



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 4, 2022 – 04:46 pm BST

PDB ID : 7NZZ
Title : Ras1 guanine nucleotide exchange factor Cdc25 (REM and catalytic domains)
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Deposited on : 2021-03-24
Resolution : 2.45 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)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

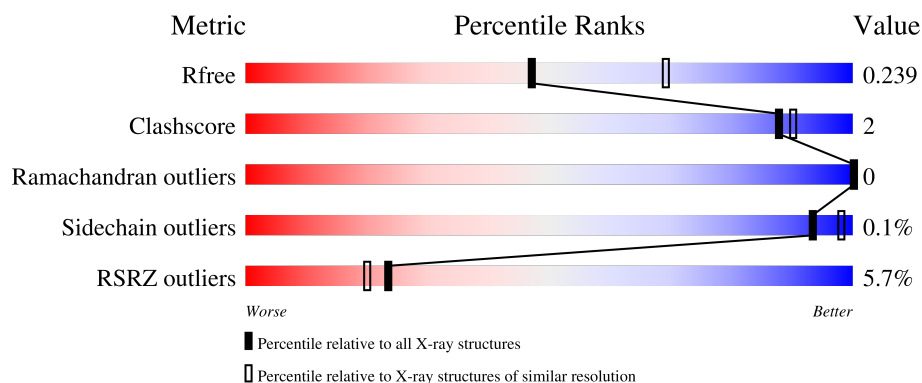
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	476	<div> <div>3%</div> <div>85%</div> <div>12%</div> </div>
1	B	476	<div> <div>7%</div> <div>80%</div> <div>8%</div> <div>12%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6860 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 Cell division control protein 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	4	0
			3393	2182	575	620	16			
1	B	419	Total	C	N	O	S	0	0	0
			3323	2144	555	608	16			

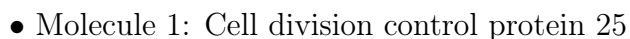
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	858	MET	-	initiating methionine	UNP P43069
A	859	GLY	-	cloning artifact	UNP P43069
A	1308	PRO	ALA	engineered mutation	UNP P43069
A	1309	ALA	VAL	engineered mutation	UNP P43069
B	858	MET	-	initiating methionine	UNP P43069
B	859	GLY	-	cloning artifact	UNP P43069
B	1308	PRO	ALA	engineered mutation	UNP P43069
B	1309	ALA	VAL	engineered mutation	UNP P43069

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	86	Total	O	0	0
			86	86		
2	B	58	Total	O	0	0
			58	58		

- Molecule 1: Cell division control protein 25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.65Å 107.21Å 196.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.22 – 2.45 43.22 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.22-2.45) 99.7 (43.22-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.194 , 0.240 0.196 , 0.239	Depositor DCC
R_{free} test set	1953 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtrriage
Anisotropy	0.409	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6860	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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	0.24	0/3482	0.44	0/4722
1	B	0.24	0/3403	0.44	0/4618
All	All	0.24	0/6885	0.44	0/9340

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 [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	3393	0	3300	8	0
1	B	3323	0	3205	20	0
2	A	86	0	0	0	0
2	B	58	0	0	0	0
All	All	6860	0	6505	27	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 2.

