



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 06:00 PM UTC

PDB ID : 3OWE / pdb_00003owe
Title : Crystal Structure of Staphylococcal Enterotoxin G (SEG) in Complex with a High Affinity Mutant Mouse T-cell Receptor Chain
Authors : Fernandez, M.M.; Cho, S.; Robinson, H.; Mariuzza, R.A.; Malchiodi, M.L.
Deposited on : 2010-09-17
Resolution : 2.60 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

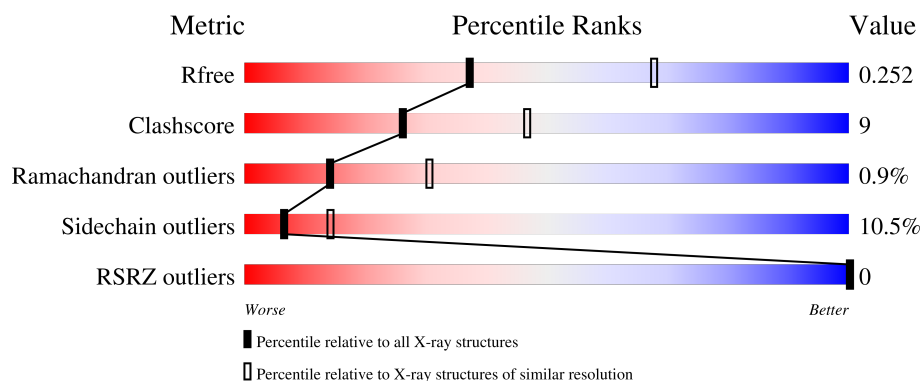
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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	112	
1	C	112	
1	E	112	
1	G	112	
1	I	112	

