



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 02:30 PM GMT

PDB ID : 2D26
Title : Active site distortion is sufficient for proteinase inhibit second crystal structure of covalent serpin-proteinase complex
Authors : Dementiev, A.; Dobo, J.; Gettins, P.G.
Deposited on : 2005-09-03
Resolution : 3.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

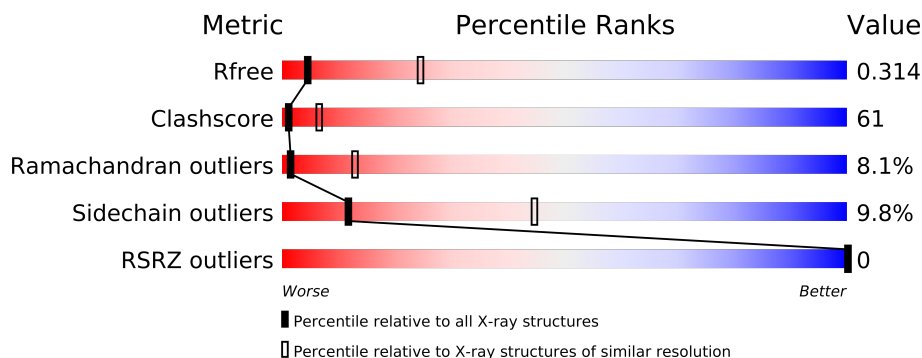
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



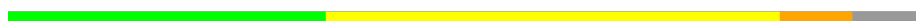
The reported resolution of this entry is 3.30 Å.

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))
R_{free}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	358	
2	B	36	
3	C	240	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4189 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Alpha-1-antitrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2302	1474	394	429	5			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	GLU	ENGINEERED	UNP P01009
A	51	LEU	PHE	ENGINEERED	UNP P01009
A	59	ALA	THR	ENGINEERED	UNP P01009
A	68	ALA	THR	ENGINEERED	UNP P01009
A	70	GLY	ALA	ENGINEERED	UNP P01009
A	101	HIS	ARG	ENGINEERED	UNP P01009
A	232	SER	CYS	ENGINEERED	UNP P01009

- Molecule 2 is a protein called Alpha-1-antitrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	30	Total	C	N	O	S	0	0	0
			221	148	34	38	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	374	ILE	MET	ENGINEERED	UNP P01009
B	381	ALA	SER	ENGINEERED	UNP P01009
B	387	ARG	LYS	ENGINEERED	UNP P01009

- Molecule 3 is a protein called Elastase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	223	Total	C	N	O	S	0	0	0
			1591	1001	288	292	10			

- Molecule 4 is water.

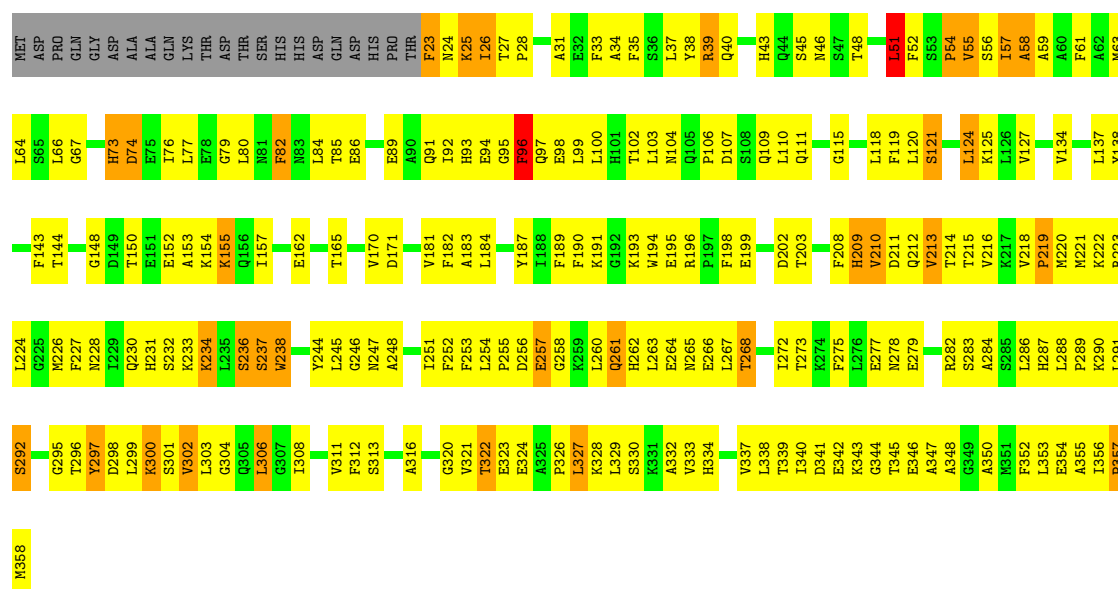
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total 43	O 43	0	0
4	B	3	Total 3	O 3	0	0
4	C	29	Total 29	O 29	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Alpha-1-antitrypsin

Chain A:



