



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 9, 2019 – 08:26 PM EDT

PDB ID : 6FPY
Title : Inter-alpha-inhibitor heavy chain 1, wild type
Authors : Briggs, D.C.; Day, A.J.
Deposited on : 2018-02-12
Resolution : 2.34 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.3.2
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

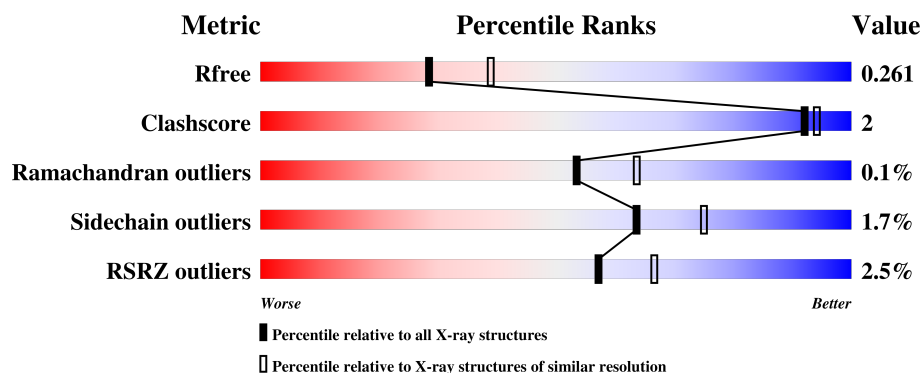
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	111664	1763 (2.36-2.32)
Clashscore	122126	1858 (2.36-2.32)
Ramachandran outliers	120053	1834 (2.36-2.32)
Sidechain outliers	120020	1835 (2.36-2.32)
RSRZ outliers	108989	1737 (2.36-2.32)

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. 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 $\leq 5\%$. 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	A	660	<div> <div>2%</div> <div>85%</div> <div>5%</div> <div>9%</div> </div>
1	B	660	<div> <div>3%</div> <div>85%</div> <div>5%</div> <div>9%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18872 atoms, of which 9170 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 Inter-alpha-trypsin inhibitor heavy chain H1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	600	Total	C	H	N	O	S	0	2	0
			9261	2954	4585	818	885	19			
1	B	599	Total	C	H	N	O	S	0	0	0
			9184	2932	4541	813	879	19			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	initiating methionine	UNP P19827
A	14	ALA	-	expression tag	UNP P19827
A	15	HIS	-	expression tag	UNP P19827
A	16	HIS	-	expression tag	UNP P19827
A	17	HIS	-	expression tag	UNP P19827
A	18	HIS	-	expression tag	UNP P19827
A	19	HIS	-	expression tag	UNP P19827
A	20	HIS	-	expression tag	UNP P19827
A	21	VAL	-	expression tag	UNP P19827
A	22	GLY	-	expression tag	UNP P19827
A	23	THR	-	expression tag	UNP P19827
A	24	GLY	-	expression tag	UNP P19827
A	25	SER	-	expression tag	UNP P19827
A	26	ASN	-	expression tag	UNP P19827
A	27	ASP	-	expression tag	UNP P19827
A	28	ASP	-	expression tag	UNP P19827
A	29	ASP	-	expression tag	UNP P19827
A	30	ASP	-	expression tag	UNP P19827
A	31	ASP	-	expression tag	UNP P19827
A	32	LYS	-	expression tag	UNP P19827
A	33	SER	-	expression tag	UNP P19827
A	34	PRO	-	expression tag	UNP P19827
B	13	MET	-	initiating methionine	UNP P19827
B	14	ALA	-	expression tag	UNP P19827
B	15	HIS	-	expression tag	UNP P19827

