



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:25 PM UTC

PDB ID : 3DPT / pdb_00003dpt
Title : COR domain of Rab family protein (Roco)
Authors : Gotthardt, K.; Weyand, M.; Kortholt, A.; Van Haastert, P.J.M.; Wittinghofer, A.
Deposited on : 2008-07-09
Resolution : 2.90 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

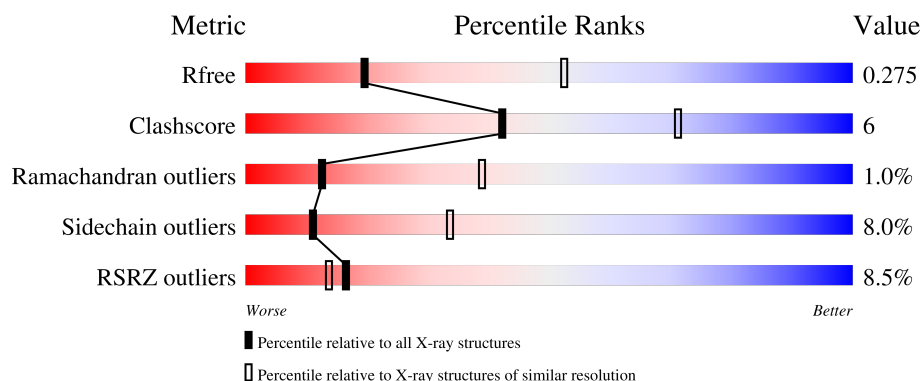
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. 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	332	5% 71% 16% • 10%
1	B	332	11% 73% 14% • 10%

2 Entry composition

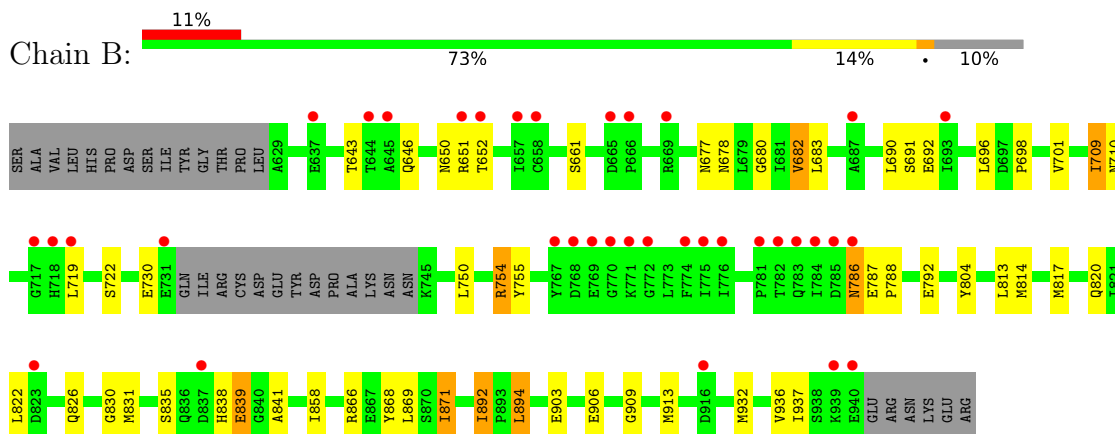
There is only 1 type of molecule in this entry. The entry contains 4643 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Rab family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2329	1502	373	443	11			
1	B	299	Total	C	N	O	S	0	0	0
			2314	1489	367	447	11			

- Molecule 1: Rab family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.11Å 130.11Å 129.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.83 – 2.90 45.83 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.83-2.90) 99.9 (45.83-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.243 (Not available) , 0.275	Depositor DCC
R_{free} test set	1422 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4643	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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	0.55	0/2375	0.83	0/3231
1	B	0.55	0/2362	0.88	2/3218 (0.1%)
All	All	0.55	0/4737	0.85	2/6449 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	830	GLY	N-CA-C	7.13	120.97	110.63
1	B	792	GLU	N-CA-C	6.35	118.29	111.36

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	2329	0	2261	31	0
1	B	2314	0	2195	28	0
All	All	4643	0	4456	57	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.

