



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:45 PM UTC

PDB ID : 9QCD / pdb_00009qcd
Title : Micro-ED structure of the NSH2-CSH2 tandem domain of SHP2 in complex with the bis-phosphorylated pY627-pY659-Gab1 (613-694) peptide
Authors : Machner, L.; Shaikhqasem, A.; Hamdi, F.; Breithaupt, C.; Parthier, C.; Kyrilis, F.L.; Kastritis, P.L.; Feller, S.M.; Stubbs, M.T.
Deposited on : 2025-03-04
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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
Mogul : 2022.3.0, CSD as543be (2022)
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

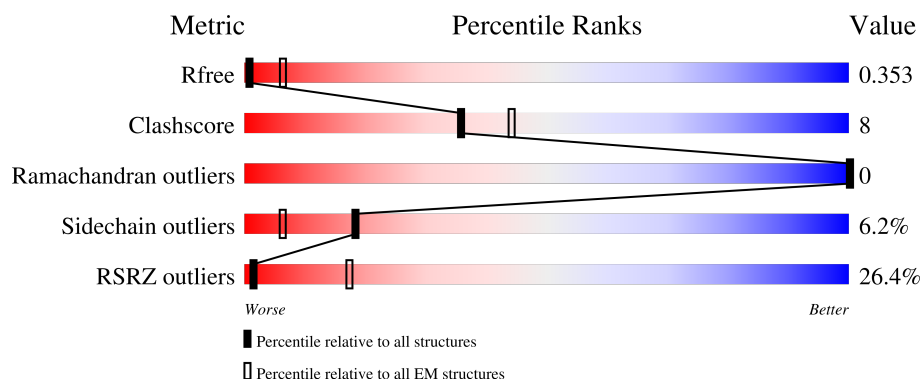
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.20 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)	EM structures (#Entries)
R_{free}	180332	208
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RSRZ outliers	180361	209

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	223	25% 78% 13% 8%
2	C	69	10% 38% 12% 49%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3821 atoms, of which 1889 are hydrogens and 0 are deuteriums.

In the tables below, 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 Tyrosine-protein phosphatase non-receptor type 11.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	206	Total	C	H	N	O	S	0	0
			3262	1038	1620	290	309	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP Q06124

- Molecule 2 is a protein called GRB2-associated-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	35	Total	C	H	N	O	P	0	0
			559	174	269	46	68	2		

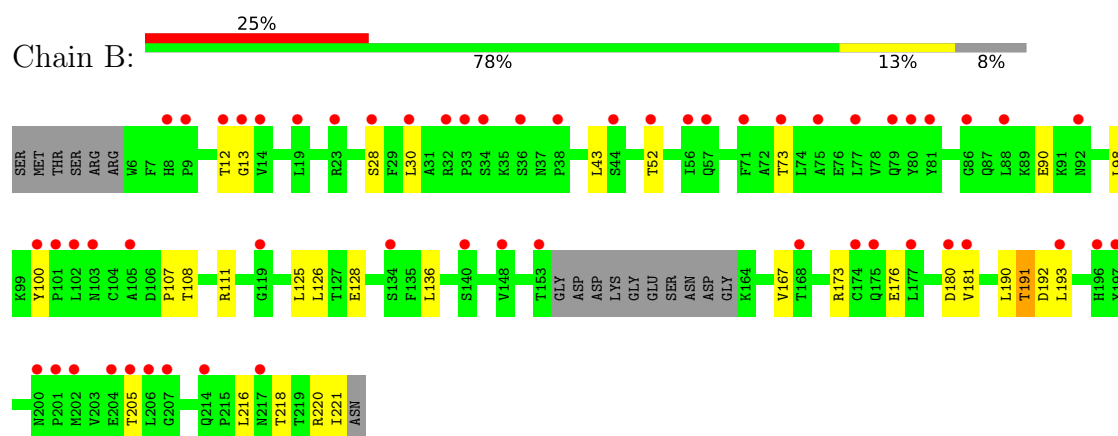
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	615	GLY	-	expression tag	UNP Q13480
C	616	PRO	-	expression tag	UNP Q13480

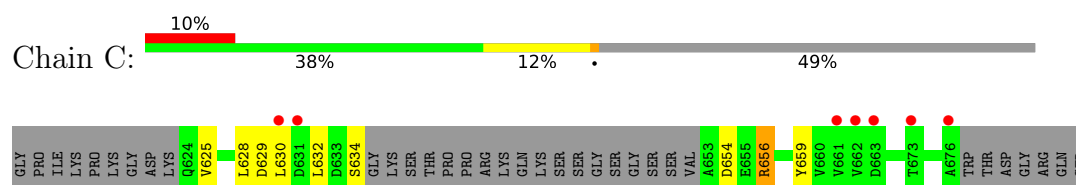
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: Tyrosine-protein phosphatase non-receptor type 11



