



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:26 am GMT

PDB ID : 1HA5
Title : STRUCTURAL FEATURES OF A ZINC-BINDING SITE IN THE SUPER-ANTIGEN STREPTOCOCCAL PYROGENIC EXOTOXIN A (SPEA1): IMPLICATIONS FOR MHC CLASS II RECOGNITION.
Authors : Baker, M.D.; Gutman, D.M.; Papageorgiou, A.C.; Collins, C.M.; Acharya, K.R.
Deposited on : 2001-03-28
Resolution : 2.82 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

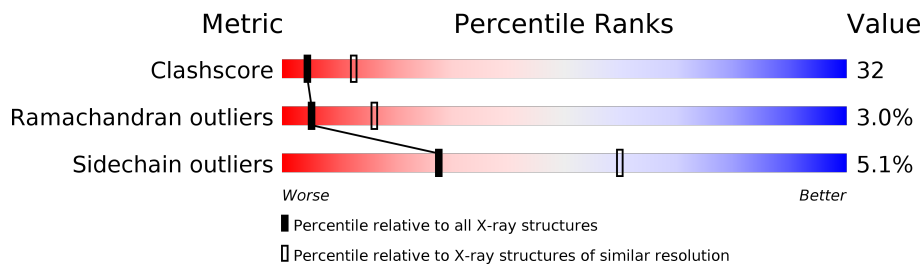
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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))
Clashscore	112137	3382 (2.84-2.80)
Ramachandran outliers	110173	3324 (2.84-2.80)
Sidechain outliers	110143	3326 (2.84-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	218	
1	B	218	
1	C	218	
1	D	218	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7180 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 STREPTOCOCCAL PYOGENIC EXOTOXIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1763	1128	284	345	6			
1	B	218	Total	C	N	O	S	0	0	0
			1759	1126	284	343	6			
1	C	218	Total	C	N	O	S	0	0	0
			1756	1125	283	342	6			
1	D	218	Total	C	N	O	S	0	0	0
			1756	1125	283	342	6			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

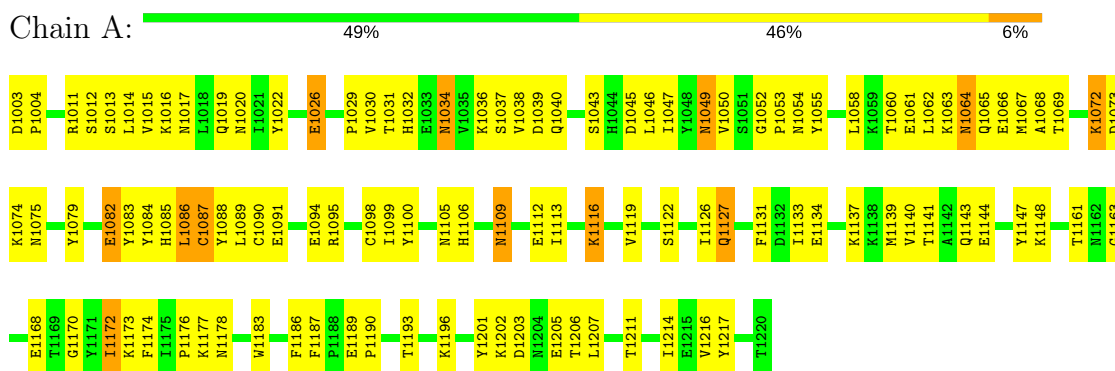
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	33	Total	O	0	0
			33	33		
3	C	54	Total	O	0	0
			54	54		
3	D	14	Total	O	0	0
			14	14		

3 Residue-property plots

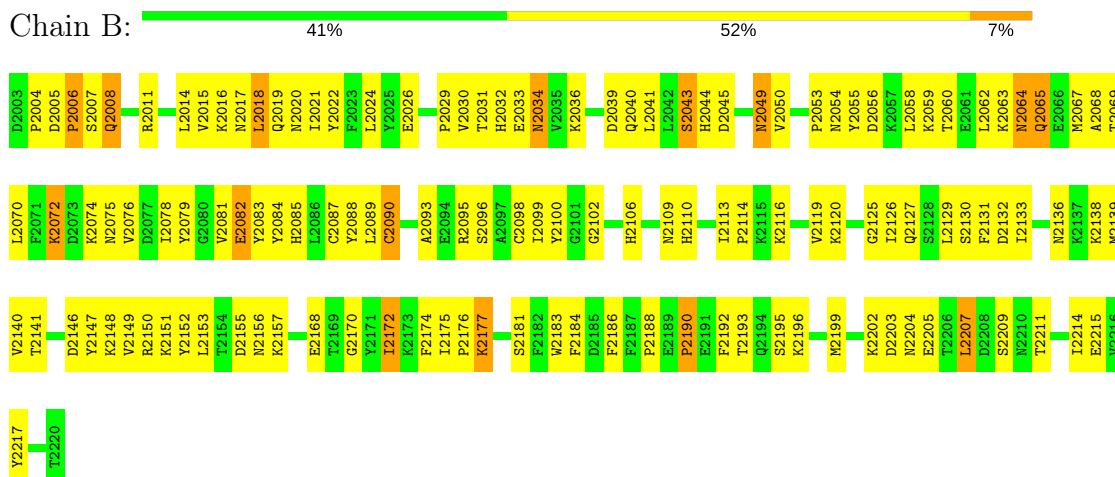
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

