



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:26 AM GMT

PDB ID : 3OWE  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

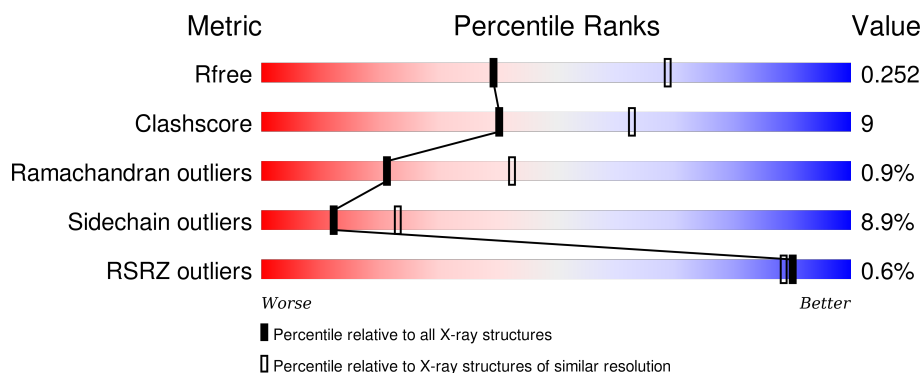
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	112	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• •</div> </div> </div>
1	C	112	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>33%</div> <div>6%</div> <div>• •</div> </div> </div>
1	E	112	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• • •</div> </div> </div>
1	G	112	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• •</div> </div> </div>
1	I	112	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>• •</div> </div> </div>

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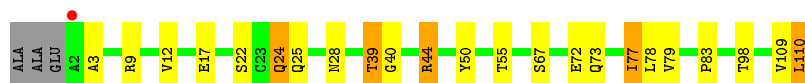
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	K	6	Total 6	O 6	0	0
3	L	22	Total 22	O 22	0	0
3	M	3	Total 3	O 3	0	0
3	N	20	Total 20	O 20	0	0
3	O	4	Total 4	O 4	0	0
3	P	20	Total 20	O 20	0	0

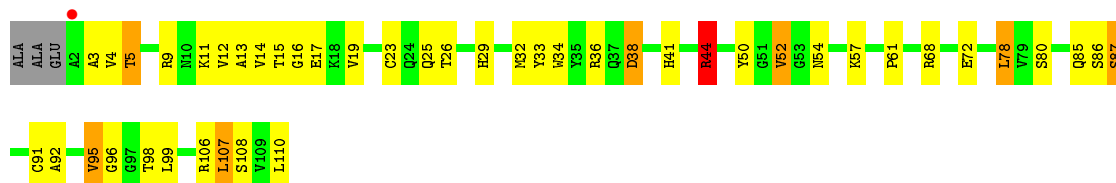
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

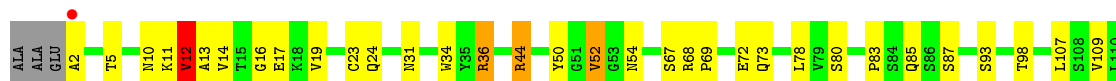
- Molecule 1: Beta-chain



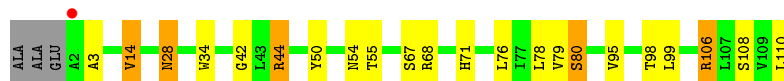
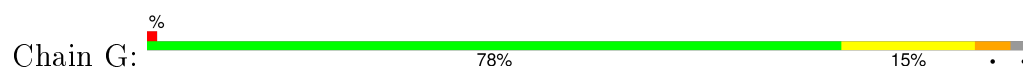
- Molecule 1: Beta-chain



