Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 04:08 PM EDT

PDB ID	:	4C9R
Title	:	Xenopus ZNRF3 ectodomain in complex with Xenopus RSPO2 Fu1-Fu2 crystal form I
Authors	:	Zebisch, M.; Jones, E.Y.
Deposited on	:	2013-10-02
Resolution	:	2.10 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:

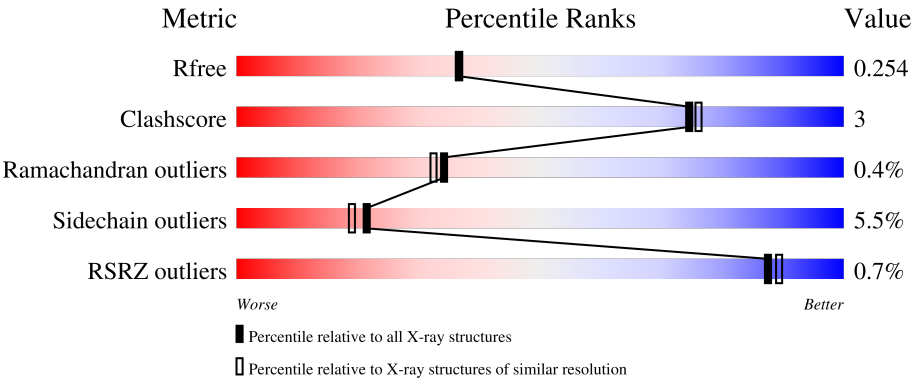
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	182	82% 12%
1	C	182	84% 12%
2	B	121	75% 10% 13%
2	D	121	76% 12% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4365 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 E3 UBIQUITIN-PROTEIN LIGASE ZNRF3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1243	776	219	241	7			
1	C	161	Total	C	N	O	S	0	0	0
			1233	772	217	237	7			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLU	-	expression tag	UNP Q08D68
A	23	THR	-	expression tag	UNP Q08D68
A	192	GLY	-	expression tag	UNP Q08D68
A	193	THR	-	expression tag	UNP Q08D68
A	194	HIS	-	expression tag	UNP Q08D68
A	195	HIS	-	expression tag	UNP Q08D68
A	196	HIS	-	expression tag	UNP Q08D68
A	197	HIS	-	expression tag	UNP Q08D68
A	198	HIS	-	expression tag	UNP Q08D68
A	199	HIS	-	expression tag	UNP Q08D68
A	200	HIS	-	expression tag	UNP Q08D68
A	201	HIS	-	expression tag	UNP Q08D68
A	202	HIS	-	expression tag	UNP Q08D68
A	203	HIS	-	expression tag	UNP Q08D68
C	22	GLU	-	expression tag	UNP Q08D68
C	23	THR	-	expression tag	UNP Q08D68
C	192	GLY	-	expression tag	UNP Q08D68
C	193	THR	-	expression tag	UNP Q08D68
C	194	HIS	-	expression tag	UNP Q08D68
C	195	HIS	-	expression tag	UNP Q08D68
C	196	HIS	-	expression tag	UNP Q08D68
C	197	HIS	-	expression tag	UNP Q08D68
C	198	HIS	-	expression tag	UNP Q08D68
C	199	HIS	-	expression tag	UNP Q08D68
C	200	HIS	-	expression tag	UNP Q08D68

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Chain	Residue	Modelled	Actual	Comment	Reference
C	201	HIS	-	expression tag	UNP Q08D68
C	202	HIS	-	expression tag	UNP Q08D68
C	203	HIS	-	expression tag	UNP Q08D68

- Molecule 2 is a protein called R-SPONDIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	105	Total	C	N	O	S	0	1	0
			833	512	150	152	19			
2	D	107	Total	C	N	O	S	0	0	0
			836	513	149	155	19			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	32	GLU	-	expression tag	UNP Q5M7L6
B	33	THR	-	expression tag	UNP Q5M7L6
B	34	GLY	-	expression tag	UNP Q5M7L6
B	145	THR	-	expression tag	UNP Q5M7L6
B	146	LYS	-	expression tag	UNP Q5M7L6
B	147	HIS	-	expression tag	UNP Q5M7L6
B	148	HIS	-	expression tag	UNP Q5M7L6
B	149	HIS	-	expression tag	UNP Q5M7L6
B	150	HIS	-	expression tag	UNP Q5M7L6
B	151	HIS	-	expression tag	UNP Q5M7L6
B	152	HIS	-	expression tag	UNP Q5M7L6
D	32	GLU	-	expression tag	UNP Q5M7L6
D	33	THR	-	expression tag	UNP Q5M7L6
D	34	GLY	-	expression tag	UNP Q5M7L6
D	145	THR	-	expression tag	UNP Q5M7L6
D	146	LYS	-	expression tag	UNP Q5M7L6
D	147	HIS	-	expression tag	UNP Q5M7L6
D	148	HIS	-	expression tag	UNP Q5M7L6
D	149	HIS	-	expression tag	UNP Q5M7L6
D	150	HIS	-	expression tag	UNP Q5M7L6
D	151	HIS	-	expression tag	UNP Q5M7L6
D	152	HIS	-	expression tag	UNP Q5M7L6

- Molecule 3 is water.