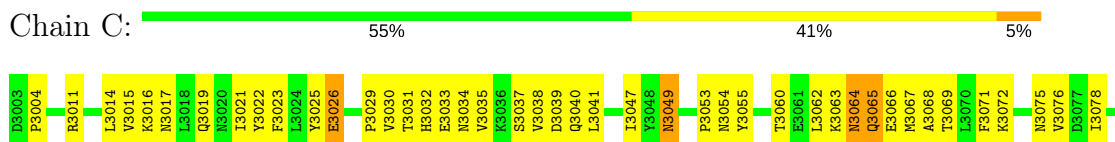
• Molecule 1: STREPTOCOCCAL PYOGENIC EXOTOXIN A1

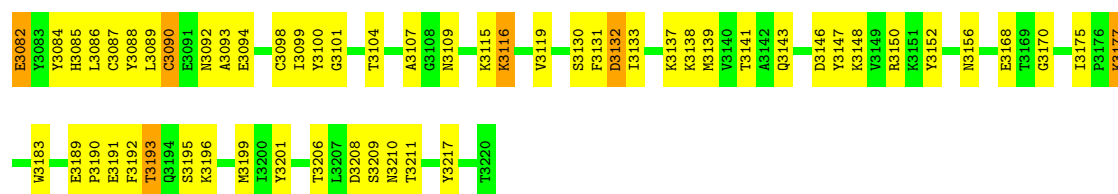


• Molecule 1: STREPTOCOCCAL PYOGENIC EXOTOXIN A1



• Molecule 1: STREPTOCOCCAL PYOGENIC EXOTOXIN A1





• Molecule 1: STREPTOCOCCAL PYOGENIC EXOTOXIN A1

Chain D: 44% 49% 7%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.95Å 101.32Å 82.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.60 – 2.82	Depositor
% Data completeness (in resolution range)	95.3 (39.60-2.82)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7180	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.41	0/1804	0.64	0/2446
1	B	0.39	0/1800	0.63	0/2441
1	C	0.40	0/1797	0.65	0/2437
1	D	0.36	0/1797	0.62	0/2437
All	All	0.39	0/7198	0.63	0/9761

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 [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	1763	0	1701	103	0
1	B	1759	0	1697	123	0
1	C	1756	0	1693	97	0
1	D	1756	0	1693	125	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	41	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	0	3	0
3	C	54	0	0	6	0
3	D	14	0	0	2	0
All	All	7180	0	6784	432	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 32.

The worst 5 of 432 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:D:4129:LEU:HD12	1:D:4130:SER:H	1.26	1.01
1:C:3193:THR:HG22	1:C:3196:LYS:H	1.25	1.00
1:D:4121:VAL:HG12	1:D:4122:SER:H	1.22	0.99
1:A:1062:LEU:HB3	1:A:1067:MET:HE2	1.45	0.98
1:D:4062:LEU:HB3	1:D:4067:MET:HE2	1.46	0.94

There are no symmetry-related clashes.

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	216/218 (99%)	191 (88%)	22 (10%)	3 (1%)	13	38
1	B	216/218 (99%)	190 (88%)	19 (9%)	7 (3%)	5	15
1	C	216/218 (99%)	186 (86%)	24 (11%)	6 (3%)	6	18
1	D	216/218 (99%)	181 (84%)	25 (12%)	10 (5%)	3	8
All	All	864/872 (99%)	748 (87%)	90 (10%)	26 (3%)	5	16

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2072	LYS
1	C	3093	ALA
1	D	4020	ASN
1	D	4090	CYS
1	D	4122	SER

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	198/204 (97%)	186 (94%)	12 (6%)	22	51
1	B	197/204 (97%)	186 (94%)	11 (6%)	25	55
1	C	196/204 (96%)	188 (96%)	8 (4%)	35	68
1	D	196/204 (96%)	187 (95%)	9 (5%)	31	64
All	All	787/816 (96%)	747 (95%)	40 (5%)	28	60

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2082	GLU
1	B	2207	LEU
1	D	4109	ASN
1	B	2188	PRO
1	C	3026	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2092	ASN
1	C	3019	GLN
1	D	4049	ASN
1	B	2109	ASN
1	B	2127	GLN

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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.

5.7 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.