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Mol	Chain	Length	Quality of chain
1	K	112	
1	M	112	
1	O	112	
2	B	234	
2	D	234	
2	F	234	
2	H	234	
2	J	234	
2	L	234	
2	N	234	
2	P	234	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21680 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 Beta-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			833	518	148	164	3			
1	C	109	Total	C	N	O	S	0	0	0
			833	518	148	164	3			
1	E	109	Total	C	N	O	S	0	0	0
			833	518	148	164	3			
1	G	109	Total	C	N	O	S	0	0	0
			833	518	148	164	3			
1	I	109	Total	C	N	O	S	0	0	0
			833	518	148	164	3			
1	K	109	Total	C	N	O	S	0	0	0
			833	518	148	164	3			
1	M	109	Total	C	N	O	S	0	0	0
			833	518	148	164	3			
1	O	109	Total	C	N	O	S	0	0	0
			833	518	148	164	3			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP A2NTY6
A	0	ALA	MET	engineered mutation	UNP A2NTY6
A	17	GLU	GLY	engineered mutation	UNP A2NTY6
A	24	GLN	ASN	engineered mutation	UNP A2NTY6
A	52	VAL	ALA	engineered mutation	UNP A2NTY6
A	54	ASN	SER	engineered mutation	UNP A2NTY6
A	65	GLU	LYS	engineered mutation	UNP A2NTY6
A	71	HIS	GLN	engineered mutation	UNP A2NTY6
A	73	GLN	ASN	engineered mutation	UNP A2NTY6
A	79	VAL	GLU	engineered mutation	UNP A2NTY6
A	80	SER	LEU	engineered mutation	UNP A2NTY6
A	86	SER	THR	engineered mutation	UNP A2NTY6
A	?	-	GLU	deletion	UNP A2NTY6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	95	VAL	LEU	engineered mutation	UNP A2NTY6
A	?	-	PHE	deletion	UNP A2NTY6
A	?	-	ASN	deletion	UNP A2NTY6
A	?	-	GLN	deletion	UNP A2NTY6
A	?	-	ASP	deletion	UNP A2NTY6
A	99	LEU	GLN	engineered mutation	UNP A2NTY6
A	103	ALA	PRO	engineered mutation	UNP A2NTY6
A	108	SER	LEU	engineered mutation	UNP A2NTY6
C	-1	ALA	-	expression tag	UNP A2NTY6
C	0	ALA	MET	engineered mutation	UNP A2NTY6
C	17	GLU	GLY	engineered mutation	UNP A2NTY6
C	24	GLN	ASN	engineered mutation	UNP A2NTY6
C	52	VAL	ALA	engineered mutation	UNP A2NTY6
C	54	ASN	SER	engineered mutation	UNP A2NTY6
C	65	GLU	LYS	engineered mutation	UNP A2NTY6
C	71	HIS	GLN	engineered mutation	UNP A2NTY6
C	73	GLN	ASN	engineered mutation	UNP A2NTY6
C	79	VAL	GLU	engineered mutation	UNP A2NTY6
C	80	SER	LEU	engineered mutation	UNP A2NTY6
C	86	SER	THR	engineered mutation	UNP A2NTY6
C	?	-	GLU	deletion	UNP A2NTY6
C	95	VAL	LEU	engineered mutation	UNP A2NTY6
C	?	-	PHE	deletion	UNP A2NTY6
C	?	-	ASN	deletion	UNP A2NTY6
C	?	-	GLN	deletion	UNP A2NTY6
C	?	-	ASP	deletion	UNP A2NTY6
C	99	LEU	GLN	engineered mutation	UNP A2NTY6
C	103	ALA	PRO	engineered mutation	UNP A2NTY6
C	108	SER	LEU	engineered mutation	UNP A2NTY6
E	-1	ALA	-	expression tag	UNP A2NTY6
E	0	ALA	MET	engineered mutation	UNP A2NTY6
E	17	GLU	GLY	engineered mutation	UNP A2NTY6
E	24	GLN	ASN	engineered mutation	UNP A2NTY6
E	52	VAL	ALA	engineered mutation	UNP A2NTY6
E	54	ASN	SER	engineered mutation	UNP A2NTY6
E	65	GLU	LYS	engineered mutation	UNP A2NTY6
E	71	HIS	GLN	engineered mutation	UNP A2NTY6
E	73	GLN	ASN	engineered mutation	UNP A2NTY6
E	79	VAL	GLU	engineered mutation	UNP A2NTY6
E	80	SER	LEU	engineered mutation	UNP A2NTY6
E	86	SER	THR	engineered mutation	UNP A2NTY6
E	?	-	GLU	deletion	UNP A2NTY6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	95	VAL	LEU	engineered mutation	UNP A2NTY6
E	?	-	PHE	deletion	UNP A2NTY6
E	?	-	ASN	deletion	UNP A2NTY6
E	?	-	GLN	deletion	UNP A2NTY6
E	?	-	ASP	deletion	UNP A2NTY6
E	99	LEU	GLN	engineered mutation	UNP A2NTY6
E	103	ALA	PRO	engineered mutation	UNP A2NTY6
E	108	SER	LEU	engineered mutation	UNP A2NTY6
G	-1	ALA	-	expression tag	UNP A2NTY6
G	0	ALA	MET	engineered mutation	UNP A2NTY6
G	17	GLU	GLY	engineered mutation	UNP A2NTY6
G	24	GLN	ASN	engineered mutation	UNP A2NTY6
G	52	VAL	ALA	engineered mutation	UNP A2NTY6
G	54	ASN	SER	engineered mutation	UNP A2NTY6
G	65	GLU	LYS	engineered mutation	UNP A2NTY6
G	71	HIS	GLN	engineered mutation	UNP A2NTY6
G	73	GLN	ASN	engineered mutation	UNP A2NTY6
G	79	VAL	GLU	engineered mutation	UNP A2NTY6
G	80	SER	LEU	engineered mutation	UNP A2NTY6
G	86	SER	THR	engineered mutation	UNP A2NTY6
G	?	-	GLU	deletion	UNP A2NTY6
G	95	VAL	LEU	engineered mutation	UNP A2NTY6
G	?	-	PHE	deletion	UNP A2NTY6
G	?	-	ASN	deletion	UNP A2NTY6
G	?	-	GLN	deletion	UNP A2NTY6
G	?	-	ASP	deletion	UNP A2NTY6
G	99	LEU	GLN	engineered mutation	UNP A2NTY6
G	103	ALA	PRO	engineered mutation	UNP A2NTY6
G	108	SER	LEU	engineered mutation	UNP A2NTY6
I	-1	ALA	-	expression tag	UNP A2NTY6
I	0	ALA	MET	engineered mutation	UNP A2NTY6
I	17	GLU	GLY	engineered mutation	UNP A2NTY6
I	24	GLN	ASN	engineered mutation	UNP A2NTY6
I	52	VAL	ALA	engineered mutation	UNP A2NTY6
I	54	ASN	SER	engineered mutation	UNP A2NTY6
I	65	GLU	LYS	engineered mutation	UNP A2NTY6
I	71	HIS	GLN	engineered mutation	UNP A2NTY6
I	73	GLN	ASN	engineered mutation	UNP A2NTY6
I	79	VAL	GLU	engineered mutation	UNP A2NTY6
I	80	SER	LEU	engineered mutation	UNP A2NTY6
I	86	SER	THR	engineered mutation	UNP A2NTY6
I	?	-	GLU	deletion	UNP A2NTY6

