



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:52 PM GMT

PDB ID : 1R1I
Title : STRUCTURAL ANALYSIS OF NEPRILYSIN WITH VARIOUS SPECIFIC AND POTENT INHIBITORS
Authors : Oefner, C.; Roques, B.P.; Fournie-Zaluski, M.C.; Dale, G.E.
Deposited on : 2003-09-24
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

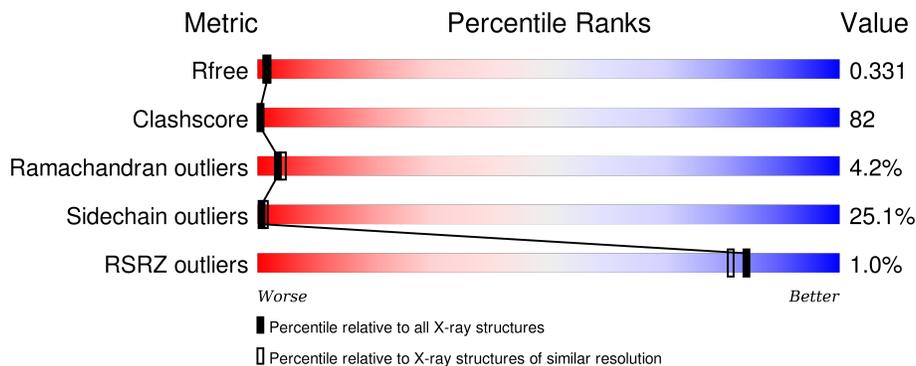
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	696	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TI1	A	2001	X	-	-	-

2 Entry composition [i](#)

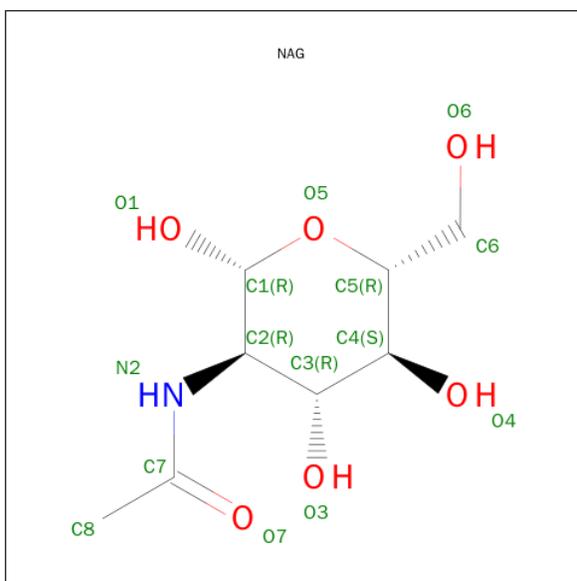
There are 5 unique types of molecules in this entry. The entry contains 5683 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nephilysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	696	5595	3538	957	1074	26	0	0	0

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

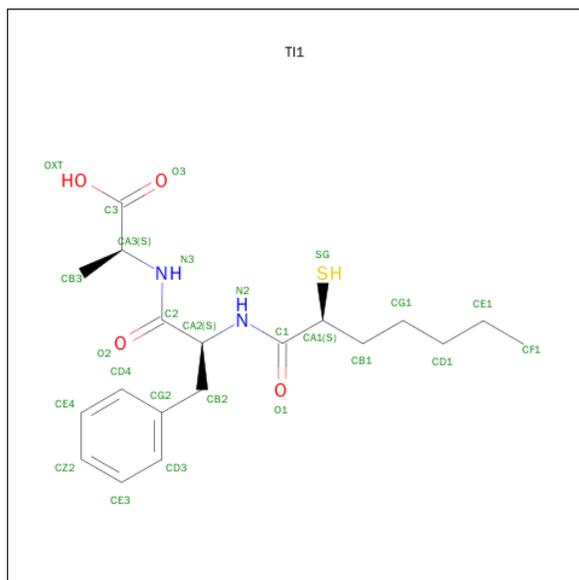


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is [2(R,S)-2-SULFANYLHEPTANOYL]-PHE-ALA (three-letter code: TI1) (formula: C₁₉H₂₈N₂O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 26 19 2 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	19	Total O 19 19	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.84Å 108.84Å 113.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-2.60) 97.2 (19.98-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.45 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.276 , 0.358 0.262 , 0.331	Depositor DCC
R_{free} test set	1186 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.5	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 23536 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5683	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, NAG, TI1

