

# Full wwPDB X-ray Structure Validation Report (i)

#### Feb 18, 2024 – 10:05 PM EST

PDB ID	:	4HN6
Title	:	GR DNA Binding Domain R460D/D462R - TSLP nGRE Complex
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Deposited on		
Resolution	:	2.55  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:

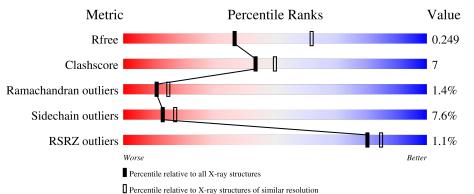
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.55 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	$1284 \ (2.56-2.52)$
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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% 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	Qual	lity of chain		
1	А	114	<sup>2%</sup> 56%	• •	37%	
1	В	114	50%	11% •	37%	
2	С	16	50%	44	4%	6%
3	D	16	38%	62%		



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1799 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 Glucocorticoid receptor.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	72	Total	С	Ν	Ο	S	10	0	0
1	A	12	549	337	105	96	11	10	0	0
1	р	72	Total	С	Ν	Ο	S	0	0	0
1	D	12	553	339	106	97	11	9	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	393	MET	-	expression tag	UNP P04150
А	394	HIS	-	expression tag	UNP P04150
А	395	HIS	-	expression tag	UNP P04150
А	396	HIS	-	expression tag	UNP P04150
А	397	HIS	-	expression tag	UNP P04150
А	398	HIS	-	expression tag	UNP P04150
А	399	HIS	-	expression tag	UNP P04150
А	400	SER	-	expression tag	UNP P04150
А	401	SER	-	expression tag	UNP P04150
А	402	GLY	-	expression tag	UNP P04150
А	403	VAL	-	expression tag	UNP P04150
А	404	ASP	-	expression tag	UNP P04150
А	405	LEU	-	expression tag	UNP P04150
А	406	GLY	-	expression tag	UNP P04150
А	407	THR	-	expression tag	UNP P04150
А	408	GLU	-	expression tag	UNP P04150
А	409	ASN	-	expression tag	UNP P04150
А	410	LEU	-	expression tag	UNP P04150
А	411	TYR	-	expression tag	UNP P04150
А	412	PHE	-	expression tag	UNP P04150
А	413	GLN	-	expression tag	UNP P04150
А	414	SER	-	expression tag	UNP P04150
А	415	ASN	-	expression tag	UNP P04150
А	416	ALA	-	expression tag	UNP P04150
А	460	ASP	ARG	engineered mutation	UNP P04150

There are 52 discrepancies between the modelled and reference sequences:

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Chain	Residue	Modelled	Actual	Comment	Reference
А	462	ARG	ASP	engineered mutation	UNP P04150
В	393	MET	-	expression tag	UNP P04150
В	394	HIS	-	expression tag	UNP P04150
В	395	HIS	-	expression tag	UNP P04150
В	396	HIS	-	expression tag	UNP P04150
В	397	HIS	-	expression tag	UNP P04150
В	398	HIS	-	expression tag	UNP P04150
В	399	HIS	-	expression tag	UNP P04150
В	400	SER	-	expression tag	UNP P04150
В	401	SER	-	expression tag	UNP P04150
В	402	GLY	-	expression tag	UNP P04150
В	403	VAL	-	expression tag	UNP P04150
В	404	ASP	-	expression tag	UNP P04150
В	405	LEU	-	expression tag	UNP P04150
В	406	GLY	-	expression tag	UNP P04150
В	407	THR	-	expression tag	UNP P04150
В	408	GLU	-	expression tag	UNP P04150
В	409	ASN	-	expression tag	UNP P04150
В	410	LEU	-	expression tag	UNP P04150
В	411	TYR	-	expression tag	UNP P04150
В	412	PHE	-	expression tag	UNP P04150
В	413	GLN	-	expression tag	UNP P04150
В	414	SER	-	expression tag	UNP P04150
В	415	ASN	-	expression tag	UNP P04150
В	416	ALA	-	expression tag	UNP P04150
В	460	ASP	ARG	engineered mutation	UNP P04150
В	462	ARG	ASP	engineered mutation	UNP P04150

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• Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*GP\*CP\*CP\*TP\*CP\*CP\*GP\*GP\*GP\*GP\*AP\*GP\*AP\*GP\*CP\*T)-3').

