



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 09:31 pm GMT

PDB ID : 1WG0
Title : Structural comparison of Nas6p protein structures in two different crystal forms
Authors : Nakamura, Y.; Umehara, T.; Tanaka, A.; Horikoshi, M.; Yokoyama, S.; Padmanabhan, B.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-05-27
Resolution : 2.53 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

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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

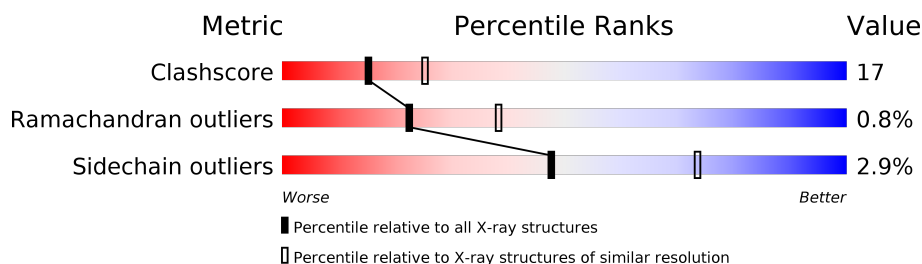
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	112137	5382 (2.54-2.50)
Ramachandran outliers	110173	5282 (2.54-2.50)
Sidechain outliers	110143	5284 (2.54-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	243	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2114 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 Probable 26S proteasome regulatory subunit p28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1932	1236	335	354	7			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	229	VAL	-	EXPRESSION TAG	UNP P50086
A	230	ASP	-	EXPRESSION TAG	UNP P50086
A	231	LYS	-	EXPRESSION TAG	UNP P50086
A	232	LEU	-	EXPRESSION TAG	UNP P50086
A	233	ALA	-	EXPRESSION TAG	UNP P50086
A	234	ALA	-	EXPRESSION TAG	UNP P50086
A	235	ALA	-	EXPRESSION TAG	UNP P50086
A	236	LEU	-	EXPRESSION TAG	UNP P50086
A	237	GLU	-	EXPRESSION TAG	UNP P50086
A	238	HIS	-	EXPRESSION TAG	UNP P50086
A	239	HIS	-	EXPRESSION TAG	UNP P50086
A	240	HIS	-	EXPRESSION TAG	UNP P50086
A	241	HIS	-	EXPRESSION TAG	UNP P50086
A	242	HIS	-	EXPRESSION TAG	UNP P50086
A	243	HIS	-	EXPRESSION TAG	UNP P50086

- Molecule 2 is water.

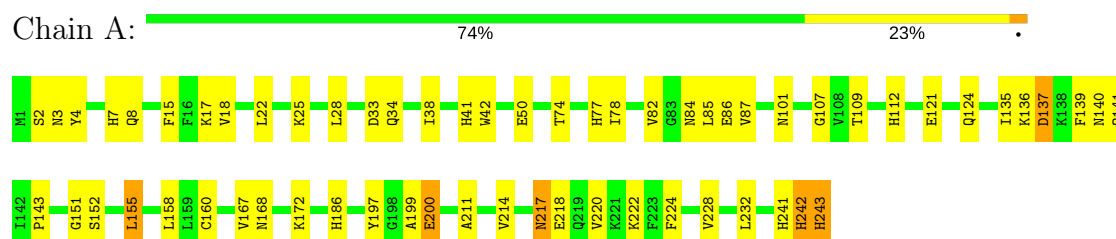
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	182	Total	O	0	0
			182	182		

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.

Note EDS was not executed.

- Molecule 1: Probable 26S proteasome regulatory subunit p28



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.44 Å 68.63 Å 46.98 Å 90.00° 108.95° 90.00°	Depositor
Resolution (Å)	20.00 – 2.53	Depositor
% Data completeness (in resolution range)	96.3 (20.00-2.53)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.179 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2114	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

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	0.36	0/1981	0.57	0/2683

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	1932	0	1903	64	0
2	A	182	0	0	4	0
All	All	2114	0	1903	64	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 17.

