

Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2023 – 09:37 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 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
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 <=5%

Mol	Chain	Length	Quality of chain					
1	А	390	54%	19% • 26%				
2	В	348	63%	26% · 10%				
3	С	16	44%	56%				
4	D	16	44%	56%				



2 Entry composition (i)

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	А	287	Total 2317	C 1457	N 412	O 431	S 17	0	0	0

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

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

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

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

• 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*T)-3').

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



3 Residue-property plots (i)

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. 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. 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: Aryl hydrocarbon receptor nuclear translocator 2

• 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%



C1 C2 C2 C2 C5 C5 C5 C11 C11

• 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%
	70	5070



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants	72.77Å 72.77Å 415.27Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	15.97 - 4.27	Depositor
Resolution (A)	25.95 - 4.27	EDS
% Data completeness	92.4 (15.97-4.27)	Depositor
(in resolution range)	92.2(25.95-4.27)	EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$3.54 (at 4.25 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
P. P.	0.249 , 0.315	Depositor
n, n_{free}	0.249 , 0.314	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 $twinning^2$	$ < L >=0.48, < L^2>=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.

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.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond angles		
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.27	0/2360	0.47	0/3178	
2	В	0.28	0/2517	0.48	0/3410	
3	С	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	А	2317	0	2302	55	0
2	В	2463	0	2443	67	0
3	С	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.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom_1	Atom_2	Interatomic	Clash	
Atom-1			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	
1:A:139:LYS:HD2	2:B:65:PRO:HG2	1.66	0.78	
2:B:148:ARG:N	2:B:327:GLN:NE2	2.33	0.77	
3:C:14:DG:H1	4:D:6:DA:H2	1.33	0.75	
2:B:168:LEU:HB2	2:B:195:LEU:HD21	1.68	0.75	
1:A:376:PRO:HA	1:A:379:GLN:HE22	1.50	0.74	
1:A:90:VAL:HG13	1:A:93:CYS:HB3	1.69	0.74	
1:A:133:LEU:HB2	1:A:137:GLU:HG3	1.71	0.73	
2:B:31:GLU:HA	2:B:34:LYS:HB2	1.68	0.73	
2:B:232:VAL:HG12	2:B:244:ARG:HG3	1.70	0.72	
2:B:34:LYS:HA	2:B:37:LEU:HD12	1.72	0.71	
1:A:376:PRO:CA	1:A:379:GLN:NE2	2.53	0.71	
2:B:39:TYR:HA	2:B:42:ILE:HD12	1.73	0.70	
1:A:376:PRO:CA	1:A:379:GLN:HE22	2.04	0.70	
4:D:11:DC:H2"	4:D:12:DG:C8	2.27	0.69	
1:A:152:VAL:HG21	2:B:68:LEU:HG	1.73	0.69	
2:B:146:LEU:HD12	2:B:170:ARG:HB2	1.72	0.69	
1:A:379:GLN:N	1:A:379:GLN:OE1	2.28	0.67	
2:B:24:LYS:HA	2:B:27:LEU:HD12	1.78	0.64	
3:C:7:DC:H2"	3:C:8:DG:C8	2.33	0.64	
1:A:375:HIS:O	1:A:379:GLN:OE1	2.17	0.63	
2:B:225:LYS:HD2	2:B:272:LEU:HD21	1.81	0.62	
2:B:98:SER:OG	2:B:100:SER:OG	2.18	0.60	
2:B:51:ARG:HH12	2:B:93:LYS:HB3	1.66	0.60	
1:A:376:PRO:HA	1:A:379:GLN:CD	2.20	0.59	
1:A:376:PRO:N	1:A:379:GLN:HE22	2.00	0.59	
2:B:148:ARG:NH2	2:B:331:GLU:OE2	2.35	0.59	
1:A:134:THR:HG22	1:A:137:GLU:HG2	1.86	0.58	
1:A:87:SER:HB2	1:A:105:ILE:HD13	1.86	0.57	
1:A:133:LEU:HD13	1:A:137:GLU:HB2	1.85	0.57	
3:C:13:DT:H2"	3:C:14:DG:N7	2.19	0.56	
2:B:224:ALA:HB2	2:B:230:LEU:HD21	1.87	0.55	
2:B:223:HIS:O	2:B:309:ILE:HB	2.06	0.55	
1:A:160:VAL:HG11	1:A:178:TRP:HD1	1.73	0.54	
1:A:411:LEU:HD11	1:A:437:ASN:OD1	2.08	0.54	
2:B:29:LEU:HD22	2:B:110:VAL:HG22	1.89	0.54	
1:A:388:GLN:O	1:A:392:LEU:HG	2.08	0.54	
2:B:225:LYS:HE3	2:B:306:GLU:HA	1.90	0.54	

Continued on next page...



