wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 07:46 am GMT

PDB ID	:	2BP3
Title	:	Crystal structure of Filamin A domain 17 and GPIb alpha cytoplasmic domain complex
Authors	:	Pudas, R.; Ylanne, J.
Deposited on	:	2005-04-18
Resolution	:	2.32 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 (1)) were used in the production of this report:

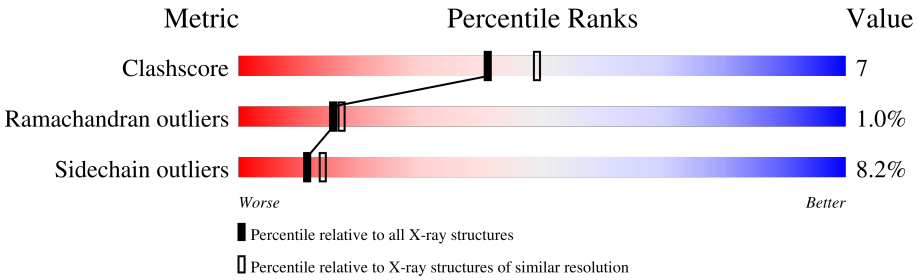
MolProbity	:	4.02b-467
Mogul	:	NOT EXECUTED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.32 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	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 1593 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.

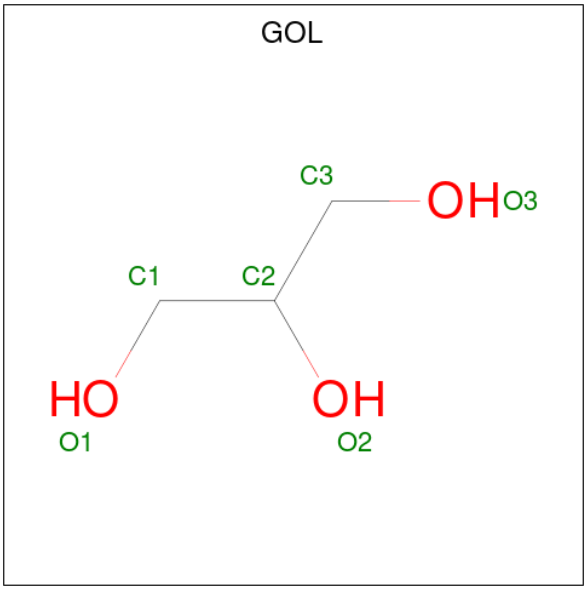
- Molecule 1 is a protein called FILAMIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	93	Total	C	N	O	S	0	0	2
			657	410	112	133	2			
1	B	91	Total	C	N	O	S	0	0	1
			651	406	110	132	3			

- Molecule 2 is a protein called PLATELET GLYCOPROTEIN IB ALPHA CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	S	12	Total	C	N	O	0	0	1
			101	68	19	14			
2	T	18	Total	C	N	O	0	0	1
			144	95	28	21			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	10	Total O 10 10	0	0
4	B	11	Total O 11 11	0	0
4	S	3	Total O 3 3	0	0
4	T	4	Total O 4 4	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	41.90Å 62.80Å 122.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 2.32	Depositor
% Data completeness (in resolution range)	100.0 (19.88-2.32)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.33Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.214 , 0.256	Depositor
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.192	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1593	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.85% 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.

4 Model quality

4.1 Standard geometry

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

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	0.63	0/671	0.72	0/918
1	B	0.65	0/666	0.68	0/911
2	S	0.77	1/104 (1.0%)	0.81	0/140
2	T	0.73	0/149	0.84	0/202
All	All	0.66	1/1590 (0.1%)	0.72	0/2171

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	572	ARG	C-N	-5.59	1.23	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	A	657	0	627	11	0
1	B	651	0	627	11	0
2	S	101	0	101	0	0
2	T	144	0	147	1	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	10	0	0	0	0
4	B	11	0	0	0	0
4	S	3	0	0	0	0
4	T	4	0	0	0	0
All	All	1593	0	1518	22	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 7.

The worst 5 of 22 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:1915:ASN:HD22	1:A:1919:THR:HG22	1.37	0.86
1:A:1939:ASN:O	1:A:1940:GLU:HG2	1.76	0.86
1:B:1935:LEU:HD22	1:B:1947:PRO:HB3	1.75	0.69
1:A:1885:THR:HG22	1:A:1923:SER:HB3	1.81	0.63
1:B:1889:ASN:C	1:B:1889:ASN:HD22	2.06	0.58

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	89/97 (92%)	87 (98%)	1 (1%)	1 (1%)	14 15
1	B	89/97 (92%)	86 (97%)	3 (3%)	0	100 100
2	S	10/22 (46%)	9 (90%)	0	1 (10%)	0 0
2	T	16/22 (73%)	16 (100%)	0	0	100 100
All	All	204/238 (86%)	198 (97%)	4 (2%)	2 (1%)	15 17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1894	GLY
2	S	572	ARG

4.3.2 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	71/77 (92%)	65 (92%)	6 (8%)	10 12
1	B	72/77 (94%)	67 (93%)	5 (7%)	15 20
2	S	11/20 (55%)	9 (82%)	2 (18%)	1 1
2	T	16/20 (80%)	15 (94%)	1 (6%)	18 24
All	All	170/194 (88%)	156 (92%)	14 (8%)	11 14

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1899	SER
1	B	1919	THR
2	T	559	SER
2	S	565	SER
2	S	569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1915	ASN
1	B	1877	HIS
1	B	1881	ASN
1	B	1889	ASN

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

Mogul was not executed - this section is therefore empty.

4.5 Carbohydrates (i)

Mogul was not executed - this section is therefore empty.

4.6 Ligand geometry (i)

Mogul was not executed - this section is therefore empty.

4.7 Other polymers (i)

Mogul was not executed - this section is therefore empty.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.