



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 03:44 PM EDT

PDB ID : 2NZ8
Title : N-terminal DHPH cassette of Trio in complex with nucleotide-free Rac1
Authors : Chhatriwala, M.K.; Betts, L.; Worthylake, D.K.; Sondek, J.
Deposited on : unknown
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

<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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

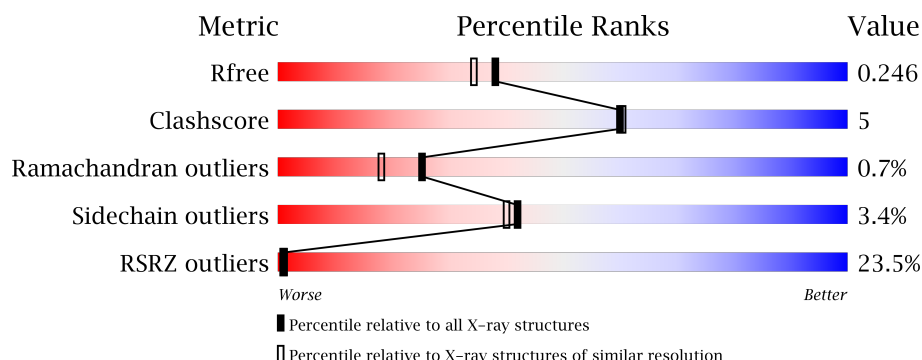
1 Overall quality at a glance

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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 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	177	<div> <div>11%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>•</div> </div> </div>
2	B	313	<div> <div>28%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3905 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 ras-related C3 botulinum toxin substrate 1 isoform Rac1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1383	889	228	258	8			

- Molecule 2 is a protein called triple functional domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	279	Total	C	N	O	S	0	0	0
			2280	1457	375	433	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1223	GLY	-	CLONING ARTIFACT	UNP O75962
B	1224	ALA	-	CLONING ARTIFACT	UNP O75962
B	1225	MET	-	INITIATING METHIONINE	UNP O75962

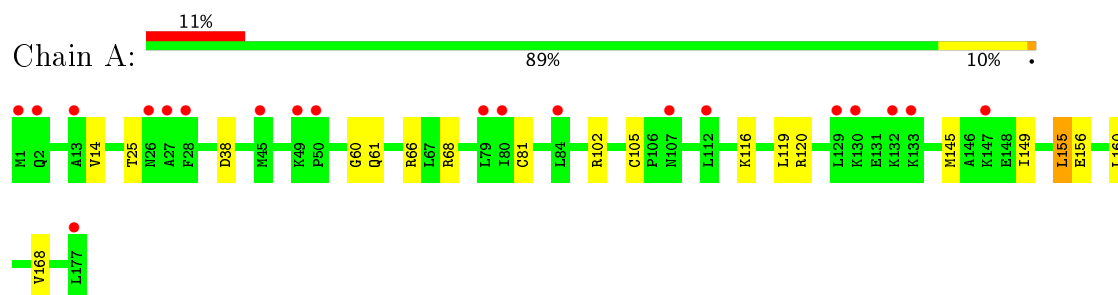
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total	O	0	0
			110	110		
3	B	132	Total	O	0	0
			132	132		

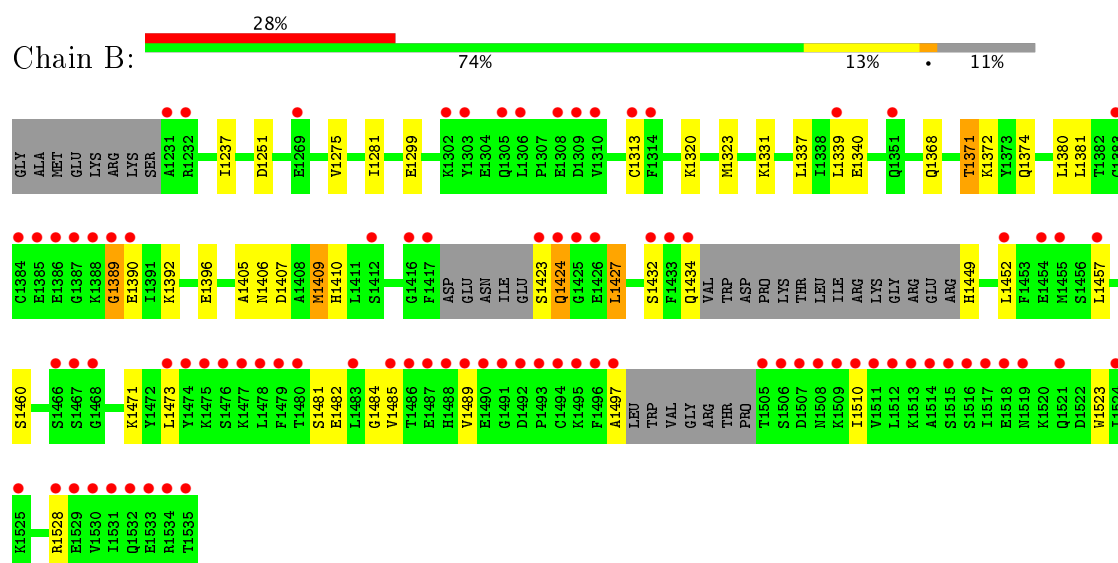
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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: ras-related C3 botulinum toxin substrate 1 isoform Rac1



