



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 13, 2024 – 01:57 am BST

PDB ID : 4ADY
Title : Crystal structure of 26S proteasome subunit Rpn2
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Deposited on : 2012-01-04
Resolution : 2.70 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

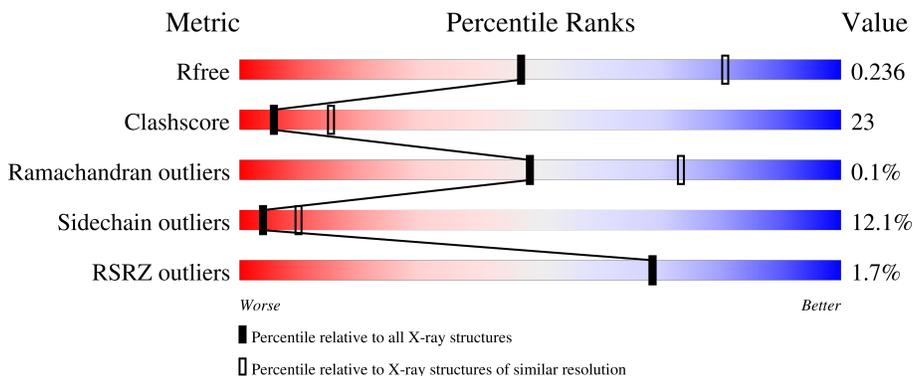
1 Overall quality at a glance

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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (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 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 $\leq 5\%$. 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	963	 % 56% 27% 5% 12%
1	B	963	 2% 50% 28% 6% 17%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 12581 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 26S PROTEASOME REGULATORY SUBUNIT RPN2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	849	6498	4138	1076	1256	8	20	0	0	0
1	B	802	6024	3851	993	1152	8	20	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MSE	-	expression tag	UNP P32565
A	-9	ARG	-	expression tag	UNP P32565
A	-8	GLY	-	expression tag	UNP P32565
A	-7	SER	-	expression tag	UNP P32565
A	-6	HIS	-	expression tag	UNP P32565
A	-5	HIS	-	expression tag	UNP P32565
A	-4	HIS	-	expression tag	UNP P32565
A	-3	HIS	-	expression tag	UNP P32565
A	-2	HIS	-	expression tag	UNP P32565
A	-1	HIS	-	expression tag	UNP P32565
A	0	GLY	-	expression tag	UNP P32565
A	1	SER	-	expression tag	UNP P32565
A	946	LEU	-	expression tag	UNP P32565
A	947	GLN	-	expression tag	UNP P32565
A	948	PRO	-	expression tag	UNP P32565
A	949	SER	-	expression tag	UNP P32565
A	950	LEU	-	expression tag	UNP P32565
A	951	ILE	-	expression tag	UNP P32565
A	952	SER	-	expression tag	UNP P32565
B	-10	MSE	-	expression tag	UNP P32565
B	-9	ARG	-	expression tag	UNP P32565
B	-8	GLY	-	expression tag	UNP P32565
B	-7	SER	-	expression tag	UNP P32565
B	-6	HIS	-	expression tag	UNP P32565
B	-5	HIS	-	expression tag	UNP P32565

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP P32565
B	-3	HIS	-	expression tag	UNP P32565
B	-2	HIS	-	expression tag	UNP P32565
B	-1	HIS	-	expression tag	UNP P32565
B	0	GLY	-	expression tag	UNP P32565
B	1	SER	-	expression tag	UNP P32565
B	946	LEU	-	expression tag	UNP P32565
B	947	GLN	-	expression tag	UNP P32565
B	948	PRO	-	expression tag	UNP P32565
B	949	SER	-	expression tag	UNP P32565
B	950	LEU	-	expression tag	UNP P32565
B	951	ILE	-	expression tag	UNP P32565
B	952	SER	-	expression tag	UNP P32565

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	30	Total O 30 30	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.96Å 148.66Å 114.03Å 90.00° 107.39° 90.00°	Depositor
Resolution (Å)	70.58 – 2.70 70.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (70.58-2.70) 99.8 (70.58-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.183 , 0.240 0.183 , 0.236	Depositor DCC
R_{free} test set	1323 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtrriage
Anisotropy	0.639	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 79.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12581	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [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	0.43	0/6586	0.60	0/8893
1	B	0.41	0/6106	0.59	0/8252
All	All	0.42	0/12692	0.60	0/17145

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	GLU	Peptide
1	A	908	ARG	Sidechain

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	6498	0	6471	249	0
1	B	6024	0	5933	323	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	29	0	0	2	0
2	B	30	0	0	1	0
All	All	12581	0	12404	570	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 23.

The worst 5 of 570 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:918:GLU:CD	1:A:923:MSE:SE	2.38	1.12
1:A:398:ARG:HD3	1:A:438:ASP:HA	1.25	1.11
1:A:919:THR:HG22	1:A:922:GLN:H	1.08	1.09
1:B:371:LEU:HB3	1:B:386:MSE:HE1	1.33	1.08
1:A:570:ARG:HG3	1:A:570:ARG:HH11	1.21	1.05

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	843/963 (88%)	829 (98%)	14 (2%)	0	100	100
1	B	798/963 (83%)	783 (98%)	14 (2%)	1 (0%)	48	73
All	All	1641/1926 (85%)	1612 (98%)	28 (2%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	910	PRO

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	694/792 (88%)	612 (88%)	82 (12%)	4 10
1	B	623/792 (79%)	546 (88%)	77 (12%)	4 9
All	All	1317/1584 (83%)	1158 (88%)	159 (12%)	4 10

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	257	ILE
1	B	600	THR
1	B	289	ILE
1	B	398	ARG
1	B	728	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	300	ASN
1	B	681	ASN
1	B	329	HIS
1	B	899	ASN
1	B	510	HIS

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 oligosaccharides 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 [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	829/963 (86%)	-0.27	5 (0%) 85 85	40, 73, 114, 144	0
1	B	782/963 (81%)	-0.13	23 (2%) 54 52	35, 80, 136, 173	0
All	All	1611/1926 (83%)	-0.20	28 (1%) 69 68	35, 75, 129, 173	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	LEU	3.0
1	A	4	THR	3.0
1	B	789	GLU	2.9
1	B	884	PHE	2.8
1	B	149	GLU	2.7

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 monosaccharides 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.