



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:23 pm GMT

PDB ID : 1N1T
Title : Trypanosoma rangeli sialidase in complex with DANA at 1.6 Å
Authors : Amaya, M.F.; Buschiazzi, A.; Nguyen, T.; Alzari, P.M.
Deposited on : 2002-10-20
Resolution : 1.60 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

<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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

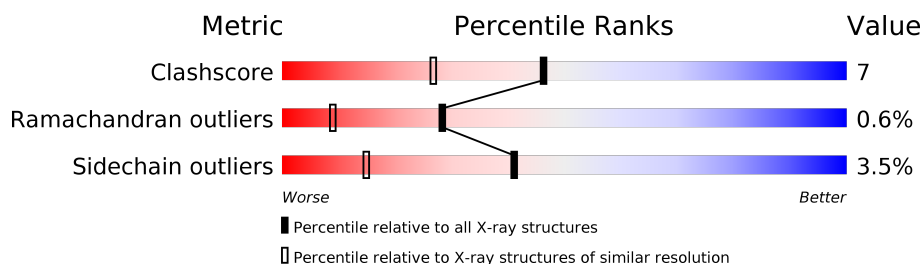
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	641	 87% 9% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5522 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 Sialidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	628	4831	3049	853	913	16	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

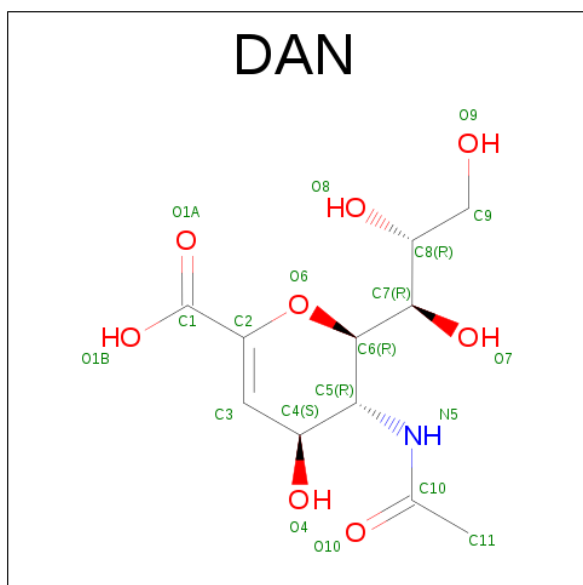
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	CLONING ARTIFACT	UNP O44049
A	2	ALA	-	CLONING ARTIFACT	UNP O44049
A	3	SER	-	CLONING ARTIFACT	UNP O44049
A	53	ILE	THR	SEE REMARK 999	UNP O44049
A	180	VAL	ILE	SEE REMARK 999	UNP O44049
A	189	ALA	GLY	SEE REMARK 999	UNP O44049
A	375	LEU	PHE	SEE REMARK 999	UNP O44049
A	609	VAL	ILE	SEE REMARK 999	UNP O44049

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (three-letter code: DAN) (formula: $C_{11}H_{17}NO_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 4 is water.

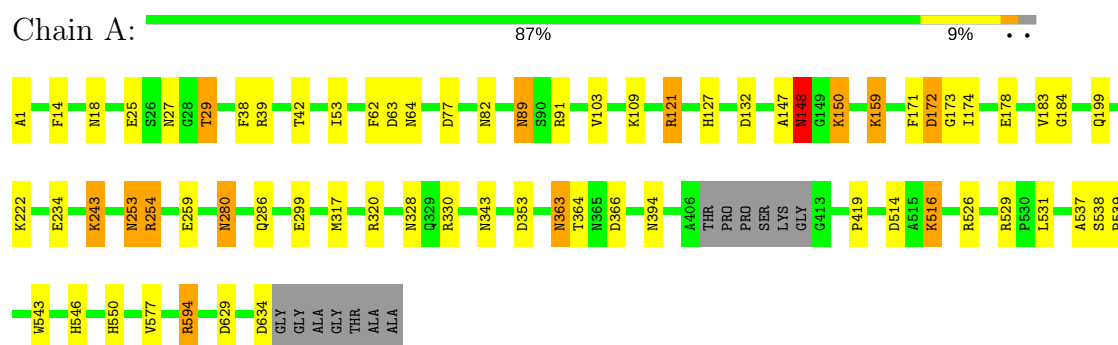
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	661	Total	O	0	0
			661	661		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

