wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 04:08 am BST

PDB ID	:	4XH9
Title	:	CRYSTAL STRUCTURE OF HUMAN RHOA IN COMPLEX WITH DH/PH FRAGMENT OF THE GUANINE NUCLEOTIDE EXCHANGE FACTOR NET1
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Deposited on	:	2015-01-05
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

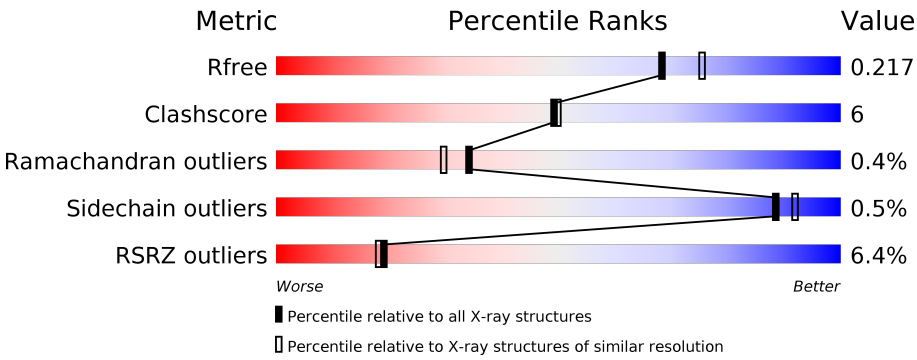
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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	361	9% 77% 16% • 7%
1	D	361	6% 81% 11% • 6%
2	B	180	4% 87% 10% •
2	E	180	3% 89% 7% • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9206 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 Neuroepithelial cell-transforming gene 1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	2753	1751	487	504	11	0	0	0
1	D	338	2784	1769	497	508	10	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	MET	-	initiating methionine	UNP Q7Z628
A	148	GLY	-	expression tag	UNP Q7Z628
A	502	HIS	-	expression tag	UNP Q7Z628
A	503	HIS	-	expression tag	UNP Q7Z628
A	504	HIS	-	expression tag	UNP Q7Z628
A	505	HIS	-	expression tag	UNP Q7Z628
A	506	HIS	-	expression tag	UNP Q7Z628
A	507	HIS	-	expression tag	UNP Q7Z628
D	147	MET	-	initiating methionine	UNP Q7Z628
D	148	GLY	-	expression tag	UNP Q7Z628
D	502	HIS	-	expression tag	UNP Q7Z628
D	503	HIS	-	expression tag	UNP Q7Z628
D	504	HIS	-	expression tag	UNP Q7Z628
D	505	HIS	-	expression tag	UNP Q7Z628
D	506	HIS	-	expression tag	UNP Q7Z628
D	507	HIS	-	expression tag	UNP Q7Z628

- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	174	1374	865	234	265	10	0	0	0
2	E	174	1374	865	234	265	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	expression tag	UNP P61586
B	25	ASN	PHE	engineered mutation	UNP P61586
E	1	GLY	-	expression tag	UNP P61586
E	25	ASN	PHE	engineered mutation	UNP P61586

- Molecule 3 is water.

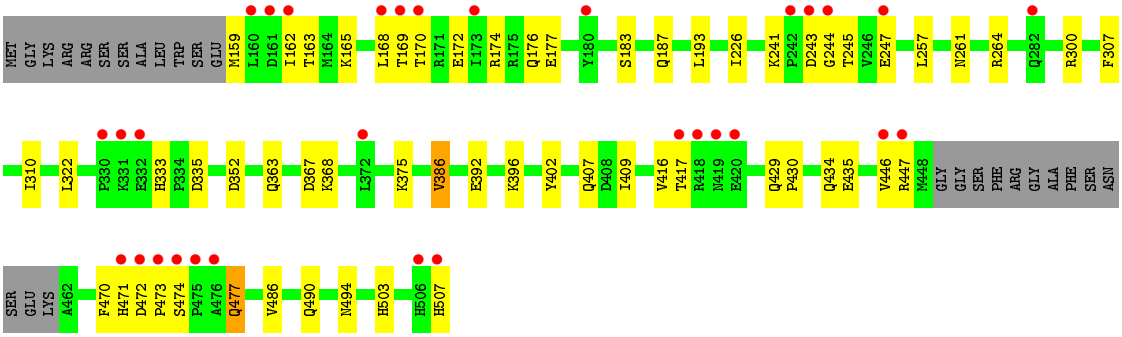
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	337	337	337	0	0
			Total	O		
3	B	170	170	170	0	0
			Total	O		
3	D	291	291	291	0	0
			Total	O		
3	E	123	123	123	0	0

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.