- Molecule 1: Beta-chain



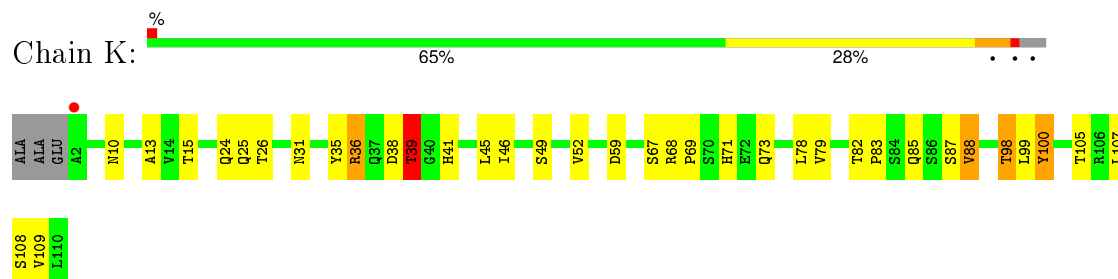
- Molecule 1: Beta-chain



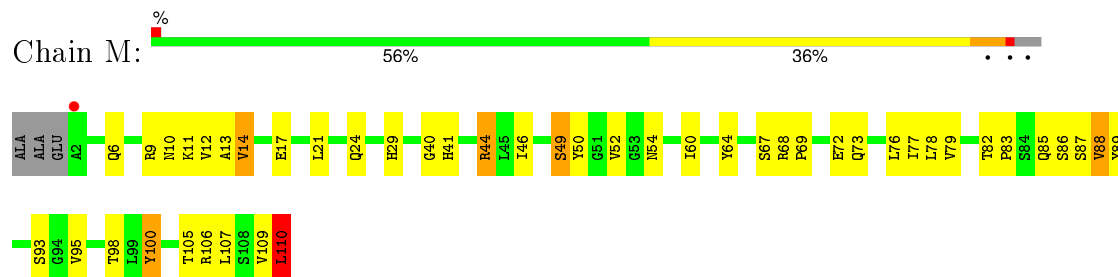
- Molecule 1: Beta-chain



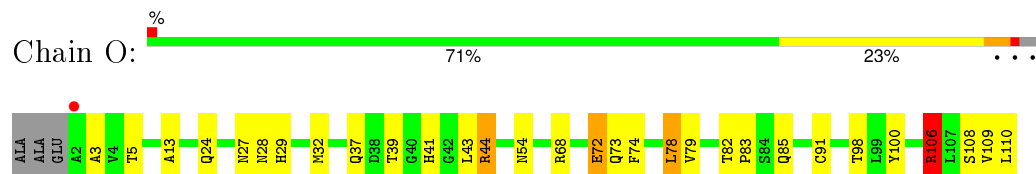
- Molecule 1: Beta-chain



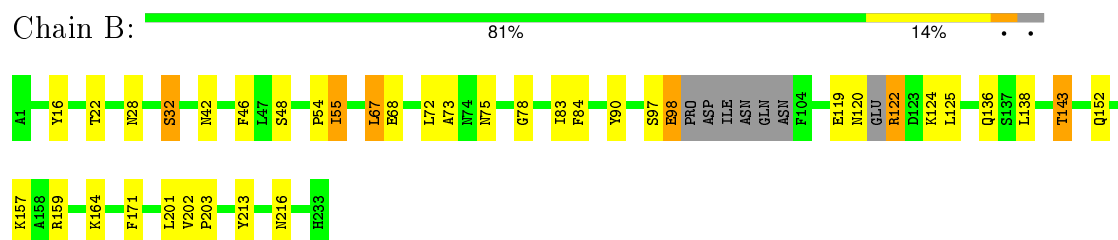
- Molecule 1: Beta-chain



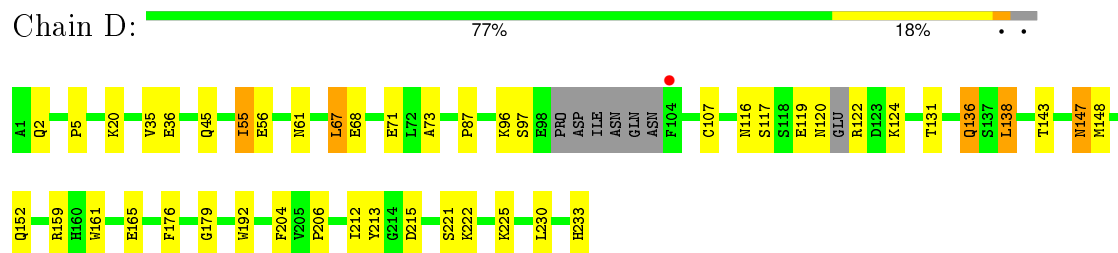