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Chain	Residue	Modelled	Actual	Comment	Reference
I	95	VAL	LEU	engineered mutation	UNP A2NTY6
I	?	-	PHE	deletion	UNP A2NTY6
I	?	-	ASN	deletion	UNP A2NTY6
I	?	-	GLN	deletion	UNP A2NTY6
I	?	-	ASP	deletion	UNP A2NTY6
I	99	LEU	GLN	engineered mutation	UNP A2NTY6
I	103	ALA	PRO	engineered mutation	UNP A2NTY6
I	108	SER	LEU	engineered mutation	UNP A2NTY6
K	-1	ALA	-	expression tag	UNP A2NTY6
K	0	ALA	MET	engineered mutation	UNP A2NTY6
K	17	GLU	GLY	engineered mutation	UNP A2NTY6
K	24	GLN	ASN	engineered mutation	UNP A2NTY6
K	52	VAL	ALA	engineered mutation	UNP A2NTY6
K	54	ASN	SER	engineered mutation	UNP A2NTY6
K	65	GLU	LYS	engineered mutation	UNP A2NTY6
K	71	HIS	GLN	engineered mutation	UNP A2NTY6
K	73	GLN	ASN	engineered mutation	UNP A2NTY6
K	79	VAL	GLU	engineered mutation	UNP A2NTY6
K	80	SER	LEU	engineered mutation	UNP A2NTY6
K	86	SER	THR	engineered mutation	UNP A2NTY6
K	?	-	GLU	deletion	UNP A2NTY6
K	95	VAL	LEU	engineered mutation	UNP A2NTY6
K	?	-	PHE	deletion	UNP A2NTY6
K	?	-	ASN	deletion	UNP A2NTY6
K	?	-	GLN	deletion	UNP A2NTY6
K	?	-	ASP	deletion	UNP A2NTY6
K	99	LEU	GLN	engineered mutation	UNP A2NTY6
K	103	ALA	PRO	engineered mutation	UNP A2NTY6
K	108	SER	LEU	engineered mutation	UNP A2NTY6
M	-1	ALA	-	expression tag	UNP A2NTY6
M	0	ALA	MET	engineered mutation	UNP A2NTY6
M	17	GLU	GLY	engineered mutation	UNP A2NTY6
M	24	GLN	ASN	engineered mutation	UNP A2NTY6
M	52	VAL	ALA	engineered mutation	UNP A2NTY6
M	54	ASN	SER	engineered mutation	UNP A2NTY6
M	65	GLU	LYS	engineered mutation	UNP A2NTY6
M	71	HIS	GLN	engineered mutation	UNP A2NTY6
M	73	GLN	ASN	engineered mutation	UNP A2NTY6
M	79	VAL	GLU	engineered mutation	UNP A2NTY6
M	80	SER	LEU	engineered mutation	UNP A2NTY6
M	86	SER	THR	engineered mutation	UNP A2NTY6
M	?	-	GLU	deletion	UNP A2NTY6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	95	VAL	LEU	engineered mutation	UNP A2NTY6
M	?	-	PHE	deletion	UNP A2NTY6
M	?	-	ASN	deletion	UNP A2NTY6
M	?	-	GLN	deletion	UNP A2NTY6
M	?	-	ASP	deletion	UNP A2NTY6
M	99	LEU	GLN	engineered mutation	UNP A2NTY6
M	103	ALA	PRO	engineered mutation	UNP A2NTY6
M	108	SER	LEU	engineered mutation	UNP A2NTY6
O	-1	ALA	-	expression tag	UNP A2NTY6
O	0	ALA	MET	engineered mutation	UNP A2NTY6
O	17	GLU	GLY	engineered mutation	UNP A2NTY6
O	24	GLN	ASN	engineered mutation	UNP A2NTY6
O	52	VAL	ALA	engineered mutation	UNP A2NTY6
O	54	ASN	SER	engineered mutation	UNP A2NTY6
O	65	GLU	LYS	engineered mutation	UNP A2NTY6
O	71	HIS	GLN	engineered mutation	UNP A2NTY6
O	73	GLN	ASN	engineered mutation	UNP A2NTY6
O	79	VAL	GLU	engineered mutation	UNP A2NTY6
O	80	SER	LEU	engineered mutation	UNP A2NTY6
O	86	SER	THR	engineered mutation	UNP A2NTY6
O	?	-	GLU	deletion	UNP A2NTY6
O	95	VAL	LEU	engineered mutation	UNP A2NTY6
O	?	-	PHE	deletion	UNP A2NTY6
O	?	-	ASN	deletion	UNP A2NTY6
O	?	-	GLN	deletion	UNP A2NTY6
O	?	-	ASP	deletion	UNP A2NTY6
O	99	LEU	GLN	engineered mutation	UNP A2NTY6
O	103	ALA	PRO	engineered mutation	UNP A2NTY6
O	108	SER	LEU	engineered mutation	UNP A2NTY6