All (57) 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:B:786:ASN:H	1:B:786:ASN:HD22	1.17	0.90
1:A:631:SER:O	1:A:635:VAL:HG23	1.81	0.81
1:A:635:VAL:HG22	1:A:661:SER:HB2	1.69	0.75
1:A:635:VAL:HG21	1:A:663:ILE:HD12	1.69	0.73
1:A:895:PRO:HD3	1:A:932:MET:HE3	1.69	0.73
1:A:894:LEU:HD12	1:A:932:MET:HE1	1.71	0.72
1:B:696:LEU:HD11	1:B:755:TYR:HE2	1.61	0.65
1:A:682:VAL:HG13	1:A:695:VAL:HG13	1.78	0.65
1:A:780:LEU:HD11	1:A:814:MET:HE1	1.79	0.64
1:A:707:ARG:NH1	1:A:728:LEU:O	2.32	0.63
1:A:754:ARG:CZ	1:B:871:ILE:HD12	2.29	0.62
1:A:823:ASP:H	1:A:825:MET:HG3	1.64	0.62
1:B:813:LEU:HD23	1:B:831:MET:HE1	1.82	0.61
1:A:635:VAL:HG22	1:A:661:SER:CB	2.30	0.61
1:A:835:SER:HB2	1:A:838:HIS:HD2	1.64	0.61
1:B:814:MET:HE3	1:B:826:GLN:OE1	2.05	0.57
1:A:814:MET:HE3	1:A:826:GLN:OE1	2.05	0.56
1:B:817:MET:HE2	1:B:820:GLN:NE2	2.24	0.52
1:B:696:LEU:HD11	1:B:755:TYR:CE2	2.43	0.52
1:B:786:ASN:H	1:B:786:ASN:ND2	1.98	0.51
1:B:786:ASN:HD22	1:B:786:ASN:N	1.92	0.51
1:A:909:GLY:O	1:A:913:MET:HG3	2.11	0.50
1:A:642:ALA:HB1	1:A:649:LEU:HD21	1.93	0.50
1:B:909:GLY:O	1:B:913:MET:HG2	2.13	0.49
1:A:863:ARG:HA	1:A:866:ARG:NH1	2.28	0.49
1:A:808:THR:C	1:A:811:PRO:HD2	2.38	0.48
1:B:683:LEU:HD12	1:B:698:PRO:HA	1.94	0.48
1:B:858:ILE:HD12	1:B:869:LEU:HB2	1.95	0.48
1:A:835:SER:CB	1:A:838:HIS:HD2	2.27	0.47
1:A:803:ASP:HB2	1:A:887:ASP:HB3	1.96	0.46
1:B:838:HIS:O	1:B:839:GLU:C	2.58	0.46
1:A:769:GLU:OE2	1:A:824:ARG:HD3	2.15	0.46
1:A:786:ASN:ND2	1:A:825:MET:HE3	2.30	0.46
1:A:777:PRO:HB2	1:A:811:PRO:HB3	1.98	0.46
1:A:775:ILE:O	1:A:777:PRO:HD3	2.16	0.46
1:A:643:THR:O	1:A:646:GLN:O	2.34	0.45
1:B:817:MET:HE2	1:B:820:GLN:HE21	1.82	0.45
1:A:682:VAL:HG13	1:A:695:VAL:CG1	2.45	0.45
1:B:709:ILE:HG13	1:B:710:ASN:ND2	2.31	0.45
1:A:875:GLU:OE2	1:B:754:ARG:NH1	2.50	0.44
1:B:678:ASN:C	1:B:680:GLY:H	2.25	0.44
1:B:892:ILE:HD13	1:B:892:ILE:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:ILE:HD11	1:B:936:VAL:HG21	2.00	0.43
1:A:817:MET:HE1	1:A:872:ILE:HG12	2.00	0.43
1:B:894:LEU:HD12	1:B:932:MET:HE1	2.01	0.43
1:B:643:THR:O	1:B:646:GLN:O	2.36	0.43
1:B:677:ASN:HA	1:B:682:VAL:O	2.19	0.43
1:B:650:ASN:HA	1:B:691:SER:O	2.20	0.42
1:A:749:THR:O	1:A:753:GLN:HG3	2.20	0.42
1:A:759:ILE:O	1:A:762:GLN:HB3	2.20	0.41
1:B:786:ASN:ND2	1:B:786:ASN:N	2.63	0.41
1:B:903:GLU:O	1:B:906:GLU:HB2	2.20	0.41
1:B:787:GLU:HA	1:B:788:PRO:HD3	1.96	0.41
1:A:692:GLU:H	1:A:692:GLU:HG2	1.45	0.41
1:B:650:ASN:O	1:B:651:ARG:C	2.64	0.41
1:B:835:SER:HB3	1:B:868:TYR:CZ	2.56	0.41
1:A:632:TRP:CD1	1:A:663:ILE:HD11	2.57	0.40

