WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2024 – 09:30 pm BST

PDB ID	:	5MJT
Title	:	Thrombin Mutant A190S in complex with (S) -1 - ((R) -2-amino-3,3-diphenyl propanoyl) -N- (3-chlorobenzyl) pyrrolidine-2-carboxamide
Authors	:	Marca, A.; Sandner, A.; Heine, A.; Klebe, G.
Deposited on	:	2016-12-01
Resolution	:	1.40 Å(reported)

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

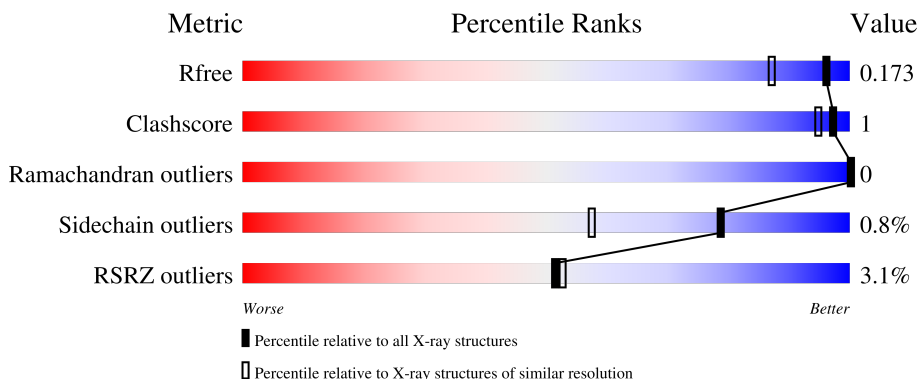|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.40 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	Percentile Ranks	Value
Rfree		0.173
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		3.1%

Worse *Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	2247 (1.40-1.40)
Clashscore	180529	2446 (1.40-1.40)
Ramachandran outliers	177936	2398 (1.40-1.40)
Sidechain outliers	177891	2397 (1.40-1.40)
RSRZ outliers	164620	2246 (1.40-1.40)

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% 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	L	36	6% / 81% 6% 14%
2	H	259	2% / 94% · ·
3	D	12	17% / 83% 8% 8%

2　Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 4942 atoms, of which 2283 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
1	L	31	Total	C	H	N	O	S	0	0	0
			493	156	242	42	52	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	250	Total	C	H	N	O	S	0	8	0
			4006	1298	1975	358	361	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	190	SER	ALA	conflict	UNP P00734

- Molecule 3 is a protein called Hirudin variant-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	11	Total	C	H	N	O	S	0	0	0
			154	57	66	11	19	1			

- Molecule 4 is beta-phenyl-D-phenylalanyl-N-(3-chlorobenzyl)-L-prolinamide (three-letter code: 23U) (formula: $C_{27}H_{28}ClN_3O_2$).
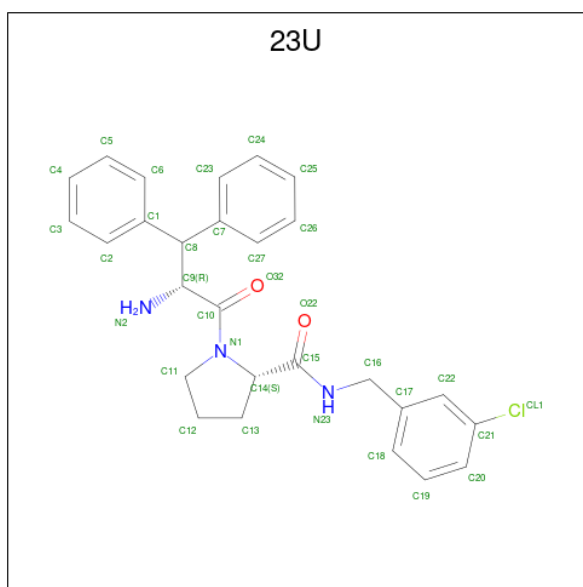
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	H	1	33	27	1	3	2	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	H	1	4	2	1	1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O2   P   O1

O4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total 5	O 4	P 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1   C2

HO

OH

O1   O2

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

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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	2	Total 2	Na 2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	32	Total 32	O 32	0	0
9	H	180	Total 180	O 180	0	0
9	D	3	Total 3	O 3	0	0

# 3 Residue-property plots ⓘ

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.
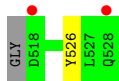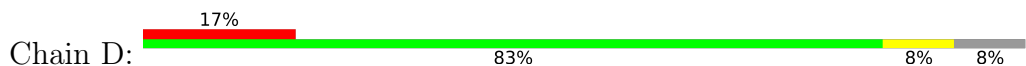
• Molecule 1: Thrombin light chain
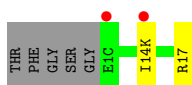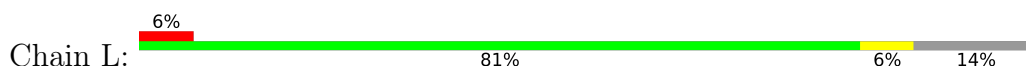
Chain L:

• Molecule 2: Thrombin heavy chain

Chain H:
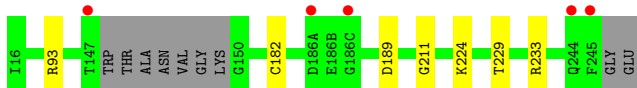
• Molecule 3: Hirudin variant-2