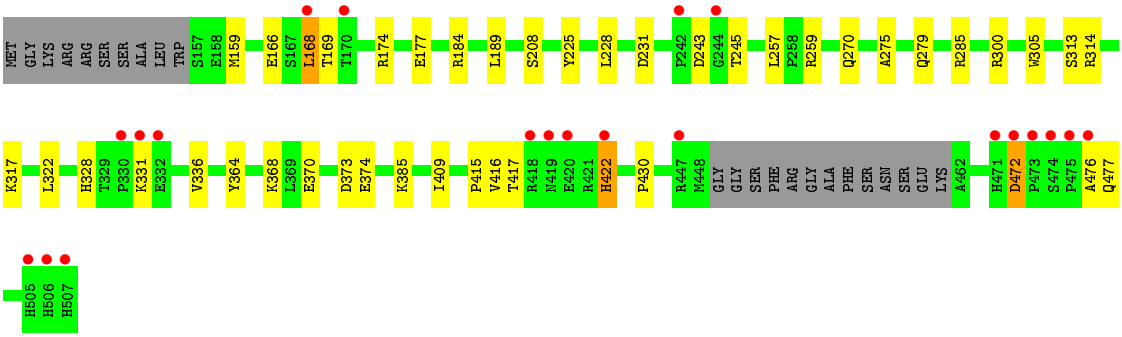
- Molecule 1: Neuroepithelial cell-transforming gene 1 protein

Chain A:



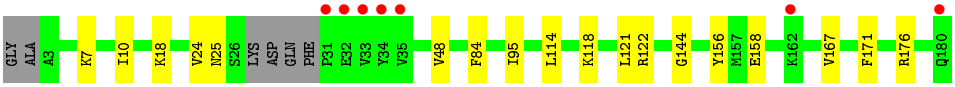
- Molecule 1: Neuroepithelial cell-transforming gene 1 protein

Chain D:



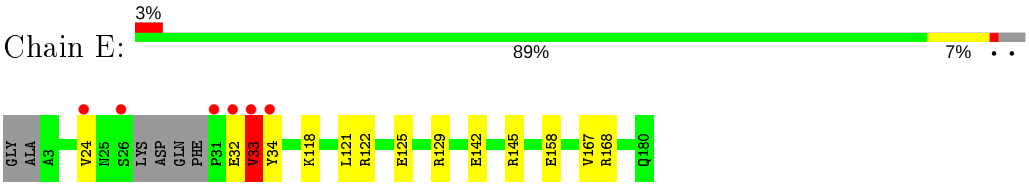
- Molecule 2: Transforming protein RhoA

Chain B:



- Molecule 2: Transforming protein RhoA

Chain E:


3%
89%
7%
GLY
ALA
A3
V24
N25
S26
LYS
ASP
GLN
PHE
P31
E32
V33
Y34
K118
L121
R122
E125
R129
E142
R145
E158
V167
R168
Q180

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.10Å 101.40Å 116.20Å 90.00° 94.30° 90.00°	Depositor
Resolution (Å)	34.69 – 2.00 34.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.69-2.00) 99.4 (34.69-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.189 , 0.217 0.190 , 0.217	Depositor DCC
R_{free} test set	4195 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9206	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 3.84% 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 (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	0.28	0/2813	0.45	0/3803
1	D	0.27	0/2850	0.46	0/3851
2	B	0.27	0/1399	0.46	0/1890
2	E	0.34	0/1399	0.47	0/1890
All	All	0.28	0/8461	0.46	0/11434

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	D	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	472	ASP	Peptide
2	E	33	VAL	Peptide

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	2753	0	2745	45	0
1	D	2784	0	2782	32	0
2	B	1374	0	1368	13	0
2	E	1374	0	1368	11	0
3	A	337	0	0	6	0
3	B	170	0	0	5	0
3	D	291	0	0	5	0
3	E	123	0	0	0	0
All	All	9206	0	8263	98	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 6.

The worst 5 of 98 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:241:LYS:NZ	1:A:247:GLU:OE2	2.02	0.92
1:A:392:GLU:OE1	3:A:601:HOH:O	1.97	0.82
1:A:429:GLN:H	1:A:477:GLN:HE22	1.30	0.79
1:A:300:ARG:NH1	3:A:694:HOH:O	2.18	0.76
1:A:470:PHE:CD1	1:A:477:GLN:HG2	2.22	0.75

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	332/361 (92%)	321 (97%)	10 (3%)	1 (0%)	41 37
1	D	336/361 (93%)	328 (98%)	6 (2%)	2 (1%)	25 19
2	B	170/180 (94%)	168 (99%)	2 (1%)	0	100 100
2	E	170/180 (94%)	164 (96%)	5 (3%)	1 (1%)	25 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1008/1082 (93%)	981 (97%)	23 (2%)	4 (0%)	34 30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	ASP
1	D	472	ASP
1	D	166	GLU
2	E	33	VAL

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	304/328 (93%)	301 (99%)	3 (1%)	76 81
1	D	307/328 (94%)	305 (99%)	2 (1%)	84 88
2	B	152/156 (97%)	152 (100%)	0	100 100
2	E	152/156 (97%)	152 (100%)	0	100 100
All	All	915/968 (94%)	910 (100%)	5 (0%)	88 92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	386	VAL
1	A	447	ARG
1	A	477	GLN
1	D	168	LEU
1	D	422	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	477	GLN

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Mol	Chain	Res	Type
2	E	52	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 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 (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	336/361 (93%)	0.17	31 (9%)	9	8	16, 29, 69, 81	0
1	D	338/361 (93%)	0.09	21 (6%)	20	19	18, 31, 67, 80	0
2	B	174/180 (96%)	0.05	7 (4%)	38	37	14, 29, 57, 121	0
2	E	174/180 (96%)	-0.10	6 (3%)	45	44	16, 31, 60, 122	0
All	All	1022/1082 (94%)	0.08	65 (6%)	19	18	14, 30, 67, 122	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	34	TYR	10.9
1	D	473	PRO	9.1
2	B	33	VAL	8.9
2	E	33	VAL	8.8
1	D	474	SER	8.2

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.