



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 26, 2019 – 10:53 AM EDT

PDB ID : 3A98
Title : Crystal structure of the complex of the interacting regions of DOCK2 and ELMO1
Authors : Hanawa-Suetsugu, K.; Kukimoto-Niino, M.; Sekine, S.; Ito, T.; Mishima-Tsumagari, C.; Terada, T.; Shirouzu, M.; Fukui, Y.; Yokoyama, S.
Deposited on : 2009-10-21
Resolution : 2.10 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
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

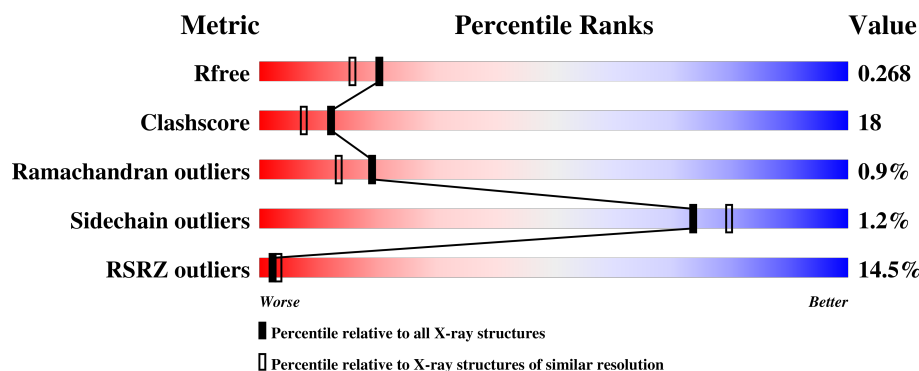
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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. 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	184	<div> <div>5%</div> <div>65% 20% • 15%</div> </div>
1	C	184	<div> <div>4%</div> <div>61% 21% • 17%</div> </div>
2	B	203	<div> <div>14%</div> <div>64% 29% • 6%</div> </div>
2	D	203	<div> <div>24%</div> <div>49% 33% • 18%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5550 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 Deducator of cytokinesis protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	Se	0	0	0
			1286	833	218	229	1	5			
1	C	152	Total	C	N	O	S	Se	0	0	0
			1243	804	210	223	1	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP Q92608
A	-5	SER	-	EXPRESSION TAG	UNP Q92608
A	-4	SER	-	EXPRESSION TAG	UNP Q92608
A	-3	GLY	-	EXPRESSION TAG	UNP Q92608
A	-2	SER	-	EXPRESSION TAG	UNP Q92608
A	-1	SER	-	EXPRESSION TAG	UNP Q92608
A	0	GLY	-	EXPRESSION TAG	UNP Q92608
C	-6	GLY	-	EXPRESSION TAG	UNP Q92608
C	-5	SER	-	EXPRESSION TAG	UNP Q92608
C	-4	SER	-	EXPRESSION TAG	UNP Q92608
C	-3	GLY	-	EXPRESSION TAG	UNP Q92608
C	-2	SER	-	EXPRESSION TAG	UNP Q92608
C	-1	SER	-	EXPRESSION TAG	UNP Q92608
C	0	GLY	-	EXPRESSION TAG	UNP Q92608

- Molecule 2 is a protein called Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S	Se	0	0	0
			1539	975	262	292	6	4			
2	D	167	Total	C	N	O	S	Se	0	0	0
			1349	862	223	254	6	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	525	GLY	-	EXPRESSION TAG	UNP Q92556
B	526	SER	-	EXPRESSION TAG	UNP Q92556
B	527	SER	-	EXPRESSION TAG	UNP Q92556
B	528	GLY	-	EXPRESSION TAG	UNP Q92556
B	529	SER	-	EXPRESSION TAG	UNP Q92556
B	530	SER	-	EXPRESSION TAG	UNP Q92556
B	531	GLY	-	EXPRESSION TAG	UNP Q92556
D	525	GLY	-	EXPRESSION TAG	UNP Q92556
D	526	SER	-	EXPRESSION TAG	UNP Q92556
D	527	SER	-	EXPRESSION TAG	UNP Q92556
D	528	GLY	-	EXPRESSION TAG	UNP Q92556
D	529	SER	-	EXPRESSION TAG	UNP Q92556
D	530	SER	-	EXPRESSION TAG	UNP Q92556
D	531	GLY	-	EXPRESSION TAG	UNP Q92556