All (64) 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:167:VAL:H	1:A:243:HIS:CE1	1.72	1.06
1:A:84:ASN:HD22	1:A:87:VAL:H	1.09	0.99
1:A:38:ILE:H	1:A:41:HIS:HD2	1.29	0.81
1:A:74:THR:H	1:A:77:HIS:HD2	1.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASN:ND2	1:A:87:VAL:H	1.84	0.75
1:A:168:ASN:HD21	1:A:200:GLU:H	1.36	0.71
1:A:25:LYS:HE3	1:A:28:LEU:HD21	1.72	0.70
1:A:38:ILE:H	1:A:41:HIS:CD2	2.09	0.70
1:A:18:VAL:O	1:A:22:LEU:HD23	1.92	0.69
1:A:168:ASN:ND2	1:A:200:GLU:H	1.92	0.67
1:A:74:THR:H	1:A:77:HIS:CD2	2.13	0.67
1:A:2:SER:O	1:A:3:ASN:HB2	1.97	0.64
1:A:136:LYS:HB2	1:A:140:ASN:HA	1.80	0.63
1:A:168:ASN:N	1:A:243:HIS:NE2	2.35	0.63
1:A:139:PHE:HB3	2:A:295:HOH:O	1.98	0.62
1:A:109:THR:H	1:A:112:HIS:CD2	2.18	0.61
1:A:25:LYS:O	1:A:28:LEU:HD13	2.00	0.61
1:A:168:ASN:HD21	1:A:199:ALA:HA	1.68	0.59
1:A:4:TYR:CE2	1:A:33:ASP:HA	2.38	0.59
1:A:2:SER:O	1:A:3:ASN:CB	2.52	0.57
1:A:217:ASN:ND2	1:A:220:VAL:HG23	2.19	0.57
1:A:241:HIS:O	1:A:242:HIS:CB	2.53	0.57
1:A:84:ASN:HD22	1:A:87:VAL:N	1.92	0.56
1:A:15:PHE:CD2	1:A:50:GLU:HG2	2.41	0.55
1:A:168:ASN:HD21	1:A:200:GLU:N	2.04	0.55
1:A:217:ASN:ND2	1:A:220:VAL:H	2.05	0.53
1:A:109:THR:H	1:A:112:HIS:HD2	1.57	0.52
1:A:33:ASP:HB2	1:A:34:GLN:OE1	2.08	0.52
1:A:218:GLU:O	1:A:222:LYS:HB2	2.10	0.52
1:A:217:ASN:HD21	1:A:220:VAL:HG23	1.75	0.52
1:A:107:GLY:O	1:A:137:ASP:HA	2.10	0.51
1:A:121:GLU:HG3	2:A:401:HOH:O	2.10	0.51
1:A:85:LEU:HD22	1:A:121:GLU:HB3	1.91	0.51
1:A:241:HIS:O	1:A:242:HIS:HB2	2.11	0.50
1:A:139:PHE:HA	1:A:172:LYS:HG3	1.94	0.49
1:A:152:SER:OG	1:A:155:LEU:HD23	2.13	0.49
1:A:167:VAL:N	1:A:243:HIS:NE2	2.57	0.48
1:A:224:PHE:CE1	1:A:228:VAL:HG11	2.48	0.48
1:A:242:HIS:C	1:A:243:HIS:ND1	2.67	0.47
1:A:28:LEU:N	1:A:28:LEU:HD12	2.28	0.47
1:A:140:ASN:ND2	1:A:172:LYS:HG2	2.29	0.47
1:A:242:HIS:O	1:A:243:HIS:CB	2.64	0.46
1:A:160:CYS:HB3	1:A:197:TYR:CD1	2.50	0.46
1:A:242:HIS:O	1:A:243:HIS:CG	2.68	0.46
1:A:243:HIS:N	1:A:243:HIS:HD1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:HIS:HE1	1:A:141:GLN:O	1.98	0.45
1:A:84:ASN:HD21	1:A:86:GLU:HB2	1.81	0.45
1:A:8:GLN:HG2	2:A:301:HOH:O	2.17	0.45
1:A:167:VAL:N	1:A:243:HIS:CE1	2.58	0.45
1:A:78:ILE:O	1:A:82:VAL:HG23	2.16	0.45
1:A:241:HIS:HB3	2:A:327:HOH:O	2.16	0.45
1:A:151:GLY:HA3	1:A:186:HIS:CG	2.53	0.45
1:A:124:GLN:HG3	1:A:158:LEU:HD11	1.99	0.44
1:A:84:ASN:ND2	1:A:87:VAL:N	2.59	0.44
1:A:140:ASN:HD22	1:A:172:LYS:HG2	1.83	0.43
1:A:211:ALA:O	1:A:214:VAL:HG22	2.18	0.43
1:A:242:HIS:C	1:A:243:HIS:HD1	2.22	0.42
1:A:25:LYS:HE3	1:A:28:LEU:CD2	2.46	0.42
1:A:25:LYS:HG3	1:A:28:LEU:HD13	2.03	0.41
1:A:28:LEU:N	1:A:28:LEU:CD1	2.83	0.41
1:A:7:HIS:HB3	1:A:42:TRP:CD1	2.56	0.41
1:A:101:ASN:HB3	1:A:135:ILE:CD1	2.51	0.41
1:A:17:LYS:HB2	1:A:17:LYS:HE3	1.93	0.41
1:A:18:VAL:O	1:A:22:LEU:CD2	2.63	0.41

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	241/243 (99%)	227 (94%)	12 (5%)	2 (1%)	22 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	A	137	ASP

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	210/210 (100%)	204 (97%)	6 (3%)	48 73

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	PRO
1	A	155	LEU
1	A	200	GLU
1	A	217	ASN
1	A	232	LEU
1	A	243	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	7	HIS
1	A	23	HIS
1	A	41	HIS
1	A	77	HIS
1	A	84	ASN
1	A	112	HIS
1	A	124	GLN
1	A	140	ASN
1	A	168	ASN
1	A	173	GLN
1	A	217	ASN
1	A	219	GLN
1	A	238	HIS

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](#)

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.