- Molecule 2 is a protein called Enterotoxin SEG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1851	1193	298	351	9			
2	D	227	Total	C	N	O	S	0	0	0
			1851	1193	298	351	9			
2	F	227	Total	C	N	O	S	0	0	0
			1851	1193	298	351	9			
2	H	227	Total	C	N	O	S	0	0	0
			1851	1193	298	351	9			
2	J	227	Total	C	N	O	S	0	0	0
			1851	1193	298	351	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	228	Total	C	N	O	S	0	0	0
			1860	1198	299	354	9			
2	N	228	Total	C	N	O	S	0	0	0
			1860	1198	299	354	9			
2	P	228	Total	C	N	O	S	0	0	0
			1860	1198	299	354	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	expression tag	UNP D0EMB6
D	1	ALA	-	expression tag	UNP D0EMB6
F	1	ALA	-	expression tag	UNP D0EMB6
H	1	ALA	-	expression tag	UNP D0EMB6
J	1	ALA	-	expression tag	UNP D0EMB6
L	1	ALA	-	expression tag	UNP D0EMB6
N	1	ALA	-	expression tag	UNP D0EMB6
P	1	ALA	-	expression tag	UNP D0EMB6

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	17	Total	O	0	0
			17	17		
3	C	4	Total	O	0	0
			4	4		
3	D	17	Total	O	0	0
			17	17		
3	E	3	Total	O	0	0
			3	3		
3	F	17	Total	O	0	0
			17	17		
3	G	1	Total	O	0	0
			1	1		
3	H	19	Total	O	0	0
			19	19		
3	I	5	Total	O	0	0
			5	5		
3	J	20	Total	O	0	0
			20	20		

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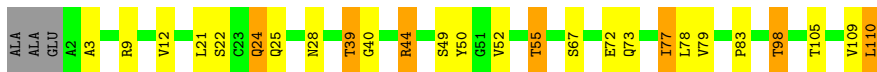
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	6	Total 6	O 6	0	0
3	L	22	Total 22	O 22	0	0
3	M	3	Total 3	O 3	0	0
3	N	20	Total 20	O 20	0	0
3	O	4	Total 4	O 4	0	0
3	P	20	Total 20	O 20	0	0

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.

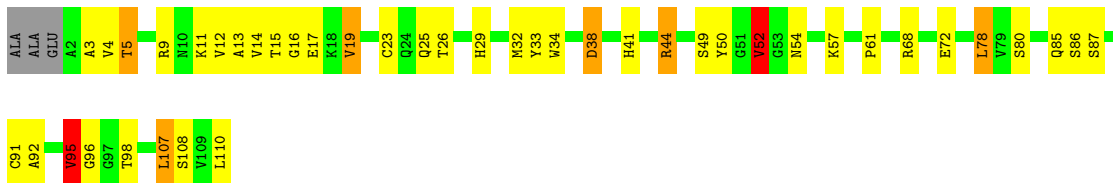
- Molecule 1: Beta-chain

Chain A: 



