wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:42 AM GMT

PDB ID	:	3BUW
Title	:	Crystal structure of c-Cbl-TKB domain complexed with its binding motif in Syk
Authors	:	Ng, C.; Jackson, R.A.; Buschdorf, J.P.; Sun, Q.; Guy, G.R.; Sivaraman, J.
Deposited on	:	2008-01-03
Resolution	:	1.45 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

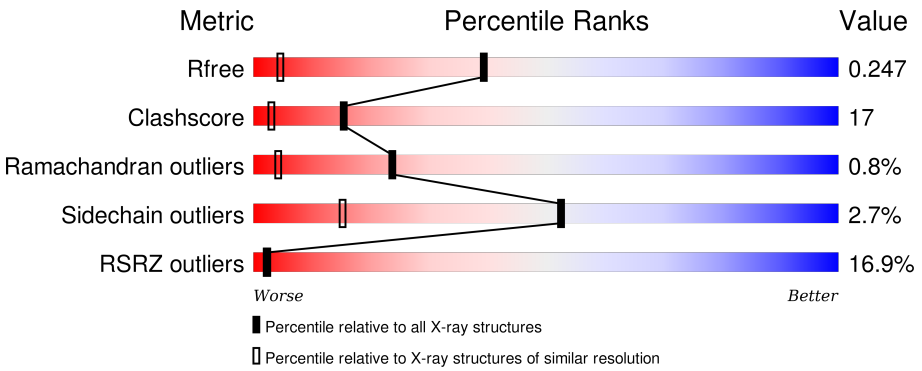
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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}	91344	1278 (1.48-1.44)
Clashscore	102246	1336 (1.48-1.44)
Ramachandran outliers	100387	1320 (1.48-1.44)
Sidechain outliers	100360	1320 (1.48-1.44)
RSRZ outliers	91569	1279 (1.48-1.44)

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 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 <=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	13	38%; 46%; 23%; 31%
1	C	13	38%; 23%; 46%; 31%
2	B	329	15%; 65%; 26%; • ; 7%
2	D	329	14%; 64%; 27%; • ; 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5731 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 13-meric peptide from Tyrosine-protein kinase SYK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	9	81	51	10	19	1	0	0	0
1	C	9	81	51	10	19	1	0	0	0

- Molecule 2 is a protein called E3 ubiquitin-protein ligase CBL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	305	2497	1617	425	442	13	0	0	0
2	D	305	2497	1617	425	442	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	SER	GLY	CLONING ARTIFACT	UNP P22681
D	24	SER	GLY	CLONING ARTIFACT	UNP P22681

- Molecule 3 is water.

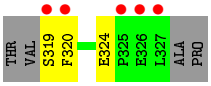
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	7	7	7	0	0
3	B	291	291	291	0	0
3	C	14	14	14	0	0
3	D	263	263	263	0	0

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 errors 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.

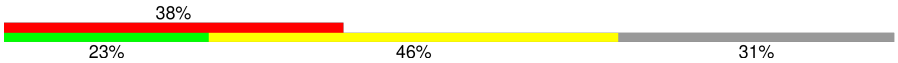
- Molecule 1: 13-meric peptide from Tyrosine-protein kinase SYK

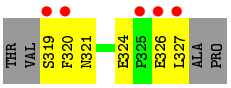
Chain A:



- Molecule 1: 13-meric peptide from Tyrosine-protein kinase SYK

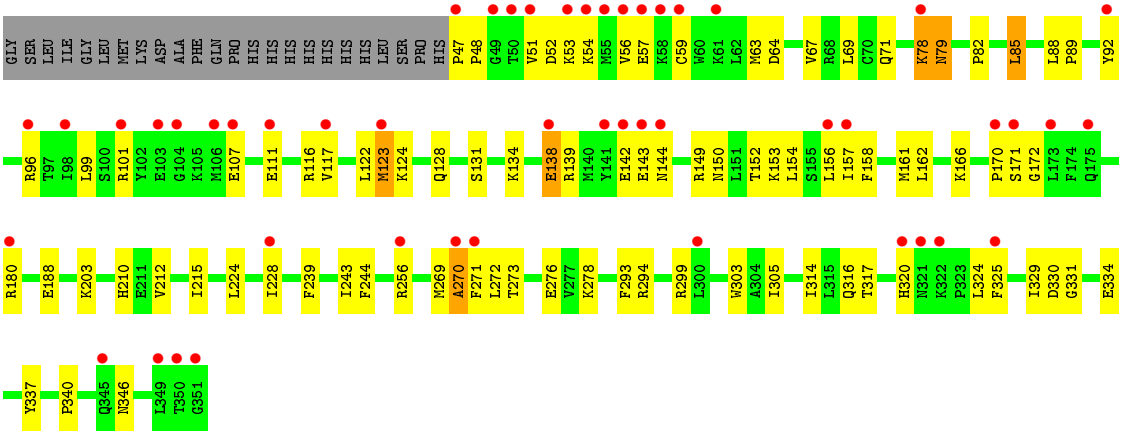
Chain C:





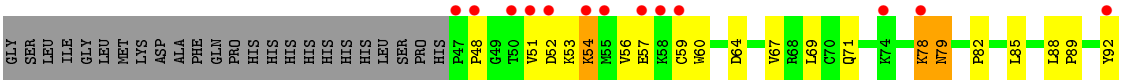
- Molecule 2: E3 ubiquitin-protein ligase CBL

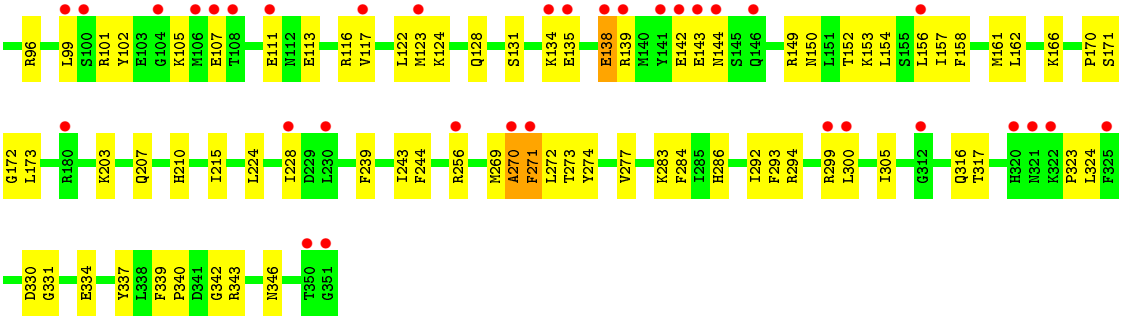
Chain B:



- Molecule 2: E3 ubiquitin-protein ligase CBL

Chain D:




R96
L99 S100 R101 Y102 E103 G104 K105 M106 E107 T108
E111 N112 E113
R116 Y117
L122 M123 K124
Q128
S131
K134 E135
E138 R139 M140 Y141 E142 E143 N144 S145 Q146
R149 N150 L151 T152 K153 L154 S155 L156 I157 F158
M161 L162
K166
P170 S171
G172 L173 R180 K203 Q207 H210 I215 L224 I228 D229 L230 F239 I243 F244 R256 M269 A270 F271 L272 T273 Y274 V277 K283 F284 I285 H286 I292 F293 R294 R299 L300 I305 G312 Q316 T317 H320 N321 K322 P323 L324 F325
D330 G331 E334 Y337 L338 F339 P340 D341 G342 R343 N346 T350 G351

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.79Å 104.81Å 52.78Å 90.00° 89.83° 90.00°	Depositor
Resolution (Å)	20.00 – 1.45 32.16 – 1.45	Depositor EDS
% Data completeness (in resolution range)	79.8 (20.00-1.45) 92.3 (32.16-1.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 1.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.238 0.233 , 0.247	Depositor DCC
R_{free} test set	2538 reflections (2.24%)	DCC
Wilson B-factor (Å^2)	14.4	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 47.0	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 113542 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5731	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.82 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6694e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR