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
2	С	16	Total 325	C 154	N 62	0 94	Р 15	2	0	0

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

Mol	Chain	Residues		Ate	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
3	D	16	Total 325	C 154	N 62	0 94	Р 15	3	0	0



• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total Zn 2 2	0	0
4	В	2	Total Zn 2 2	0	0

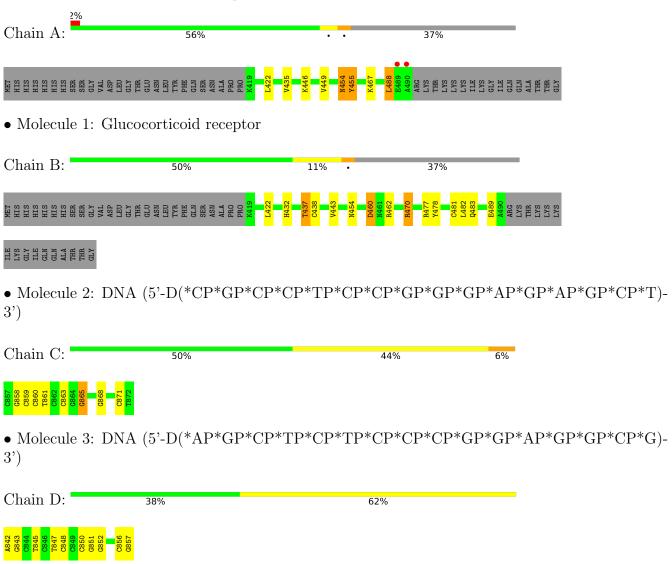
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	9	Total O 9 9	0	0
5	С	10	Total         O           10         10	0	0
5	D	7	Total O 7 7	0	0
5	В	17	Total         O           17         17	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 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.



• Molecule 1: Glucocorticoid receptor



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	38.74Å 87.87Å 103.15Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	44.48 - 2.55	Depositor
Resolution (A)	44.48 - 2.55	EDS
% Data completeness	96.6 (44.48-2.55)	Depositor
(in resolution range)	96.7 (44.48 - 2.55)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.70 (at 2.54 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
$R, R_{free}$	0.195 , $0.248$	Depositor
$10, 10_{free}$	0.200 , $0.249$	DCC
$R_{free}$ test set	1169 reflections $(10.00\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	36.8	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.33 , $42.2$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	1799	wwPDB-VP
Average B, all atoms $(Å^2)$	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.60% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: 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	А	0.43	0/556	0.55	0/742
1	В	0.45	0/560	0.58	0/747
2	С	0.73	0/364	1.45	6/560~(1.1%)
3	D	0.70	0/364	1.35	5/560~(0.9%)
All	All	0.57	0/1844	1.01	11/2609~(0.4%)

There are no bond length outliers.

All (	(11)	bond ang	le outliers	are listed	below:
\	()			0110 110 0 0 0 0	10 01 0 11 1

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	863	DC	O4'-C1'-N1	7.57	113.30	108.00
2	С	859	DC	O4'-C4'-C3'	-6.57	101.87	104.50
2	С	871	DC	O4'-C1'-N1	6.21	112.35	108.00
3	D	850	DC	O4'-C1'-C2'	-5.93	101.15	105.90
3	D	848	DC	C6-N1-C2	5.54	122.52	120.30
2	С	868	DG	C3'-C2'-C1'	-5.51	95.89	102.50
3	D	847	DT	N3-C4-O4	5.35	123.11	119.90
3	D	845	DT	N3-C4-O4	5.31	123.09	119.90
2	С	859	DC	C1'-O4'-C4'	-5.23	104.87	110.10
2	С	865	DG	C1'-O4'-C4'	-5.13	104.97	110.10
3	D	845	DT	C5-C4-O4	-5.03	121.38	124.90

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	549	0	541	6	0
1	В	553	0	547	8	0
2	С	325	0	180	4	0
3	D	325	0	180	3	0
4	А	2	0	0	0	0
4	В	2	0	0	0	0
5	А	9	0	0	1	0
5	В	17	0	0	0	0
5	С	10	0	0	0	0
5	D	7	0	0	0	0
All	All	1799	0	1448	19	0

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.

