



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:28 AM UTC

PDB ID : 6XAR / pdb_00006xar
Title : Structure of CBL tyrosine kinase binding domain (TKBD) with C-terminal tail of Src-like kinase protein 2 (SLAP2)
Authors : Wybenga-Groot, L.E.; McGlade, C.J.
Deposited on : 2020-06-04
Resolution : 2.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

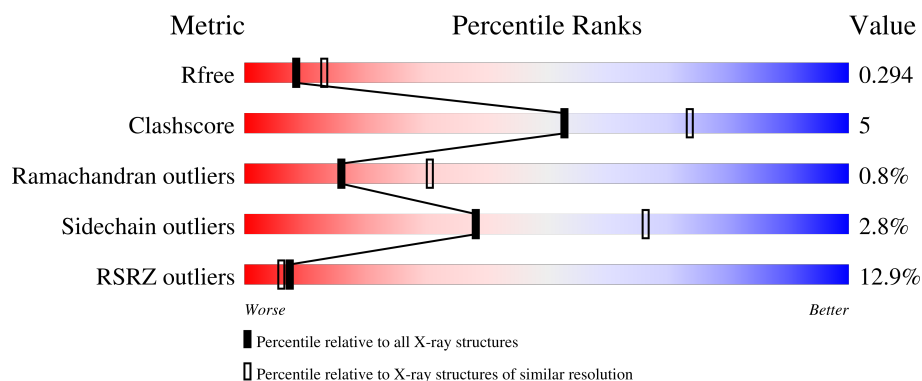
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of 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	335	
1	B	335	
2	C	19	
2	D	19	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5002 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 E3 ubiquitin-protein ligase CBL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2399	1561	399	426	13			
1	B	300	Total	C	N	O	S	0	0	0
			2281	1487	376	408	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP P22681
A	24	SER	-	expression tag	UNP P22681
B	23	GLY	-	expression tag	UNP P22681
B	24	SER	-	expression tag	UNP P22681

- Molecule 2 is a protein called Src-like-adapter 2.

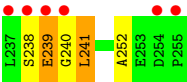
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	19	Total	C	N	O	0	0	0
			140	87	22	31			
2	D	19	Total	C	N	O	0	0	0
			133	82	22	29			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total 28	O 28	0	0
4	B	15	Total 15	O 15	0	0
4	C	1	Total 1	O 1	0	0
4	D	3	Total 3	O 3	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.73Å 86.96Å 65.26Å 90.00° 112.31° 90.00°	Depositor
Resolution (Å)	45.32 – 2.50 45.32 – 2.50	Depositor EDS
% Data completeness (in resolution range)	83.8 (45.32-2.50) 83.8 (45.32-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX dev	Depositor
R, R_{free}	0.249 , 0.293 0.251 , 0.294	Depositor DCC
R_{free} test set	943 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5002	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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: CA

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	0.27	0/2464	0.65	0/3345
1	B	0.26	0/2345	0.67	0/3200
2	C	0.32	0/141	0.72	0/190
2	D	0.27	0/134	0.70	0/181
All	All	0.27	0/5084	0.66	0/6916

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	2399	0	2326	29	1
1	B	2281	0	2125	15	1
2	C	140	0	134	5	0
2	D	133	0	121	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	28	0	0	0	0
4	B	15	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	3	0	0	0	0
All	All	5002	0	4706	48	1

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 5.

