



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 01:54 pm BST

PDB ID : 3BUO
Title : Crystal structure of c-Cbl-TKB domain complexed with its binding motif in EGF receptor'
Authors : Ng, C.; Jackson, R.A.; Buschdorf, J.P.; Sun, Q.; Guy, G.R.; Sivaraman, J.
Deposited on : 2008-01-03
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

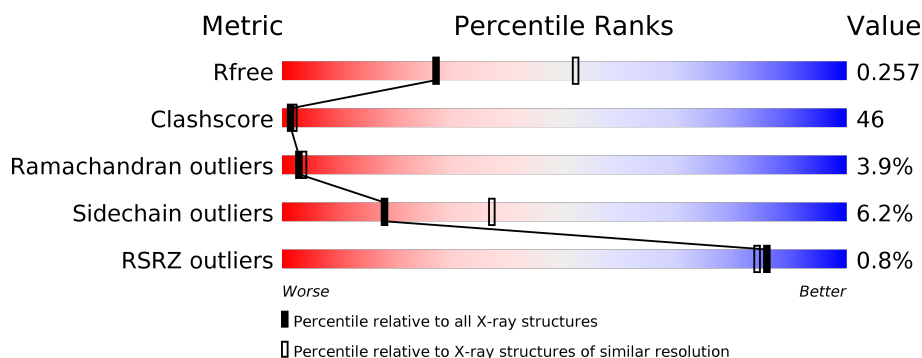
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	13	<div> <div>15%</div> <div> <div>38%</div> <div>23%</div> <div>23%</div> <div>15%</div> </div> </div>
1	C	13	<div> <div>15%</div> <div> <div>38%</div> <div>23%</div> <div>23%</div> <div>15%</div> </div> </div>
2	B	329	<div> <div>38%</div> <div>48%</div> <div>6%</div> <div>8%</div> </div>
2	D	329	<div> <div>36%</div> <div>49%</div> <div>6%</div> <div>8%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5405 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	11	Total	C	N	O	P	0	0	0
			95	57	15	22	1			
1	C	11	Total	C	N	O	P	0	0	0
			95	57	15	22	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	304	Total	C	N	O	S	0	0	0
			2490	1612	424	441	13			
2	D	304	Total	C	N	O	S	0	0	0
			2490	1612	424	441	13			

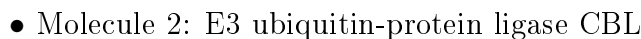
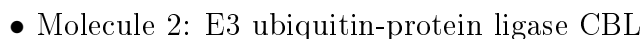
There are 2 discrepancies between the modelled and reference sequences:

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
3	A	6	Total	O	0	0
			6	6		
3	B	111	Total	O	0	0
			111	111		
3	C	6	Total	O	0	0
			6	6		
3	D	112	Total	O	0	0
			112	112		

- Molecule 1: 13-meric peptide from Epidermal growth factor receptor



GLY	GLY			
SER	SER			
LEU	LEU			
ILE	ILE			
GLY	GLY			
LEU	LEU			
MET	MET			
LYS	LYS			
ASP	ASP			
ALA	ALA			
PHE	PHE			
GLN	GLN			
PRO	PRO			
HIS	HIS			
HIS	HIS			
HIS	HIS			
HIS	HIS			
HIS	HIS			
LEU	LEU			
SER	SER			
PRO	PRO			
HIS	HIS			
PRO	PRO			
P48	P48			
G49	G49			
V51	V51			
D52	D52			
K53	K53			
K54	K54			
K55	K55			
V56	V56			
E57	E57			
K58	K58			
C59	C59			
K60	K60			
K61	K61			
L62	L62			
M63	M63			
D64	D64			
K65	K65			
V66	V66			
V67	V67			
R68	R68			
L69	L69			
C70	C70			
Q71	Q71			
N72	N72			
F73	F73			
K74	K74			
L75	L75			
A76	A76			
L77	L77			
K78	K78			
N79	N79			
S80	S80			
P81	P81			
P82	P82			
Y83	Y83			
R84	R84			
L85	L85			
D86	D86			
L87	L87			
L88	L88			
P89	P89			
D90	D90			
T91	T91			
H94	H94			
L95	L95			
L99	L99			
S100	S100			
R101	R101			
E102	E102			
H103	H103			
G104	G104			
K105	K105			
M106	M106			
E107	E107			
E111	E111			
M112	M112			
F115	F115			
R116	R116			
V117	V117			
E120	E120			
M121	M121			
L122	L122			
M123	M123			
K127	K127			
Q128	Q128			
T129	T129			
I130	I130			
S131	S131			
L132	L132			
F133	F133			
K134	K134			
E135	E135			
G136	G136			
K137	K137			
E138	E138			
R139	R139			
M140	M140			
Y141	Y141			
E142	E142			
E143	E143			
M144	M144			
S145	S145			
Q146	Q146			
P147	P147			
R148	R148			
R149	R149			
M150	M150			
L151	L151			
T152	T152			
K153	K153			
L154	L154			
S155	S155			
L156	L156			
I157	I157			
F158	F158			
S159	S159			
H160	H160			
M161	M161			
L162	L162			
L165	L165			
K166	K166			
G167	G167			
I168	I168			
F169	F169			
P170	P170			
S171	S171			
G172	G172			
L173	L173			
F174	F174			
Q175	Q175			
T182	T182			
K183	K183			
E188	E188			
F189	F189			
H190	H190			
R191	R191			
G195	G195			
E196	E196			
K197	K197			
T198	T198			
I199	I199			
V200	V200			
P201	P201			
W202	W202			
K203	K203			
L209	L209			
H210	H210			
T215	T215			
S216	S216			
A221	A221			
L224	L224			
K225	K225			
L228	L228			
D229	D229			
L230	L230			
T231	T231			
C232	C232			
Y235	Y235			
T243	T243			
F244	F244			
L247	L247			
F248	F248			
Q249	Q249			
P250	P250			
L254	L254			
L255	L255			
R256	R256			
N257	N257			
W258	W258			
N259	N259			
V263	V263			
T264	T264			
R265	R265			
P266	P266			
G267	G267			
Y268	Y268			
N269	N269			
A270	A270			
T271	T271			
L272	L272			
T273	T273			
Y274	Y274			
D275	D275			
E276	E276			
V277	V277			
R280	R280			
L281	L281			
Q282	Q282			
K283	K283			
F284	F284			
T285	T285			
H286	H286			
K287	K287			
P288	P288			
Y291	Y291			
T292	T292			
F293	F293			
R294	R294			
L295	L295			
T298	T298			
R299	R299			
L300	L300			
W303	W303			
A304	A304			
I305	I305			
G306	G306			
Y307	Y307			
V308	V308			
T309	T309			
A310	A310			
D311	D311			
G312	G312			
N313	N313			
I314	I314			
L315	L315			
Q316	Q316			
T317	T317			
I318	I318			
P319	P319			
H320	H320			
N321	N321			
K322	K322			
P323	P323			
L324	L324			
F325	F325			
I329	I329			
D330	D330			
G331	G331			
Y337	Y337			
L338	L338			
F339	F339			
P340	P340			
D341	D341			
G342	G342			
R343	R343			
N344	N344			
Q345	Q345			
N346	N346			
P347	P347			
D348	D348			
L349	L349			
T350	T350			
G351	G351			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.86Å 110.17Å 55.82Å 90.00° 89.94° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 39.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	51.8 (20.00-2.60) 91.3 (39.29-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.278 0.249 , 0.257	Depositor DCC
R_{free} test set	2860 reflections (13.04%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.458 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5405	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.08% 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](#)