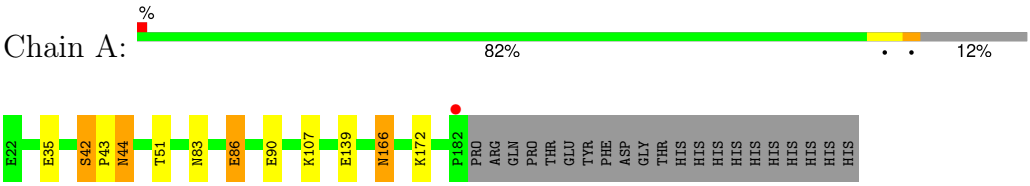
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	95	Total O 95 95	0	0
3	B	24	Total O 24 24	0	0
3	C	71	Total O 71 71	0	0
3	D	30	Total O 30 30	0	0

3 Residue-property plots (i)

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.

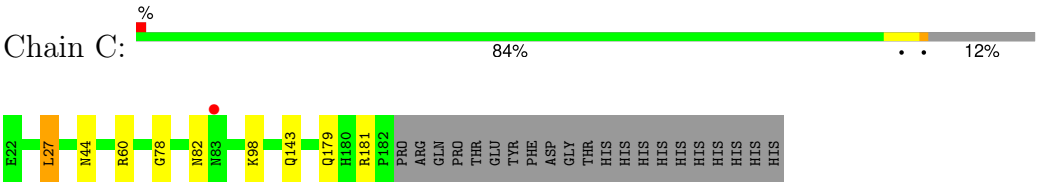
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3

Chain A:



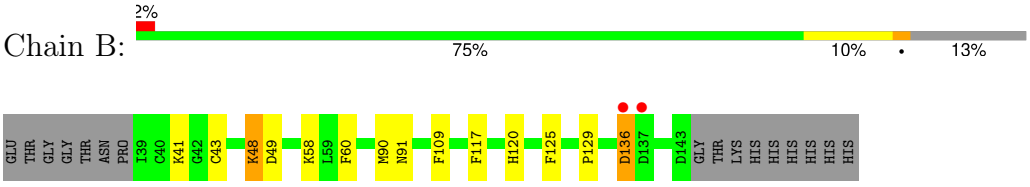
• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE ZNRF3

Chain C:



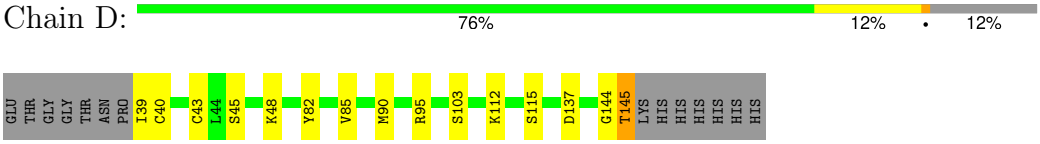
• Molecule 2: R-SPONDIN-2

Chain B:



• Molecule 2: R-SPONDIN-2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.99Å 81.23Å 71.63Å 90.00° 113.00° 90.00°	Depositor
Resolution (Å)	65.94 – 2.10 65.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.0 (65.94-2.10) 93.0 (65.94-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.188 , 0.246 0.196 , 0.254	Depositor DCC
R_{free} test set	1128 reflections (3.51%)	wwPDB-VP
Wilson B-factor (Å^2)	27.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 22.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.128 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4365	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.72	0/1264	0.83	0/1709
1	C	0.71	0/1254	0.80	0/1696
2	B	0.61	0/854	0.81	0/1140
2	D	0.63	0/854	0.75	0/1141
All	All	0.68	0/4226	0.80	0/5686

