wwPDB X-ray Structure Validation Summary Report (i)

Jul 26, 2023 – 12:33 AM EDT

PDB ID	:	1BBZ
Title	:	CRYSTAL STRUCTURE OF THE ABL-SH3 DOMAIN COMPLEXED WITH A DESIGNED HIGH-AFFINITY PEPTIDE LIGAND: IMPLICATIONS FOR SH3-LIGAND INTERACTIONS
Authors	:	Pisabarro, M.T.; Serrano, L.; Wilmanns, M.
Deposited on	:	1998-04-28
Resolution	:	1.65 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

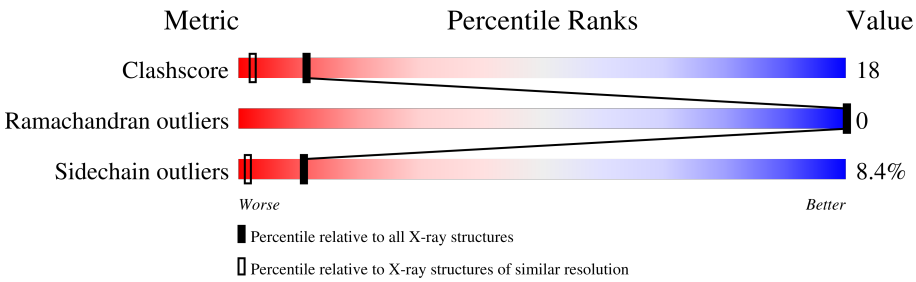
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.65 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))
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	58	66% 28% 5% •
1	C	58	59% 34% 5% •
1	E	58	66% 31% •
1	G	58	67% 24% 9%
2	B	11	91% 9%
2	D	11	100%
2	F	11	100%
2	H	11	91% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2415 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.

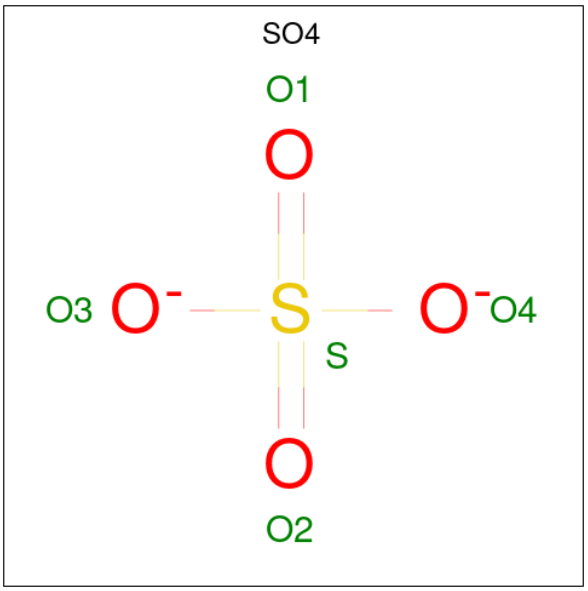
- Molecule 1 is a protein called ABL TYROSINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	58	457	291	78	86	2	0	3	0
1	C	58	463	293	80	89	1	0	2	0
1	E	58	452	288	75	87	2	0	2	0
1	G	58	454	289	76	88	1	0	1	0

- Molecule 2 is a protein called PEPTIDE P41.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	11	75	50	10	15	0	0	0
2	D	11	75	50	10	15	0	0	0
2	F	11	75	50	10	15	0	0	0
2	H	11	75	50	10	15	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

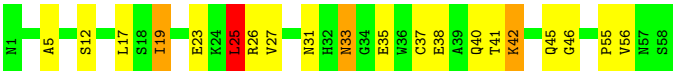
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	63	Total O 63 63	0	0
4	B	11	Total O 11 11	0	0
4	C	46	Total O 46 46	0	0
4	D	13	Total O 13 13	0	0
4	E	56	Total O 56 56	0	0
4	F	11	Total O 11 11	0	0
4	G	61	Total O 61 61	0	0
4	H	8	Total O 8 8	0	0

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.

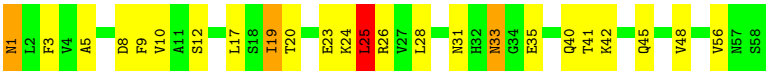
• Molecule 1: ABL TYROSINE KINASE

Chain A:



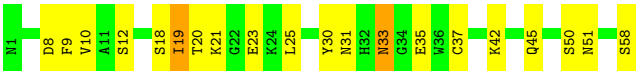
• Molecule 1: ABL TYROSINE KINASE

Chain C:



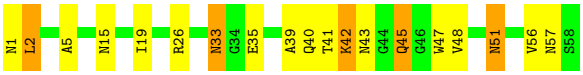
• Molecule 1: ABL TYROSINE KINASE

Chain E:



• Molecule 1: ABL TYROSINE KINASE

Chain G:

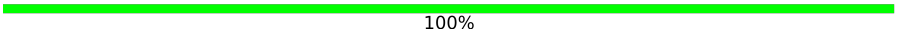


• Molecule 2: PEPTIDE P41

Chain B:

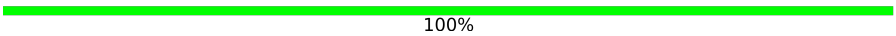
• Molecule 2: PEPTIDE P41

Chain D:



There are no outlier residues recorded for this chain.

