



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:46 AM UTC

PDB ID : 3M7F / pdb_00003m7f
Title : Crystal structure of the Nedd4 C2/Grb10 SH2 complex
Authors : Huang, Q.; Szebenyi, M.
Deposited on : 2010-03-16
Resolution : 2.00 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
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

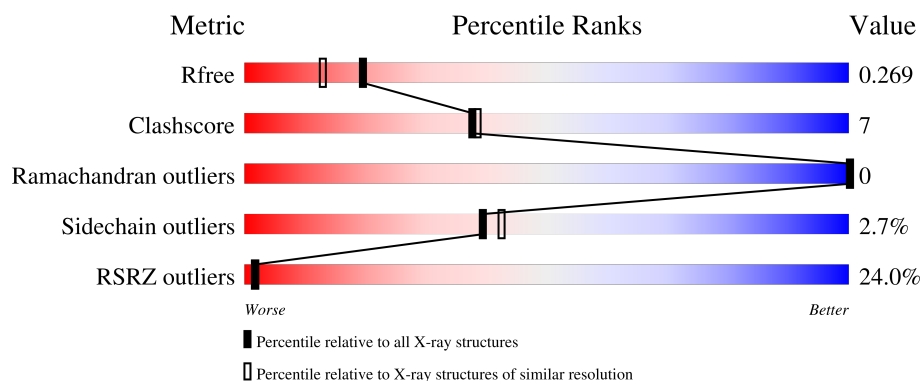
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	108	9% 87% 12%
2	B	176	27% 64% 12% 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2126 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 Growth factor receptor-bound protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	0	0	0
			879	560	163	152	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	SER	THR	SEE REMARK 999	UNP Q60760

- Molecule 2 is a protein called E3 ubiquitin-protein ligase NEDD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	135	Total	C	N	O	S	0	0	0
			1106	719	191	194	2			

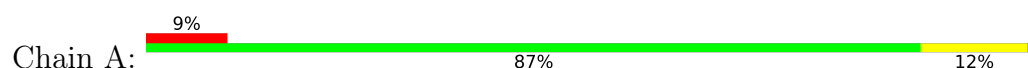
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	79	Total	O	0	0
			79	79		

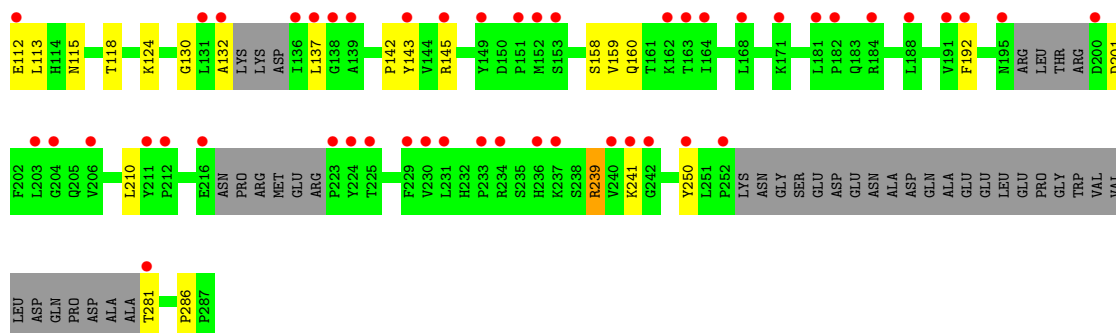
3 Residue-property plots

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 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: Growth factor receptor-bound protein 10



- Molecule 2: E3 ubiquitin-protein ligase NEDD4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.16Å 70.09Å 86.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.12 – 2.00 43.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (43.12-2.00) 95.6 (43.12-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.193 , 0.232 0.253 , 0.269	Depositor DCC
R_{free} test set	1120 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2126	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 6.75% 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

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	0.45	0/900	0.68	0/1210
2	B	0.38	0/1134	0.72	0/1536
All	All	0.41	0/2034	0.70	0/2746

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

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	879	0	871	16	0
2	B	1106	0	1126	13	0
3	A	62	0	0	5	0
3	B	79	0	0	3	2
All	All	2126	0	1997	28	2

