wwPDB X-ray Structure Validation Summary Report (i)

Nov 2, 2026 – 07:18 PM JST

PDB ID	:	9XJB / pdb_00009xjb
Title	:	CRM197 mutant-P226E, R458P,G510D (Named CRM197-Mut3)
Authors	:	Hu, E.; Yu, R.; Mao, Y.; Chen, C.
Deposited on	:	2025-11-04
Resolution	:	2.68 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 (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:

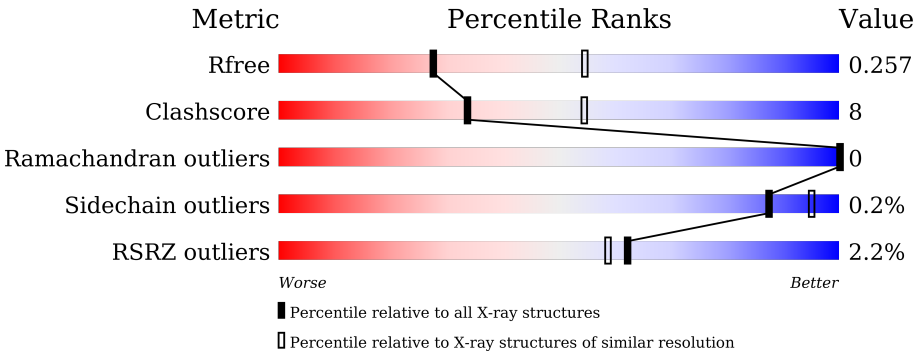
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.68 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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	A	542	2% 79% 18% .
1	B	542	2% 80% 15% 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8049 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 Diphtheria toxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4051	2551	686	802	12			
1	B	515	Total	C	N	O	S	0	0	0
			3978	2508	675	783	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	GLU	GLY	conflict	UNP Q5PY51
A	226	GLU	PRO	engineered mutation	UNP Q5PY51
A	459	PRO	ARG	engineered mutation	UNP Q5PY51
A	511	ASP	GLY	engineered mutation	UNP Q5PY51
A	537	HIS	-	expression tag	UNP Q5PY51
A	538	HIS	-	expression tag	UNP Q5PY51
A	539	HIS	-	expression tag	UNP Q5PY51
A	540	HIS	-	expression tag	UNP Q5PY51
A	541	HIS	-	expression tag	UNP Q5PY51
A	542	HIS	-	expression tag	UNP Q5PY51
B	53	GLU	GLY	conflict	UNP Q5PY51
B	226	GLU	PRO	engineered mutation	UNP Q5PY51
B	459	PRO	ARG	engineered mutation	UNP Q5PY51
B	511	ASP	GLY	engineered mutation	UNP Q5PY51
B	537	HIS	-	expression tag	UNP Q5PY51
B	538	HIS	-	expression tag	UNP Q5PY51
B	539	HIS	-	expression tag	UNP Q5PY51
B	540	HIS	-	expression tag	UNP Q5PY51
B	541	HIS	-	expression tag	UNP Q5PY51
B	542	HIS	-	expression tag	UNP Q5PY51

- Molecule 2 is water.

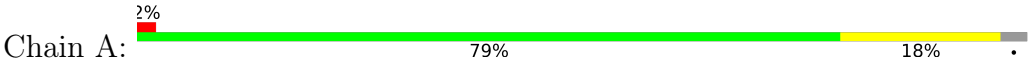
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	11	Total O 11 11	0	0
2	B	9	Total O 9 9	0	0

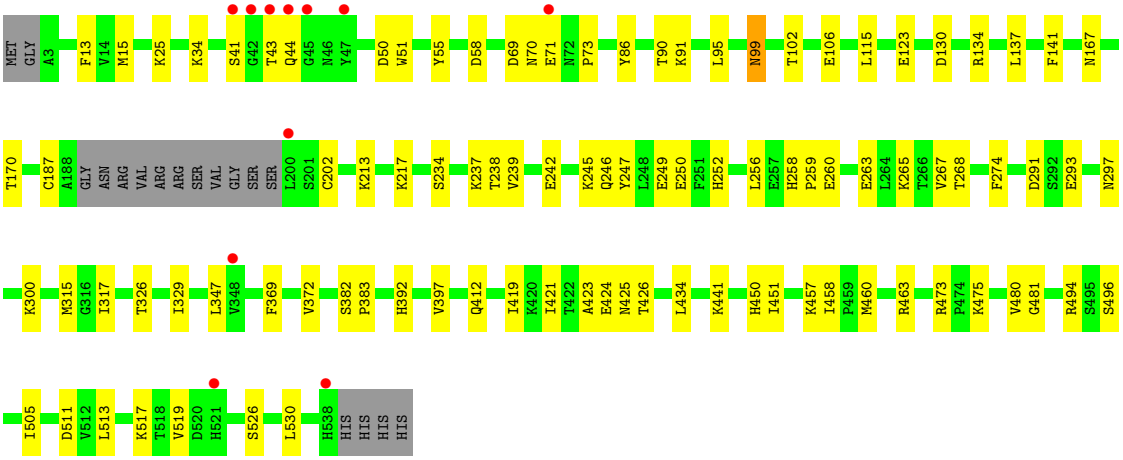
3 Residue-property plots (i)

