



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:57 AM GMT

PDB ID : 2VAK
Title : CRYSTAL STRUCTURE OF THE AVIAN REOVIRUS INNER CAPSID
PROTEIN SIGMAA
Authors : Guardado-Calvo, P.; Llamas-Saiz, A.L.; Fox, G.C.; Hermo-Parrado, X.L.;
Vazquez-Iglesias, L.; Martinez-Costas, J.; Benavente, J.; Van Raaij, M.J.
Deposited on : 2007-09-01
Resolution : 2.34 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
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

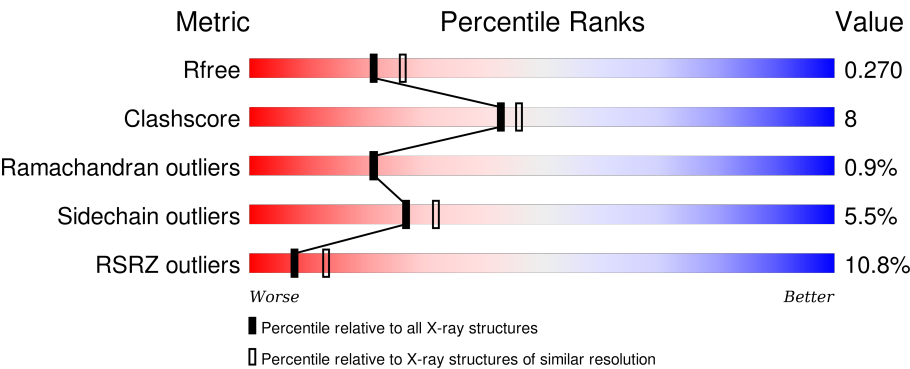
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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.

Mol	Chain	Length	Quality of chain
1	A	423	<div><div>9%</div><div>82%</div><div>13%</div><div>• •</div></div>
1	B	423	<div><div>17%</div><div>75%</div><div>18%</div><div>• •</div></div>
1	C	423	<div><div>13%</div><div>76%</div><div>18%</div><div>• •</div></div>
1	D	423	<div><div>28%</div><div>74%</div><div>20%</div><div>• •</div></div>
1	E	423	<div><div>12%</div><div>79%</div><div>16%</div><div>• •</div></div>

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Mol	Chain	Length	Quality of chain
1	F	423	
1	G	423	
1	H	423	
1	I	423	
1	J	423	
1	K	423	
1	L	423	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	1427	-	-	-	X
2	SO4	F	1427	-	-	-	X
2	SO4	H	1427	-	-	X	-
2	SO4	J	1427	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41224 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 SIGMA A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3198	2023	559	598	18			
1	B	409	Total	C	N	O	S	0	0	0
			3190	2017	558	597	18			
1	C	404	Total	C	N	O	S	0	0	0
			3154	1995	553	588	18			
1	D	409	Total	C	N	O	S	0	0	0
			3190	2017	558	597	18			
1	E	409	Total	C	N	O	S	0	0	0
			3190	2017	558	597	18			
1	F	404	Total	C	N	O	S	0	0	0
			3154	1995	553	588	18			
1	G	403	Total	C	N	O	S	0	0	0
			3147	1991	552	586	18			
1	H	409	Total	C	N	O	S	0	0	0
			3190	2017	558	597	18			
1	I	410	Total	C	N	O	S	0	0	0
			3198	2023	559	598	18			
1	J	404	Total	C	N	O	S	0	0	0
			3154	1995	553	588	18			
1	K	410	Total	C	N	O	S	0	0	0
			3198	2023	559	598	18			
1	L	410	Total	C	N	O	S	0	0	0
			3198	2023	559	598	18			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

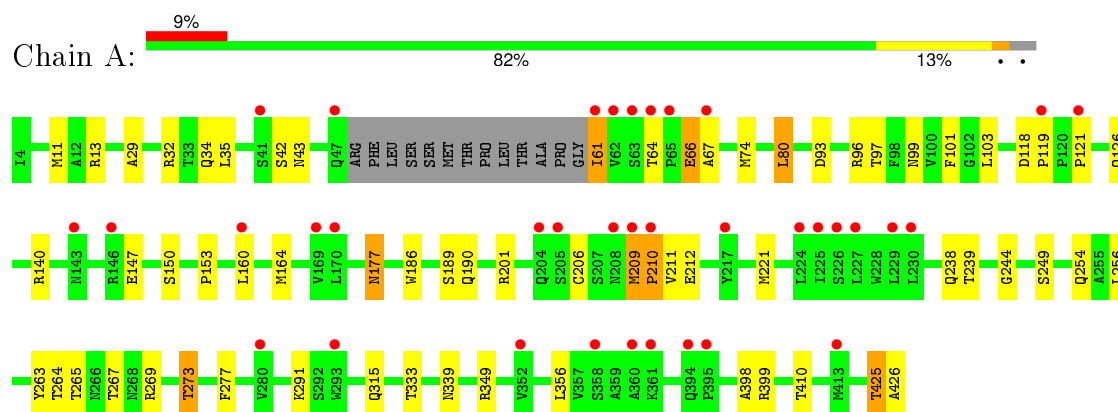
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	262	Total 262	O 262	0	0
3	B	180	Total 180	O 180	0	0
3	C	186	Total 186	O 186	0	0
3	D	160	Total 160	O 160	0	0
3	E	223	Total 223	O 223	0	0
3	F	314	Total 314	O 314	0	0
3	G	305	Total 305	O 305	0	0
3	H	272	Total 272	O 272	0	0
3	I	226	Total 226	O 226	0	0
3	J	247	Total 247	O 247	0	0
3	K	301	Total 301	O 301	0	0
3	L	327	Total 327	O 327	0	0