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:308:VAL:HG12	1:A:314:ILE:HG12	1.76	0.68
1:A:335:GLY:HA2	1:A:338:LEU:HD21	1.82	0.62
1:A:219:LEU:HD23	1:B:219:LEU:HD23	1.81	0.62
1:B:311:ASP:N	1:B:312:GLY:HA2	2.16	0.59
1:A:255:LEU:O	1:A:259:ASN:ND2	2.31	0.58
1:B:272:LEU:HB2	1:B:294:ARG:HD3	1.86	0.56
2:C:238:SER:HB2	2:C:242:ARG:HE	1.71	0.55
1:A:311:ASP:N	1:A:312:GLY:HA2	2.21	0.55
1:A:266:PRO:HG2	1:A:340:PRO:HB2	1.90	0.53
1:A:277:VAL:HG13	1:A:292:ILE:HD11	1.91	0.53
1:A:178:THR:O	1:A:178:THR:OG1	2.16	0.53
1:A:56:VAL:HG11	1:A:99:LEU:HD11	1.90	0.53
1:B:296:SER:HB3	1:B:299:ARG:HB2	1.90	0.52
1:A:181:ILE:HB	1:A:187:ALA:HB2	1.92	0.52
1:A:288:PRO:HA	1:A:308:VAL:HG23	1.92	0.51
1:A:340:PRO:HG3	1:A:347:PRO:HD3	1.92	0.51
1:B:261:LEU:HD13	1:B:324:LEU:HD12	1.93	0.50
1:A:265:HIS:O	2:C:239:GLU:HG3	2.13	0.49
1:A:101:ARG:HD3	1:A:173:LEU:HD13	1.94	0.49
1:A:179:PHE:HD2	1:A:181:ILE:HG13	1.78	0.49
1:B:82:PRO:HB3	1:B:159:SER:HB2	1.95	0.49
1:B:282:GLN:C	1:B:284:PHE:H	2.20	0.49
1:B:294:ARG:HG3	1:B:304:ALA:HB3	1.97	0.46
1:A:290:SER:HA	1:A:339:PHE:HB2	1.97	0.46
1:A:121:ASN:ND2	1:A:161:MET:SD	2.88	0.46
1:B:277:VAL:HG21	1:B:294:ARG:HE	1.81	0.45
1:A:114:TYR:CZ	1:A:168:ILE:HD12	2.52	0.45
1:B:131:SER:O	1:B:135:GLU:HG2	2.17	0.44
1:A:263:VAL:HA	2:C:241:LEU:HD12	1.98	0.44
2:D:239:GLU:OE1	2:D:240:GLY:N	2.49	0.44
2:D:239:GLU:OE2	2:D:241:LEU:HB2	2.19	0.43
2:C:242:ARG:NH2	2:D:252:ALA:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:PHE:O	1:B:243:ILE:HG12	2.18	0.43
1:A:303:TRP:CD2	1:A:324:LEU:HD22	2.54	0.43
1:A:65:LYS:HD3	1:A:130:ILE:HD13	2.01	0.42
1:B:294:ARG:HH12	1:B:296:SER:HB2	1.84	0.42
1:B:335:GLY:HA2	1:B:338:LEU:HD21	2.01	0.42
1:A:83:TYR:CE2	1:A:85:LEU:HB2	2.54	0.42
1:A:261:LEU:HD13	1:A:324:LEU:HB3	2.02	0.42
1:A:92:TYR:CZ	1:A:96:ARG:HD2	2.55	0.42
1:B:84:ILE:HA	1:B:87:LEU:HB2	2.02	0.42
1:A:209:LEU:O	1:A:213:HIS:N	2.44	0.41
1:A:331:GLY:HA3	1:A:337:TYR:CD2	2.55	0.41
1:A:247:LEU:HD12	1:A:247:LEU:HA	1.84	0.41
1:B:168:ILE:C	1:B:170:PRO:HD3	2.45	0.41
1:A:349:LEU:C	1:A:351:GLY:H	2.29	0.41
2:C:239:GLU:CD	2:C:240:GLY:H	2.28	0.41
1:A:162:LEU:HD11	1:A:166:LYS:HE2	2.03	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:OG1	1:B:274:TYR:OH[1_556]	2.18	0.02

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	303/335 (90%)	286 (94%)	15 (5%)	2 (1%)	18	34
1	B	298/335 (89%)	278 (93%)	18 (6%)	2 (1%)	18	34
2	C	17/19 (90%)	15 (88%)	2 (12%)	0	100	100
2	D	17/19 (90%)	15 (88%)	1 (6%)	1 (6%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	635/708 (90%)	594 (94%)	36 (6%)	5 (1%)	16	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	LYS
2	D	239	GLU
1	A	350	THR
1	B	263	VAL
1	B	196	GLU

