



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:26 am BST

PDB ID : 3WOZ
Title : Crystal structure of CLASP2 TOG domain (TOG3)
Authors : Hayashi, I.; Maki, T.
Deposited on : 2014-01-06
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

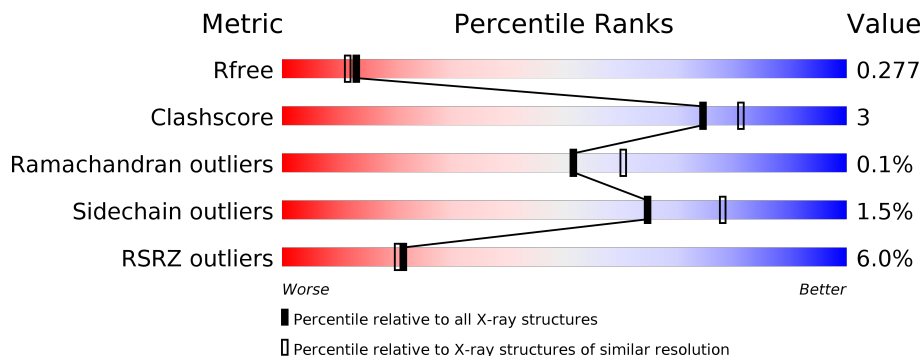
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	232	 3% 88% 8% . .
1	B	232	 3% 90% 9% .
1	C	232	 6% 89% 9% .
1	D	232	 11% 86% 9% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7722 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 CLIP-associating protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	225	Total 1820	C 1161	N 315	O 336	S 2	Se 6	0	2	0
1	B	229	Total 1842	C 1174	N 319	O 341	S 2	Se 6	0	0	0
1	C	229	Total 1842	C 1174	N 319	O 341	S 2	Se 6	0	0	0
1	D	222	Total 1795	C 1143	N 309	O 333	S 2	Se 8	0	2	0

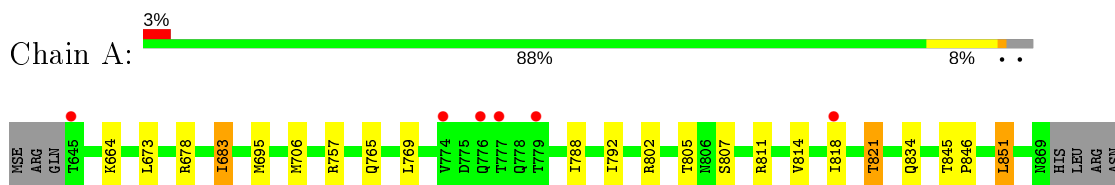
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	115	Total 115	O 115	0	0
2	B	139	Total 139	O 139	0	0
2	C	91	Total 91	O 91	0	0
2	D	78	Total 78	O 78	0	0

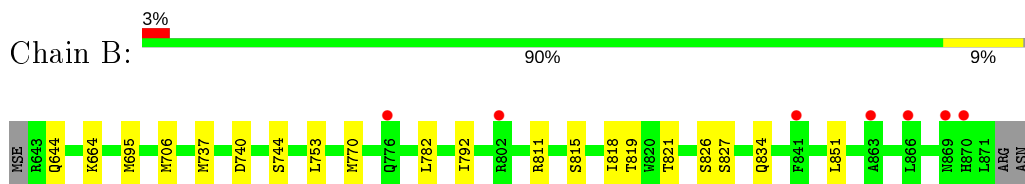
3 Residue-property plots [i](#)

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.

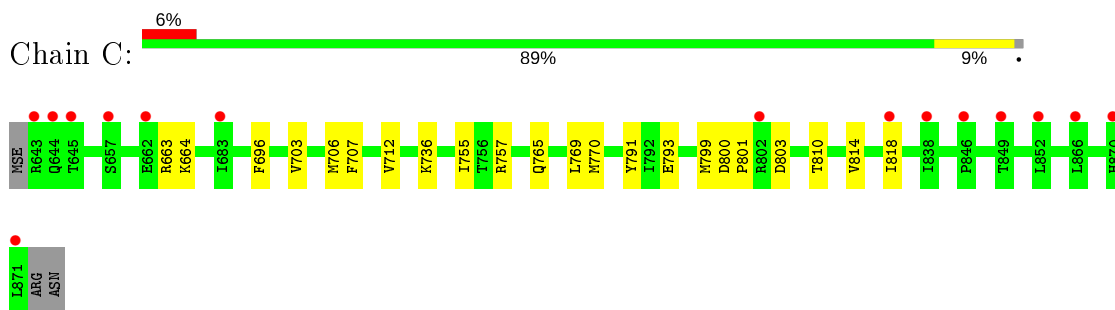
- Molecule 1: CLIP-associating protein 2