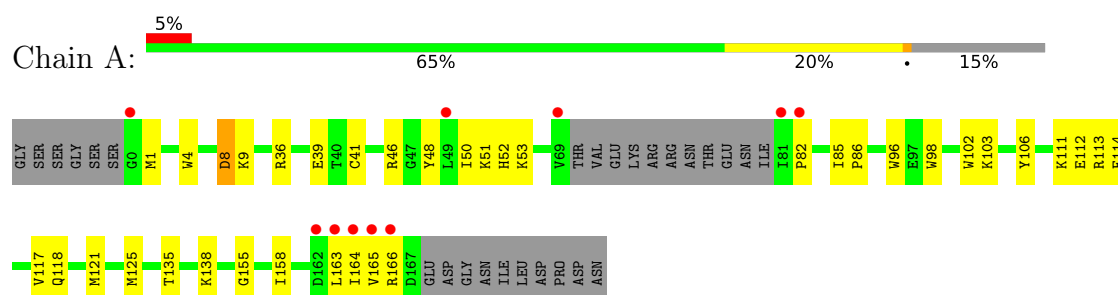
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	52	Total O 52 52	0	0
3	B	35	Total O 35 35	0	0
3	C	23	Total O 23 23	0	0
3	D	23	Total O 23 23	0	0

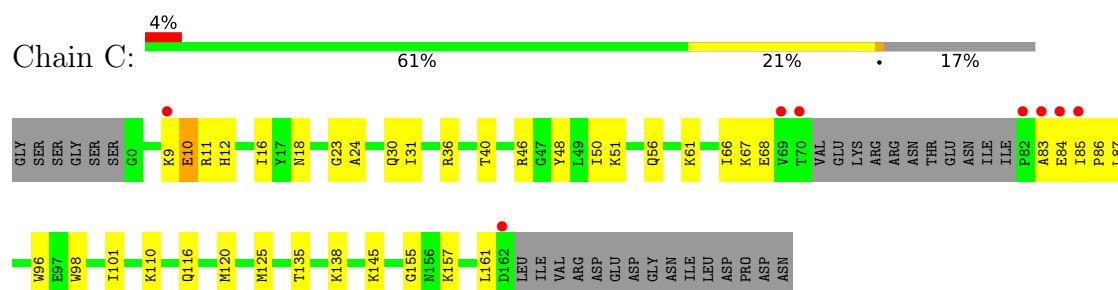
3 Residue-property plots [i](#)

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.

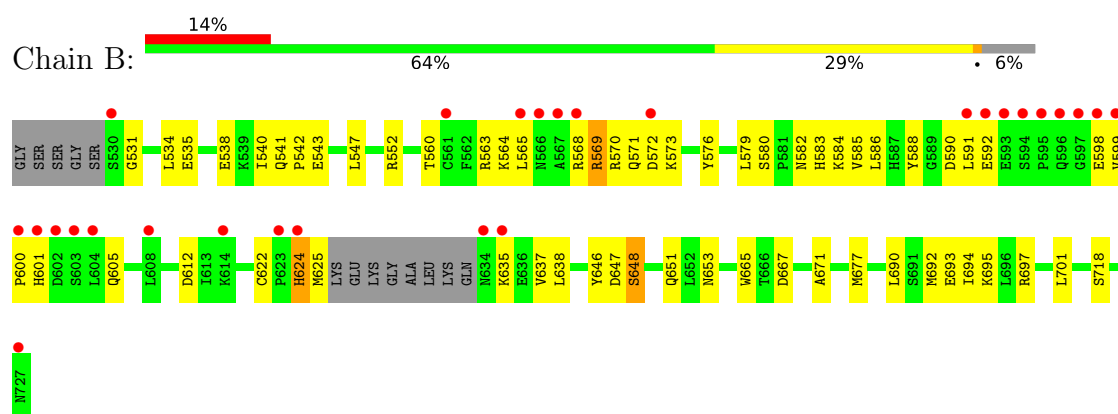
• Molecule 1: Dedicator of cytokinesis protein 2