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 (28) 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:429:ILE:HG23	1:A:431:ARG:H	1.31	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:HIS:HA	1:A:433:GLN:HG2	1.72	0.70
2:B:145:ARG:HD2	2:B:158:SER:OG	1.95	0.66
2:B:239:ARG:HD3	3:B:53:HOH:O	1.99	0.62
2:B:132:ALA:HB2	2:B:241:LYS:HG2	1.80	0.62
1:A:439:ARG:CZ	3:A:63:HOH:O	2.52	0.57
1:A:503:ASN:HB2	3:A:131:HOH:O	2.05	0.55
2:B:239:ARG:HA	3:B:53:HOH:O	2.11	0.49
1:A:429:ILE:N	3:A:95:HOH:O	2.45	0.49
1:A:439:ARG:NH2	3:A:63:HOH:O	2.45	0.49
2:B:286:PRO:HD2	3:B:58:HOH:O	2.11	0.48
1:A:449:ILE:CD1	1:A:474:THR:HG22	2.46	0.46
2:B:130:GLY:O	2:B:241:LYS:HG3	2.16	0.46
1:A:512:LEU:C	1:A:512:LEU:HD23	2.42	0.45
1:A:433:GLN:OE1	2:B:112:GLU:N	2.51	0.44
2:B:239:ARG:HD3	2:B:239:ARG:HA	1.42	0.43
1:A:429:ILE:HG23	1:A:431:ARG:N	2.14	0.43
1:A:460:LEU:HD12	1:A:460:LEU:C	2.44	0.43
2:B:142:PRO:HA	2:B:192:PHE:O	2.19	0.43
2:B:210:LEU:O	2:B:250:TYR:OH	2.32	0.43
2:B:124:LYS:HE3	2:B:124:LYS:HB3	1.87	0.42
1:A:449:ILE:HD12	1:A:474:THR:HG22	2.00	0.42
1:A:437:HIS:CE1	1:A:533:ARG:HA	2.55	0.42
2:B:115:ASN:HB3	2:B:118:THR:HG23	2.02	0.41
1:A:503:ASN:CB	3:A:131:HOH:O	2.67	0.41
1:A:429:ILE:CG2	1:A:431:ARG:HB2	2.51	0.41
1:A:449:ILE:HG23	1:A:458:LEU:HD23	2.03	0.40
2:B:143:TYR:CD1	2:B:160:GLN:HG3	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:108:HOH:O	3:B:109:HOH:O[2_555]	1.59	0.61
3:B:108:HOH:O	3:B:340:HOH:O[2_555]	1.93	0.27

5.3 Torsion angles

5.3.1 Protein backbone

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	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	B	125/176 (71%)	124 (99%)	1 (1%)	0	100	100
All	All	230/284 (81%)	227 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	98/100 (98%)	98 (100%)	0	100	100
2	B	126/161 (78%)	120 (95%)	6 (5%)	23	21
All	All	224/261 (86%)	218 (97%)	6 (3%)	39	42

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	113	LEU
2	B	137	LEU
2	B	159	VAL
2	B	201	ASP
2	B	239	ARG
2	B	281	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	477	HIS
1	A	485	GLN
2	B	232	HIS
2	B	282	HIS

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

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	107/108 (99%)	1.01	10 (9%) 14 13	20, 31, 54, 63	0
2	B	135/176 (76%)	1.85	48 (35%) 1 1	21, 36, 71, 97	0
All	All	242/284 (85%)	1.48	58 (23%) 2 2	20, 34, 63, 97	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	136	ILE	6.3
2	B	224	TYR	5.2
2	B	192	PHE	4.7
2	B	225	THR	4.3
2	B	137	LEU	4.2
1	A	429	ILE	4.2
2	B	152	MET	4.1
1	A	431	ARG	4.0
2	B	132	ALA	3.9
2	B	200	ASP	3.9
1	A	493	GLY	3.7
2	B	281	THR	3.7
2	B	236	HIS	3.6
2	B	143	TYR	3.6
2	B	131	LEU	3.5
2	B	151	PRO	3.4
2	B	163	THR	3.4
2	B	138	GLY	3.2
2	B	211	TYR	3.2
2	B	231	LEU	3.1
2	B	184	ARG	3.0
2	B	145	ARG	3.0
2	B	229	PHE	2.9
2	B	195	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	490	GLU	2.9
1	A	535	ALA	2.8
2	B	139	ALA	2.8
2	B	233	PRO	2.8
2	B	191	VAL	2.7
2	B	223	PRO	2.7
2	B	241	LYS	2.7
2	B	250	TYR	2.7
1	A	501	ASP	2.6
2	B	181	LEU	2.6
2	B	240	VAL	2.5
2	B	112	GLU	2.5
1	A	503	ASN	2.4
2	B	171	LYS	2.3
2	B	164	ILE	2.3
2	B	252	PRO	2.3
2	B	237	LYS	2.3
2	B	153	SER	2.3
2	B	188	LEU	2.3
2	B	234	ARG	2.2
2	B	149	TYR	2.2
2	B	168	LEU	2.2
2	B	162	LYS	2.2
2	B	216	GLU	2.1
2	B	204	GLY	2.1
2	B	203	LEU	2.1
2	B	182	PRO	2.1
2	B	242	GLY	2.1
1	A	451	GLN	2.0
2	B	212	PRO	2.0
1	A	438	GLY	2.0
1	A	532	ILE	2.0
2	B	206	VAL	2.0
2	B	230	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.