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	0.65	0/5713	0.85	21/7727 (0.3%)

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	23

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	504	ASP	CB-CG-OD2	7.07	124.66	118.30
1	A	631	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	365	ASP	CB-CG-OD2	6.95	124.55	118.30
1	A	489	ASP	CB-CG-OD2	6.83	124.45	118.30
1	A	111	ASP	CB-CG-OD2	6.77	124.39	118.30

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	THR	Peptide
1	A	181	TRP	Peptide
1	A	182	THR	Peptide
1	A	316	ASN	Peptide
1	A	54	GLY	Peptide

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	5595	0	5444	914	4
2	A	42	0	39	1	0
3	A	1	0	0	0	0
4	A	26	0	26	6	0
5	A	19	0	0	2	1
All	All	5683	0	5509	916	5

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 82.

The worst 5 of 916 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:68:LEU:HD22	1:A:687:LEU:CD1	1.29	1.59
1:A:68:LEU:CD2	1:A:687:LEU:CD1	1.88	1.45
1:A:68:LEU:CD2	1:A:687:LEU:HD13	1.45	1.44
1:A:502:LYS:HD2	1:A:505:GLU:OE2	1.22	1.38
1:A:62:ILE:CD1	1:A:63:LYS:N	1.88	1.35

All (5) 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)
5:A:16:HOH:O	5:A:16:HOH:O[4_556]	1.18	1.02
1:A:175:GLN:NE2	1:A:261:LEU:C[6_765]	1.74	0.46
1:A:175:GLN:NE2	1:A:261:LEU:O[6_765]	1.91	0.29
1:A:490:ASN:ND2	1:A:609:GLN:OE1[5_665]	2.02	0.18
1:A:175:GLN:NE2	1:A:261:LEU:CA[6_765]	2.08	0.12

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	694/696 (100%)	584 (84%)	81 (12%)	29 (4%)	3 4

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	TRP
1	A	183	ALA
1	A	269	ALA
1	A	304	LEU
1	A	318	LYS

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	A	605/605 (100%)	453 (75%)	152 (25%)	1 1

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	339	ASN
1	A	419	GLU
1	A	687	LEU
1	A	349	GLU
1	A	369	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	ASN
1	A	550	ASN
1	A	704	ASN
1	A	518	GLN
1	A	570	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	TI1	A	2001	3	21,26,26	0.82	1 (4%)	25,33,33	1.28	3 (12%)
2	NAG	A	752	1	14,14,15	0.69	0	15,19,21	1.76	2 (13%)
2	NAG	A	753	1	14,14,15	0.71	0	15,19,21	1.64	5 (33%)
2	NAG	A	754	1	14,14,15	0.68	0	15,19,21	2.26	4 (26%)

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	TI1	A	2001	3	1/1/6/8	0/23/29/29	0/1/1/1
2	NAG	A	752	1	-	0/6/23/26	0/1/1/1
2	NAG	A	753	1	-	0/6/23/26	0/1/1/1
2	NAG	A	754	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2001	TI1	CA1-C1	-2.16	1.49	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	752	NAG	C1-O5-C5	-6.10	104.51	112.25
2	A	754	NAG	C1-O5-C5	-6.01	104.62	112.25
2	A	754	NAG	C2-N2-C7	-3.80	118.16	123.04
4	A	2001	TI1	CA3-N3-C2	-3.30	118.48	123.04
4	A	2001	TI1	CA2-N2-C1	-3.24	114.36	121.62

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	2001	TI1	CA1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	TI1	6	0
2	A	754	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	696/696 (100%)	-0.16	7 (1%) 84 81	25, 52, 78, 93	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	PRO	2.9
1	A	735	ARG	2.7
1	A	334	ASN	2.7
1	A	564	PHE	2.7
1	A	433	GLY	2.5

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	753	14/15	0.83	0.29	0.76	72,83,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	TI1	A	2001	26/26	0.95	0.14	0.12	35,46,55,56	0
2	NAG	A	752	14/15	0.93	0.15	-	56,62,67,69	0
2	NAG	A	754	14/15	0.87	0.25	-	56,59,69,71	0
3	ZN	A	1001	1/1	0.99	0.02	-	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.