wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 05:29 am BST

PDB ID	:	5TGI
Title	:	Structure of the SNX5 PX domain in complex with chlamydial protein IncE in space group P212121
Authors	:	Collins, B.; Paul, B.
Deposited on	:	2016-09-28
Resolution	:	1.98 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 following versions of software and data (see references (1)) were used in the production of this report:

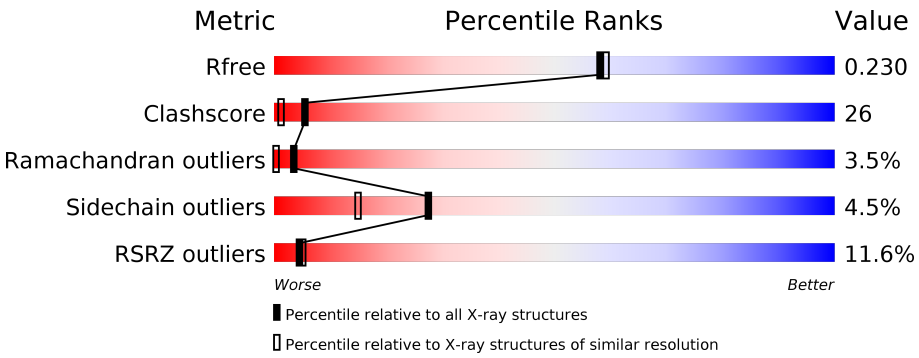
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.98 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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 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% 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	152	14% 75% 11% • • 8%
1	B	152	7% 80% 9% • 8%
2	C	22	9% 50% 32% 5% 5% 9%
2	D	22	14% 50% 27% 14% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5394 atoms, of which 2539 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-5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	140	2255	729	1116	187	220	3	0	0	0
1	B	140	2254	729	1115	187	220	3	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	expression tag	UNP Q9Y5X3
A	171	PRO	-	expression tag	UNP Q9Y5X3
A	172	ALA	-	expression tag	UNP Q9Y5X3
B	21	GLY	-	expression tag	UNP Q9Y5X3
B	171	PRO	-	expression tag	UNP Q9Y5X3
B	172	ALA	-	expression tag	UNP Q9Y5X3

- Molecule 2 is a protein called IncE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
2	C	20	306	97	154	26	29	0	0	0
2	D	20	303	97	154	25	27	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	121	121	121	0	0
3	B	113	113	113	0	0
3	C	21	21	21	0	0

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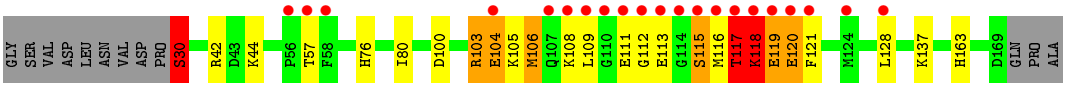
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	D	21	21	21	0	0

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 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.

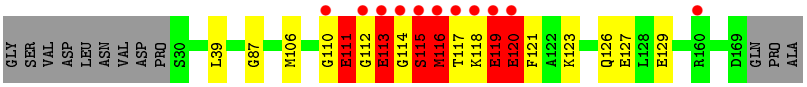
- Molecule 1: Sorting nexin-5

Chain A:



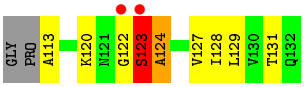
- Molecule 1: Sorting nexin-5

Chain B:



- Molecule 2: IncE

Chain C:



- Molecule 2: IncE

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.71Å 67.54Å 88.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.15 – 1.98 45.15 – 1.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.15-1.98) 100.0 (45.15-1.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 1.98Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.181 , 0.226 0.184 , 0.230	Depositor DCC
R_{free} test set	2000 reflections (7.69%)	wwPDB-VP
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 59.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5394	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.95	3/1168 (0.3%)	0.88	7/1580 (0.4%)
1	B	0.59	0/1168	0.74	2/1580 (0.1%)
2	C	0.59	0/153	1.15	1/203 (0.5%)
2	D	0.55	0/151	0.83	0/202
All	All	0.77	3/2640 (0.1%)	0.84	10/3565 (0.3%)

