



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 11:13 PM EDT

PDB ID : 5B86
Title : Crystal structure of M-Sec
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Deposited on : 2016-06-12
Resolution : 3.02 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

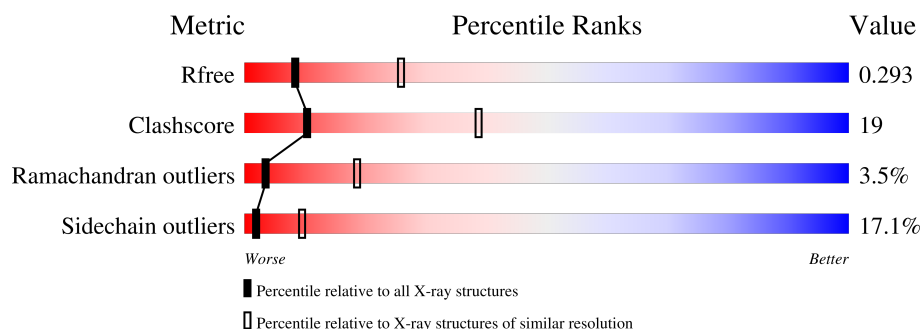
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	600	<div> <div>52%</div> <div>38%</div> <div>6%</div> <div>.</div> </div>
1	B	600	<div> <div>49%</div> <div>38%</div> <div>9%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9312 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 Tumor necrosis factor alpha-induced protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	Se	0	0	0
			4638	2948	814	859	8	9			
1	B	578	Total	C	N	O	S	Se	0	0	0
			4628	2942	811	858	8	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLY	-	expression tag	UNP Q61333
A	52	PRO	-	expression tag	UNP Q61333
B	51	GLY	-	expression tag	UNP Q61333
B	52	PRO	-	expression tag	UNP Q61333

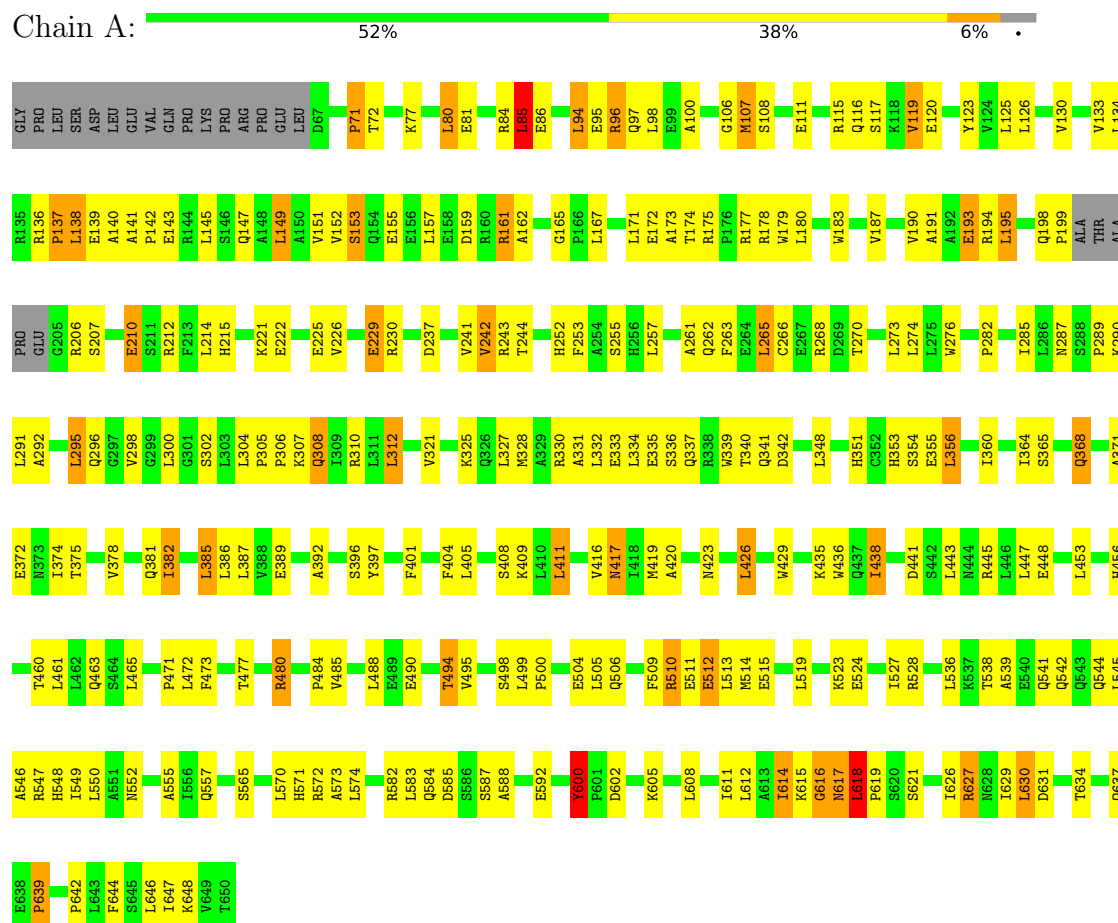
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	30	Total	O	0	0
			30	30		