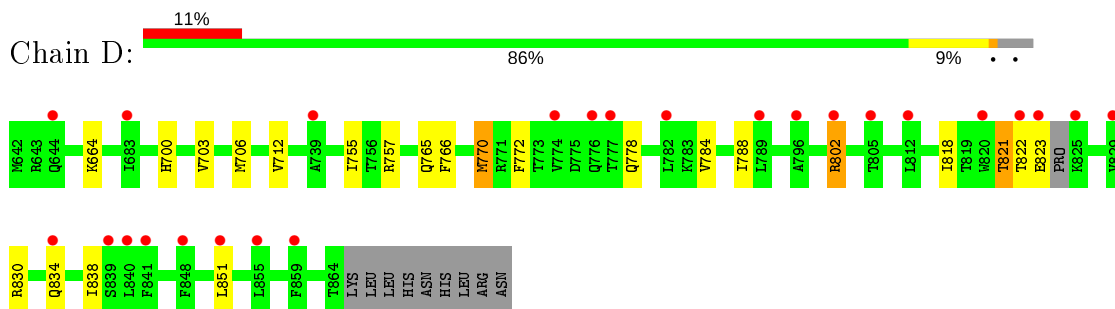
- Molecule 1: CLIP-associating protein 2



- Molecule 1: CLIP-associating protein 2



- Molecule 1: CLIP-associating protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.90Å 122.32Å 86.51Å 90.00° 94.67° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 49.88 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.20) 99.7 (49.88-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.14Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.241 , 0.279 0.238 , 0.277	Depositor DCC
R_{free} test set	2917 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtrriage
Anisotropy	0.242	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7722	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.35	0/1848	0.50	1/2483 (0.0%)
1	B	0.37	0/1866	0.48	0/2510
1	C	0.35	0/1866	0.49	0/2510
1	D	0.34	0/1821	0.50	1/2444 (0.0%)
All	All	0.36	0/7401	0.49	2/9947 (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	D	851	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	851	LEU	CA-CB-CG	5.05	126.91	115.30

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	1820	0	1886	12	0
1	B	1842	0	1899	12	0
1	C	1842	0	1899	11	0
1	D	1795	0	1855	15	0
2	A	115	0	0	0	0
2	B	139	0	0	1	0
2	C	91	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	78	0	0	1	0
All	All	7722	0	7539	48	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 3.

All (48) 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:821:THR:CG2	1:A:834:GLN:HG3	2.09	0.82
1:A:814:VAL:O	1:A:818:ILE:HG12	1.86	0.75
1:B:818:ILE:O	1:B:821:THR:HG22	1.88	0.73
1:A:788:ILE:O	1:A:792:ILE:HG12	1.89	0.71
1:A:769:LEU:HD13	1:A:792:ILE:HD13	1.72	0.70
1:C:712:VAL:HG13	1:C:755:ILE:HD13	1.73	0.69
1:C:814:VAL:O	1:C:818:ILE:HG12	1.96	0.64
1:B:664:LYS:HG3	1:B:706:MSE:SE	2.51	0.61
1:D:757:ARG:HA	1:D:765:GLN:HE22	1.66	0.61
1:B:770:MSE:HE1	1:B:792:ILE:HD13	1.84	0.59
1:D:822:THR:O	1:D:823:GLU:HB3	2.02	0.59
1:C:757:ARG:HA	1:C:765:GLN:HE22	1.68	0.59
1:A:845:THR:HB	1:A:846:PRO:HD3	1.84	0.58
1:C:712:VAL:HG13	1:C:755:ILE:CD1	2.34	0.58
1:A:664:LYS:HG3	1:A:706:MSE:SE	2.56	0.56
1:D:834:GLN:O	1:D:838:ILE:HG12	2.06	0.56
1:D:766:PHE:CZ	1:D:770:MSE:HE2	2.42	0.55
1:B:821:THR:OG1	1:B:834:GLN:HG3	2.07	0.54
1:B:782:LEU:HD13	1:B:826:SER:HB2	1.90	0.53
1:B:644:GLN:NE2	2:B:1015:HOH:O	2.37	0.51
1:D:830:ARG:HD2	2:D:944:HOH:O	2.12	0.50
1:D:757:ARG:HA	1:D:765:GLN:NE2	2.25	0.49
1:D:818:ILE:O	1:D:821:THR:HG22	2.12	0.49
1:A:673:LEU:HD22	1:A:678:ARG:HG2	1.95	0.49
1:A:821:THR:HG23	1:A:834:GLN:HG3	1.91	0.49
1:C:663:ARG:HE	1:C:703:VAL:HG11	1.77	0.49
1:C:757:ARG:HA	1:C:765:GLN:NE2	2.28	0.48
1:C:770:MSE:HE3	1:C:810:THR:HA	1.95	0.48
1:A:807:SER:O	1:A:811:ARG:HB2	2.14	0.47
1:A:802:ARG:HH11	1:A:805:THR:HG22	1.80	0.47
1:C:664:LYS:HG3	1:C:706:MSE:SE	2.64	0.47
1:D:700:HIS:HD2	1:D:703:VAL:H	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:ARG:HA	1:A:765:GLN:HE22	1.79	0.47
1:B:827:SER:HB3	1:D:802:ARG:HB2	1.98	0.45
1:C:799:MSE:HE3	1:C:803:ASP:HB3	1.99	0.45
1:D:664:LYS:HE3	1:D:706:MSE:SE	2.67	0.45
1:B:770:MSE:HE1	1:B:792:ILE:CD1	2.48	0.44
1:D:712:VAL:HG22	1:D:755:ILE:HG13	2.00	0.44
1:C:696:PHE:O	1:C:736:LYS:HE3	2.18	0.44
1:D:821:THR:O	1:D:830:ARG:HG3	2.19	0.43
1:D:784:VAL:O	1:D:788:ILE:HG12	2.19	0.43
1:C:769:LEU:HD11	1:C:791:TYR:CD2	2.54	0.42
1:B:737:MSE:HG3	1:B:753:LEU:CD1	2.50	0.41
1:A:683:ILE:HG23	1:B:740:ASP:OD1	2.21	0.41
1:B:815:SER:O	1:B:819:THR:HG23	2.20	0.41
1:B:811:ARG:HG2	1:B:851:LEU:HG	2.02	0.41
1:D:700:HIS:CD2	1:D:703:VAL:HG23	2.56	0.40
1:D:772:PHE:HE2	1:D:778:GLN:HE22	1.70	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	225/232 (97%)	220 (98%)	5 (2%)	0	100	100
1	B	227/232 (98%)	225 (99%)	2 (1%)	0	100	100
1	C	227/232 (98%)	225 (99%)	1 (0%)	1 (0%)	34	37
1	D	219/232 (94%)	216 (99%)	3 (1%)	0	100	100
All	All	898/928 (97%)	886 (99%)	11 (1%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	801	PRO

