



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 7XI3 / pdb_00007xi3
Title : Crystal Structure of the NPAS4-ARNT2 heterodimer in complex with DNA
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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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

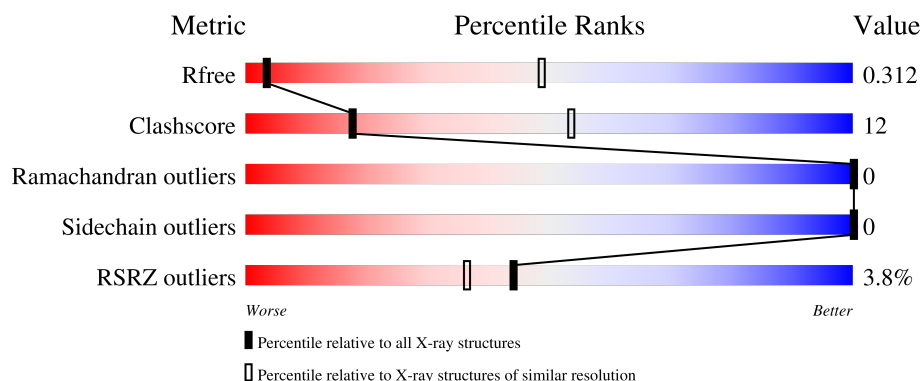
1 Overall quality at a glance

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}	180053	1036 (4.66-3.90)
Clashscore	190562	1081 (4.66-3.90)
Ramachandran outliers	187476	1007 (4.68-3.88)
Sidechain outliers	187428	1034 (4.70-3.86)
RSRZ outliers	180081	1033 (4.66-3.90)

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	390	2% 55% 19% 26%
2	B	348	4% 63% 27% 10%
3	C	16	44% 56%
4	D	16	44% 56%

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			

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

- Chain A:
-
- 2% 55% 19% 26%
- Met
ASP
PHE
ASP
GLU
ASP
GLY
GLU
GLY
PRO
S61
E70
R73
K78
Y82
S87
M89
V90
C93
D101
K102
L103
T104
I105
L106
R107
V110
M113
M116
R117
G118
T118
GLY
ASN
LYS
SER
THR
ASP
GLY
ALA
TYR
K129
P130
L133
T134
F135
C136
- E137
L138
K139
I142
L143
A146
D147
G148
F149
L150
F151
V152
A155
E156
V160
I161
Y162
V170
W178
S181
T182
L183
Y184
E185
L195
L199
K204
SER
MET
THR
GLY
ARG
ILE
LEU
ASP
LYS
LEU
THR
VAL
LYS
LYS
GLU
GLY
GLN
SER
SER
MET
- ARG
MET
CYS
M231
R242
M245
ALA
PRO
LEU
ASP
HIS
LEU
PRO
LEU
ASN
ARG
ILE
THR
THR
MET
SER
ARG
LYS
ARG
PHE
ASN
GLY
LEU
GLY
GLY
PRO
VAL
GLY
GLU
GLY
GLU
M275
Q276
V277
Y286
L286
K287
P290
PRO
ALA
GLY
MET
THR
ILE
PRO
GLU
GLU
ASP
ALA
ASP
VAL
CYS
- GLN
G306
V312
A313
I314
Q318
V319
T320
S321
SER
PRO
VAL
CYS
MET
ASP
MET
SER
GLY
MET
SER
VAL
P334
T335
E336
R340
D351
P352
R353
Q363
L366
H375
P376
Q379
L382
S385
Q388
V389
L392
Q395
Y401
L411
S417
N422
- E429
Y430
C433
N437
V438
K439

- [illegible]

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

Chain C:  44% 56%



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

Chain D:  44% 56%



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 15.97 – 4.27	Depositor EDS
% Data completeness (in resolution range)	92.4 (15.97-4.27) 90.1 (15.97-4.27)	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 0.253 , 0.312	Depositor DCC
R_{free} test set	390 reflections (4.60%)	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)	0.23 , 18.2	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	0.84	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	0.17	0/2360	0.40	0/3178
2	B	0.18	0/2517	0.42	0/3410
3	C	0.21	0/380	0.38	0/587
4	D	0.23	0/354	0.42	0/541
All	All	0.18	0/5611	0.41	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	56	0
2	B	2463	0	2443	68	0
3	C	338	0	181	9	0
4	D	318	0	180	6	0
All	All	5436	0	5106	130	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 130 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%)	263 (100%)	0	100	100
2	B	262/286 (92%)	262 (100%)	0	100	100
All	All	525/635 (83%)	525 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	204	ASN
2	B	15	GLN
2	B	133	GLN
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 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	287/390 (73%)	0.68	9 (3%) 51 40	27, 55, 88, 96	0
2	B	314/348 (90%)	0.71	15 (4%) 35 32	23, 36, 76, 104	0
3	C	16/16 (100%)	0.75	0 100 100	40, 58, 70, 78	0
4	D	16/16 (100%)	0.66	0 100 100	36, 59, 77, 78	0
All	All	633/770 (82%)	0.70	24 (3%) 44 36	23, 46, 83, 104	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	65	PRO	5.4
2	B	60	THR	3.8
2	B	4	SER	3.7
2	B	335	ALA	3.3
2	B	75	GLU	3.1

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 oligosaccharides 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.