- Molecule 2: PEPTIDE P41

Chain F: 

There are no outlier residues recorded for this chain.

- Molecule 2: PEPTIDE P41

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	46.68Å 73.79Å 80.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.65 40.32 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-1.65) 92.1 (40.32-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 1.60Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.205 , 0.266 0.429 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	2415	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, ACE

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	0.50	0/483	0.71	1/656 (0.2%)
1	C	0.51	0/484	0.80	3/657 (0.5%)
1	E	0.52	0/473	0.65	0/643
1	G	0.51	0/470	0.62	0/639
2	B	0.40	0/79	0.60	0/112
2	D	0.51	0/79	0.72	0/112
2	F	0.38	0/79	0.64	0/112
2	H	0.51	0/79	0.63	0/112
All	All	0.50	0/2226	0.69	4/3043 (0.1%)

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	C	25	LEU	CA-CB-CG	6.82	130.98	115.30
1	A	25	LEU	CA-CB-CG	6.46	130.17	115.30
1	C	19[A]	ILE	CG1-CB-CG2	-5.60	99.08	111.40
1	C	19[B]	ILE	CG1-CB-CG2	-5.60	99.08	111.40

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	457	0	438	23	18
1	C	463	0	448	20	10
1	E	452	0	432	13	5
1	G	454	0	435	21	21
2	B	75	0	69	1	0
2	D	75	0	69	0	0
2	F	75	0	69	0	0
2	H	75	0	69	0	1
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
3	G	5	0	0	0	1
4	A	63	0	0	4	3
4	B	11	0	0	0	0
4	C	46	0	0	1	9
4	D	13	0	0	0	0
4	E	56	0	0	2	3
4	F	11	0	0	0	0
4	G	61	0	0	4	9
4	H	8	0	0	0	0
All	All	2415	0	2029	75	40

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 18.

The worst 5 of 75 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:C:1:ASN:HB2	1:C:3:PHE:HE1	1.29	0.93
1:G:19[A]:ILE:HD11	1:G:41:THR:HG21	1.50	0.91
1:C:1:ASN:HB2	1:C:3:PHE:CE1	2.15	0.82
1:C:24:LYS:HE3	1:C:56:VAL:HG11	1.66	0.77
1:A:42:LYS:H	1:A:42:LYS:HD2	1.63	0.64

The worst 5 of 40 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:G:56:VAL:CG2	4:C:1123:HOH:O[3_555]	0.82	1.38
1:C:20:THR:OG1	1:E:10:VAL:CG1[3_545]	1.00	1.20
1:A:40:GLN:NE2	1:G:15:ASN:CG[3_645]	1.06	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:SER:CB	4:C:2024:HOH:O[3_555]	1.21	0.99
1:A:38:GLU:OE1	1:G:45:GLN:CD[3_645]	1.37	0.83

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	59/58 (102%)	58 (98%)	1 (2%)	0	100	100
1	C	58/58 (100%)	56 (97%)	2 (3%)	0	100	100
1	E	58/58 (100%)	57 (98%)	1 (2%)	0	100	100
1	G	57/58 (98%)	57 (100%)	0	0	100	100
2	B	9/11 (82%)	9 (100%)	0	0	100	100
2	D	9/11 (82%)	9 (100%)	0	0	100	100
2	F	9/11 (82%)	9 (100%)	0	0	100	100
2	H	9/11 (82%)	9 (100%)	0	0	100	100
All	All	268/276 (97%)	264 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	49/49 (100%)	43 (88%)	6 (12%)	5	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	51/49 (104%)	46 (90%)	5 (10%)	8 1
1	E	49/49 (100%)	44 (90%)	5 (10%)	7 1
1	G	49/49 (100%)	44 (90%)	5 (10%)	7 1
2	B	9/9 (100%)	9 (100%)	0	100 100
2	D	9/9 (100%)	9 (100%)	0	100 100
2	F	9/9 (100%)	9 (100%)	0	100 100
2	H	9/9 (100%)	9 (100%)	0	100 100
All	All	234/232 (101%)	213 (91%)	21 (9%)	11 1

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	25	LEU
1	G	33	ASN
1	G	51	ASN
1	G	42	LYS
1	G	2	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	51	ASN
1	G	45	GLN
1	E	33	ASN
1	C	33	ASN
1	G	33	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands 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	$\#\|Z\| > 2$
3	SO4	A	3000	-	4,4,4	0.41	0	6,6,6	0.58	0
3	SO4	G	3002	-	4,4,4	0.24	0	6,6,6	1.90	3 (50%)
3	SO4	E	3003	-	4,4,4	0.46	0	6,6,6	0.90	0
3	SO4	C	3001	-	4,4,4	0.29	0	6,6,6	1.46	1 (16%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	3002	SO4	O3-S-O1	-2.94	93.98	109.31
3	G	3002	SO4	O4-S-O3	2.20	118.43	109.06
3	G	3002	SO4	O3-S-O2	2.06	120.08	109.31
3	C	3001	SO4	O4-S-O2	2.05	120.03	109.31

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
3	G	3002	SO4	0	1

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.