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Chain	Residue	Modelled	Actual	Comment	Reference
B	16	HIS	-	expression tag	UNP P19827
B	17	HIS	-	expression tag	UNP P19827
B	18	HIS	-	expression tag	UNP P19827
B	19	HIS	-	expression tag	UNP P19827
B	20	HIS	-	expression tag	UNP P19827
B	21	VAL	-	expression tag	UNP P19827
B	22	GLY	-	expression tag	UNP P19827
B	23	THR	-	expression tag	UNP P19827
B	24	GLY	-	expression tag	UNP P19827
B	25	SER	-	expression tag	UNP P19827
B	26	ASN	-	expression tag	UNP P19827
B	27	ASP	-	expression tag	UNP P19827
B	28	ASP	-	expression tag	UNP P19827
B	29	ASP	-	expression tag	UNP P19827
B	30	ASP	-	expression tag	UNP P19827
B	31	ASP	-	expression tag	UNP P19827
B	32	LYS	-	expression tag	UNP P19827
B	33	SER	-	expression tag	UNP P19827
B	34	PRO	-	expression tag	UNP P19827

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			13	3	7	3		
3	A	1	Total	C	H	O	0	0
			13	3	7	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			13	3	7	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			13	3	7	3		

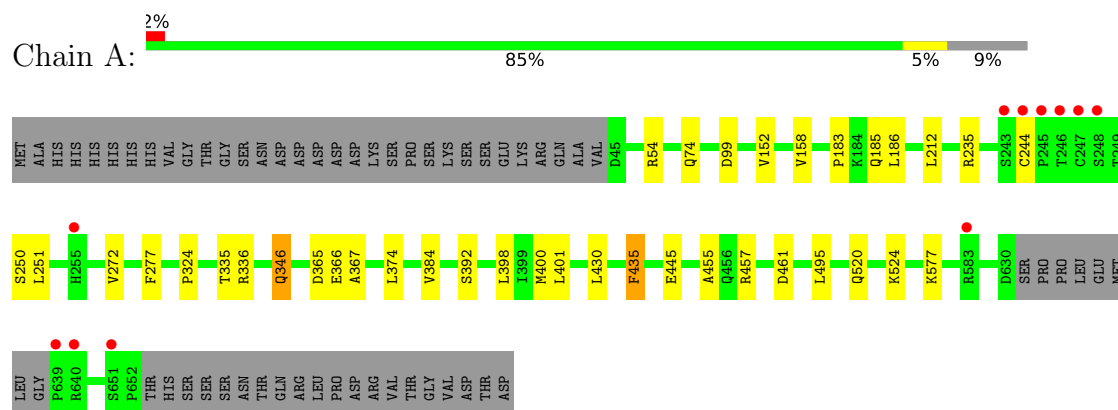
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	180	Total	O	0	0
			180	180		
4	B	165	Total	O	0	0
			165	165		

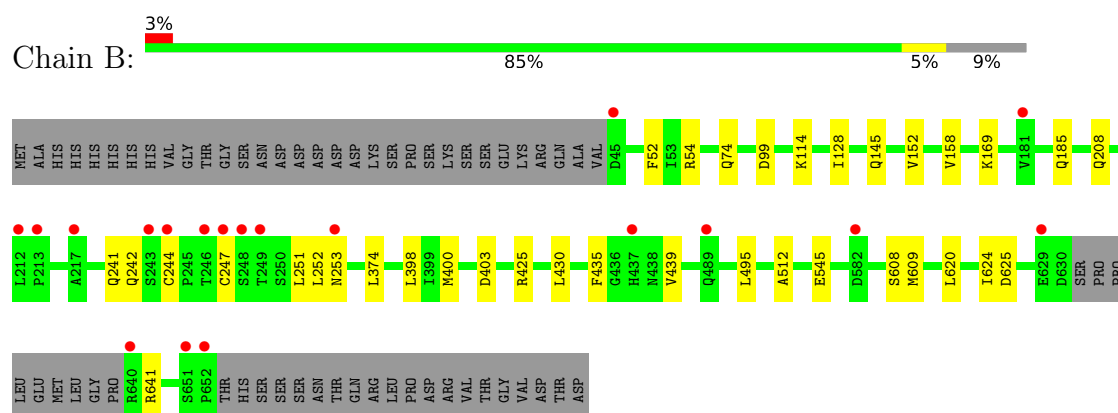
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Inter-alpha-trypsin inhibitor heavy chain H1



- Molecule 1: Inter-alpha-trypsin inhibitor heavy chain H1



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	158.77Å 158.77Å 65.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.38 – 2.34 79.38 – 2.34	Depositor EDS
% Data completeness (in resolution range)	91.9 (79.38-2.34) 91.9 (79.38-2.34)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.231 , 0.261 0.231 , 0.261	Depositor DCC
R_{free} test set	3194 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18872	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.26	0/4769	0.48	0/6456
1	B	0.26	0/4728	0.49	0/6404
All	All	0.26	0/9497	0.49	0/12860

There are no bond length outliers.