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 7.

All (19) 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:B:432:HIS:HD2	1:B:437:THR:HG22	1.45	0.81
1:B:432:HIS:CD2	1:B:437:THR:HG22	2.28	0.68
1:A:454:ASN:N	1:A:454:ASN:OD1	2.39	0.55
3:D:842:DA:H2'	3:D:843:DG:C8	2.40	0.55
1:A:422:LEU:HD12	1:A:435:VAL:HG13	1.92	0.52
3:D:851:DG:H2'	3:D:852:DG:C8	2.46	0.50
1:A:449:VAL:HG11	1:A:488:LEU:HD22	1.94	0.49
1:B:470:ARG:HD3	1:B:477:ARG:CZ	2.43	0.49
3:D:856:DC:H2"	3:D:857:DG:C8	2.47	0.48
1:B:437:THR:HG23	1:B:438:CYS:O	2.15	0.46
1:B:460:ASP:O	1:B:462:ARG:N	2.44	0.45
2:C:858:DG:OP1	1:B:470:ARG:HD2	2.17	0.44
1:B:478:TYR:O	1:B:481:CYS:HB2	2.18	0.44
2:C:860:DC:H2'	2:C:861:DT:C6	2.53	0.44
1:B:454:ASN:OD1	1:B:454:ASN:N	2.52	0.42
1:A:454:ASN:CG	1:A:455:TYR:H	2.23	0.42
2:C:860:DC:H2"	2:C:861:DT:H5'	2.00	0.42
1:A:446:LYS:HE3	2:C:865:DG:OP2	2.21	0.40
1:A:467:LYS:HB2	5:A:701:HOH:O	2.21	0.40

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	ntiles
1	А	70/114~(61%)	62~(89%)	6 (9%)	2(3%)	4	4
1	В	70/114~(61%)	65~(93%)	5(7%)	0	100	100
All	All	140/228~(61%)	127~(91%)	11 (8%)	2(1%)	11	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	454	ASN
1	А	455	TYR

#### 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	А	59/96~(62%)	58~(98%)	1 (2%)	60 75
1	В	60/96~(62%)	52 (87%)	8 (13%)	4 3
All	All	119/192~(62%)	110~(92%)	9~(8%)	13 17

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	488	LEU
1	В	422	LEU
1	В	437	THR
1	В	443	VAL

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Mol	Chain	Res	Type
1	В	460	ASP
1	В	470	ARG
1	В	482	LEU
1	В	483	GLN
1	В	489	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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)

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)

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,  $95^{th}$  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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	72/114~(63%)	0.39	2 (2%) 53 60	20, 36, 55, 72	9 (12%)
1	В	72/114~(63%)	0.06	0 100 100	18, 26, 41, 49	6 (8%)
2	С	16/16~(100%)	0.11	0 100 100	38, 47, 51, 52	0
3	D	16/16~(100%)	0.16	0 100 100	33, 41, 58, 59	0
All	All	176/260~(67%)	0.21	2 (1%) 80 85	18, 33, 54, 72	15 (8%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	490	ALA	6.9
1	А	489	GLU	4.7

### 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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
4	ZN	А	601	1/1	0.99	0.12	$35,\!35,\!35,\!35$	0
4	ZN	А	602	1/1	0.99	0.15	20,20,20,20	0
4	ZN	В	601	1/1	0.99	0.13	23,23,23,23	0
4	ZN	В	602	1/1	1.00	0.15	18,18,18,18	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