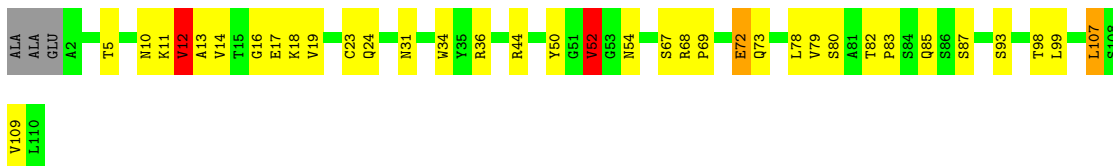
- Molecule 1: Beta-chain

Chain C: 



- Molecule 1: Beta-chain

Chain E: 



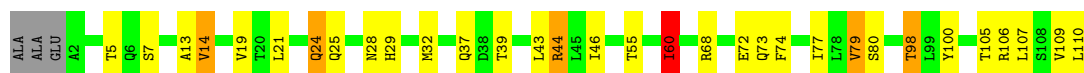
- Molecule 1: Beta-chain

Chain G: 

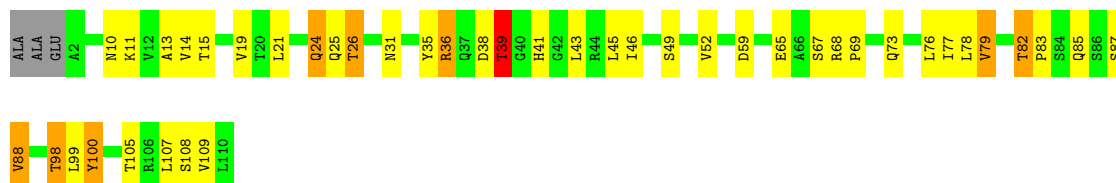


- Molecule 1: Beta-chain

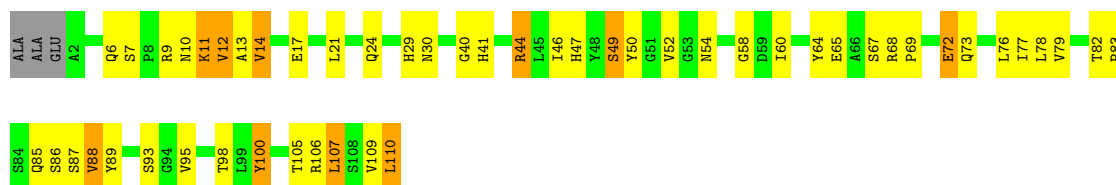
Chain I: 



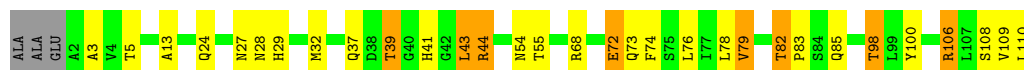
• Molecule 1: Beta-chain



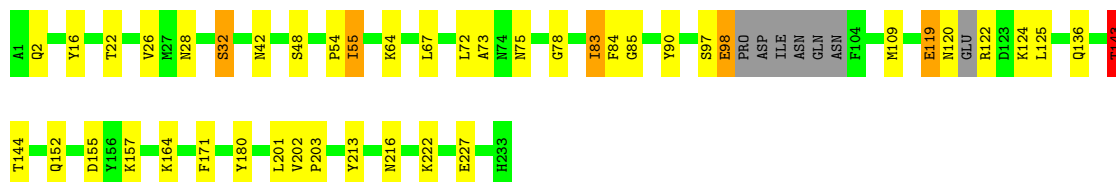
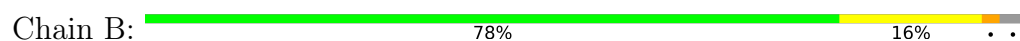
• Molecule 1: Beta-chain



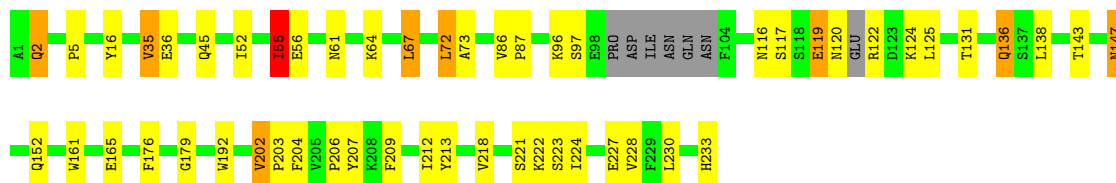
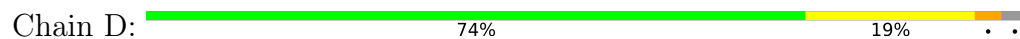
• Molecule 1: Beta-chain