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	0.43	0/66	0.55	0/88
1	C	0.44	0/66	0.56	0/88
2	B	0.38	0/2564	0.54	0/3461
2	D	0.38	0/2564	0.54	0/3461
All	All	0.38	0/5260	0.54	0/7098

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	81	0	63	3	0
1	C	81	0	63	7	0
2	B	2497	0	2506	84	0
2	D	2497	0	2506	89	0
3	A	7	0	0	0	0
3	B	291	0	0	9	0
3	C	14	0	0	3	0
3	D	263	0	0	9	0
All	All	5731	0	5138	178	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 17.

The worst 5 of 178 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:157:ILE:HG22	2:B:161:MET:HE2	1.19	1.15
1:C:324:GLU:HB2	2:D:317:THR:HG22	1.32	1.11
2:D:157:ILE:HG22	2:D:161:MET:HE2	1.31	1.07
1:A:324:GLU:HB2	2:B:317:THR:HG22	1.35	1.06
2:B:158:PHE:HA	2:B:161:MET:HE3	1.33	1.04

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	6/13 (46%)	4 (67%)	2 (33%)	0	100	100
1	C	6/13 (46%)	4 (67%)	2 (33%)	0	100	100
2	B	303/329 (92%)	287 (95%)	14 (5%)	2 (1%)	26	5
2	D	303/329 (92%)	289 (95%)	11 (4%)	3 (1%)	19	3
All	All	618/684 (90%)	584 (94%)	29 (5%)	5 (1%)	24	4

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	270	ALA
2	D	270	ALA
2	B	271	PHE
2	D	271	PHE
2	D	54	LYS

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	8/11 (73%)	8 (100%)	0	100	100
1	C	8/11 (73%)	8 (100%)	0	100	100
2	B	272/293 (93%)	264 (97%)	8 (3%)	50	13
2	D	272/293 (93%)	265 (97%)	7 (3%)	54	17
All	All	560/608 (92%)	545 (97%)	15 (3%)	52	15

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	138	GLU
2	B	299	ARG
2	D	85	LEU
2	B	123	MET
2	D	79	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	345	GLN
2	D	146	GLN
2	D	345	GLN
2	B	346	ASN
2	D	79	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PTR	A	323	1	14,16,17	1.45	0	18,22,24	1.14	2 (11%)
1	PTR	C	323	1	14,16,17	1.45	0	18,22,24	1.09	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	323	1	-	0/9/11/13	0/1/1/1
1	PTR	C	323	1	-	0/9/11/13	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	323	PTR	CD2-CE2-CZ	-2.28	116.87	119.74
1	C	323	PTR	CD2-CE2-CZ	-2.24	116.93	119.74
1	A	323	PTR	O-C-CA	-2.12	119.98	125.49
1	C	323	PTR	O-C-CA	-2.04	120.17	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	8/13 (61%)	4.84	5 (62%)	0	0	21, 34, 51, 52	0
1	C	8/13 (61%)	5.65	5 (62%)	0	0	21, 34, 51, 52	0
2	B	305/329 (92%)	0.96	49 (16%)	3	3	9, 18, 48, 57	0
2	D	305/329 (92%)	0.94	47 (15%)	3	3	9, 18, 48, 57	0
All	All	626/684 (91%)	1.06	106 (16%)	2	2	9, 19, 48, 57	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	327	LEU	19.3
1	A	327	LEU	18.4
2	D	350	THR	12.0
2	D	47	PRO	11.2
2	D	351	GLY	9.6

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	PTR	C	323	16/17	0.97	0.09	-	12,16,26,26	0
1	PTR	A	323	16/17	0.97	0.09	-	12,16,26,26	0

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.