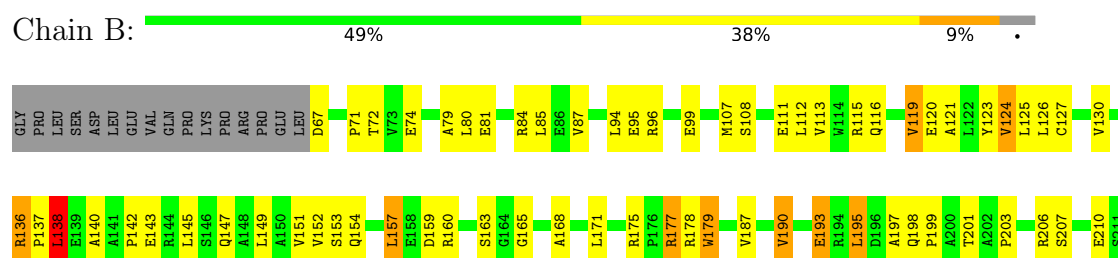
3 Residue-property plots

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. 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. 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: Tumor necrosis factor alpha-induced protein 2



- Molecule 1: Tumor necrosis factor alpha-induced protein 2



N617	K523	L446	D359	P282	R212
P619	E524	L447	I360	N283	F214
S620		E448	L361	D284	L213
G621	I527	P449	D362	I285	H215
E622	R528	L450	I363	I286	N216
V623	L529	L453	I364	N287	G217
R624	R533	K454		S288	R218
S625	L534		Q368	P289	T219
I626	V635	F458		K290	M220
R627	L536		E372	L291	K221
N628	L537		N373		
I629	Q537	L461	I374	E294	L224
L630	T538	L462	T375	L303	V227
D631	A539	Q463	S376	L304	V228
I632	E540	A564	D377	P305	E229
ASN	Q541	L465	V378	P306	E230
THR	Q542	L467		K307	L231
GLY	Q543	D468		Q308	
VAL	Q544	L469	K383	I309	L234
GLN		K470	Q384	R310	P236
E638	L550	P471	L385	L311	P235
	A551	L472	L386	L312	D237
P639	N552	F473	L387	E313	E238
		K474			F239
P642		K475		F316	N240
L643	Q557	F476	L393	L317	V241
F644	G558		L394	S318	V242
S645	F559	T477	R395	N319	F243
L646		Q478		E320	T244
L647	E562	T479	Q398	V321	
R648		R480		T322	E247
V649	A567	L481	S408	S323	
T650	T568		L410	V324	
		T487	L411		
	M576	L488		K325	Y251
		E489		Q326	H252
E579		Q490	R415	L327	P253
I580	I581	L491	V416	M328	A254
I581	I581	L492	A329	H256	S255
R582	T583	T493	M419	R330	H256
L583		T494	A420		L257
		V495		L334	C258
	A588	S496	N423	E335	A259
	I589		N424		L260
	K590	E501	C425	W339	F263
		F502	L426		E264
V593		S503	F427	D342	L265
		E504	F428	V343	C266
D602		L505	W429	A344	
		Q506		P345	
K605		D507	W436		D269
G606		G508	Q437	G350	L272
H607		F509	L438	R351	L273
L608		R510	S439	G352	L274
			H440	H353	L275
			D441	S354	W276
L612		L513	L442	E355	
A613		E514	L443	L356	N279
I614			L444	A357	L280
V645		K615	W445	T357	Y281
		C616			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.41Å 107.83Å 229.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.44 – 3.02 46.44 – 3.02	Depositor EDS
% Data completeness (in resolution range)	86.1 (46.44-3.02) 87.3 (46.44-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.229 , 0.292 0.230 , 0.293	Depositor DCC
R_{free} test set	1981 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9312	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.50	0/4717	0.71	2/6380 (0.0%)
1	B	0.46	0/4708	0.69	2/6369 (0.0%)
All	All	0.48	0/9425	0.70	4/12749 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LEU	CA-CB-CG	7.45	132.44	115.30
1	B	265	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	618	LEU	CA-CB-CG	6.03	129.17	115.30
1	A	85	LEU	CA-CB-CG	5.41	127.74	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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	4638	0	4693	166	1
1	B	4628	0	4679	183	1
2	A	16	0	0	3	0
2	B	30	0	0	9	0
All	All	9312	0	9372	349	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 19.

The worst 5 of 349 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:605:LYS:HE3	1:B:630:LEU:HB2	1.52	0.92
1:B:179:TRP:NE1	2:B:701:HOH:O	2.00	0.91
1:A:608:LEU:HD23	1:A:626:ILE:HG12	1.51	0.91
1:A:328:MSE:HE2	1:A:360:ILE:HG23	1.53	0.90
1:B:615:LYS:HB3	1:B:618:LEU:HD21	1.55	0.89

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:A:480:ARG:NH1	1:B:264:GLU:OE2[4_455]	2.17	0.03

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	575/600 (96%)	483 (84%)	67 (12%)	25 (4%)	2	14
1	B	574/600 (96%)	496 (86%)	63 (11%)	15 (3%)	5	26
All	All	1149/1200 (96%)	979 (85%)	130 (11%)	40 (4%)	3	18

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	463	GLN
1	A	639	PRO
1	B	286	LEU
1	B	616	GLY

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	504/513 (98%)	429 (85%)	75 (15%)	3	13
1	B	502/513 (98%)	405 (81%)	97 (19%)	1	7
All	All	1006/1026 (98%)	834 (83%)	172 (17%)	2	9

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	309	ILE
1	B	448	GLU
1	B	322	THR
1	B	376	SER
1	B	489	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	541	GLN
1	B	518	HIS
1	B	250	HIS
1	A	552	ASN
1	B	256	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.