Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 06:47 PM EDT

PDB ID	:	6PXJ
Title	:	Crystal structure of human thrombin mutant I16T
Authors	:	Stojanovski, B.; Chen, Z.; Koester, S.K.; Pelc, L.A.; Di Cera, E.
Deposited on	:	2019-07-26
Resolution	:	1.70 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 (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:

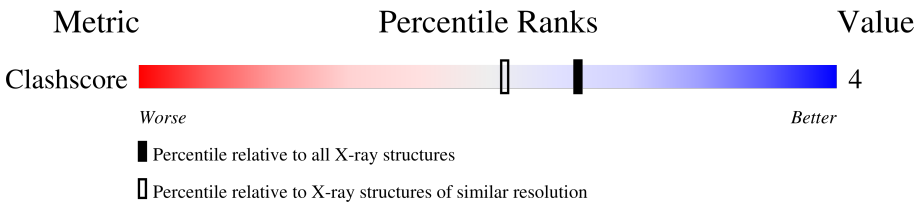
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.70 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	4695 (1.70-1.70)

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4968 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 Thrombin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	34	271	169	43	58	1	0	0	0
1	A	28	231	145	37	48	1	0	0	0

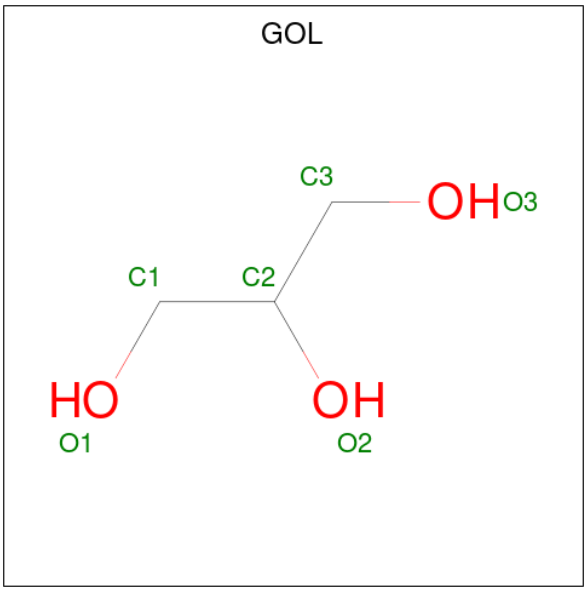
- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	245	1987	1267	352	354	14	0	0	0
2	B	245	2003	1274	353	360	16	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	16	THR	ILE	engineered mutation	UNP P00734
B	16	THR	ILE	engineered mutation	UNP P00734

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



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	B	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	L	28	28	28	0	0
			Total	O		
5	H	198	198	198	0	0
			Total	O		
5	B	214	214	214	0	0
			Total	O		
5	A	23	23	23	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 2	Depositor
Cell constants a, b, c, α, β, γ	81.59Å 151.40Å 50.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.77 – 1.70	Depositor
% Data completeness (in resolution range)	98.3 (31.77-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.173 , 0.203	Depositor
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.035	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	4968	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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 (i)

4.1 Standard geometry (i)

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

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	0.79	0/233	1.08	0/310
1	L	0.81	0/274	1.00	0/365
2	B	0.77	0/2060	0.93	0/2781
2	H	0.76	0/2039	0.92	0/2756
All	All	0.77	0/4606	0.94	0/6212

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	231	0	231	1	0
1	L	271	0	262	0	0
2	B	2003	0	1967	17	0
2	H	1987	0	1957	23	0
3	H	12	0	16	0	0
4	B	1	0	0	0	0
5	A	23	0	0	0	0
5	B	214	0	0	2	0
5	H	198	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	28	0	0	0	0
All	All	4968	0	4433	38	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 4.

All (38) 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:H:185:LYS:HG3	2:H:186:PRO:HD2	1.44	0.96
2:H:186(D):LYS:H	2:H:186(D):LYS:CE	1.87	0.88
2:H:186(D):LYS:H	2:H:186(D):LYS:HE2	1.40	0.85
2:H:185:LYS:HG3	2:H:186:PRO:CD	2.11	0.79
2:B:77(A):ARG:C	2:B:77(A):ARG:HD3	2.05	0.77
2:B:77(A):ARG:HD3	2:B:77(A):ARG:O	1.84	0.76
2:B:60(F):LYS:HE3	5:B:476:HOH:O	1.88	0.73
2:B:77(A):ARG:NH1	2:B:77(A):ARG:HG2	2.07	0.68
2:H:186(D):LYS:H	2:H:186(D):LYS:CD	2.07	0.67
2:B:77(A):ARG:HG2	2:B:77(A):ARG:HH11	1.60	0.67
2:B:77(A):ARG:HH11	2:B:77(A):ARG:CG	2.12	0.62
2:H:224:LYS:NZ	2:B:60(E):ASP:OD2	2.25	0.61
2:H:165:ARG:HB3	2:H:166:PRO:HD3	1.83	0.61
2:H:186(D):LYS:HD2	2:H:186(D):LYS:O	2.00	0.60
2:H:186(B):GLU:HG2	2:H:187:ARG:HD3	1.84	0.59
2:H:128:THR:HG23	2:H:129(C):LEU:HD22	1.82	0.59
2:H:165:ARG:NH2	2:H:177:THR:O	2.41	0.53
2:H:186(D):LYS:CD	2:H:186(D):LYS:N	2.71	0.52
2:B:186(D):LYS:NZ	5:B:405:HOH:O	2.42	0.52
2:H:18:GLU:OE1	2:H:186(D):LYS:HB2	2.10	0.52
2:B:206:ARG:NH2	1:A:1(B):ALA:O	2.42	0.52
2:H:33:LEU:HD13	2:H:41:LEU:HD23	1.92	0.51
2:H:139:THR:HG22	2:H:157:VAL:HG12	1.94	0.50
2:H:24:ILE:HD12	2:H:24:ILE:H	1.78	0.48
2:H:186(D):LYS:HD2	2:H:186(D):LYS:N	2.30	0.47
2:H:60(D):TRP:CG	2:B:223:GLY:HA2	2.50	0.46
2:B:77:GLU:HB3	2:B:79:ILE:HB	1.99	0.44
2:H:33:LEU:HD11	2:H:59:LEU:HD21	2.00	0.43
2:B:17:VAL:HG13	2:B:220:CYS:SG	2.58	0.43
2:B:185:LYS:N	2:B:186(B):GLU:OE1	2.50	0.43
2:B:35:ARG:HH21	2:B:35:ARG:CG	2.32	0.43
2:H:18:GLU:OE1	2:H:186(D):LYS:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:186(D):LYS:HE2	2:H:186(D):LYS:N	2.21	0.42
2:H:35:ARG:HE	2:H:35:ARG:HB3	1.70	0.42
2:B:129(C):LEU:HD12	2:B:129(C):LEU:HA	1.82	0.42
2:H:211:GLY:HA2	2:H:229:THR:O	2.20	0.41
2:B:94:TYR:CZ	2:B:96:TRP:HB3	2.56	0.40
2:B:50:ARG:HD3	2:B:111:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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