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	1243	0	1233	7	0
1	C	1233	0	1221	4	0
2	B	833	0	777	7	0
2	D	836	0	774	8	0
3	A	95	0	0	4	0
3	B	24	0	0	1	0
3	C	71	0	0	2	0
3	D	30	0	0	3	0
All	All	4365	0	4005	26	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 (26) 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:35:GLU:HG3	1:A:51:THR:HG23	1.76	0.65
2:D:85:VAL:HG22	3:D:2008:HOH:O	1.97	0.65
3:A:2022:HOH:O	1:C:179:GLN:NE2	2.33	0.61
1:A:86:GLU:HG3	3:A:2038:HOH:O	1.99	0.61
2:D:48:LYS:NZ	3:D:2005:HOH:O	2.32	0.61
2:D:103:SER:HB3	2:D:112:LYS:HB2	1.82	0.61
2:D:82:TYR:OH	2:D:95:ARG:NH1	2.34	0.60
1:C:27:LEU:HD12	1:C:27:LEU:H	1.65	0.60
1:A:42:SER:HB2	1:A:43:PRO:CD	2.35	0.57
2:D:90:MET:HG3	3:D:2007:HOH:O	2.05	0.54
1:A:42:SER:HB2	1:A:43:PRO:HD2	1.90	0.54
1:A:44:ASN:ND2	1:A:44:ASN:H	2.09	0.50
1:C:78:GLY:HA3	3:C:2032:HOH:O	2.13	0.48
3:A:2090:HOH:O	2:B:48:LYS:NZ	2.47	0.46
1:C:98:LYS:HE3	3:C:2043:HOH:O	2.16	0.45
2:D:39:ILE:HG22	2:D:40:CYS:N	2.32	0.43
2:D:144:GLY:O	2:D:145:THR:C	2.56	0.43
1:A:166:ASN:ND2	3:A:2090:HOH:O	2.52	0.43
2:B:120:HIS:CD2	2:B:129:PRO:HG3	2.54	0.42
2:D:39:ILE:HD12	2:D:39:ILE:N	2.35	0.42
2:B:60:PHE:CD2	2:B:91:ASN:HB3	2.55	0.41
2:B:58:LYS:HA	2:B:58:LYS:CE	2.51	0.41
1:A:42:SER:CB	1:A:43:PRO:CD	2.99	0.41
2:B:117:PHE:HA	2:B:125:PHE:O	2.21	0.40
2:B:48:LYS:HB3	3:B:2005:HOH:O	2.20	0.40
2:B:48:LYS:HG2	2:B:49:ASP:N	2.35	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	159/182 (87%)	156 (98%)	3 (2%)	0	100 100
1	C	159/182 (87%)	155 (98%)	3 (2%)	1 (1%)	25 21
2	B	104/121 (86%)	103 (99%)	0	1 (1%)	15 11
2	D	105/121 (87%)	103 (98%)	2 (2%)	0	100 100
All	All	527/606 (87%)	517 (98%)	8 (2%)	2 (0%)	34 32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	82	ASN
2	B	136	ASP

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	134/155 (86%)	125 (93%)	9 (7%)	16 13
1	C	131/155 (84%)	126 (96%)	5 (4%)	33 34
2	B	95/107 (89%)	89 (94%)	6 (6%)	18 15
2	D	95/107 (89%)	90 (95%)	5 (5%)	22 20
All	All	455/524 (87%)	430 (94%)	25 (6%)	21 19

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	SER
1	A	44	ASN
1	A	83	ASN
1	A	86	GLU
1	A	90	GLU
1	A	107	LYS
1	A	139	GLU
1	A	166	ASN
1	A	172	LYS

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Mol	Chain	Res	Type
2	B	41	LYS
2	B	43	CYS
2	B	48	LYS
2	B	90	MET
2	B	109	PHE
2	B	136	ASP
1	C	27	LEU
1	C	44	ASN
1	C	60	ARG
1	C	143	GLN
1	C	181	ARG
2	D	43	CYS
2	D	45	SER
2	D	115	SER
2	D	137	ASP
2	D	145	THR

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

Mol	Chain	Res	Type
1	A	44	ASN
1	A	50	HIS
1	A	166	ASN
2	B	120	HIS
1	C	101	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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, 95^{th} 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	161/182 (88%)	-0.40	1 (0%)	89	91	13, 27, 56, 84	0
1	C	161/182 (88%)	-0.43	1 (0%)	89	91	14, 26, 56, 97	0
2	B	105/121 (86%)	-0.05	2 (1%)	66	71	19, 44, 68, 89	0
2	D	107/121 (88%)	-0.29	0	100	100	19, 35, 60, 77	0
All	All	534/606 (88%)	-0.32	4 (0%)	87	89	13, 32, 65, 97	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	83	ASN	3.3
2	B	137	ASP	2.7
1	A	182	PRO	2.6
2	B	136	ASP	2.5

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

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.