYS:HA	2:C:120:LYS:HE3	1.96	0.47
1:B:112:THR:CG2	1:B:115:GLU:HB3	2.35	0.46
1:B:99:GLU:O	1:B:103:LYS:HG3	2.16	0.45
1:B:111:VAL:HG22	1:B:112:THR:O	2.17	0.44
1:B:116:PHE:CD2	1:B:116:PHE:C	2.90	0.44
1:B:66:GLU:HA	1:B:66:GLU:OE1	2.19	0.42
1:B:127:TYR:CZ	2:D:114:VAL:HG21	2.55	0.42
1:A:93:ASP:OD1	1:A:95:GLU:HG3	2.20	0.42
2:C:120:LYS:O	2:C:121:ASN:C	2.58	0.42
2:C:121:ASN:HA	2:C:122:GLY:HA2	1.73	0.42
1:B:36:GLU:O	1:B:36:GLU:CG	2.68	0.41
1:B:106:GLU:OE1	1:B:107:GLY:N	2.53	0.41
1:A:24:SER:N	3:A:212:HOH:O	2.53	0.41
1:A:38:ASP:OD1	1:A:39:LYS:HG3	2.21	0.41
2:D:119:GLY:HA3	2:D:123:SER:O	2.21	0.41
1:B:111:VAL:CG2	1:B:112:THR:N	2.80	0.40
1:B:52:HIS:CE1	1:B:158:PHE:CE2	3.09	0.40

All (9) 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:A:118:LYS:HZ1	2:D:123:SER:H[2_555]	1.08	0.52
1:A:118:LYS:HZ3	2:D:120:LYS:O[2_555]	1.13	0.47
3:A:316:HOH:O	3:A:331:HOH:O[4_444]	1.86	0.34
1:A:118:LYS:HZ2	2:D:123:SER:OG[2_555]	1.30	0.30
1:A:118:LYS:NZ	2:D:120:LYS:O[2_555]	2.01	0.19
1:A:118:LYS:NZ	2:D:123:SER:OG[2_555]	2.06	0.14
3:B:207:HOH:O	3:B:247:HOH:O[4_544]	2.11	0.09
1:A:118:LYS:NZ	2:D:123:SER:H[2_555]	1.55	0.05
1:A:118:LYS:CE	2:D:123:SER:N[2_555]	2.17	0.03



## 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	140/150 (93%)	139 (99%)	0	1 (1%)	24	23
1	B	139/150 (93%)	137 (99%)	1 (1%)	1 (1%)	24	23
2	C	18/25 (72%)	18 (100%)	0	0	100	100
2	D	17/25 (68%)	15 (88%)	2 (12%)	0	100	100
All	All	314/350 (90%)	309 (98%)	3 (1%)	2 (1%)	27	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	ASP
1	B	108	ASP

### 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	
1	A	126/133 (95%)	119 (94%)	7 (6%)	23	23
1	B	125/133 (94%)	117 (94%)	8 (6%)	19	18
2	C	15/19 (79%)	15 (100%)	0	100	100
2	D	15/19 (79%)	14 (93%)	1 (7%)	18	16
All	All	281/304 (92%)	265 (94%)	16 (6%)	23	23

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	38	ASP
1	A	39	LYS
1	A	55	GLN
1	A	59	SER
1	A	103	LYS
1	A	165	GLN
1	B	24	SER
1	B	37	ARG
1	B	104	LEU
1	B	106	GLU
1	B	112	THR
1	B	113	ARG
1	B	118	LYS
1	B	122	GLU
2	D	118	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates 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 ⓘ

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, 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	142/150 (94%)	0.31	5 (3%) 44 47	16, 25, 62, 101	0
1	B	141/150 (94%)	0.79	18 (12%) 3 3	23, 38, 117, 142	0
2	C	20/25 (80%)	0.22	1 (5%) 29 32	20, 30, 58, 69	0
2	D	19/25 (76%)	0.70	1 (5%) 26 30	38, 49, 68, 76	0
All	All	322/350 (92%)	0.54	25 (7%) 13 14	16, 32, 100, 142	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	VAL	7.8
1	B	108	ASP	6.4
1	A	107	GLY	5.6
1	B	110	SER	5.4
1	B	114	GLU	4.9
1	B	107	GLY	4.5
1	A	108	ASP	4.5
1	B	116	PHE	4.4
1	B	109	SER	4.4
1	B	119	MET	4.2
1	B	115	GLU	4.1
1	A	109	SER	3.6
1	B	117	ALA	3.5
1	B	38	ASP	3.4
1	B	103	LYS	3.3
1	B	104	LEU	3.1
1	B	106	GLU	3.1
1	B	105	GLY	3.1
2	C	121	ASN	2.7
1	B	37	ARG	2.6
1	A	37	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	122	GLY	2.3
1	B	118	LYS	2.2
1	B	112	THR	2.2
1	A	110	SER	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.