



wwPDB X-ray Structure Validation Summary Report

Feb 10, 2024 – 10:07 PM EST

PDB ID : 2NLL
Title : RETINOID X RECEPTOR-THYROID HORMONE RECEPTOR DNA-BINDING DOMAIN HETERODIMER BOUND TO THYROID RESPONSE ELEMENT DNA
Authors : Rastinejad, F.; Perlmann, T.; Evans, R.M.; Sigler, P.B.
Deposited on : 1996-11-20
Resolution : 1.90 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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

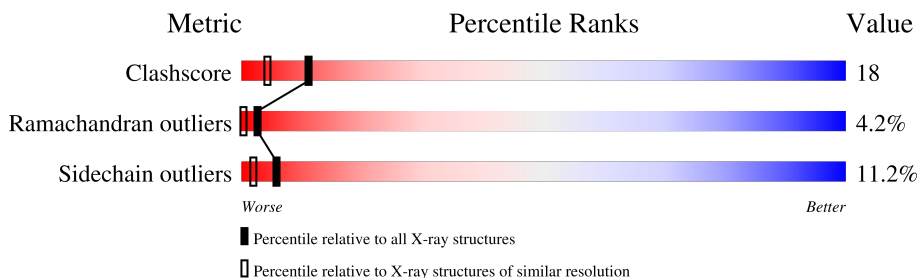
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	18	44% 33% 22%
2	D	18	33% 67%
3	A	66	50% 41% 9%
4	B	103	75% 20% 5%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2351 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 DNA chain called DNA (5'-D(*CP*AP*GP*GP*TP*CP*AP*TP*TP*(5IU)P*CP*AP*GP*GP*TP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	I	N	O				P
1	C	18	367	175	1	67	107	17	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*GP*AP*CP*CP*TP*GP*AP*AP*AP*TP*GP*AP*CP*CP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	18	365	175	68	105	17	0	0	0

- Molecule 3 is a protein called PROTEIN (RETINOIC ACID RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	66	533	323	104	95	11	0	0	0

- Molecule 4 is a protein called PROTEIN (THYROID HORMONE RECEPTOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	103	846	521	159	155	11	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	401	GLU	GLN	conflict	UNP P10828

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Zn 2	0	0
5	B	2	Total 2	Zn 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	58	Total 58	O 58	0	0
6	D	43	Total 43	O 43	0	0
6	A	52	Total 52	O 52	0	0
6	B	83	Total 83	O 83	0	0

3 Residue-property plots

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.

Note EDS was not executed.

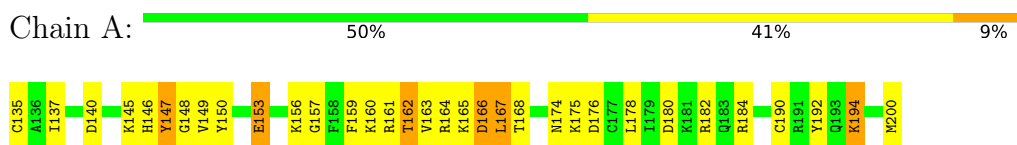
- Molecule 1: DNA (5'-D(*CP*AP*GP*GP*TP*CP*AP*TP*TP*(5IU)P*CP*AP*GP*GP*TP*CP*AP*G)-3')



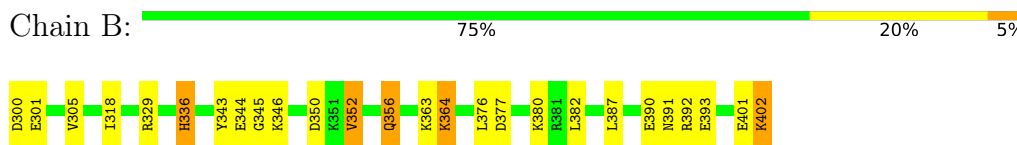
- Molecule 2: DNA (5'-D(*CP*TP*GP*AP*CP*CP*TP*GP*AP*AP*AP*TP*GP*AP*CP*CP*T P*G)-3')



- Molecule 3: PROTEIN (RETINOIC ACID RECEPTOR)



- Molecule 4: PROTEIN (THYROID HORMONE RECEPTOR)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	40.90Å 65.60Å 125.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.90	Depositor
% Data completeness (in resolution range)	87.0 (6.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.206 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2351	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 5IU, ZN

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	C	3.06	40/388 (10.3%)	2.35	31/595 (5.2%)
2	D	2.90	33/409 (8.1%)	2.58	43/629 (6.8%)
3	A	0.52	0/540	0.70	0/713
4	B	0.67	0/856	0.84	0/1136
All	All	1.86	73/2193 (3.3%)	1.68	74/3073 (2.4%)

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	C	0	4
2	D	0	5
All	All	0	9

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	524	DA	N9-C4	14.38	1.46	1.37
1	C	504	DG	P-O5'	13.23	1.73	1.59
1	C	503	DA	P-O5'	12.52	1.72	1.59
1	C	504	DG	O3'-P	11.71	1.75	1.61
1	C	516	DT	C5-C7	-10.33	1.43	1.50

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	521	DC	P-O3'-C3'	19.60	143.22	119.70
1	C	509	DT	P-O3'-C3'	15.71	138.55	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	530	DA	P-O3'-C3'	12.30	134.46	119.70
2	D	529	DA	P-O3'-C3'	12.04	134.14	119.70
1	C	518	DA	P-O3'-C3'	11.35	133.32	119.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	503	DA	Sidechain
1	C	505	DG	Sidechain
1	C	507	DC	Sidechain
1	C	518	DA	Sidechain
2	D	524	DA	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	C	367	0	202	15	0
2	D	365	0	202	8	0
3	A	533	0	518	31	0
4	B	846	0	850	20	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	52	0	0	3	0
6	B	83	0	0	1	0
6	C	58	0	0	0	0
6	D	43	0	0	0	0
All	All	2351	0	1772	68	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 18.

The worst 5 of 68 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)
3:A:175:LYS:HD2	3:A:190:CYS:SG	2.00	1.01
3:A:159:PHE:HB3	6:A:838:HOH:O	1.73	0.89
3:A:148:GLY:HA3	3:A:200:MET:HA	1.56	0.87
3:A:157:GLY:HA2	3:A:160:LYS:HE3	1.54	0.87
4:B:377:ASP:H	4:B:380:LYS:HZ3	1.22	0.84

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	
3	A	64/66 (97%)	48 (75%)	12 (19%)	4 (6%)	1	0
4	B	101/103 (98%)	94 (93%)	4 (4%)	3 (3%)	4	0
All	All	165/169 (98%)	142 (86%)	16 (10%)	7 (4%)	3	0

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	147	TYR
3	A	164	ARG
4	B	301	GLU
4	B	392	ARG
4	B	345	GLY

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	
3	A	58/58 (100%)	50 (86%)	8 (14%)	3	1
4	B	94/94 (100%)	85 (90%)	9 (10%)	8	3
All	All	152/152 (100%)	135 (89%)	17 (11%)	6	2

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	382	LEU
4	B	402	LYS
3	A	194	LYS
4	B	336	HIS
4	B	352	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	185	ASN
4	B	336	HIS
4	B	355	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	5IU	C	511	1,2	18,21,22	1.58	2 (11%)	26,30,33	1.04	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5IU	C	511	1,2	-	0/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	511	5IU	C2-N1	4.71	1.46	1.38
1	C	511	5IU	O3'-C3'	2.71	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	511	5IU	C6-C5-I5	-2.62	116.48	120.97
1	C	511	5IU	C2'-C3'-C4'	2.04	107.01	102.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.