- Molecule 2: GRB2-associated-binding protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	30.59Å 82.25Å 117.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.72 – 3.20 33.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	88.9 (33.72-3.20) 88.8 (33.72-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.300 , 0.353 0.308 , 0.353	Depositor DCC
R_{free} test set	238 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.888	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	3821	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.90% 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

5.1 Standard geometry

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	B	0.13	0/1678	0.28	0/2264
2	C	0.16	0/254	0.28	0/338
All	All	0.14	0/1932	0.28	0/2602

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

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	B	1642	1620	1620	24	0
2	C	290	269	269	7	0
All	All	1932	1889	1889	28	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 8.

All (28) 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:B:125:LEU:HD21	1:B:216:LEU:HD22	1.48	0.92
1:B:125:LEU:HD23	1:B:126:LEU:HD23	1.58	0.85
1:B:125:LEU:CD2	1:B:216:LEU:HD22	2.27	0.62
1:B:126:LEU:CD2	1:B:216:LEU:HD13	2.30	0.61
1:B:181:VAL:HG23	1:B:193:LEU:HD11	1.82	0.61
1:B:126:LEU:HD23	1:B:216:LEU:HD13	1.81	0.61
1:B:125:LEU:HD23	1:B:126:LEU:CD2	2.33	0.57
1:B:12:THR:HG22	1:B:13:GLY:N	2.20	0.57
1:B:126:LEU:HD12	1:B:167:VAL:HG11	1.87	0.57
1:B:125:LEU:HD22	1:B:136:LEU:CD2	2.39	0.52
2:C:628:LEU:HD23	2:C:630:LEU:HD21	1.91	0.52
1:B:180:ASP:O	1:B:180:ASP:OD1	2.30	0.50
2:C:656:ARG:NH2	2:C:659:PTR:O3P	2.45	0.50
1:B:191:THR:HG22	1:B:192:ASP:N	2.28	0.48
2:C:628:LEU:HD23	2:C:630:LEU:CD2	2.43	0.48
1:B:111:ARG:NH2	1:B:218:THR:O	2.47	0.48
1:B:52:THR:HG23	2:C:628:LEU:HD13	1.97	0.46
1:B:43:LEU:HD21	1:B:98:LEU:CD1	2.46	0.45
1:B:126:LEU:HD21	1:B:136:LEU:HD23	2.00	0.44
1:B:52:THR:HG21	2:C:628:LEU:HD22	2.00	0.43
1:B:107:PRO:HB2	1:B:190:LEU:HD12	2.01	0.42
1:B:12:THR:HG22	1:B:13:GLY:H	1.85	0.41
1:B:173:ARG:HB2	1:B:180:ASP:OD1	2.21	0.41
1:B:43:LEU:HD21	1:B:98:LEU:HD11	2.02	0.41
1:B:30:LEU:HD12	1:B:30:LEU:C	2.46	0.41
2:C:654:ASP:OD1	2:C:654:ASP:N	2.54	0.40
1:B:28:SER:HA	1:B:100:TYR:O	2.21	0.40
1:B:90:GLU:HA	2:C:630:LEU:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	B	202/223 (91%)	193 (96%)	9 (4%)	0	100	100
2	C	29/69 (42%)	27 (93%)	2 (7%)	0	100	100
All	All	231/292 (79%)	220 (95%)	11 (5%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	B	180/194 (93%)	172 (96%)	8 (4%)	25	59
2	C	30/58 (52%)	25 (83%)	5 (17%)	2	11
All	All	210/252 (83%)	197 (94%)	13 (6%)	18	49

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	73	THR
1	B	108	THR
1	B	128	GLU
1	B	176	GLU
1	B	191	THR
1	B	205	THR
1	B	220	ARG
1	B	221	ILE
2	C	625	VAL
2	C	629	ASP
2	C	632	LEU
2	C	634	SER
2	C	656	ARG

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

Mol	Chain	Res	Type
1	B	18	ASN
1	B	143	HIS
2	C	665	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
2	PTR	C	659	2	15,16,17	0.52	0	17,22,24	0.62	0
2	PTR	C	627	2	15,16,17	0.54	0	17,22,24	0.69	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
2	PTR	C	659	2	-	0/10/11/13	0/1/1/1
2	PTR	C	627	2	-	0/10/11/13	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	659	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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.