- Molecule 2: triple functional domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.49 Å 108.56 Å 53.42 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.41 – 2.00 19.41 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.41-2.00) 99.6 (19.41-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.01 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.223 , 0.249 0.223 , 0.246	Depositor DCC
R_{free} test set	1968 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3905	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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 [i](#)

5.1 Standard geometry [i](#)

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	0/1413	0.62	0/1922
2	B	0.59	3/2322 (0.1%)	0.54	0/3117
All	All	0.54	3/3735 (0.1%)	0.57	0/5039

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1482	GLU	CD-OE1	13.10	1.40	1.25
2	B	1482	GLU	CD-OE2	13.08	1.40	1.25
2	B	1434	GLN	C-O	6.92	1.36	1.23

There are no bond angle outliers.

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	1383	0	1405	18	0
2	B	2280	0	2265	27	0
3	A	110	0	0	3	0
3	B	132	0	0	2	0
All	All	3905	0	3670	39	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 5.

All (39) 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:66:ARG:H	2:B:1406:ASN:HD21	1.08	1.01
1:A:38:ASP:OD2	3:A:2199:HOH:O	2.06	0.73
1:A:105:CYS:SG	3:A:2139:HOH:O	2.48	0.71
1:A:66:ARG:H	2:B:1406:ASN:ND2	1.87	0.67
2:B:1251:ASP:OD1	3:B:2156:HOH:O	2.13	0.65
1:A:61:GLN:HG3	2:B:1371:THR:HG21	1.79	0.64
2:B:1368:GLN:O	2:B:1372:LYS:HG2	1.97	0.63
2:B:1485:VAL:HG21	2:B:1528:ARG:HH21	1.64	0.62
2:B:1281:ILE:HG13	2:B:1337:LEU:HD23	1.86	0.58
2:B:1389:GLY:O	2:B:1390:GLU:HB2	2.04	0.57
1:A:145:MET:CE	1:A:149:ILE:HG23	2.35	0.57
2:B:1405:ALA:O	2:B:1409:MET:HG2	2.05	0.56
1:A:155:LEU:HD23	1:A:168:VAL:HA	1.88	0.55
1:A:145:MET:HE1	1:A:149:ILE:HG23	1.89	0.55
1:A:68:ARG:NH2	3:A:2133:HOH:O	2.04	0.54
2:B:1484:GLY:HA3	2:B:1497:ALA:HB3	1.90	0.52
1:A:116:LYS:HB3	1:A:119:LEU:HD23	1.92	0.51
2:B:1407:ASP:HB3	2:B:1427:LEU:HD13	1.94	0.50
1:A:14:VAL:HG11	1:A:81:CYS:CB	2.42	0.50
1:A:61:GLN:CG	2:B:1371:THR:HG21	2.40	0.50
2:B:1432:SER:HA	2:B:1449:HIS:HA	1.93	0.50
1:A:102:ARG:HA	1:A:102:ARG:HE	1.76	0.49
2:B:1299:GLU:HB3	2:B:1313:CYS:SG	2.54	0.48
2:B:1485:VAL:HG21	2:B:1528:ARG:NH2	2.30	0.47
1:A:66:ARG:HG2	2:B:1410:HIS:NE2	2.30	0.46
2:B:1423:SER:HA	2:B:1424:GLN:HA	1.59	0.46
1:A:60:GLY:C	2:B:1371:THR:HG23	2.37	0.45
2:B:1424:GLN:O	2:B:1424:GLN:HG2	2.16	0.45
2:B:1237:ILE:HG21	2:B:1380:LEU:HG	1.99	0.45
1:A:14:VAL:HG11	1:A:81:CYS:HB3	2.00	0.43
2:B:1392:LYS:O	2:B:1396:GLU:HG3	2.19	0.43
2:B:1339:LEU:HD12	2:B:1340:GLU:HG2	2.00	0.43
1:A:14:VAL:HG11	1:A:81:CYS:HB2	2.01	0.42
2:B:1320:LYS:O	2:B:1323:MET:HG2	2.19	0.42
1:A:120:ARG:NH2	1:A:156:GLU:OE2	2.47	0.41
2:B:1409:MET:HG2	2:B:1409:MET:H	1.76	0.41
2:B:1510:ILE:HD13	3:B:2232:HOH:O	2.21	0.41
2:B:1452:LEU:HD23	2:B:1457:LEU:HG	2.03	0.40
2:B:1452:LEU:HB2	2:B:1523:TRP:CZ3	2.56	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	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
2	B	271/313 (87%)	260 (96%)	8 (3%)	3 (1%)	17	9
All	All	446/490 (91%)	431 (97%)	12 (3%)	3 (1%)	25	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1481	SER
2	B	1489	VAL
2	B	1389	GLY

