W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2021 – 03:10 PM EDT

PDB ID	:	1XCG
Title	:	Crystal Structure of Human RhoA in complex with DH/PH fragment of PDZRHOGEF
Authors	:	Derewenda, U.; Oleksy, A.; Stevenson, A.S.; Korczynska, J.; Dauter, Z; Somlyo, A.P.; Otlewski, J.; Somlyo, A.V.; Derewenda, Z.S.
Deposited on	:	2004-09-01
Resolution	:	2.50 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 ⓘ symbol.

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

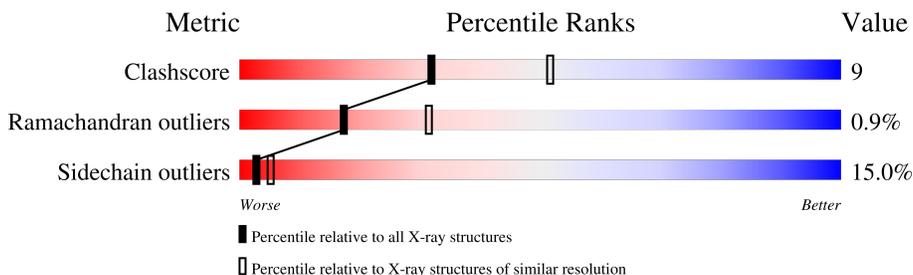|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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	Percentile Ranks	Value
Clashscore		9
Ramachandran outliers		0.9%
Sidechain outliers		15.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	368	67% — 25% • • •
1	E	368	64% — 31% • •
2	B	178	69% — 29% • •
2	F	178	77% — 19% •

2　Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8750 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 guanine nucleotide exchange factor 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total 2906	C 1837	N 519	O 535	S 15	0	0	0
1	E	358	Total 2931	C 1852	N 525	O 539	S 15	0	0	0

- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	178	Total 1411	C 889	N 240	O 272	S 10	0	0	0
2	F	178	Total 1411	C 889	N 240	O 272	S 10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ASN	PHE	engineered mutation	UNP P61586
F	25	ASN	PHE	engineered mutation	UNP P61586

- Molecule 3 is water.

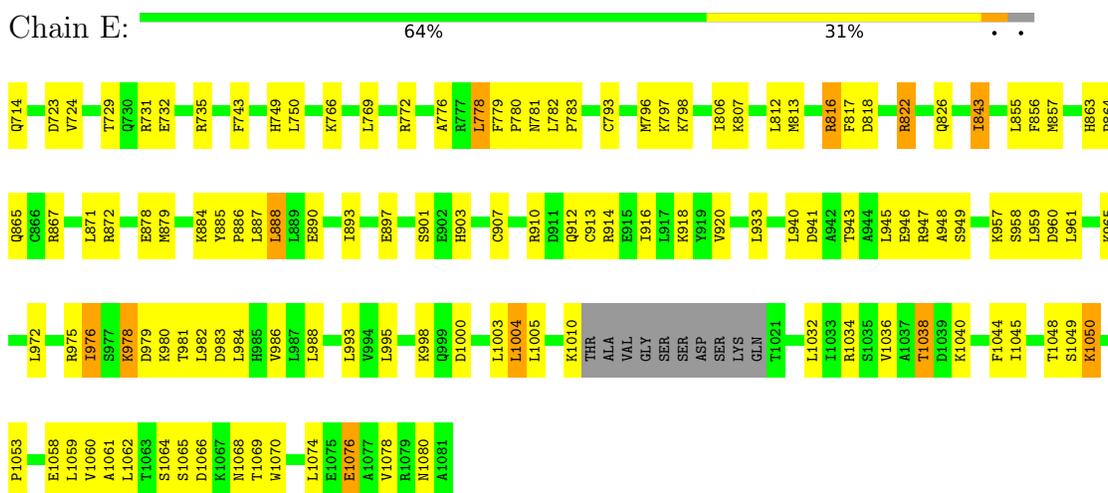| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	B	17	Total 17	O 17	0	0
3	E	30	Total 30	O 30	0	0
3	F	14	Total 14	O 14	0	0