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	207/205 (101%)	203 (98%)	4 (2%)	57	71
1	B	209/205 (102%)	207 (99%)	2 (1%)	76	86
1	C	209/205 (102%)	206 (99%)	3 (1%)	67	80
1	D	204/205 (100%)	201 (98%)	3 (2%)	65	78
All	All	829/820 (101%)	817 (99%)	12 (1%)	65	80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	683	ILE
1	A	695	MSE
1	A	821	THR
1	A	851	LEU
1	B	695	MSE
1	B	744	SER
1	C	707	PHE
1	C	793	GLU
1	C	800	ASP
1	D	770	MSE
1	D	802	ARG
1	D	821	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	671	GLN
1	A	677	GLN
1	A	765	GLN
1	A	767	ASN

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Mol	Chain	Res	Type
1	A	834	GLN
1	C	671	GLN
1	C	765	GLN
1	C	869	ASN
1	D	700	HIS
1	D	723	GLN
1	D	762	ASN
1	D	765	GLN
1	D	860	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

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	219/232 (94%)	0.34	6 (2%) 54 52	34, 51, 82, 94	0
1	B	223/232 (96%)	0.27	7 (3%) 49 47	35, 48, 82, 91	0
1	C	223/232 (96%)	0.57	15 (6%) 17 16	38, 57, 76, 95	0
1	D	215/232 (92%)	0.74	25 (11%) 4 4	46, 62, 103, 107	0
All	All	880/928 (94%)	0.48	53 (6%) 21 20	34, 54, 96, 107	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	645	THR	7.9
1	D	820	TRP	7.8
1	D	802	ARG	5.9
1	C	871	LEU	5.3
1	D	822	THR	4.9
1	D	777	THR	4.4
1	D	789	LEU	3.8
1	A	776	GLN	3.7
1	D	840	LEU	3.6
1	C	870	HIS	3.3
1	C	643	ARG	3.2
1	D	644	GLN	3.0
1	D	829	VAL	3.0
1	A	777	THR	3.0
1	D	851	LEU	3.0
1	D	823	GLU	3.0
1	D	805	THR	3.0
1	B	802	ARG	2.9
1	D	776	GLN	2.8
1	B	863	ALA	2.8
1	D	782	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	848	PHE	2.7
1	D	812	LEU	2.6
1	C	683	ILE	2.6
1	D	683	ILE	2.6
1	D	859	PHE	2.5
1	B	776	GLN	2.5
1	C	802	ARG	2.5
1	D	774	VAL	2.5
1	B	866	LEU	2.5
1	B	869	ASN	2.5
1	C	662	GLU	2.5
1	D	739	ALA	2.4
1	C	644	GLN	2.4
1	C	818	ILE	2.4
1	D	841	PHE	2.4
1	A	645	THR	2.3
1	B	841	PHE	2.3
1	D	855	LEU	2.3
1	C	849	THR	2.2
1	D	796	ALA	2.2
1	D	834	GLN	2.2
1	A	774	VAL	2.2
1	A	779	THR	2.2
1	A	818	ILE	2.2
1	B	870	HIS	2.2
1	C	838	ILE	2.2
1	C	852	LEU	2.2
1	C	846	PRO	2.1
1	D	839	SER	2.1
1	C	866	LEU	2.1
1	D	825	LYS	2.1
1	C	657	SER	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.