• Molecule 2: Enterotoxin SEG

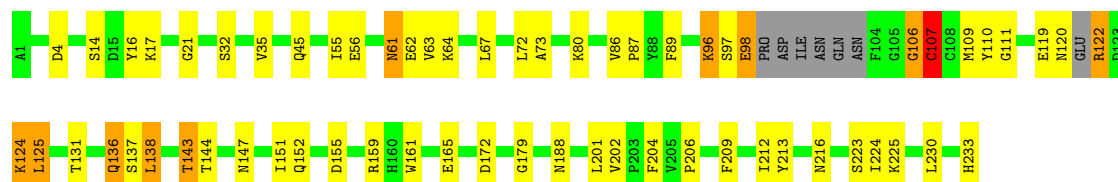


• Molecule 2: Enterotoxin SEG



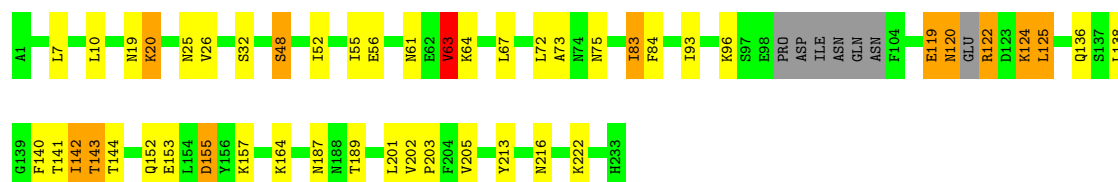
- Molecule 2: Enterotoxin SEG

Chain F: 



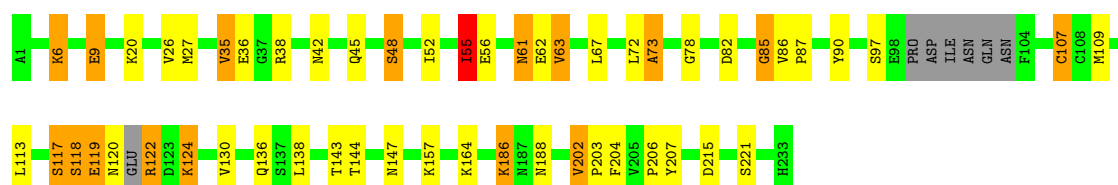
- Molecule 2: Enterotoxin SEG

Chain H: 



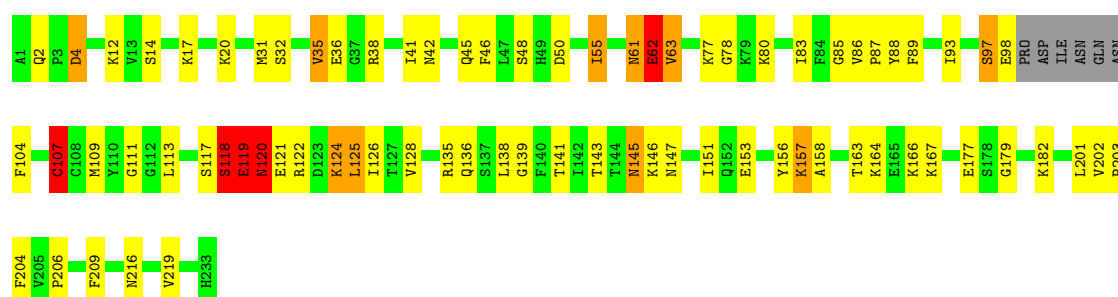
- Molecule 2: Enterotoxin SEG

Chain J: 



- Molecule 2: Enterotoxin SEG

Chain L: 



- Molecule 2: Enterotoxin SEG

Chain N: 