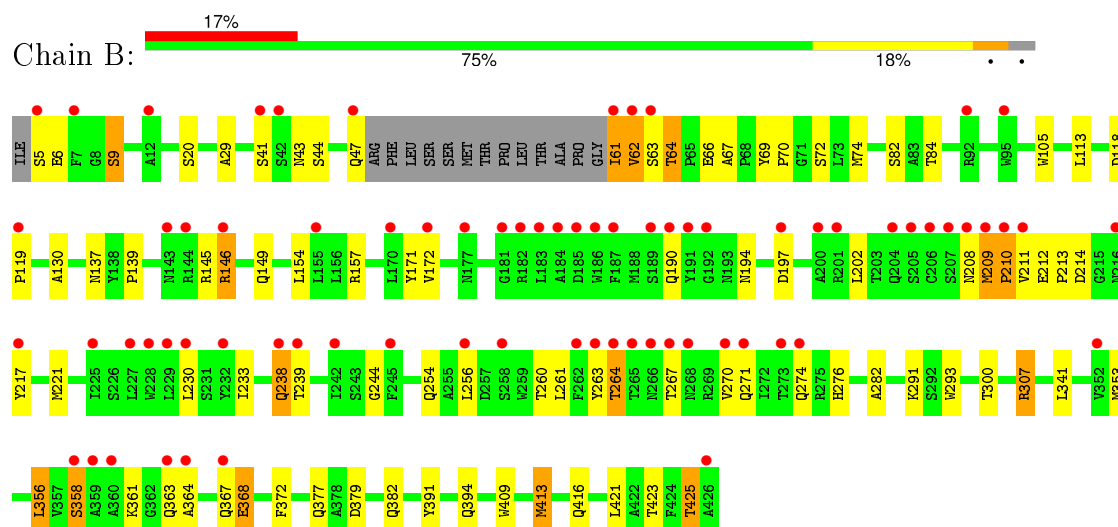
3 Residue-property plots

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

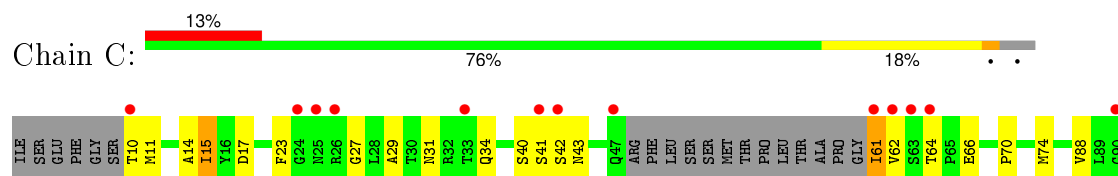
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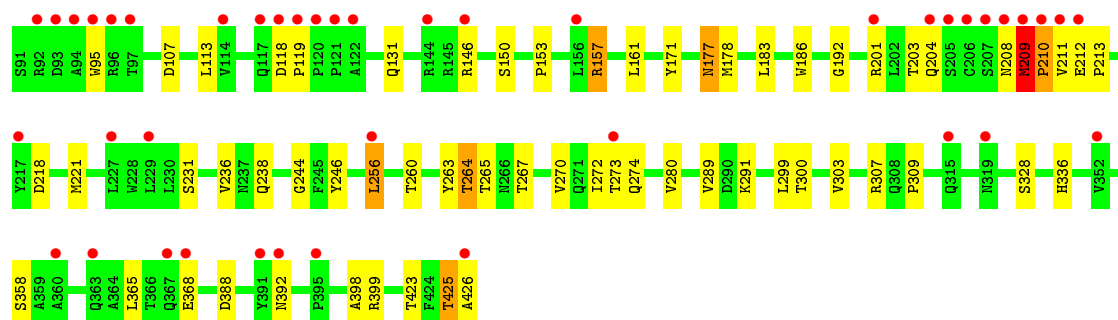