Chain D:

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	69.49Å 71.61Å 72.13Å 90.00° 99.73° 90.00°	Depositor
Resolution (Å)	49.50 – 1.40 49.50 – 1.40	Depositor EDS
% Data completeness (in resolution range)	93.6 (49.50-1.40) 93.9 (49.50-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 1.40Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.148 , 0.172 0.148 , 0.173	Depositor DCC
R_{free} test set	3217 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	12.8	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 39.8	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4942	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TYS, GOL, NA, 23U, DMS, PO4

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	L	0.68	0/253	0.79	0/335
2	H	0.54	0/2117	0.74	1/2864 (0.0%)
3	D	0.40	0/72	0.38	0/96
All	All	0.55	0/2442	0.74	1/3295 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	189	ASP	CB-CG-OD1	5.14	122.92	118.30

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	L	251	242	244	1	0
2	H	2031	1975	1948	3	0
3	D	88	66	66	0	0
4	H	33	0	28	0	0
5	H	4	0	6	0	0
6	H	5	0	0	0	0
7	H	30	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	2	0	0	0	0
9	D	3	0	0	0	0
9	H	180	0	0	0	0
9	L	32	0	0	0	0
All	All	2659	2283	2332	4	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 1.

All (4) 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:224:LYS:HD2	7:H:305:GOL:H12	1.54	0.89
2:H:211:GLY:HA2	2:H:229:THR:O	2.11	0.51
2:H:93:ARG:HG2	7:H:304:GOL:H32	1.93	0.50
1:L:14(K):ILE:O	1:L:17:ARG:HG2	2.17	0.44

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 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	L	29/36 (81%)	28 (97%)	1 (3%)	0	100	100
2	H	254/259 (98%)	246 (97%)	8 (3%)	0	100	100
3	D	8/12 (67%)	8 (100%)	0	0	100	100
All	All	291/307 (95%)	282 (97%)	9 (3%)	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	L	26/31 (84%)	26 (100%)	0	100	100
2	H	215/226 (95%)	213 (99%)	2 (1%)	75	53
3	D	6/10 (60%)	6 (100%)	0	100	100
All	All	247/267 (92%)	245 (99%)	2 (1%)	79	57

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	182	CYS
2	H	233	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TYS	D	526	3	15,16,17	1.25	2 (13%)	18,22,24	0.95	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
3	TYS	D	526	3	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	526	TYS	OH-CZ	-3.39	1.37	1.42
3	D	526	TYS	OH-S	-2.67	1.54	1.58

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.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	$\#|Z| > 2$
7	GOL	H	310	-	5,5,5	0.30	0	5,5,5	0.26	0
7	GOL	H	305	-	5,5,5	0.77	0	5,5,5	1.28	0
4	23U	H	301	-	35,36,36	0.30	0	46,49,49	0.44	0
5	DMS	H	302	-	3,3,3	0.58	0	3,3,3	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	GOL	H	306	-	5,5,5	0.23	0	5,5,5	0.66	0
6	PO4	H	303	-	4,4,4	0.79	0	6,6,6	1.48	1 (16%)
7	GOL	H	304	-	5,5,5	0.42	0	5,5,5	0.63	0
7	GOL	H	307	-	5,5,5	0.46	0	5,5,5	0.65	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
7	GOL	H	310	-	-	0/4/4/4	-
7	GOL	H	305	-	-	0/4/4/4	-
4	23U	H	301	-	-	0/29/39/39	0/4/4/4
7	GOL	H	306	-	-	0/4/4/4	-
7	GOL	H	304	-	-	1/4/4/4	-
7	GOL	H	307	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	303	PO4	O4-P-O3	2.58	116.27	107.97

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	H	307	GOL	C1-C2-C3-O3
7	H	307	GOL	O2-C2-C3-O3
7	H	304	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	305	GOL	1	0
7	H	304	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	L	31/36 (86%)	-0.11	2 (6%)	26	26	11, 16, 38, 43	0
2	H	250/259 (96%)	-0.38	5 (2%)	64	66	7, 16, 38, 49	5 (2%)
3	D	10/12 (83%)	1.57	2 (20%)	3	3	31, 36, 49, 65	0
All	All	291/307 (94%)	-0.28	9 (3%)	51	53	7, 17, 39, 65	5 (1%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	186(C)	GLY	4.9
2	H	245	PHE	4.3
3	D	528	GLN	4.1
3	D	518	ASP	4.0
2	H	186(A)	ASP	3.9

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

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(Å²)	Q<0.9
3	TYS	D	526	16/17	0.95	0.10	29,32,37,44	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å^2)	Q<0.9
7	GOL	H	304	6/6	0.80	0.18	27,28,35,40	0
7	GOL	H	310	6/6	0.89	0.14	15,20,24,27	6
7	GOL	H	307	6/6	0.92	0.10	19,23,26,27	0
7	GOL	H	305	6/6	0.93	0.13	11,17,18,20	6
7	GOL	H	306	6/6	0.94	0.10	14,18,26,30	0
6	PO4	H	303	5/5	0.98	0.07	17,17,19,21	0
4	23U	H	301	33/33	0.98	0.06	9,12,18,20	0
5	DMS	H	302	4/4	0.98	0.11	12,15,18,19	4
8	NA	H	308	1/1	0.98	0.04	14,14,14,14	0
8	NA	H	309	1/1	0.99	0.03	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.