There are no bond angle outliers.

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	A	4676	4585	4586	16	0
1	B	4643	4541	4541	16	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	18	22	24	0	0
3	B	18	22	24	1	0
4	A	180	0	0	0	0
4	B	165	0	0	1	0
All	All	9702	9170	9175	32	1

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 2.

The worst 5 of 32 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:B:241:GLN:OE1	4:B:1101:HOH:O	2.05	0.75
1:B:244:CYS:SG	1:B:247:CYS:N	2.68	0.67
1:B:54:ARG:NH1	1:B:74:GLN:OE1	2.27	0.67
1:A:398:LEU:HD23	1:A:430:LEU:HD13	1.87	0.56
1:B:398:LEU:HD23	1:B:430:LEU:HD13	1.87	0.56

All (1) 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:B:54:ARG:HH22	1:B:545:GLU:OE1[3_555]	1.52	0.08

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	598/660 (91%)	586 (98%)	12 (2%)	0	100	100
1	B	595/660 (90%)	579 (97%)	15 (2%)	1 (0%)	49	58
All	All	1193/1320 (90%)	1165 (98%)	27 (2%)	1 (0%)	53	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	252	LEU

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	503/575 (88%)	493 (98%)	10 (2%)	58	70
1	B	497/575 (86%)	490 (99%)	7 (1%)	69	80
All	All	1000/1150 (87%)	983 (98%)	17 (2%)	63	75

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	ASP
1	A	524	LYS
1	B	208	GLN
1	A	457	ARG
1	B	425	ARG

Some 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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
3	GOL	A	1002	-	5,5,5	0.88	0	5,5,5	0.96	0
3	GOL	A	1003	-	5,5,5	0.91	0	5,5,5	1.01	0
3	GOL	A	1004	-	5,5,5	0.90	0	5,5,5	0.89	0
3	GOL	B	1002	-	5,5,5	0.93	0	5,5,5	0.87	0
3	GOL	B	1003	-	5,5,5	0.90	0	5,5,5	0.99	0
3	GOL	B	1004	-	5,5,5	0.93	0	5,5,5	0.90	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	GOL	A	1002	-	-	2/4/4/4	-
3	GOL	A	1003	-	-	0/4/4/4	-
3	GOL	A	1004	-	-	2/4/4/4	-
3	GOL	B	1002	-	-	0/4/4/4	-
3	GOL	B	1003	-	-	3/4/4/4	-
3	GOL	B	1004	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	GOL	C1-C2-C3-O3
3	B	1003	GOL	O2-C2-C3-O3
3	A	1002	GOL	O2-C2-C3-O3
3	B	1003	GOL	C1-C2-C3-O3
3	A	1004	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	GOL	1	0

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](#)

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	600/660 (90%)	0.33	11 (1%) 68 76	27, 45, 83, 160	0
1	B	599/660 (90%)	0.41	19 (3%) 47 58	24, 47, 83, 140	0
All	All	1199/1320 (90%)	0.37	30 (2%) 57 66	24, 46, 83, 160	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	THR	5.2
1	B	652	PRO	4.8
1	A	247	CYS	4.5
1	A	243	SER	3.9
1	A	244	CYS	3.9

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
3	GOL	B	1002	6/6	0.70	0.37	65,71,86,86	0
2	MG	B	1001	1/1	0.77	0.06	50,50,50,50	0
3	GOL	A	1004	6/6	0.81	0.34	75,90,93,94	0
2	MG	A	1001	1/1	0.87	0.09	43,43,43,43	0
3	GOL	B	1004	6/6	0.90	0.23	68,73,86,86	0
3	GOL	A	1002	6/6	0.90	0.23	45,53,60,63	0
3	GOL	B	1003	6/6	0.91	0.21	50,61,69,69	0
3	GOL	A	1003	6/6	0.94	0.17	55,64,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.