● Molecule 2: Enterotoxin SEG



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	141.21Å 141.21Å 255.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.60) 99.7 (50.00-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.261 0.205 , 0.252	Depositor DCC
R_{free} test set	7725 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 3.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21680	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5433e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	1.31	1/852 (0.1%)	1.29	4/1156 (0.3%)
1	C	1.30	2/852 (0.2%)	1.25	1/1156 (0.1%)
1	E	1.34	2/852 (0.2%)	1.36	3/1156 (0.3%)
1	G	1.35	1/852 (0.1%)	1.33	4/1156 (0.3%)
1	I	1.34	4/852 (0.5%)	1.32	7/1156 (0.6%)
1	K	1.35	2/852 (0.2%)	1.32	6/1156 (0.5%)
1	M	1.35	0/852	1.37	6/1156 (0.5%)
1	O	1.38	0/852	1.40	12/1156 (1.0%)
2	B	1.34	2/1894 (0.1%)	1.35	17/2551 (0.7%)
2	D	1.35	8/1894 (0.4%)	1.34	14/2551 (0.5%)
2	F	1.33	5/1894 (0.3%)	1.34	11/2551 (0.4%)
2	H	1.32	3/1894 (0.2%)	1.36	16/2551 (0.6%)
2	J	1.40	7/1894 (0.4%)	1.32	9/2551 (0.4%)
2	L	1.40	8/1904 (0.4%)	1.43	15/2566 (0.6%)
2	N	1.40	8/1904 (0.4%)	1.36	12/2566 (0.5%)
2	P	1.39	6/1904 (0.3%)	1.31	11/2566 (0.4%)
All	All	1.36	59/21998 (0.3%)	1.34	148/29701 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
2	H	0	1
2	L	0	3
All	All	0	6

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	202	VAL	CA-CB	8.40	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	86	VAL	N-CA	-7.91	1.40	1.46
1	E	52	VAL	CA-CB	7.89	1.63	1.54
2	J	86	VAL	N-CA	-7.87	1.40	1.46
2	P	107	CYS	N-CA	7.67	1.55	1.46

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	107	CYS	N-CA-C	11.31	127.34	108.90
2	B	32	SER	CA-C-N	-10.87	109.19	120.38
2	B	32	SER	C-N-CA	-10.87	109.19	120.38
2	D	2	GLN	CB-CA-C	9.18	119.25	110.17
2	N	107	CYS	N-CA-C	9.01	123.58	108.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	38	ASP	Peptide
1	C	96	GLY	Peptide
2	H	119	GLU	Peptide
2	L	117	SER	Peptide
2	L	118	SER	Peptide

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	833	0	792	10	0
1	C	833	0	792	23	0
1	E	833	0	792	16	0
1	G	833	0	792	14	0
1	I	833	0	792	17	0
1	K	833	0	792	22	0
1	M	833	0	792	34	0
1	O	833	0	792	19	0
2	B	1851	0	1821	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1851	0	1821	31	0
2	F	1851	0	1821	38	0
2	H	1851	0	1821	23	0
2	J	1851	0	1821	31	0
2	L	1860	0	1828	49	0
2	N	1860	0	1828	32	0
2	P	1860	0	1828	26	0
3	A	3	0	0	0	0
3	B	17	0	0	0	0
3	C	4	0	0	0	0
3	D	17	0	0	0	0
3	E	3	0	0	0	0
3	F	17	0	0	1	0
3	G	1	0	0	0	0
3	H	19	0	0	1	0
3	I	5	0	0	0	0
3	J	20	0	0	1	0
3	K	6	0	0	0	0
3	L	22	0	0	1	0
3	M	3	0	0	0	0
3	N	20	0	0	0	0
3	O	4	0	0	1	0
3	P	20	0	0	0	0
All	All	21680	0	20925	399	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 9.

The worst 5 of 399 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)
2:J:120:ASN:C	2:J:122:ARG:N	2.11	1.09
2:F:55:ILE:HG21	2:F:63:VAL:HG23	1.36	1.02
1:O:108:SER:HB2	3:O:165:HOH:O	1.60	1.02
1:G:44:ARG:HG3	1:G:44:ARG:HH11	1.27	0.98
1:G:50:TYR:H	1:G:54:ASN:ND2	1.63	0.97

There are no symmetry-related clashes.