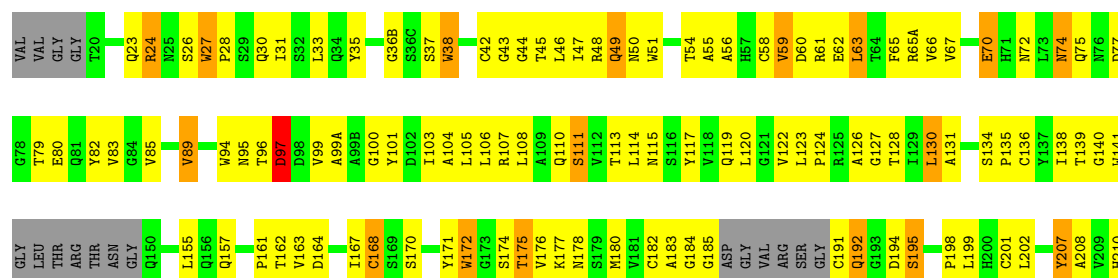
• Molecule 2: Alpha-1-antitrypsin

Chain B:



• Molecule 3: Elastase-1

Chain C:



G211	V212	T213	S214	F215	V216	S217	R217A	L218	R223	K224	P225	T226	V227	F228	T229	R230	V231	S232	A233	Y234	I235	S236	W237	N240	V241	I242	N245
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.83Å 85.18Å 76.26Å 90.00° 121.01° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 39.16 – 2.93	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.30) 91.3 (39.16-2.93)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.312 0.252 , 0.314	Depositor DCC
R_{free} test set	821 reflections (10.09%)	DCC
Wilson B-factor (Å ²)	80.8	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 143.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 12476 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4189	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.49	1/2353 (0.0%)	0.82	5/3222 (0.2%)
2	B	0.56	0/228	0.83	0/311
3	C	0.62	3/1628 (0.2%)	0.79	0/2229
All	All	0.55	4/4209 (0.1%)	0.81	5/5762 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	TRP	NE1-CE2	8.70	1.48	1.37
3	C	38	TRP	NE1-CE2	8.69	1.48	1.37
3	C	27	TRP	NE1-CE2	8.67	1.48	1.37
3	C	172	TRP	NE1-CE2	8.66	1.48	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	LEU	CB-CG-CD2	10.07	128.12	111.00
1	A	278	ASN	N-CA-C	-9.67	84.90	111.00
1	A	278	ASN	CB-CA-C	-9.25	91.89	110.40
1	A	279	GLU	N-CA-CB	-9.00	94.40	110.60
1	A	51	LEU	CA-CB-CG	-6.20	101.04	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2302	0	1920	271	2
2	B	221	0	198	39	0
3	C	1591	0	1401	171	1
4	A	43	0	0	5	0
4	B	3	0	0	0	0
4	C	29	0	0	5	1
All	All	4189	0	3519	468	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 61.

The worst 5 of 468 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:299:LEU:HB2	1:A:332:ALA:CB	1.54	1.37
1:A:299:LEU:CD1	1:A:332:ALA:HB1	1.57	1.33
3:C:122:VAL:O	3:C:208:ALA:HB1	1.43	1.16
1:A:299:LEU:HB2	1:A:332:ALA:HB3	1.19	1.14
1:A:45:SER:O	1:A:46:ASN:ND2	1.79	1.14

All (2) 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	Distance(Å)	Clash(Å)
1:A:23:PHE:N	3:C:127:GLY:CA[3_445]	1.71	0.49
1:A:24:ASN:ND2	4:C:269:HOH:O[3_445]	1.80	0.40

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	A	334/358 (93%)	244 (73%)	57 (17%)	33 (10%)	1 8
2	B	28/36 (78%)	18 (64%)	7 (25%)	3 (11%)	1 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	217/240 (90%)	152 (70%)	54 (25%)	11 (5%)	3	28
All	All	579/634 (91%)	414 (72%)	118 (20%)	47 (8%)	1	13

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	55	VAL
1	A	210	VAL
1	A	213	VAL
1	A	257	GLU

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 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	182/311 (58%)	166 (91%)	16 (9%)	14	52
2	B	21/34 (62%)	15 (71%)	6 (29%)	0	2
3	C	144/198 (73%)	132 (92%)	12 (8%)	16	56
All	All	347/543 (64%)	313 (90%)	34 (10%)	12	45

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	358	MET
2	B	382	PRO
3	C	207	TYR
2	B	376	GLU
1	A	107	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	367	ASN
3	C	23	GLN

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Mol	Chain	Res	Type
3	C	200	HIS
1	A	287	HIS
3	C	210	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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(Å ²)	Q<0.9
1	A	336/358 (93%)	-0.25	0 100 100	31, 71, 96, 98	0
2	B	30/36 (83%)	-0.25	0 100 100	29, 52, 86, 92	0
3	C	223/240 (92%)	-0.21	0 100 100	29, 54, 91, 99	5 (2%)
All	All	589/634 (92%)	-0.23	0 100 100	29, 62, 95, 99	5 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.