



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 25, 2022 – 06:07 PM JST

PDB ID : 7XI3
Title : Crystal Structure of the NPAS4-ARNT2 heterodimer in complex with DNA
Authors : Sun, X.N.; Jing, L.Q.; Li, F.W.; Wu, D.L.
Deposited on : 2022-04-11
Resolution : 4.27 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
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

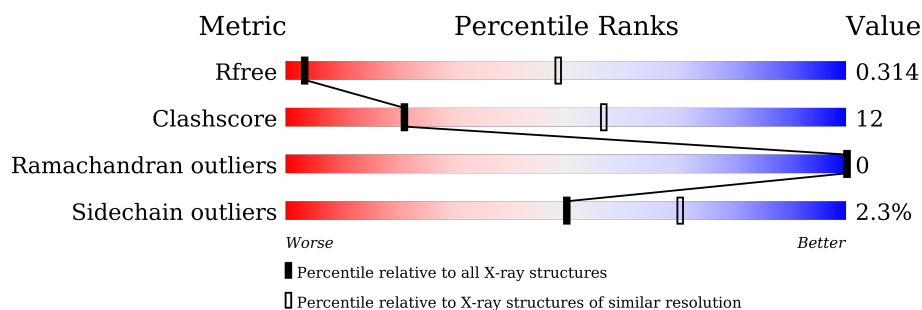
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.27 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}	130704	1001 (4.76-3.80)
Clashscore	141614	1063 (4.76-3.80)
Ramachandran outliers	138981	1018 (4.76-3.80)
Sidechain outliers	138945	1002 (4.76-3.80)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	390	
2	B	348	
3	C	16	
4	D	16	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5436 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 Aryl hydrocarbon receptor nuclear translocator 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2317	1457	412	431	17			

- Molecule 2 is a protein called Neuronal PAS domain protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	314	Total	C	N	O	S	0	0	0
			2463	1567	429	456	11			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*GP*AP*GP*GP*TP*CP*GP*TP*GP*AP*GP*TP*GP*AP*T)-3').

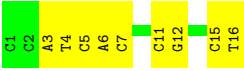
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	16	Total	C	N	O	P	0	0	0
			338	159	66	97	16			

- Molecule 4 is a DNA chain called DNA (5'-D(P*CP*CP*AP*TP*CP*AP*CP*TP*CP*AP*CP*GP*AP*CP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	16	Total	C	N	O	P	0	0	0
			318	152	55	95	16			



● Molecule 4: DNA (5'-D(P*CP*CP*AP*TP*CP*AP*CP*TP*CP*AP*CP*GP*AP*CP*CP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.77Å 72.77Å 415.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.97 – 4.27 25.95 – 4.27	Depositor EDS
% Data completeness (in resolution range)	92.4 (15.97-4.27) 92.2 (25.95-4.27)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 4.25Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.249 , 0.315 0.249 , 0.314	Depositor DCC
R_{free} test set	390 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	5436	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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	0.27	0/2360	0.47	0/3178
2	B	0.28	0/2517	0.48	0/3410
3	C	0.56	0/380	0.92	0/587
4	D	0.58	0/354	0.89	0/541
All	All	0.33	0/5611	0.56	0/7716

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	2317	0	2302	55	0
2	B	2463	0	2443	67	0
3	C	338	0	181	9	0
4	D	318	0	180	6	0
All	All	5436	0	5106	127	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 12.

The worst 5 of 127 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)
2:B:147:PHE:HB2	2:B:327:GLN:HE21	1.07	1.09
1:A:376:PRO:HA	1:A:379:GLN:NE2	1.71	1.06
2:B:147:PHE:HB2	2:B:327:GLN:NE2	1.82	0.93
2:B:147:PHE:CB	2:B:327:GLN:HE21	1.86	0.88
2:B:148:ARG:H	2:B:327:GLN:NE2	1.80	0.78

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	275/390 (70%)	263 (96%)	12 (4%)	0	100	100
2	B	308/348 (88%)	290 (94%)	18 (6%)	0	100	100
All	All	583/738 (79%)	553 (95%)	30 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	263/349 (75%)	257 (98%)	6 (2%)	50	70
2	B	262/286 (92%)	256 (98%)	6 (2%)	50	70
All	All	525/635 (83%)	513 (98%)	12 (2%)	50	70

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	52	LYS
2	B	152	ASN
2	B	298	CYS
2	B	155	LYS
1	A	131	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	128	HIS
2	B	327	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 monosaccharides 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.