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	0.68	0/79	0.96	0/104
1	C	0.65	0/79	0.95	0/104
2	B	0.52	0/2556	0.65	0/3449
2	D	0.51	0/2556	0.65	0/3449
All	All	0.52	0/5270	0.66	0/7106

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	95	0	80	16	0
1	C	95	0	80	19	0
2	B	2490	0	2499	232	0
2	D	2490	0	2499	232	0
3	A	6	0	0	0	0
3	B	111	0	0	16	0
3	C	6	0	0	1	0
3	D	112	0	0	18	0
All	All	5405	0	5158	478	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 46.

The worst 5 of 478 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:D:82:PRO:HG3	2:D:156:LEU:HD12	1.33	1.09
2:D:277:VAL:HG13	2:D:292:ILE:HD11	1.37	1.05
2:B:82:PRO:HG3	2:B:156:LEU:HD12	1.33	1.04
2:B:282:GLN:HE22	2:B:285:ILE:HD12	1.23	1.00
2:D:282:GLN:HE22	2:D:285:ILE:HD12	1.22	1.00

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	8/13 (62%)	4 (50%)	2 (25%)	2 (25%)	0	0
1	C	8/13 (62%)	4 (50%)	2 (25%)	2 (25%)	0	0
2	B	302/329 (92%)	248 (82%)	44 (15%)	10 (3%)	4	6
2	D	302/329 (92%)	248 (82%)	44 (15%)	10 (3%)	4	6
All	All	620/684 (91%)	504 (81%)	92 (15%)	24 (4%)	3	4

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	103	GLU
2	B	270	ALA
2	B	285	ILE
2	D	103	GLU
2	D	270	ALA

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	10/11 (91%)	9 (90%)	1 (10%)	7	14
1	C	10/11 (91%)	9 (90%)	1 (10%)	7	14
2	B	271/293 (92%)	254 (94%)	17 (6%)	18	36
2	D	271/293 (92%)	255 (94%)	16 (6%)	19	39
All	All	562/608 (92%)	527 (94%)	35 (6%)	18	37

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	313	ASN
2	D	53	LYS
2	D	313	ASN
2	B	325	PHE
2	B	343	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	346	ASN
2	D	94	HIS
2	D	345	GLN
2	D	79	ASN
2	D	160	HIS

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	C	1069	1	15,16,17	1.47	1 (6%)	19,22,24	0.98	0
1	PTR	A	1069	1	15,16,17	1.48	2 (13%)	19,22,24	0.99	0

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	C	1069	1	-	1/10/11/13	0/1/1/1
1	PTR	A	1069	1	-	1/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1069	PTR	P-OH	3.43	1.64	1.59
1	C	1069	PTR	P-OH	3.37	1.64	1.59
1	A	1069	PTR	CE1-CD1	2.07	1.42	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	1069	PTR	O-C-CA-CB
1	A	1069	PTR	O-C-CA-CB

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	10/13 (76%)	0.12	2 (20%) 1 0	22, 32, 48, 51	0
1	C	10/13 (76%)	0.10	2 (20%) 1 0	22, 32, 48, 51	0
2	B	304/329 (92%)	-0.43	1 (0%) 94 93	16, 32, 52, 71	0
2	D	304/329 (92%)	-0.43	0 100 100	16, 32, 52, 71	0
All	All	628/684 (91%)	-0.42	5 (0%) 86 84	16, 32, 52, 71	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1065	PHE	2.8
1	C	1064	SER	2.7
1	A	1064	SER	2.4
2	B	173	LEU	2.1
1	C	1065	PHE	2.0

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. 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	B-factors(Å ²)	Q<0.9
1	PTR	C	1069	16/17	0.96	0.14	27,28,29,30	0
1	PTR	A	1069	16/17	0.97	0.13	27,28,29,30	0

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.