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	153/153 (100%)	150 (98%)	3 (2%)	60	64
2	B	255/285 (90%)	244 (96%)	11 (4%)	33	29
All	All	408/438 (93%)	394 (97%)	14 (3%)	42	40

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	THR
1	A	155	LEU
1	A	160	LEU
2	B	1275	VAL
2	B	1331	LYS
2	B	1371	THR
2	B	1374	GLN
2	B	1381	LEU
2	B	1409	MET
2	B	1424	GLN
2	B	1427	LEU
2	B	1460	SER
2	B	1471	LYS
2	B	1473	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1286	GLN
2	B	1294	ASN
2	B	1353	HIS
2	B	1374	GLN
2	B	1406	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](#)

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	177/177 (100%)	0.44	20 (11%) 6 6	23, 36, 63, 80	0
2	B	279/313 (89%)	1.84	87 (31%) 0 1	23, 45, 224, 402	5 (1%)
All	All	456/490 (93%)	1.30	107 (23%) 1 1	23, 40, 198, 402	5 (1%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1509	LYS	21.7
2	B	1492	ASP	15.2
2	B	1389	GLY	12.9
2	B	1493	PRO	12.7
2	B	1534	ARG	12.3
2	B	1491	GLY	11.5
2	B	1488	HIS	11.0
2	B	1505	THR	10.6
2	B	1510	ILE	10.0
2	B	1485	VAL	9.9
2	B	1535	THR	9.7
2	B	1511	VAL	9.3
2	B	1387	GLY	9.1
2	B	1490	GLU	8.7
2	B	1507	ASP	8.5
2	B	1530	VAL	7.3
2	B	1518	GLU	7.2
2	B	1386	GLU	6.7
2	B	1480	THR	6.6
2	B	1489	VAL	6.6
2	B	1385	GLU	6.5
2	B	1517	ILE	6.4
1	A	26	ASN	6.1
2	B	1479	PHE	6.0

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Mol	Chain	Res	Type	RSRZ
2	B	1433	PHE	5.7
2	B	1519	ASN	5.4
2	B	1506	SER	5.2
2	B	1417	PHE	5.2
2	B	1308	GLU	5.2
2	B	1478	LEU	5.2
2	B	1532	GLN	4.9
2	B	1483	LEU	4.8
2	B	1494	CYS	4.7
2	B	1486	THR	4.7
2	B	1454	GLU	4.7
2	B	1388	LYS	4.5
2	B	1515	SER	4.4
2	B	1529	GLU	4.4
2	B	1384	CYS	4.3
2	B	1477	LYS	4.3
2	B	1508	ASN	4.2
2	B	1467	SER	4.2
1	A	1	MET	4.1
2	B	1513	LYS	3.9
2	B	1434	GLN	3.9
2	B	1516	SER	3.9
2	B	1303	TYR	3.9
2	B	1533	GLU	3.8
2	B	1512	LEU	3.7
2	B	1495	LYS	3.6
2	B	1468	GLY	3.6
1	A	27	ALA	3.6
2	B	1496	PHE	3.5
2	B	1412	SER	3.5
2	B	1457	LEU	3.4
2	B	1432	SER	3.3
2	B	1531	ILE	3.3
2	B	1383	CYS	3.3
2	B	1426	GLU	3.3
2	B	1476	SER	3.3
2	B	1521	GLN	3.3
2	B	1514	ALA	3.3
2	B	1474	TYR	3.3
1	A	50	PRO	3.3
2	B	1475	LYS	3.2
1	A	107	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	1416	GLY	3.1
2	B	1231	ALA	3.0
2	B	1310	VAL	2.9
2	B	1455	MET	2.9
2	B	1232	ARG	2.9
1	A	79	LEU	2.8
2	B	1452	LEU	2.8
1	A	177	LEU	2.8
2	B	1302	LYS	2.8
1	A	49	LYS	2.7
1	A	80	ILE	2.7
2	B	1423	SER	2.7
2	B	1425	GLY	2.7
2	B	1390	GLU	2.7
1	A	147	LYS	2.7
1	A	45	MET	2.6
2	B	1309	ASP	2.5
2	B	1339	LEU	2.5
1	A	132	LYS	2.5
2	B	1313	CYS	2.4
1	A	13	ALA	2.4
1	A	133	LYS	2.4
2	B	1314	PHE	2.4
1	A	112	LEU	2.3
2	B	1424	GLN	2.3
2	B	1528	ARG	2.3
1	A	28	PHE	2.3
2	B	1269	GLU	2.3
2	B	1487	GLU	2.3
1	A	84	LEU	2.2
2	B	1466	SER	2.2
2	B	1351	GLN	2.2
1	A	2	GLN	2.1
1	A	129	LEU	2.1
1	A	130	LYS	2.1
2	B	1473	LEU	2.1
2	B	1525	LYS	2.1
2	B	1305	GLN	2.0
2	B	1497	ALA	2.0
2	B	1524	ILE	2.0
2	B	1306	LEU	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.