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
4:D:3:DA:H2'	4:D:4:DT:H71	1.90	0.54	
1:A:143:LEU:HD11	1:A:150:LEU:HD12	1.89	0.53	
4:D:4:DT:H2"	4:D:5:DC:C5	2.45	0.52	
2:B:148:ARG:N	2:B:327:GLN:HE22	2.05	0.52	
1:A:242:ARG:HG3	1:A:277:TYR:CE1	2.45	0.52	
1:A:392:LEU:HB3	1:A:395:GLN:HB2	1.91	0.51	
2:B:172:ARG:HG3	2:B:174:HIS:CE1	2.45	0.51	
2:B:236:VAL:HG23	2:B:240:LEU:HD23	1.92	0.51	
2:B:322:TRP:O	2:B:326:GLN:HG2	2.11	0.51	
4:D:6:DA:H2"	4:D:7:DC:O4'	2.12	0.50	
2:B:221:SER:OG	2:B:223:HIS:NE2	2.30	0.49	
1:A:319:VAL:HG12	1:A:321:SER:H	1.77	0.49	
1:A:102:LYS:O	1:A:106:LEU:HD12	2.12	0.49	
1:A:287:LYS:HE2	1:A:290:PRO:HG3	1.95	0.49	
3:C:3:DA:H2'	3:C:4:DG:C8	2.48	0.48	
2:B:41:HIS:CE1	2:B:114:ALA:HB1	2.49	0.48	
1:A:162:TYR:CE2	2:B:65:PRO:HA	2.49	0.47	
1:A:136:GLN:HA	1:A:139:LYS:HE3	1.96	0.47	
1:A:155:ALA:HA	1:A:199:LEU:HD22	1.97	0.47	
1:A:363:GLN:HA	1:A:366:LEU:HD12	1.96	0.47	
1:A:82:TYR:CE2	2:B:44:SER:HB2	2.50	0.47	
3:C:15:DA:H2"	3:C:16:DT:C5	2.50	0.47	
2:B:188:PHE:CE2	2:B:190:ALA:HB2	2.49	0.47	
1:A:336:GLU:O	1:A:353:ARG:HD2	2.15	0.47	
2:B:27:LEU:HD21	2:B:46:ALA:HA	1.96	0.46	
1:A:107:ARG:O	1:A:110:VAL:HG12	2.16	0.46	
1:A:89:MET:HE3	2:B:51:ARG:HD2	1.98	0.46	
1:A:417:SER:HB3	1:A:433:CYS:SG	2.56	0.46	
2:B:153:THR:HG23	2:B:165:LYS:H	1.81	0.46	
2:B:287:GLN:HB2	2:B:293:TRP:CZ3	2.51	0.46	
3:C:3:DA:H2'	3:C:4:DG:H8	1.80	0.46	
2:B:285:ARG:HG2	2:B:295:TRP:CZ3	2.51	0.45	
2:B:169:ILE:HG12	2:B:192:CYS:SG	2.56	0.45	
1:A:422:ASN:HB2	1:A:429:GLU:OE2	2.17	0.45	
2:B:60:THR:O	2:B:62:LEU:N	2.46	0.45	
2:B:11:ALA:O	2:B:15:GLN:HB2	2.16	0.45	
1:A:152:VAL:HG22	1:A:312:VAL:HG22	2.00	0.45	
1:A:340:ARG:HD2	1:A:430:TYR:CE1	2.52	0.45	
1:A:382:LEU:HD21	1:A:401:TYR:HB3	1.99	0.45	
2:B:146:LEU:CD2	2:B:324:LEU:HD12	2.47	0.45	
2:B:81:LEU:HA	2:B:82:PRO:HD3	1.83	0.44	

Continued from previous page...

Continued on next page...



