



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:36 AM UTC

PDB ID : 8IVX / pdb_00008ivx
Title : Crystal structure of NRP2 in complex with aNRP2-14 Fab fragment
Authors : Geng, Y.; Zhai, L.
Deposited on : 2023-03-29
Resolution : 1.90 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 ⓘ 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
Mogul : 2022.3.0, CSD as543be (2022)
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

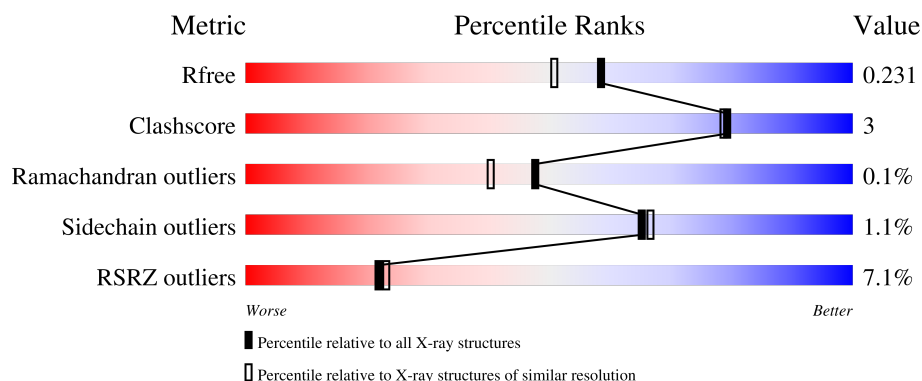
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 $\leq 5\%$. 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	583	
2	H	231	
3	L	215	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6954 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 aNRP2-14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3251	2069	564	602	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	HIS	-	expression tag	UNP O60462
A	14	HIS	-	expression tag	UNP O60462
A	15	HIS	-	expression tag	UNP O60462
A	16	HIS	-	expression tag	UNP O60462
A	17	HIS	-	expression tag	UNP O60462
A	18	HIS	-	expression tag	UNP O60462
A	19	GLU	-	expression tag	UNP O60462
A	20	ASN	-	expression tag	UNP O60462
A	21	LEU	-	expression tag	UNP O60462
A	22	TYR	-	expression tag	UNP O60462
A	23	PHE	-	expression tag	UNP O60462
A	24	GLN	-	expression tag	UNP O60462

- Molecule 2 is a protein called Heavy chain of antibody 14V4 Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1621	1030	263	321	7			

- Molecule 3 is a protein called Light chain of antibody 14V4 Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	1	0
			1662	1034	279	341	8			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	102	Total	O	0	0
			102	102		
5	H	178	Total	O	0	0
			178	178		
5	L	136	Total	O	0	0
			136	136		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.50Å 89.41Å 130.88Å 90.00° 94.18° 90.00°	Depositor
Resolution (Å)	46.65 – 1.90 46.65 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.65-1.90) 97.2 (46.65-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.191 , 0.225 0.199 , 0.231	Depositor DCC
R_{free} test set	4067 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6954	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

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	0.48	0/3335	0.72	0/4522
2	H	0.50	1/1666 (0.1%)	0.73	1/2278 (0.0%)
3	L	0.48	0/1699	0.73	0/2306
All	All	0.48	1/6700 (0.0%)	0.73	1/9106 (0.0%)

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	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	107	MET	SD-CE	-5.79	1.65	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	108	ASP	CA-CB-CG	6.47	119.07	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	239	ARG	Sidechain
1	A	263	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	3251	0	3155	21	0
2	H	1621	0	1575	6	0
3	L	1662	0	1586	9	0
4	H	4	0	6	0	0
5	A	102	0	0	3	0
5	H	178	0	0	0	0
5	L	136	0	0	0	0
All	All	6954	0	6322	34	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 3.