• Molecule 1: Dedicator of cytokinesis protein 2

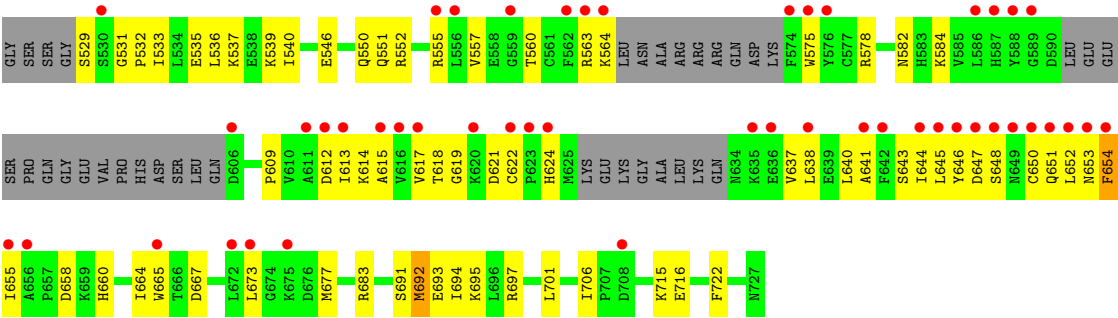


• Molecule 2: Engulfment and cell motility protein 1



• Molecule 2: Engulfment and cell motility protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.84Å 104.03Å 124.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.87 – 2.10 49.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.87-2.10) 99.6 (49.87-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.268 0.227 , 0.268	Depositor DCC
R_{free} test set	2455 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5550	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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	0.41	0/1310	0.60	0/1757
1	C	0.40	0/1267	0.60	0/1698
2	B	0.33	0/1567	0.60	0/2114
2	D	0.30	0/1372	0.56	0/1848
All	All	0.36	0/5516	0.59	0/7417

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	1286	0	1314	39	0
1	C	1243	0	1263	40	0
2	B	1539	0	1534	66	0
2	D	1349	0	1348	75	0
3	A	52	0	0	0	0
3	B	35	0	0	0	0
3	C	23	0	0	0	0
3	D	23	0	0	3	0
All	All	5550	0	5459	199	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 18.

The worst 5 of 199 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)
2:B:625:MSE:HE1	2:B:637:VAL:HG23	1.51	0.93
2:D:651:GLN:HE21	2:D:653:ASN:HD21	1.16	0.90
2:B:671:ALA:HB2	2:B:677:MSE:HE3	1.57	0.86
2:B:625:MSE:HE3	2:B:638:LEU:HD13	1.60	0.82
2:B:651:GLN:HE21	2:B:653:ASN:HD21	1.27	0.82

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	153/184 (83%)	149 (97%)	2 (1%)	2 (1%)	13	8
1	C	148/184 (80%)	140 (95%)	7 (5%)	1 (1%)	24	19
2	B	186/203 (92%)	172 (92%)	12 (6%)	2 (1%)	16	10
2	D	159/203 (78%)	150 (94%)	8 (5%)	1 (1%)	27	23
All	All	646/774 (84%)	611 (95%)	29 (4%)	6 (1%)	19	13

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	648	SER
2	D	648	SER
1	A	166	ARG
1	C	9	LYS
1	A	8	ASP

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	139/158 (88%)	139 (100%)	0	100	100
1	C	134/158 (85%)	133 (99%)	1 (1%)	85	89
2	B	176/181 (97%)	174 (99%)	2 (1%)	76	81
2	D	155/181 (86%)	151 (97%)	4 (3%)	49	53
All	All	604/678 (89%)	597 (99%)	7 (1%)	74	80

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	652	LEU
2	D	716	GLU
2	D	654	PHE
2	B	701	LEU
2	D	692	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	703	ASN
1	C	30	GLN
2	D	624	HIS
2	B	651	GLN
2	D	550	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	152/184 (82%)	0.55	10 (6%)	18 23	25, 38, 80, 105	0
1	C	147/184 (79%)	0.54	8 (5%)	26 32	27, 40, 79, 104	0
2	B	186/203 (91%)	0.92	28 (15%)	2 3	27, 50, 98, 114	0
2	D	163/203 (80%)	1.51	48 (29%)	0 0	28, 65, 108, 124	0
All	All	648/774 (83%)	0.90	94 (14%)	2 3	25, 47, 102, 124	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	LEU	10.7
2	B	599	VAL	9.0
1	C	69	VAL	8.8
2	D	616	VAL	8.6
2	B	593	GLU	7.7

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.