5.3.2 Protein sidechains ⓘ

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	249/299 (83%)	244 (98%)	5 (2%)	48	75
1	B	225/299 (75%)	220 (98%)	5 (2%)	45	73
2	C	16/17 (94%)	14 (88%)	2 (12%)	4	9
2	D	14/17 (82%)	12 (86%)	2 (14%)	3	6
All	All	504/632 (80%)	490 (97%)	14 (3%)	38	66

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	LEU
1	A	173	LEU
1	A	178	THR
1	A	247	LEU
1	A	292	ILE
1	B	106	MET
1	B	178	THR
1	B	183	LYS
1	B	274	TYR
1	B	324	LEU

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Mol	Chain	Res	Type
2	C	239	GLU
2	C	241	LEU
2	D	238	SER
2	D	241	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	HIS
1	B	150	ASN
1	B	259	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	305/335 (91%)	0.70	25 (8%) 17 15	24, 42, 71, 81	0
1	B	300/335 (89%)	1.19	48 (16%) 5 4	26, 56, 80, 92	0
2	C	19/19 (100%)	1.02	4 (21%) 2 2	30, 36, 51, 57	0
2	D	19/19 (100%)	1.31	6 (31%) 1 1	26, 34, 56, 63	0
All	All	643/708 (90%)	0.96	83 (12%) 7 6	24, 47, 76, 92	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	351	GLY	6.5
1	A	177	ASP	4.8
1	A	139	ARG	4.8
1	B	181	ILE	4.0
1	A	179	PHE	3.9
2	C	255	PRO	3.7
2	D	255	PRO	3.7
1	B	55	MET	3.7
1	A	76	ALA	3.5
1	B	177	ASP	3.5
1	B	250	PRO	3.4
1	B	309	THR	3.4
1	B	111	GLU	3.3
1	B	194	PHE	3.3
2	C	254	ASP	3.3
2	D	239	GLU	3.2
1	B	286	HIS	3.2
1	B	108	THR	3.1
2	D	254	ASP	3.1
1	A	352	LEU	3.0
1	A	80	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	234	ASP	3.0
1	A	77	LEU	2.9
1	A	79	ASN	2.9
1	B	137	LYS	2.8
1	A	180	ARG	2.8
2	D	238	SER	2.7
1	A	136	GLY	2.7
1	B	212	VAL	2.6
1	A	141	TYR	2.6
1	B	110	GLY	2.6
1	B	114	TYR	2.6
1	B	313	ASN	2.6
2	D	237	LEU	2.5
1	A	104	GLY	2.5
1	B	136	GLY	2.5
1	B	133	PHE	2.5
1	B	207	GLN	2.5
1	B	56	VAL	2.4
1	B	187	ALA	2.4
1	B	77	LEU	2.4
1	A	273	THR	2.4
1	B	178	THR	2.4
2	C	239	GLU	2.4
1	A	178	THR	2.3
1	A	49	GLY	2.3
1	B	107	GLU	2.3
1	B	144	ASN	2.3
1	B	200	VAL	2.3
1	B	109	LEU	2.3
1	B	142	GLU	2.3
2	D	240	GLY	2.2
1	B	199	ILE	2.2
1	B	105	LYS	2.2
1	B	190	TRP	2.2
1	B	104	GLY	2.2
1	A	181	ILE	2.2
1	A	145	SER	2.2
1	B	196	GLU	2.2
1	B	81	PRO	2.2
1	B	262	ALA	2.2
1	A	313	ASN	2.1
1	B	253	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	310	ALA	2.1
1	A	351	GLY	2.1
1	B	99	LEU	2.1
1	B	172	GLY	2.1
1	A	83	TYR	2.1
1	A	138	GLU	2.1
1	B	57	GLU	2.1
1	B	102	TYR	2.1
1	A	50	THR	2.1
1	A	176	GLY	2.1
1	B	315	LEU	2.1
1	B	180	ARG	2.1
1	B	103	GLU	2.1
1	B	314	ILE	2.1
2	C	253	GLU	2.1
1	B	310	ALA	2.1
1	B	75	LEU	2.0
1	B	145	SER	2.0
1	A	110	GLY	2.0
1	B	106	MET	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 oligosaccharides in this entry.

6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
3	CA	A	401	1/1	0.91	0.10	48,48,48,48	0
3	CA	B	401	1/1	0.93	0.09	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.