All (27) 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:1296:TYR:OH	1:A:1305:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1137:ARG:NH2	1:B:1303:GLU:OE2	2.34	0.60
1:A:919:HIS:HB3	1:A:975:ILE:HG13	1.84	0.60
1:B:1090:PHE:HB3	1:B:1105:GLU:HG3	1.86	0.56
1:B:1138:VAL:HG11	1:B:1181:TYR:HB2	1.86	0.56
1:A:1087:ILE:O	1:A:1266:LYS:NZ	2.31	0.55
1:A:885:PRO:HD2	1:A:888:LEU:HD12	1.89	0.54
1:A:918:HIS:O	1:A:978:ARG:NH1	2.41	0.54
1:B:1071:GLU:OE2	1:B:1075:GLN:NE2	2.41	0.49
1:B:1233:TYR:HA	1:B:1251:LYS:HE3	1.95	0.49
1:B:896:LEU:HG	1:B:911:ALA:HB1	1.94	0.48
1:A:1052:LEU:HD12	1:A:1070:VAL:HB	1.96	0.47
1:B:980:ILE:HG23	1:B:1022:LEU:HD11	1.97	0.46
1:B:1097:TRP:HB2	1:B:1101:SER:HB3	1.98	0.46
1:B:1078:LEU:HD21	1:B:1272:PHE:HB2	1.98	0.46
1:A:1243:ARG:NH2	1:B:1212:PHE:O	2.49	0.45
1:B:899:ASP:OD1	1:B:903:ASN:N	2.49	0.45
1:B:1228:ASP:HB3	1:B:1258:ILE:HD13	1.99	0.44
1:A:1121:THR:HG23	1:A:1166:ALA:HB2	1.99	0.43
1:B:1150:LYS:HD2	1:B:1150:LYS:HA	1.85	0.43
1:B:1070:VAL:HG13	1:B:1150:LYS:HE2	1.99	0.43
1:B:1089:LYS:HG2	1:B:1259:VAL:HG22	2.00	0.43
1:B:919:HIS:HB3	1:B:975:ILE:HG13	2.01	0.43
1:B:894:TYR:CE2	1:B:895:GLU:HG3	2.55	0.42
1:B:1087:ILE:O	1:B:1266:LYS:NZ	2.40	0.41
1:B:1072:LEU:HD23	1:B:1147:VAL:HG21	2.02	0.41
1:B:1214:GLY:HA2	1:B:1264:ARG:HH11	1.85	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	421/476 (88%)	414 (98%)	7 (2%)	0	100	100
1	B	415/476 (87%)	407 (98%)	8 (2%)	0	100	100
All	All	836/952 (88%)	821 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	365/433 (84%)	364 (100%)	1 (0%)	92	95
1	B	352/433 (81%)	352 (100%)	0	100	100
All	All	717/866 (83%)	716 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1105	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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	421/476 (88%)	0.51	16 (3%) 40 37	34, 50, 79, 122	0
1	B	419/476 (88%)	0.72	32 (7%) 13 10	37, 53, 87, 113	0
All	All	840/952 (88%)	0.62	48 (5%) 23 20	34, 52, 83, 122	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1045	ASN	6.5
1	B	1032	GLY	6.0
1	B	1296	TYR	5.2
1	A	900	VAL	5.2
1	A	901	LYS	5.0
1	A	1056	SER	4.9
1	B	1056	SER	4.9
1	B	1292	ILE	4.7
1	A	925	ASN	4.6
1	B	1184	ALA	4.1
1	A	1057	SER	4.1
1	B	1300	LEU	4.0
1	B	1293	ASP	3.9
1	A	1047	LYS	3.7
1	B	902	GLY	3.6
1	B	996	TYR	3.3
1	A	1213	ILE	3.3
1	B	1134	PRO	3.2
1	B	1304	PRO	3.1
1	B	1175	LEU	3.1
1	B	1302	LEU	3.1
1	B	894	TYR	2.9
1	A	1214	GLY	2.8
1	B	1108	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	1132	ALA	2.8
1	B	1294	GLU	2.7
1	B	900	VAL	2.6
1	B	1214	GLY	2.6
1	B	899	ASP	2.6
1	B	921	SER	2.5
1	A	1048	PRO	2.5
1	B	1170	SER	2.5
1	B	1080	GLU	2.5
1	A	1215	SER	2.4
1	B	1239	TYR	2.4
1	A	1050	ALA	2.4
1	A	985	LEU	2.4
1	B	1031	ARG	2.3
1	B	1182	MET	2.3
1	A	922	LEU	2.3
1	B	883	ASP	2.3
1	B	1291	THR	2.3
1	B	1174	ARG	2.2
1	A	903	ASN	2.2
1	A	1268	THR	2.1
1	B	1105	GLU	2.1
1	B	1121	THR	2.1
1	B	1213	ILE	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 monosaccharides 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.