

Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 - 06:05 am GMT

PDB ID : 2JHU

Title : CRYSTAL STRUCTURE OF RHOGDI E154A,E155A MUTANT

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Deposited on : 2007-02-23

Resolution : 1.65 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 (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

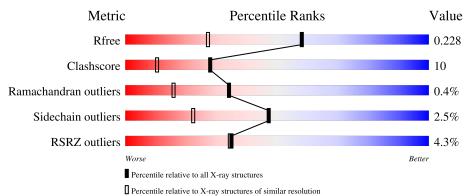
 $\begin{tabular}{lll} Validation Pipeline (wwPDB-VP) & : & 2.36 \end{tabular}$

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 1.65 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	138	88%	12%	•		
1	В	138	7% 82%	16%	•		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2599 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.

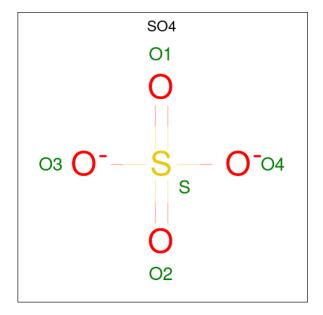
• Molecule 1 is a protein called RHO GDP-DISSOCIATION INHIBITOR 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	138	Total	С	N	О	S	0	0	0
1	1 A	130	1102	707	184	206	5	U		
1	В	138	Total	С	N	О	S	0	0	0
	138	1102	707	184	206	5			U	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	ALA	GLU	engineered mutation	UNP P52565
A	155	ALA	GLU	engineered mutation	UNP P52565
В	154	ALA	GLU	engineered mutation	UNP P52565
В	155	ALA	GLU	engineered mutation	UNP P52565

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





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

• Molecule 3 is water.

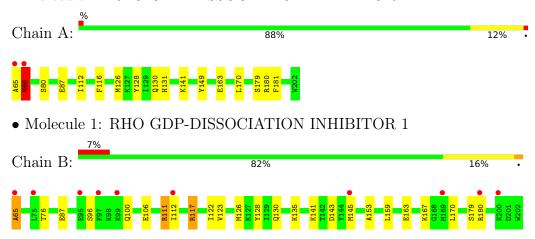
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	201	Total O 201 201	0	0
3	В	179	Total O 179 179	0	0



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: RHO GDP-DISSOCIATION INHIBITOR 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	130.78Å 130.78Å 162.31Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	1
Resolution (Å)	92.85 - 1.65	Depositor
resolution (11)	29.45 - 1.65	EDS
% Data completeness	98.9 (92.85-1.65)	Depositor
(in resolution range)	98.9 (29.45-1.65)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.16 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.233	Depositor
it, itfree	0.205 , 0.228	DCC
R_{free} test set	1039 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 51.2	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
	0.023 for -2/3 +h-1/3 +k+2/3 +l,-1/3 +h-2/3 +k-	
	2/3*1,2/3*h-2/3*k+1/3*l	
Estimated twinning fraction	0.015 for $-h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*$	Xtriage
	k+1/3*l 0.014 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3	
	*k+1/3*l	
F_o, F_c correlation	0.95	EDS
Total number of atoms	2599	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: 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).

Mal	Clasia	Bond lengths		Bond angles	
IVIOI	Mol Chain		# Z > 5	RMSZ	# Z > 5
1	A	0.58	0/1127	0.70	0/1522
1	В	0.58	0/1127	0.83	$2/1522 \ (0.1\%)$
All	All	0.58	0/2254	0.77	2/3044 (0.1%)

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	В	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
1	В	111	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	В	111	ARG	NE-CZ-NH2	-9.66	115.47	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	65	ALA	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	1102	0	1107	21	0
1	В	1102	0	1107	24	0
2	A	10	0	0	0	0
2	В	5	0	0	1	0
3	A	201	0	0	8	0
3	В	179	0	0	13	0
All	All	2599	0	2214	44	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 10.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance} ({f A})$	overlap (Å)
1:A:126:MET:SD	3:A:2182:HOH:O	2.33	0.85
1:B:128:TYR:OH	1:B:130:GLN:NE2	2.10	0.82
1:B:159:LEU:HD21	3:B:2134:HOH:O	1.81	0.80
1:A:112:ILE:HD13	1:A:130:GLN:HE22	1.46	0.79
1:A:116:PHE:CZ	1:A:126:MET:HE1	2.23	0.74
1:A:65:ALA:HA	1:A:66:MET:HB3	1.68	0.74
1:A:66:MET:HB2	3:A:2035:HOH:O	1.86	0.73
1:A:126:MET:CG	3:A:2182:HOH:O	2.39	0.69
1:A:126:MET:HG2	3:A:2182:HOH:O	1.94	0.68
1:B:117:ARG:HD2	3:B:2074:HOH:O	1.93	0.68
1:A:180:ARG:HD3	3:A:2174:HOH:O	1.94	0.68
1:A:116:PHE:CE2	1:A:126:MET:HE1	2.33	0.63
1:A:131:HIS:HD2	3:A:2174:HOH:O	1.82	0.63
1:B:163:GLU:HB3	3:B:2138:HOH:O	1.99	0.62
1:B:135:LYS:HE2	3:B:2103:HOH:O	2.00	0.61
1:B:122:ILE:HB	3:B:2063:HOH:O	2.00	0.61
1:B:117:ARG:NH2	1:B:153:ALA:O	2.33	0.60
1:B:122:ILE:HG22	3:B:2091:HOH:O	2.00	0.59
1:A:112:ILE:HD13	1:A:130:GLN:NE2	2.17	0.59
1:A:80:SER:O	1:B:111:ARG:HD2	2.02	0.59
1:B:122:ILE:CG2	3:B:2091:HOH:O	2.51	0.58
1:B:65:ALA:HB1	3:B:2004:HOH:O	2.02	0.58
1:A:179:SER:C	1:A:180:ARG:HD2	2.26	0.56
1:B:123:VAL:HG11	1:B:126:MET:SD	2.45	0.56
1:B:76:THR:OG1	1:B:87:GLU:OE1	2.19	0.55