• Molecule 1: Sialidase



4 Data and refinement statistics

Xtriage (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	73.94Å 96.26Å 106.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.60	Depositor
% Data completeness (in resolution range)	94.6 (15.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.173 , 0.197	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5522	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: DAN, SO4

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	0.62	0/4937	0.90	10/6710 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ARG	NE-CZ-NH2	12.31	126.46	120.30
1	A	254	ARG	NE-CZ-NH1	-10.90	114.85	120.30
1	A	353	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	634	ASP	N-CA-C	5.67	126.30	111.00
1	A	77	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	63	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	132	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	320	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	629	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	39	ARG	NE-CZ-NH1	-5.05	117.78	120.30

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 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	4831	0	4764	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	0	0	0
3	A	20	0	16	0	0
4	A	661	0	0	10	1
All	All	5522	0	4780	69	1

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 (69) 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:27:ASN:OD1	1:A:29:THR:HG22	1.31	1.23
1:A:394:ASN:HB3	4:A:1407:HOH:O	1.36	1.19
1:A:109:LYS:HE2	4:A:1214:HOH:O	1.52	1.07
1:A:159:LYS:HB2	1:A:159:LYS:NZ	1.62	1.06
1:A:243:LYS:NZ	1:A:259:GLU:HB3	1.79	0.97
1:A:159:LYS:HB2	1:A:159:LYS:HZ2	1.17	0.96
1:A:243:LYS:NZ	1:A:243:LYS:HB3	1.88	0.88
1:A:243:LYS:HZ2	1:A:243:LYS:HB3	1.42	0.83
1:A:253:ASN:HD22	1:A:254:ARG:H	1.26	0.81
1:A:27:ASN:OD1	1:A:29:THR:CG2	2.24	0.79
1:A:148:ASN:O	1:A:148:ASN:ND2	2.14	0.77
1:A:159:LYS:CB	1:A:159:LYS:NZ	2.44	0.74
1:A:363:ASN:HD21	1:A:366:ASP:H	1.37	0.73
1:A:53:ILE:HD13	1:A:103:VAL:HG21	1.73	0.71
1:A:531:LEU:HD23	1:A:537:ALA:CB	2.22	0.70
1:A:317:MET:CE	1:A:343:ASN:HD21	2.05	0.69
1:A:109:LYS:CE	4:A:1214:HOH:O	2.22	0.69
1:A:243:LYS:HZ2	1:A:259:GLU:HB3	1.56	0.69
1:A:89:ASN:HD22	1:A:91:ARG:H	1.39	0.69
1:A:317:MET:CE	1:A:343:ASN:ND2	2.57	0.67
1:A:317:MET:HE1	1:A:343:ASN:ND2	2.10	0.66
1:A:243:LYS:CE	1:A:259:GLU:HB3	2.26	0.64
1:A:243:LYS:HD3	4:A:1175:HOH:O	1.98	0.63
1:A:363:ASN:C	1:A:363:ASN:HD22	2.03	0.62
1:A:531:LEU:HD23	1:A:537:ALA:HB1	1.83	0.60
1:A:546:HIS:HD2	4:A:1043:HOH:O	1.84	0.60
1:A:253:ASN:HD22	1:A:254:ARG:N	2.01	0.58
1:A:529:ARG:CZ	1:A:539:PRO:HG3	2.34	0.58
1:A:171:PHE:O	1:A:172:ASP:C	2.42	0.58
1:A:531:LEU:CD2	1:A:537:ALA:CB	2.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LYS:CB	1:A:243:LYS:NZ	2.58	0.57
1:A:243:LYS:HZ1	1:A:259:GLU:HB3	1.65	0.57
1:A:1:ALA:N	4:A:1081:HOH:O	2.38	0.56
1:A:82:ASN:ND2	4:A:1378:HOH:O	2.37	0.56
1:A:253:ASN:ND2	1:A:254:ARG:H	2.02	0.56
1:A:89:ASN:ND2	1:A:91:ARG:H	2.05	0.55
1:A:89:ASN:HD21	1:A:91:ARG:HD3	1.73	0.54
1:A:199:GLN:NE2	1:A:234:GLU:H	2.07	0.52
1:A:150:LYS:HB2	1:A:150:LYS:NZ	2.24	0.52
1:A:531:LEU:HD23	1:A:537:ALA:HB2	1.91	0.52
1:A:243:LYS:HE3	1:A:259:GLU:HB3	1.92	0.51
1:A:317:MET:HE3	1:A:343:ASN:ND2	2.24	0.51
1:A:243:LYS:HZ3	1:A:243:LYS:HB3	1.74	0.50
1:A:127:HIS:HD2	1:A:178:GLU:OE2	1.95	0.50
1:A:514:ASP:O	1:A:516:LYS:HE2	2.11	0.50
1:A:280:ASN:ND2	1:A:286:GLN:H	2.10	0.49
1:A:317:MET:HE3	1:A:343:ASN:HD21	1.75	0.49
1:A:550:HIS:HE1	4:A:812:HOH:O	1.95	0.48
1:A:171:PHE:O	1:A:174:ILE:N	2.47	0.48
1:A:531:LEU:CD2	1:A:537:ALA:HB2	2.44	0.48
1:A:363:ASN:HD22	1:A:364:THR:N	2.12	0.47
1:A:363:ASN:C	1:A:363:ASN:ND2	2.68	0.46
1:A:363:ASN:HD21	1:A:366:ASP:N	2.10	0.46
1:A:363:ASN:ND2	1:A:366:ASP:H	2.09	0.44
1:A:159:LYS:HZ3	1:A:159:LYS:HB2	1.69	0.44
1:A:14:PHE:HB3	1:A:38:PHE:CG	2.53	0.43
1:A:62:PHE:CE1	1:A:64:ASN:HB2	2.54	0.43
1:A:594:ARG:HD3	1:A:594:ARG:O	2.19	0.43
1:A:538:SER:HA	1:A:539:PRO:HD3	1.87	0.42
1:A:147:ALA:O	1:A:148:ASN:C	2.58	0.42
1:A:280:ASN:HD21	1:A:286:GLN:H	1.68	0.42
1:A:89:ASN:C	1:A:89:ASN:HD22	2.22	0.42
1:A:171:PHE:O	1:A:173:GLY:N	2.54	0.41
1:A:526:ARG:HA	1:A:543:TRP:CZ2	2.55	0.41
1:A:121:ARG:NH2	4:A:1219:HOH:O	2.44	0.41
1:A:529:ARG:NE	1:A:539:PRO:HG3	2.35	0.41
1:A:25:GLU:HB2	1:A:29:THR:HG23	2.03	0.40
1:A:516:LYS:HE3	4:A:1310:HOH:O	2.21	0.40
1:A:42:THR:OG1	1:A:184:GLY:HA2	2.21	0.40