	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:351:ASP:OD2	1:A:353:ARG:HB2	2.18	0.44	
2:B:303:GLU:HB2	2:B:308:PRO:HG2	2.00	0.44	
1:A:148:GLY:HA2	1:A:170:VAL:HG21	1.99	0.44	
2:B:155:LYS:HE3	2:B:155:LYS:HB3	1.88	0.44	
1:A:70:GLU:HG2	1:A:73:ARG:HD2	2.00	0.44	
1:A:78:LYS:HD3	2:B:40:LEU:HD11	1.99	0.44	
2:B:51:ARG:HA	2:B:54:VAL:HG12	1.99	0.44	
2:B:88:PHE:HB3	2:B:94:LEU:HD23	2.00	0.43	
4:D:15:DC:H2'	4:D:16:DT:C6	2.54	0.43	
2:B:151:PHE:O	2:B:164:ASN:HB3	2.18	0.43	
1:A:101:ASP:HB3	1:A:104:THR:OG1	2.17	0.43	
2:B:22:ASN:O	2:B:26:LEU:HG	2.17	0.43	
2:B:242:PHE:CD2	2:B:247:LEU:HD21	2.54	0.43	
1:A:183:LEU:HD23	1:A:195:LEU:HD21	2.01	0.43	
1:A:385:SER:O	1:A:389:VAL:HG23	2.19	0.43	
2:B:146:LEU:HB3	2:B:320:GLU:HB3	2.01	0.42	
2:B:55:PHE:HB2	2:B:182:TRP:CZ2	2.54	0.42	
2:B:253:TYR:HA	2:B:256:LEU:HD12	2.00	0.42	
3:C:15:DA:H2"	3:C:16:DT:C6	2.54	0.42	
1:A:334:PRO:HB2	1:A:335:THR:H	1.66	0.42	
1:A:133:LEU:HD11	1:A:138:LEU:HD13	2.01	0.42	
1:A:138:LEU:O	1:A:142:ILE:HG12	2.20	0.42	
2:B:146:LEU:HA	2:B:169:ILE:O	2.19	0.42	
1:A:129:LYS:HB3	1:A:130:PRO:HD3	2.02	0.42	
1:A:134:THR:HG23	1:A:136:GLN:H	1.84	0.42	
1:A:152:VAL:HG22	1:A:312:VAL:HG13	2.01	0.42	
2:B:55:PHE:HD1	2:B:177:PRO:HG3	1.85	0.42	
2:B:157:LEU:O	2:B:161:SER:OG	2.25	0.42	
2:B:147:PHE:CA	2:B:327:GLN:HE21	2.32	0.42	
1:A:181:SER:HB2	1:A:185:GLU:OE1	2.20	0.41	
2:B:65:PRO:HB2	2:B:68:LEU:HD23	2.01	0.41	
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.81	0.41	
1:A:150:LEU:HD13	2:B:65:PRO:HG3	2.02	0.41	
2:B:24:LYS:HD3	2:B:42:ILE:HD11	2.02	0.41	
2:B:77:ILE:O	2:B:81:LEU:HG	2.21	0.41	
2:B:104:HIS:O	2:B:165:LYS:HD2	2.20	0.41	
3:C:6:DT:H2"	3:C:7:DC:C6	2.55	0.41	
2:B:142:ASP:O	2:B:144:ASP:N	2.52	0.41	
1:A:146:ALA:HB2	2:B:215:PHE:CE2	2.56	0.41	
1:A:287:LYS:NZ	2:B:68:LEU:O	2.50	0.41	
2:B:41:HIS:O	2:B:45:LEU:N	2.54	0.41	

Continued from previous page...

Continued on next page...



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)	
2:B:276:GLY:HA3	2:B:305:PRO:HA	2.02	0.41	
2:B:260:ASP:OD2	2:B:285:ARG:HG3	2.21	0.40	
3:C:14:DG:C6	3:C:15:DA:C6	3.09	0.40	

Continued from previous page...

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	Perce	entiles
1	А	275/390 (70%)	263~(96%)	12 (4%)	0	100	100
2	В	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	Perce	ntiles
1	А	263/349~(75%)	257~(98%)	6(2%)	50	70
2	В	262/286~(92%)	256~(98%)	6 (2%)	50	70
All	All	525/635~(83%)	513~(98%)	12 (2%)	50	70

All (12) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	75	ARG
1	А	93	CYS
1	А	106	LEU
1	А	131	SER
1	А	179	PHE
1	А	196	ARG
2	В	51	ARG
2	В	52	LYS
2	В	152	ASN
2	В	155	LYS
2	В	270	ARG
2	В	298	CYS

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

Mol	Chain	Res	Type
2	В	128	HIS
2	В	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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