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	107/112 (96%)	100 (94%)	5 (5%)	2 (2%)	6	13
1	C	107/112 (96%)	97 (91%)	8 (8%)	2 (2%)	6	13
1	E	107/112 (96%)	103 (96%)	4 (4%)	0	100	100
1	G	107/112 (96%)	99 (92%)	6 (6%)	2 (2%)	6	13
1	I	107/112 (96%)	103 (96%)	4 (4%)	0	100	100
1	K	107/112 (96%)	97 (91%)	8 (8%)	2 (2%)	6	13
1	M	107/112 (96%)	97 (91%)	8 (8%)	2 (2%)	6	13
1	O	107/112 (96%)	103 (96%)	4 (4%)	0	100	100
2	B	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	24	46
2	D	221/234 (94%)	210 (95%)	10 (4%)	1 (0%)	24	46
2	F	221/234 (94%)	211 (96%)	8 (4%)	2 (1%)	14	30
2	H	221/234 (94%)	211 (96%)	10 (4%)	0	100	100
2	J	221/234 (94%)	207 (94%)	13 (6%)	1 (0%)	24	46
2	L	224/234 (96%)	207 (92%)	16 (7%)	1 (0%)	30	51
2	N	224/234 (96%)	209 (93%)	12 (5%)	3 (1%)	9	21
2	P	224/234 (96%)	210 (94%)	9 (4%)	5 (2%)	5	10
All	All	2633/2768 (95%)	2475 (94%)	134 (5%)	24 (1%)	14	30

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	106	GLY
1	G	3	ALA
1	K	39	THR
1	K	41	HIS
2	L	120	ASN

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	90/91 (99%)	76 (84%)	14 (16%)	2	4
1	C	90/91 (99%)	76 (84%)	14 (16%)	2	4
1	E	90/91 (99%)	77 (86%)	13 (14%)	3	6
1	G	90/91 (99%)	74 (82%)	16 (18%)	2	3
1	I	90/91 (99%)	78 (87%)	12 (13%)	4	8
1	K	90/91 (99%)	74 (82%)	16 (18%)	2	3
1	M	90/91 (99%)	76 (84%)	14 (16%)	2	4
1	O	90/91 (99%)	79 (88%)	11 (12%)	5	10
2	B	209/216 (97%)	195 (93%)	14 (7%)	15	33
2	D	209/216 (97%)	196 (94%)	13 (6%)	16	36
2	F	209/216 (97%)	190 (91%)	19 (9%)	9	19
2	H	209/216 (97%)	191 (91%)	18 (9%)	10	22
2	J	209/216 (97%)	191 (91%)	18 (9%)	10	22
2	L	210/216 (97%)	190 (90%)	20 (10%)	8	18
2	N	210/216 (97%)	190 (90%)	20 (10%)	8	18
2	P	210/216 (97%)	191 (91%)	19 (9%)	9	20
All	All	2395/2456 (98%)	2144 (90%)	251 (10%)	6	14

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	136	GLN
1	O	5	THR
2	J	113	LEU
2	N	186	LYS
2	P	61	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	11	ASN
2	N	61	ASN
2	P	42	ASN
1	G	24	GLN
2	F	233	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, 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	109/112 (97%)	-1.53	0 100 100	23, 39, 56, 64	0
1	C	109/112 (97%)	-1.52	0 100 100	27, 42, 63, 71	0
1	E	109/112 (97%)	-1.52	0 100 100	27, 43, 62, 69	0
1	G	109/112 (97%)	-1.51	0 100 100	23, 39, 54, 64	0
1	I	109/112 (97%)	-1.59	0 100 100	19, 34, 51, 58	0
1	K	109/112 (97%)	-1.38	0 100 100	25, 50, 71, 78	0
1	M	109/112 (97%)	-1.36	0 100 100	24, 51, 71, 79	0
1	O	109/112 (97%)	-1.54	0 100 100	22, 35, 51, 58	0
2	B	227/234 (97%)	-1.64	0 100 100	15, 28, 59, 79	3 (1%)
2	D	227/234 (97%)	-1.63	0 100 100	16, 29, 57, 77	3 (1%)
2	F	227/234 (97%)	-1.64	0 100 100	17, 29, 57, 81	3 (1%)
2	H	227/234 (97%)	-1.64	0 100 100	16, 28, 56, 80	3 (1%)
2	J	227/234 (97%)	-1.68	0 100 100	12, 28, 51, 81	3 (1%)
2	L	228/234 (97%)	-1.67	0 100 100	13, 27, 52, 74	3 (1%)
2	N	228/234 (97%)	-1.66	0 100 100	13, 27, 52, 81	3 (1%)
2	P	228/234 (97%)	-1.67	0 100 100	12, 27, 52, 79	3 (1%)
All	All	2691/2768 (97%)	-1.60	0 100 100	12, 32, 62, 81	24 (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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.