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	0	1
1	B	0	3
2	C	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	ARG	C-N	-22.91	0.81	1.34
1	A	104	GLU	C-N	-7.36	1.17	1.34
1	A	117	THR	CB-CG2	5.67	1.71	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	103	ARG	O-C-N	-11.68	104.01	122.70
1	A	103	ARG	C-N-CA	10.29	147.41	121.70
2	C	122	GLY	N-CA-C	-8.73	91.28	113.10
1	A	103	ARG	CA-C-N	8.18	135.21	117.20
1	A	117	THR	N-CA-C	-7.58	90.54	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	30	SER	Mainchain
1	B	116	MET	Peptide
1	B	119	GLU	Peptide
1	B	120	GLU	Peptide
2	C	123	SER	Peptide

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	1139	1116	1114	75	0
1	B	1139	1115	1115	52	0
2	C	152	154	154	7	0
2	D	149	154	154	17	0
3	A	121	0	0	5	2
3	B	113	0	0	4	2
3	C	21	0	0	1	0
3	D	21	0	0	4	0
All	All	2855	2539	2537	133	2

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 26.

The worst 5 of 133 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:103:ARG:O	1:A:104:GLU:N	1.64	1.29
1:B:115:SER:CB	1:B:120:GLU:HG3	1.63	1.29
1:A:113:GLU:O	1:A:121:PHE:CE2	1.85	1.28
1:A:113:GLU:O	1:A:121:PHE:HE2	1.01	1.28
1:A:119:GLU:OE2	1:B:118:LYS:CD	1.89	1.21

All (2) 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)
3:A:300:HOH:O	3:B:310:HOH:O[2_465]	1.97	0.23
3:A:219:HOH:O	3:B:223:HOH:O[2_465]	1.99	0.21

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	138/152 (91%)	130 (94%)	7 (5%)	1 (1%)	22	11
1	B	138/152 (91%)	128 (93%)	4 (3%)	6 (4%)	2	0
2	C	18/22 (82%)	15 (83%)	1 (6%)	2 (11%)	0	0
2	D	18/22 (82%)	14 (78%)	2 (11%)	2 (11%)	0	0
All	All	312/348 (90%)	287 (92%)	14 (4%)	11 (4%)	3	0

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	LYS
1	B	111	GLU
1	B	113	GLU
1	B	115	SER
2	C	124	ALA

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	129/139 (93%)	123 (95%)	6 (5%)	26	13
1	B	129/139 (93%)	126 (98%)	3 (2%)	50	44
2	C	16/17 (94%)	13 (81%)	3 (19%)	1	0
2	D	16/17 (94%)	15 (94%)	1 (6%)	18	7
All	All	290/312 (93%)	277 (96%)	13 (4%)	27	15

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	GLU
1	B	111	GLU
2	C	123	SER
1	A	119	GLU
2	C	120	LYS

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

Mol	Chain	Res	Type
1	A	68	GLN

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 (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	104:GLU	C	105:LYS	N	1.17
1	A	103:ARG	C	104:GLU	N	0.81

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, 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	140/152 (92%)	0.80	21 (15%)	2	2	11, 20, 98, 114	0
1	B	140/152 (92%)	0.64	11 (7%)	12	14	12, 23, 70, 96	0
2	C	20/22 (90%)	0.94	2 (10%)	7	8	14, 25, 76, 77	0
2	D	20/22 (90%)	2.01	3 (15%)	2	2	18, 34, 80, 162	0
All	All	320/348 (91%)	0.81	37 (11%)	4	5	11, 23, 90, 162	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	131	THR	23.4
1	B	114	GLY	19.9
1	B	115	SER	11.3
1	A	121	PHE	9.8
1	A	115	SER	9.6

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.