All (1) 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)
4:A:1077:HOH:O	4:A:1249:HOH:O[4_445]	2.19	0.01

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	624/641 (97%)	595 (95%)	25 (4%)	4 (1%)	28 9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	ASP
1	A	183	VAL
1	A	18	ASN
1	A	148	ASN

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	520/531 (98%)	502 (96%)	18 (4%)	41 15

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	89	ASN

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Mol	Chain	Res	Type
1	A	121	ARG
1	A	148	ASN
1	A	150	LYS
1	A	159	LYS
1	A	222	LYS
1	A	243	LYS
1	A	253	ASN
1	A	280	ASN
1	A	299	GLU
1	A	328	ASN
1	A	330	ARG
1	A	363	ASN
1	A	419	PRO
1	A	516	LYS
1	A	577	VAL
1	A	594	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	127	HIS
1	A	199	GLN
1	A	253	ASN
1	A	276	HIS
1	A	280	ASN
1	A	343	ASN
1	A	363	ASN
1	A	546	HIS
1	A	550	HIS
1	A	608	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

3 ligands are 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	$\# Z > 2$
3	DAN	A	700	-	17,20,20	3.92	4 (23%)	18,28,28	1.70	2 (11%)
2	SO4	A	801	-	4,4,4	0.15	0	6,6,6	0.30	0
2	SO4	A	802	-	4,4,4	0.20	0	6,6,6	0.30	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
3	DAN	A	700	-	-	0/14/34/34	0/1/1/1
2	SO4	A	801	-	-	0/0/0/0	0/0/0/0
2	SO4	A	802	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	DAN	O6-C2	-5.86	1.27	1.37
3	A	700	DAN	C4-C3	2.44	1.53	1.50
3	A	700	DAN	O10-C10	6.18	1.37	1.23
3	A	700	DAN	C3-C2	13.28	1.49	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	DAN	C4-C3-C2	-5.55	112.22	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	700	DAN	O10-C10-C11	-2.12	118.21	122.06

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.