- Molecule 1: Beta-chain



- Molecule 2: Enterotoxin SEG

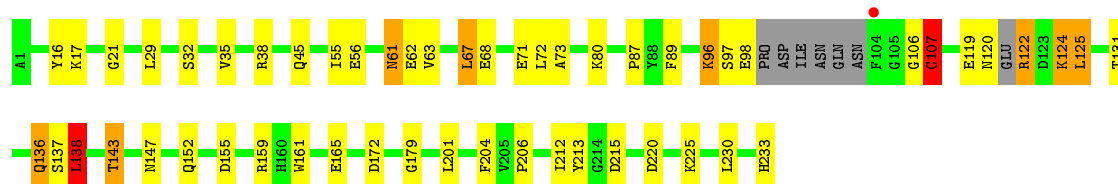


- Molecule 2: Enterotoxin SEG

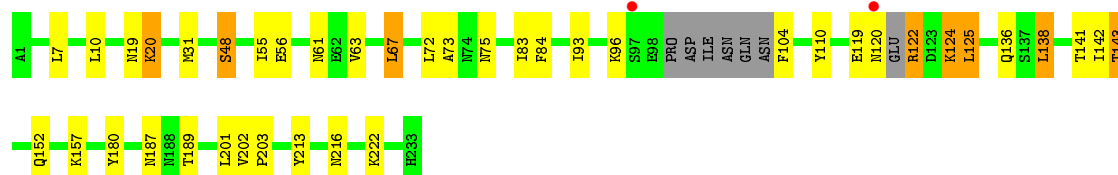
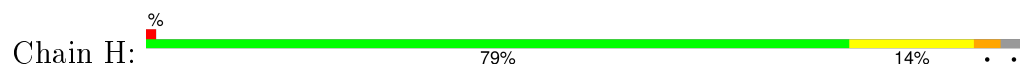


- Molecule 2: Enterotoxin SEG

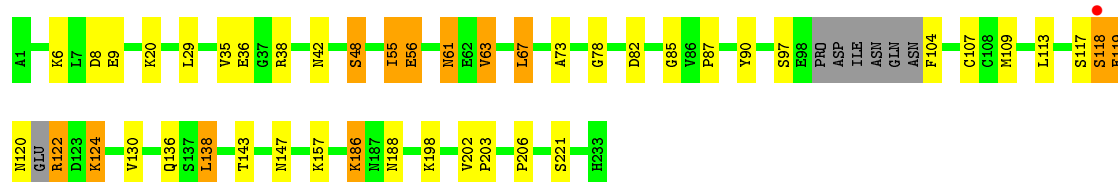
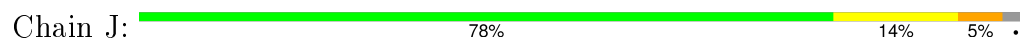