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	294/332 (89%)	280 (95%)	11 (4%)	3 (1%)	12	39
1	B	295/332 (89%)	272 (92%)	20 (7%)	3 (1%)	12	39
All	All	589/664 (89%)	552 (94%)	31 (5%)	6 (1%)	12	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	841	ALA
1	A	822	LEU
1	B	822	LEU

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Mol	Chain	Res	Type
1	A	841	ALA
1	B	839	GLU
1	A	852	SER

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	246/301 (82%)	226 (92%)	20 (8%)	11	33
1	B	239/301 (79%)	220 (92%)	19 (8%)	11	34
All	All	485/602 (81%)	446 (92%)	39 (8%)	11	34

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	651	ARG
1	A	671	THR
1	A	682	VAL
1	A	690	LEU
1	A	692	GLU
1	A	705	VAL
1	A	720	ASN
1	A	747	THR
1	A	756	LEU
1	A	762	GLN
1	A	784	ILE
1	A	799	ILE
1	A	808	THR
1	A	822	LEU
1	A	838	HIS
1	A	851	ASP
1	A	853	THR
1	A	868	TYR
1	A	894	LEU
1	A	926	VAL

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Mol	Chain	Res	Type
1	B	652	THR
1	B	661	SER
1	B	682	VAL
1	B	690	LEU
1	B	692	GLU
1	B	701	VAL
1	B	709	ILE
1	B	719	LEU
1	B	722	SER
1	B	730	GLU
1	B	750	LEU
1	B	754	ARG
1	B	786	ASN
1	B	804	TYR
1	B	866	ARG
1	B	871	ILE
1	B	892	ILE
1	B	894	LEU
1	B	937	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	699	HIS
1	A	710	ASN
1	A	716	ASN
1	A	718	HIS
1	A	838	HIS
1	A	859	GLN
1	A	880	ASN
1	B	659	ASN
1	B	720	ASN
1	B	786	ASN
1	B	820	GLN
1	B	897	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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	298/332 (89%)	0.25	15 (5%) 34 27	53, 64, 75, 81	0
1	B	299/332 (90%)	0.74	36 (12%) 9 7	53, 63, 74, 86	0
All	All	597/664 (89%)	0.49	51 (8%) 16 14	53, 64, 74, 86	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	781	PRO	4.9
1	B	783	GLN	4.7
1	B	784	ILE	4.6
1	B	782	THR	4.1
1	B	767	TYR	3.6
1	B	645	ALA	3.6
1	A	804	TYR	3.5
1	A	938	SER	3.4
1	B	786	ASN	3.4
1	B	837	ASP	3.3
1	B	669	ARG	3.2
1	A	770	GLY	3.2
1	B	666	PRO	3.2
1	B	718	HIS	3.1
1	B	652	THR	3.1
1	B	785	ASP	3.1
1	B	771	LYS	3.0
1	A	786	ASN	3.0
1	B	717	GLY	2.9
1	B	769	GLU	2.9
1	A	783	GLN	2.9
1	B	693	ILE	2.9
1	B	687	ALA	2.9
1	A	732	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	775	ILE	2.8
1	A	789	GLU	2.8
1	A	734	ARG	2.8
1	B	940	GLU	2.7
1	A	885	ASN	2.6
1	A	785	ASP	2.6
1	B	719	LEU	2.5
1	B	651	ARG	2.5
1	B	768	ASP	2.5
1	B	916	ASP	2.5
1	A	787	GLU	2.4
1	B	776	ILE	2.4
1	B	823	ASP	2.4
1	B	644	THR	2.4
1	B	770	GLY	2.3
1	B	772	GLY	2.3
1	A	631	SER	2.3
1	B	939	LYS	2.2
1	B	658	CYS	2.2
1	B	657	ILE	2.1
1	B	774	PHE	2.1
1	B	665	ASP	2.1
1	A	852	SER	2.1
1	B	731	GLU	2.1
1	A	839	GLU	2.1
1	B	637	GLU	2.1
1	A	746	PHE	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 oligosaccharides 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.