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: Diphtheria toxin

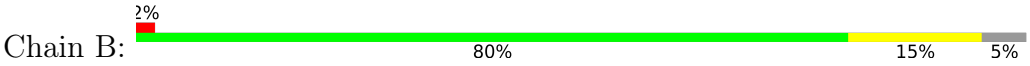
Chain A:

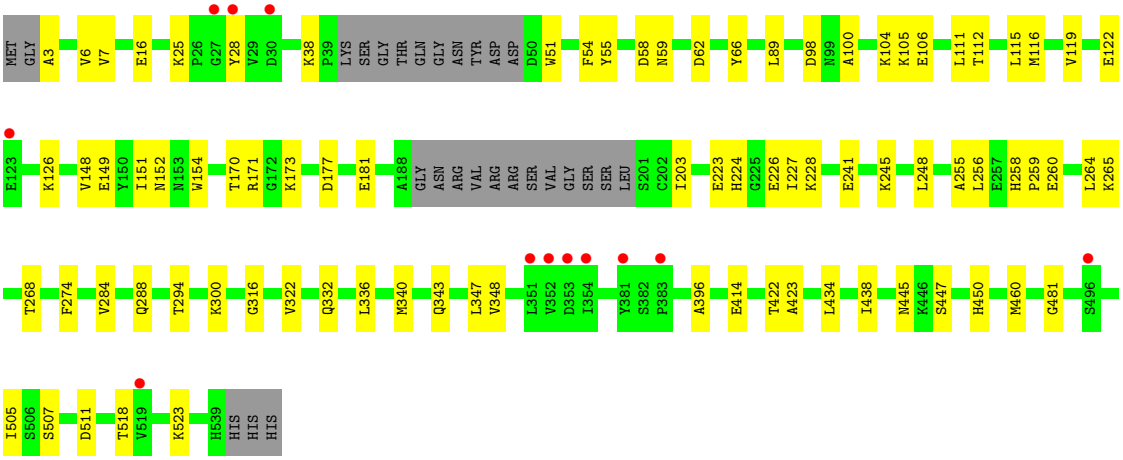




• Molecule 1: Diphtheria toxin

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.84Å 115.92Å 72.89Å 90.00° 111.38° 90.00°	Depositor
Resolution (Å)	34.44 – 2.68 34.44 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.7 (34.44-2.68) 91.5 (34.44-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.218 , 0.257 0.218 , 0.257	Depositor DCC
R_{free} test set	1992 reflections (6.29%)	wwPDB-VP
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 18.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8049	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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.

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	0.18	0/4134	0.37	0/5603
1	B	0.22	0/4060	0.40	0/5502
All	All	0.20	0/8194	0.38	0/11105

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	4051	0	3967	61	1
1	B	3978	0	3900	63	1
2	A	11	0	0	1	0
2	B	9	0	0	0	0
All	All	8049	0	7867	123	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 8.

The worst 5 of 123 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:438:ILE:HD11	1:B:505:ILE:HG13	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:GLU:H	1:B:226:GLU:CD	1.90	0.80
1:B:59:ASN:ND2	1:B:62:ASP:OD1	2.16	0.77
1:B:258:HIS:HD2	1:B:260:GLU:H	1.34	0.76
1:B:348:VAL:O	1:B:348:VAL:HG12	1.90	0.72

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:412:GLN:OE1	1:B:112:THR:OG1[2_646]	1.98	0.22

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	521/542 (96%)	507 (97%)	14 (3%)	0	100	100
1	B	509/542 (94%)	493 (97%)	16 (3%)	0	100	100
All	All	1030/1084 (95%)	1000 (97%)	30 (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	A	447/461 (97%)	445 (100%)	2 (0%)	84 93
1	B	439/461 (95%)	439 (100%)	0	100 100
All	All	886/922 (96%)	884 (100%)	2 (0%)	87 95

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

Mol	Chain	Res	Type
1	A	99	ASN
1	A	526	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	503	ASN
1	B	236	ASN
1	B	503	ASN
1	B	373	HIS
1	A	392	HIS

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 oligosaccharides 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

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, 95^{th} 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	525/542 (96%)	0.27	11 (2%)	63	60	46, 66, 108, 144	0
1	B	515/542 (95%)	0.27	12 (2%)	61	57	46, 68, 105, 177	0
All	All	1040/1084 (95%)	0.27	23 (2%)	62	59	46, 68, 107, 177	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	GLN	3.7
1	B	28	TYR	3.2
1	B	30	ASP	3.2
1	A	43	THR	3.0
1	A	47	TYR	2.8

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 oligosaccharides 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.