3 Residue-property plots ⓘ

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. 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. 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: Rho guanine nucleotide exchange factor 11
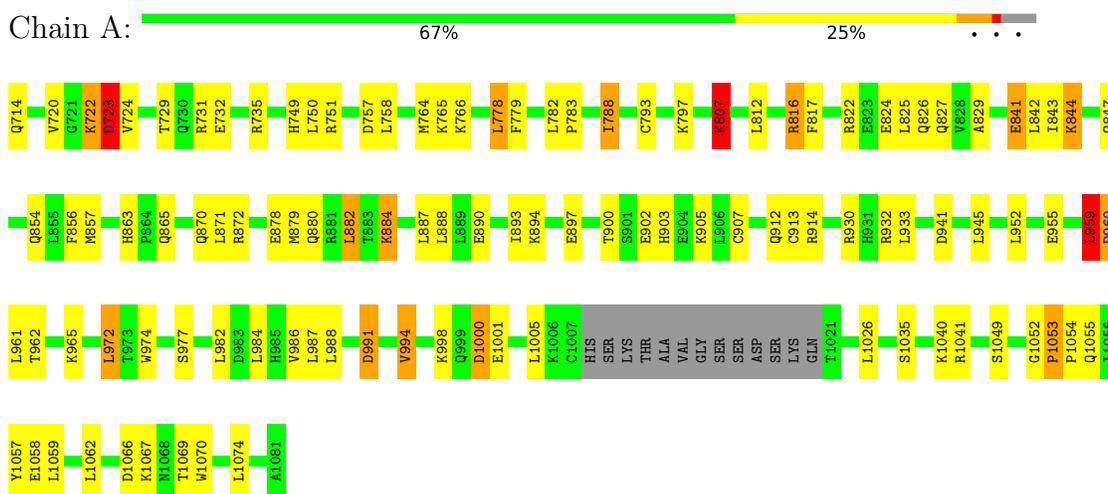
Chain A:

• Molecule 1: Rho guanine nucleotide exchange factor 11

Chain E:

• Molecule 2: Transforming protein RhoA

Chain B:

A3 I4 R5 K6 K7 L8 V11 A15 C16 C20 V24 K27 D28 Q29 F30 P31 E32 V33 N41 D45 L55 W58 Q63 E64 D65 R68 L69 R70 P71 Y74 D78 L81 M82 C83 F84 D87 I95 T100 P101 I113 L114

K118 K119 D120 L121 R122 E125 L131 A132 K133 M134 K135 R145 D146 I151 M157 E158 C159 S160 T163 K164 D165 G166 V167 V170 M173 R176 Q180

• Molecule 2: Transforming protein RhoA

Chain F:

77%   19%   •

A3 I4 I10 V11 C16 L21 V24 N25 S26 K27 D28 Q29 F30 P31 E32 V35 P36 T37 Y42 K51 L55 D59 D67 R68 L69 R70 P71 Y74 P75 D76 L81 M82 C83 I86 D87 D90 N94 E97 T100 P101 I113

N117 K118 R122 E125 L131 M134 E158 K162 V167 Q180

4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.24Å 118.78Å 90.13Å 90.00° 114.34° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50	Depositor
% Data completeness (in resolution range)	96.8 (25.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.224 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8750	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

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	0.50	0/2950	0.74	7/3970 (0.2%)
1	E	0.51	0/2976	0.78	6/4004 (0.1%)
2	B	0.56	0/1438	0.82	6/1944 (0.3%)
2	F	0.56	0/1438	0.81	6/1944 (0.3%)
All	All	0.52	0/8802	0.78	25/11862 (0.2%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	65	ASP	CB-CG-OD2	7.30	124.87	118.30
1	E	723	ASP	CB-CG-OD2	7.13	124.72	118.30
2	F	90	ASP	CB-CG-OD2	6.61	124.25	118.30
2	B	81	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	1000	ASP	CB-CG-OD2	6.02	123.72	118.30

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	2906	0	2997	55	0
1	E	2931	0	3022	62	0
2	B	1411	0	1402	28	0
2	F	1411	0	1402	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	30	0	0	4	0
3	B	17	0	0	0	0
3	E	30	0	0	2	0
3	F	14	0	0	1	0
All	All	8750	0	8823	156	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 9.

The worst 5 of 156 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:879:MET:HE3	2:B:69:LEU:HB3	1.48	0.94
1:E:822:ARG:HH11	1:E:826:GLN:HE22	1.05	0.93
1:A:879:MET:CE	2:B:69:LEU:HB3	2.03	0.88
1:E:1061:ALA:HB1	1:E:1066:ASP:HB3	1.56	0.86
1:A:822:ARG:HH11	1:A:912:GLN:HE22	1.22	0.86

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	351/368 (95%)	333 (95%)	11 (3%)	7 (2%)	7	12
1	E	354/368 (96%)	335 (95%)	18 (5%)	1 (0%)	41	61
2	B	176/178 (99%)	165 (94%)	10 (6%)	1 (1%)	25	43
2	F	176/178 (99%)	169 (96%)	6 (3%)	1 (1%)	25	43
All	All	1057/1092 (97%)	1002 (95%)	45 (4%)	10 (1%)	17	31

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1054	PRO
1	A	1000	ASP
1	A	1052	GLY
1	A	807	LYS
1	A	959	LEU

5.3.2 Protein sidechains ⓘ

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	323/334 (97%)	272 (84%)	51 (16%)	2	4
1	E	326/334 (98%)	273 (84%)	53 (16%)	2	4
2	B	156/156 (100%)	133 (85%)	23 (15%)	3	5
2	F	156/156 (100%)	139 (89%)	17 (11%)	6	12
All	All	961/980 (98%)	817 (85%)	144 (15%)	3	5

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1004	LEU
2	F	162	LYS
1	E	1036	VAL
2	F	21	LEU
1	A	1067	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	895	HIS
1	E	1080	ASN
2	F	117	ASN
2	F	41	ASN
2	B	105	HIS

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 ⓘ

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 ⓘ

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.