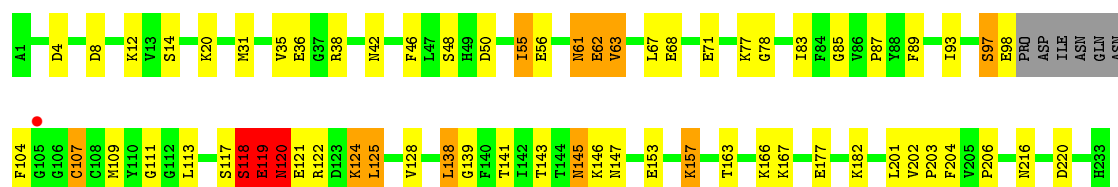
• Molecule 2: Enterotoxin SEG



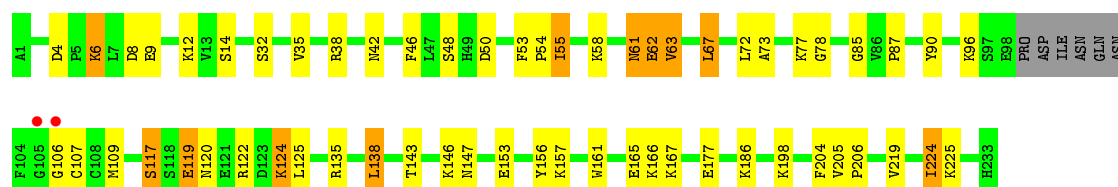
• Molecule 2: Enterotoxin SEG



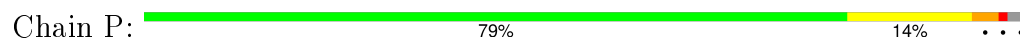
• Molecule 2: Enterotoxin SEG

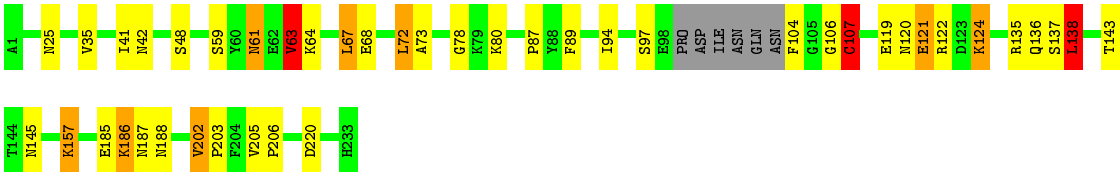


• Molecule 2: Enterotoxin SEG



• Molecule 2: Enterotoxin SEG





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.21Å 141.21Å 255.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 29.61 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.60) 99.5 (29.61-2.59)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	7668 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 1.2	EDS
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	3 of 154003 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21680	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.12	2/852 (0.2%)	1.03	1/1156 (0.1%)
1	C	1.06	1/852 (0.1%)	1.07	5/1156 (0.4%)
1	E	1.09	2/852 (0.2%)	1.06	3/1156 (0.3%)
1	G	1.16	1/852 (0.1%)	1.03	2/1156 (0.2%)
1	I	1.10	0/852	1.02	2/1156 (0.2%)
1	K	1.09	0/852	0.97	0/1156
1	M	1.12	0/852	1.02	1/1156 (0.1%)
1	O	1.14	1/852 (0.1%)	1.12	5/1156 (0.4%)
2	B	1.18	4/1894 (0.2%)	1.03	6/2551 (0.2%)
2	D	1.20	5/1894 (0.3%)	1.02	6/2551 (0.2%)
2	F	1.18	4/1894 (0.2%)	1.03	6/2551 (0.2%)
2	H	1.19	3/1894 (0.2%)	1.02	2/2551 (0.1%)
2	J	1.20	4/1894 (0.2%)	1.06	6/2551 (0.2%)
2	L	1.24	5/1904 (0.3%)	1.12	6/2566 (0.2%)
2	N	1.23	5/1904 (0.3%)	1.07	8/2566 (0.3%)
2	P	1.20	0/1904	1.03	8/2566 (0.3%)
All	All	1.17	37/21998 (0.2%)	1.05	67/29701 (0.2%)

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 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	71	GLU	CG-CD	8.35	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	198	LYS	CD-CE	8.18	1.71	1.51
2	L	68	GLU	CG-CD	8.09	1.64	1.51
2	F	68	GLU	CG-CD	7.74	1.63	1.51
2	D	71	GLU	CG-CD	7.22	1.62	1.51

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	44	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	C	44	ARG	NE-CZ-NH1	8.49	124.54	120.30
2	D	67	LEU	CA-CB-CG	-8.37	96.04	115.30
2	P	138	LEU	CB-CG-CD1	-8.04	97.34	111.00
2	J	138	LEU	CB-CG-CD2	-7.94	97.50	111.00

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

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	15	0
1	G	833	0	792	14	0
1	I	833	0	792	16	0
1	K	833	0	792	21	0
1	M	833	0	792	34	0
1	O	833	0	792	18	0
2	B	1851	0	1821	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1851	0	1821	28	0
2	F	1851	0	1821	35	0
2	H	1851	0	1821	22	0
2	J	1851	0	1821	28	0
2	L	1860	0	1828	43	0
2	N	1860	0	1828	28	0
2	P	1860	0	1828	23	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	370	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 370 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	1.04
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%)	10	19
1	C	107/112 (96%)	97 (91%)	8 (8%)	2 (2%)	10	19
1	E	107/112 (96%)	103 (96%)	4 (4%)	0	100	100
1	G	107/112 (96%)	99 (92%)	6 (6%)	2 (2%)	10	19
1	I	107/112 (96%)	103 (96%)	4 (4%)	0	100	100
1	K	107/112 (96%)	97 (91%)	8 (8%)	2 (2%)	10	19
1	M	107/112 (96%)	97 (91%)	8 (8%)	2 (2%)	10	19
1	O	107/112 (96%)	103 (96%)	4 (4%)	0	100	100
2	B	221/234 (94%)	211 (96%)	9 (4%)	1 (0%)	34	60
2	D	221/234 (94%)	210 (95%)	10 (4%)	1 (0%)	34	60
2	F	221/234 (94%)	211 (96%)	8 (4%)	2 (1%)	21	42
2	H	221/234 (94%)	211 (96%)	10 (4%)	0	100	100
2	J	221/234 (94%)	207 (94%)	13 (6%)	1 (0%)	34	60
2	L	224/234 (96%)	207 (92%)	16 (7%)	1 (0%)	39	65
2	N	224/234 (96%)	209 (93%)	12 (5%)	3 (1%)	15	30
2	P	224/234 (96%)	210 (94%)	9 (4%)	5 (2%)	8	15
All	All	2633/2768 (95%)	2475 (94%)	134 (5%)	24 (1%)	21	42