All (34) 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:A:336:LEU:HD11	1:A:468:VAL:HG21	1.74	0.70
1:A:399:HIS:N	1:A:399:HIS:ND1	2.44	0.63
1:A:185:MET:HE1	1:A:268:HIS:CD2	2.38	0.58
1:A:455:THR:HG1	1:A:460:TRP:CD1	2.21	0.58
1:A:381:HIS:N	5:A:602:HOH:O	2.37	0.57
2:H:1:GLN:N	2:H:1:GLN:OE1	2.38	0.55
3:L:36:TYR:OH	3:L:89[A]:GLN:NE2	2.43	0.52
2:H:184:LEU:HD12	2:H:184:LEU:C	2.36	0.51
2:H:107:MET:CE	3:L:89[B]:GLN:OE1	2.58	0.51
2:H:107:MET:HE2	3:L:89[B]:GLN:OE1	2.13	0.48
3:L:196:GLU:HG3	3:L:207:VAL:HG22	1.95	0.48
1:A:284:GLU:OE1	1:A:312:HIS:HD2	1.96	0.48
1:A:173:LEU:HD12	1:A:175:CYS:SG	2.53	0.48
3:L:4:MET:HE3	3:L:23:CYS:SG	2.54	0.47
3:L:138:ASN:HB3	3:L:139:ASN:HD22	1.80	0.47
1:A:184:LYS:NZ	5:A:604:HOH:O	2.49	0.46
1:A:195:ASP:C	1:A:196:LEU:HD23	2.40	0.46
3:L:80:SER:HA	3:L:107:ILE:CD1	2.45	0.46
2:H:50:LEU:C	2:H:50:LEU:HD12	2.42	0.45
1:A:185:MET:HE1	1:A:268:HIS:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ARG:C	1:A:523:LYS:HG2	2.42	0.44
1:A:338:MET:O	1:A:426:GLY:HA3	2.18	0.43
3:L:137:LEU:HD12	3:L:137:LEU:N	2.33	0.43
1:A:523:LYS:HD2	1:A:548:LEU:HD11	2.00	0.43
1:A:373:MET:HB2	1:A:554:HIS:CE1	2.54	0.42
1:A:218:GLY:HA2	1:A:244:ILE:HG23	2.01	0.42
1:A:253:MET:HE3	1:A:253:MET:HB3	1.97	0.42
1:A:521:VAL:HG21	1:A:585:MET:HE3	2.01	0.42
1:A:494:THR:CG2	1:A:495:PRO:HD2	2.50	0.42
3:L:108:LYS:HA	3:L:141:TYR:OH	2.20	0.42
1:A:455:THR:OG1	1:A:456:GLN:N	2.51	0.41
2:H:199:THR:HG23	2:H:216:LYS:HE3	2.01	0.41
1:A:149:CYS:N	5:A:607:HOH:O	2.54	0.40
1:A:441:LEU:HD23	1:A:441:LEU:C	2.47	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	Percentiles	
1	A	391/583 (67%)	372 (95%)	18 (5%)	1 (0%)	36	29
2	H	211/231 (91%)	209 (99%)	2 (1%)	0	100	100
3	L	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
All	All	814/1029 (79%)	792 (97%)	21 (3%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	GLY

5.3.2 Protein sidechains ⓘ

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	355/506 (70%)	349 (98%)	6 (2%)	53	52
2	H	188/200 (94%)	188 (100%)	0	100	100
3	L	190/191 (100%)	188 (99%)	2 (1%)	65	67
All	All	733/897 (82%)	725 (99%)	8 (1%)	65	67

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	LEU
1	A	253	MET
1	A	399	HIS
1	A	428	ARG
1	A	566	ILE
1	A	585	MET
3	L	77	ASN
3	L	200	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	221	HIS
1	A	307	GLN
1	A	312	HIS
1	A	396	ASN
1	A	415	HIS
1	A	436	ASN
1	A	545	GLN
1	A	552	ASN
2	H	13	GLN
2	H	39	GLN
3	L	38	GLN
3	L	53	ASN

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Mol	Chain	Res	Type
3	L	139	ASN
3	L	211	ASN
3	L	213	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](#)

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](#)

1 ligand 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	$\# Z > 2$
4	EDO	H	301	-	3,3,3	0.17	0	2,2,2	0.09	0

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
4	EDO	H	301	-	-	0/1/1/1	-

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	407/583 (69%)	0.83	47 (11%) 9 10	27, 50, 89, 120	0
2	H	215/231 (93%)	0.20	9 (4%) 40 43	22, 31, 55, 91	0
3	L	213/215 (99%)	0.22	3 (1%) 73 76	15, 35, 54, 78	1 (0%)
All	All	835/1029 (81%)	0.51	59 (7%) 22 23	15, 40, 79, 120	1 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	TYR	6.3
1	A	594	TRP	4.8
1	A	428	ARG	4.3
1	A	483	PRO	4.3
1	A	255	VAL	4.2
1	A	230	CYS	4.0
1	A	399	HIS	3.8
1	A	170	PRO	3.7
1	A	474	TRP	3.7
1	A	484	GLY	3.6
1	A	275	PHE	3.6
1	A	322	LEU	3.5
1	A	460	TRP	3.5
1	A	196	LEU	3.3
1	A	543	THR	3.3
1	A	488	LEU	3.2
1	A	476	PRO	3.0
1	A	169	TYR	3.0
1	A	256	ALA	3.0
2	H	178	GLN	2.8
1	A	377	HIS	2.8
1	A	583	ILE	2.7
1	A	253	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	299	TYR	2.6
1	A	475	PHE	2.6
1	A	535	TRP	2.5
1	A	455	THR	2.5
1	A	507	ARG	2.5
2	H	1	GLN	2.5
1	A	336	LEU	2.5
1	A	525	LYS	2.5
1	A	338	MET	2.4
2	H	166	LEU	2.4
2	H	168	SER	2.4
3	L	213	ASN	2.4
1	A	352	THR	2.3
1	A	538	ILE	2.3
1	A	259	GLY	2.3
1	A	471	ARG	2.2
2	H	185	SER	2.2
1	A	274	ASN	2.2
2	H	177	LEU	2.2
1	A	494	THR	2.2
1	A	495	PRO	2.2
2	H	7	SER	2.2
1	A	254	ALA	2.2
2	H	141	SER	2.1
1	A	530	LEU	2.1
1	A	553	MET	2.1
2	H	221	ASP	2.1
1	A	323	ASP	2.1
1	A	167	GLU	2.1
1	A	541	PRO	2.1
3	L	182	LEU	2.1
1	A	465	ALA	2.1
3	L	10	PHE	2.0
1	A	268	HIS	2.0
1	A	173	LEU	2.0
1	A	548	LEU	2.0

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

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](#)

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, 95th 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($\text{\AA}^2$)	Q<0.9
4	EDO	H	301	4/4	0.86	0.15	37,38,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.