



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 PM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

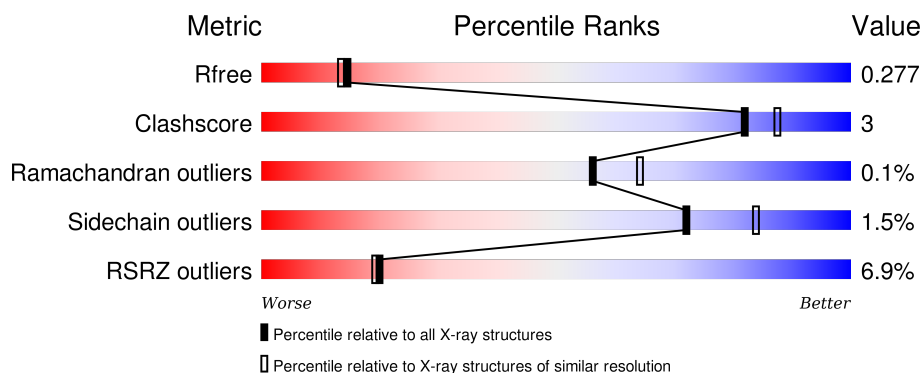
1 Overall quality at a glance ⓘ

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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. 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	<div> <div>3%</div> <div>88%</div> <div>8%</div> <div>••</div> </div>
1	B	232	<div> <div>4%</div> <div>90%</div> <div>9%</div> <div>•</div> </div>
1	C	232	<div> <div>7%</div> <div>89%</div> <div>9%</div> <div>•</div> </div>
1	D	232	<div> <div>12%</div> <div>86%</div> <div>9%</div> <div>••</div> </div>

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.

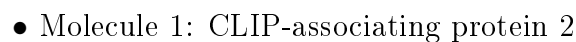
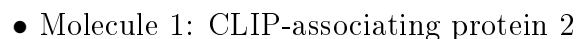
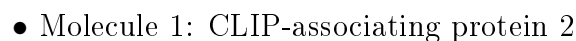
- Molecule 1 is a protein called CLIP-associating protein 2.

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

- Molecule 2 is water.

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

- 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	50.90 Å 122.32 Å 86.51 Å 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 2.14 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.241 , 0.279 0.238 , 0.277	Depositor DCC
R_{free} test set	2712 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 57449 reflections	Xtriage
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

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:B:815:SER:O	1:B:819:THR:HG23	2.20	0.41
1:A:683:ILE:HG23	1:B:740:ASP:OD1	2.21	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%)	39	42
1	D	219/232 (94%)	216 (99%)	3 (1%)	0	100	100
All	All	898/928 (97%)	886 (99%)	11 (1%)	1 (0%)	56	64

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%)	65	77
1	B	209/205 (102%)	207 (99%)	2 (1%)	82	91
1	C	209/205 (102%)	206 (99%)	3 (1%)	74	85
1	D	204/205 (100%)	201 (98%)	3 (2%)	72	84
All	All	829/820 (101%)	817 (99%)	12 (1%)	72	85

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%)	0.41	7 (3%) 51 50	34, 51, 82, 94	0
1	B	223/232 (96%)	0.33	9 (4%) 42 41	35, 48, 82, 91	0
1	C	223/232 (96%)	0.64	17 (7%) 17 16	38, 57, 76, 95	0
1	D	215/232 (92%)	0.81	28 (13%) 5 4	46, 62, 103, 107	0
All	All	880/928 (94%)	0.54	61 (6%) 20 19	34, 54, 96, 107	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	645	THR	8.2
1	D	820	TRP	8.0
1	D	802	ARG	5.9
1	C	871	LEU	5.6
1	D	822	THR	5.2
1	D	777	THR	4.6
1	D	789	LEU	4.0
1	A	776	GLN	3.7
1	D	840	LEU	3.7
1	C	870	HIS	3.4
1	C	643	ARG	3.3
1	D	851	LEU	3.2
1	D	829	VAL	3.2
1	D	644	GLN	3.1
1	D	805	THR	3.1
1	D	823	GLU	3.1
1	A	777	THR	3.0
1	B	802	ARG	3.0
1	D	782	LEU	2.9
1	D	776	GLN	2.9
1	B	863	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	848	PHE	2.8
1	D	812	LEU	2.8
1	C	683	ILE	2.7
1	D	683	ILE	2.7
1	D	774	VAL	2.7
1	D	859	PHE	2.7
1	B	866	LEU	2.6
1	B	776	GLN	2.6
1	B	869	ASN	2.6
1	C	802	ARG	2.6
1	D	739	ALA	2.6
1	C	662	GLU	2.5
1	C	818	ILE	2.5
1	D	841	PHE	2.5
1	A	645	THR	2.5
1	C	644	GLN	2.5
1	B	841	PHE	2.4
1	C	849	THR	2.4
1	D	855	LEU	2.4
1	D	796	ALA	2.3
1	A	774	VAL	2.3
1	A	818	ILE	2.3
1	A	779	THR	2.3
1	D	834	GLN	2.3
1	C	852	LEU	2.3
1	C	846	PRO	2.3
1	C	838	ILE	2.3
1	B	870	HIS	2.2
1	D	839	SER	2.2
1	C	866	LEU	2.2
1	D	825	LYS	2.2
1	C	657	SER	2.1
1	A	840	LEU	2.1
1	C	858	THR	2.1
1	B	774	VAL	2.1
1	C	698	ASP	2.1
1	D	804	PHE	2.1
1	B	871	LEU	2.1
1	D	836	VAL	2.0
1	D	837	LEU	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.