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Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance } (\text{\AA}) \end{array}$	Clash overlap (Å)
1:B:117:ARG:HD3	3:B:2073:HOH:O	2.07	0.54
1:A:131:HIS:CE1	1:A:141:LYS:HG3	2.43	0.54
1:B:112:ILE:HD13	1:B:130:GLN:HE22	1.72	0.54
1:A:116:PHE:CZ	1:A:126:MET:CE	2.90	0.53
1:A:128:TYR:CE2	1:A:130:GLN:HG3	2.49	0.47
1:B:96:SER:HB3	3:B:2044:HOH:O	2.15	0.47
1:A:180:ARG:HG2	3:A:2085:HOH:O	2.14	0.47
1:B:111:ARG:NH2	2:B:1203:SO4:O4	2.48	0.46
1:B:128:TYR:CE2	1:B:130:GLN:HG3	2.51	0.46
1:A:126:MET:HE1	1:A:181:PHE:HZ	1.81	0.46
1:A:126:MET:HE2	1:A:149:TYR:CE2	2.52	0.45
1:A:87:GLU:HG3	3:A:2023:HOH:O	2.17	0.44
1:B:122:ILE:HD12	3:B:2063:HOH:O	2.18	0.44
1:B:106:GLU:HB2	1:B:167:LYS:HA	1.99	0.43
1:B:141:LYS:NZ	1:B:143:ASP:OD2	2.51	0.43
1:A:116:PHE:CE2	1:A:126:MET:CE	3.00	0.41
1:B:65:ALA:N	3:B:2005:HOH:O	2.53	0.41
1:B:100:GLN:CD	3:B:2044:HOH:O	2.59	0.41
1:B:179:SER:C	1:B:180:ARG:HD2	2.42	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	136/138 (99%)	133 (98%)	2 (2%)	1 (1%)	22 6
1	В	136/138 (99%)	134 (98%)	2 (2%)	0	100 100
All	All	272/276 (99%)	267 (98%)	4 (2%)	1 (0%)	34 16

All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	66	MET

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	$121/121 \; (100\%)$	118 (98%)	3 (2%)	47 22		
1	В	121/121 (100%)	118 (98%)	3 (2%)	47 22		
All	All	242/242 (100%)	236 (98%)	6 (2%)	47 22		

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	MET
1	A	163	GLU
1	A	170	LEU
1	В	117	ARG
1	В	145	MET
1	В	170	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	\mathbf{Type}
1	A	130	GLN
1	A	131	HIS
1	В	130	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 (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		\mathbf{B}_{0}	ond leng	gths	В	ond ang	gles
IVIOI	туре	Cham	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1204	-	4,4,4	0.19	0	6,6,6	0.19	0
2	SO4	A	1203	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	В	1203	-	4,4,4	0.13	0	6,6,6	0.15	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1203	SO4	1	0

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, 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	138/138 (100%)	0.17	2 (1%) 75 79	17, 23, 32, 40	0
1	В	138/138 (100%)	0.33	10 (7%) 15 14	18, 24, 33, 40	0
All	All	276/276 (100%)	0.25	12 (4%) 35 34	17, 23, 33, 40	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	ALA	7.0
1	В	99	LYS	4.9
1	В	65	ALA	3.5
1	В	95	GLU	3.2
1	В	200	LYS	3.0
1	В	169	MET	2.5
1	A	66	MET	2.4
1	В	97	PHE	2.2
1	В	145	MET	2.2
1	В	112	ILE	2.2
1	В	180	ARG	2.1
1	В	75	LEU	2.1

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	SO4	В	1203	5/5	0.83	0.21	73,74,74,74	0
2	SO4	A	1203	5/5	0.89	0.28	62,63,63,64	0
2	SO4	A	1204	5/5	0.97	0.19	50,51,51,52	0

6.5 Other polymers (i)

There are no such residues in this entry.