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%)	79 (88%)	11 (12%)	6	11
1	C	90/91 (99%)	77 (86%)	13 (14%)	4	7
1	E	90/91 (99%)	81 (90%)	9 (10%)	9	18
1	G	90/91 (99%)	78 (87%)	12 (13%)	5	8
1	I	90/91 (99%)	80 (89%)	10 (11%)	8	13
1	K	90/91 (99%)	76 (84%)	14 (16%)	3	5
1	M	90/91 (99%)	79 (88%)	11 (12%)	6	11
1	O	90/91 (99%)	80 (89%)	10 (11%)	8	13
2	B	209/216 (97%)	196 (94%)	13 (6%)	23	45
2	D	209/216 (97%)	200 (96%)	9 (4%)	35	64
2	F	209/216 (97%)	191 (91%)	18 (9%)	13	25
2	H	209/216 (97%)	192 (92%)	17 (8%)	15	28
2	J	209/216 (97%)	195 (93%)	14 (7%)	20	40
2	L	210/216 (97%)	192 (91%)	18 (9%)	13	25
2	N	210/216 (97%)	191 (91%)	19 (9%)	12	23
2	P	210/216 (97%)	194 (92%)	16 (8%)	16	32
All	All	2395/2456 (98%)	2181 (91%)	214 (9%)	12	23

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	125	LEU
2	J	113	LEU
1	O	110	LEU
2	H	141	THR
1	I	55	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	233	HIS
2	J	233	HIS
2	P	11	ASN
1	I	24	GLN
2	J	11	ASN

### 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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	109/112 (97%)	-0.35	1 (0%) 85 83	23, 39, 56, 64	0
1	C	109/112 (97%)	-0.26	1 (0%) 85 83	27, 42, 63, 71	0
1	E	109/112 (97%)	-0.26	1 (0%) 85 83	27, 43, 62, 69	0
1	G	109/112 (97%)	-0.34	1 (0%) 85 83	23, 39, 54, 64	0
1	I	109/112 (97%)	-0.38	1 (0%) 85 83	19, 34, 51, 58	0
1	K	109/112 (97%)	-0.13	1 (0%) 85 83	25, 50, 71, 78	0
1	M	109/112 (97%)	-0.05	1 (0%) 85 83	24, 51, 71, 79	0
1	O	109/112 (97%)	-0.36	1 (0%) 85 83	22, 35, 51, 58	0
2	B	227/234 (97%)	-0.41	0 100 100	17, 28, 59, 79	3 (1%)
2	D	227/234 (97%)	-0.46	1 (0%) 93 91	18, 29, 57, 77	3 (1%)
2	F	227/234 (97%)	-0.41	1 (0%) 93 91	17, 29, 57, 81	3 (1%)
2	H	227/234 (97%)	-0.39	2 (0%) 85 83	16, 28, 56, 80	3 (1%)
2	J	227/234 (97%)	-0.43	1 (0%) 93 91	15, 28, 51, 81	3 (1%)
2	L	228/234 (97%)	-0.44	1 (0%) 93 91	15, 27, 52, 74	3 (1%)
2	N	228/234 (97%)	-0.45	2 (0%) 85 83	16, 27, 52, 81	3 (1%)
2	P	228/234 (97%)	-0.44	0 100 100	15, 27, 52, 79	3 (1%)
All	All	2691/2768 (97%)	-0.38	16 (0%) 90 88	15, 32, 62, 81	24 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	7.0
1	C	2	ALA	5.8
1	G	2	ALA	5.7
1	M	2	ALA	5.6
1	O	2	ALA	3.6

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.