• Molecule 1: SIGMA A

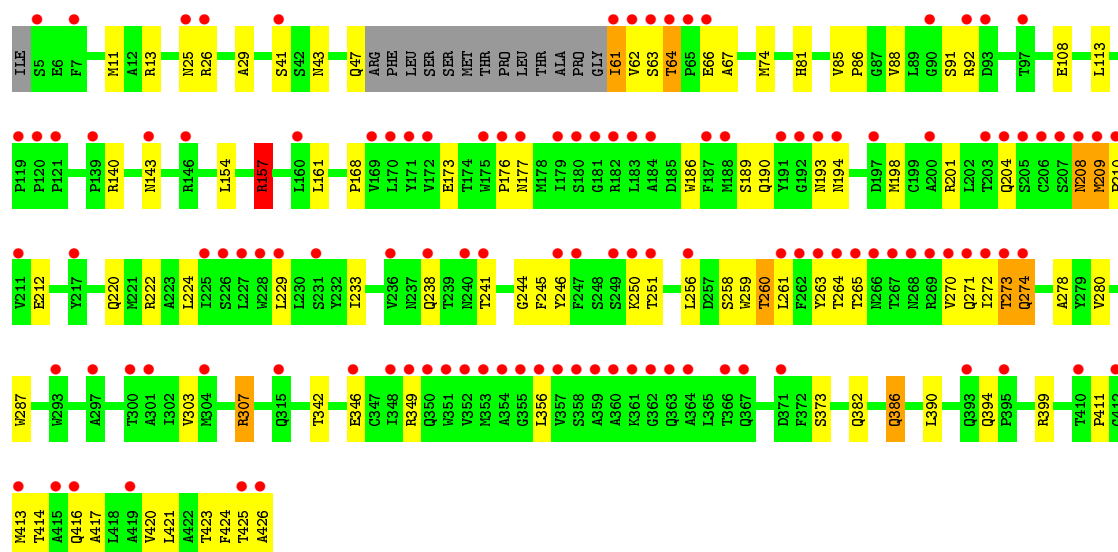
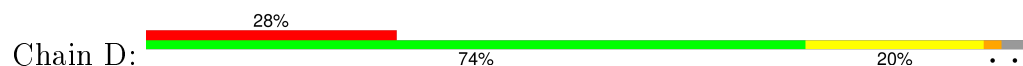


• Molecule 1: SIGMA A

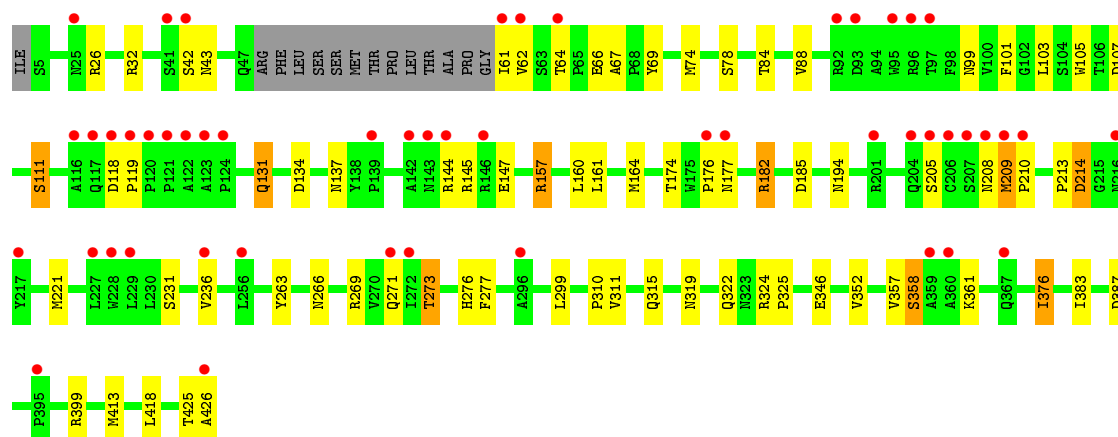
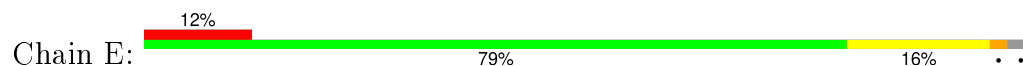




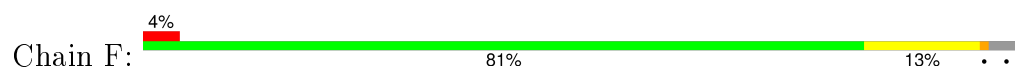
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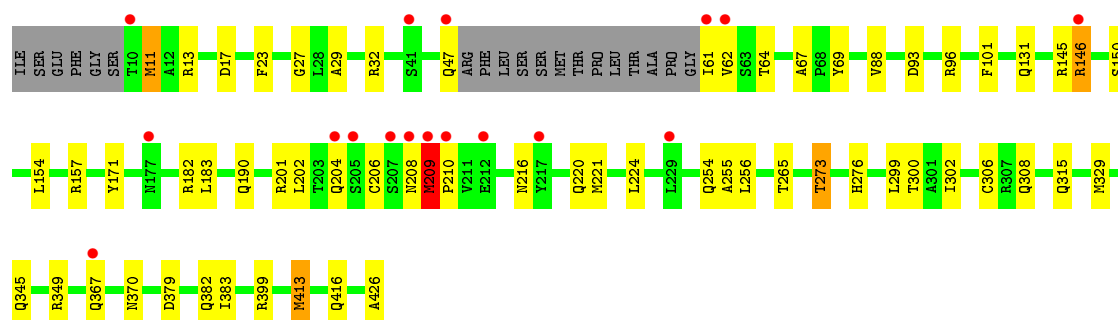


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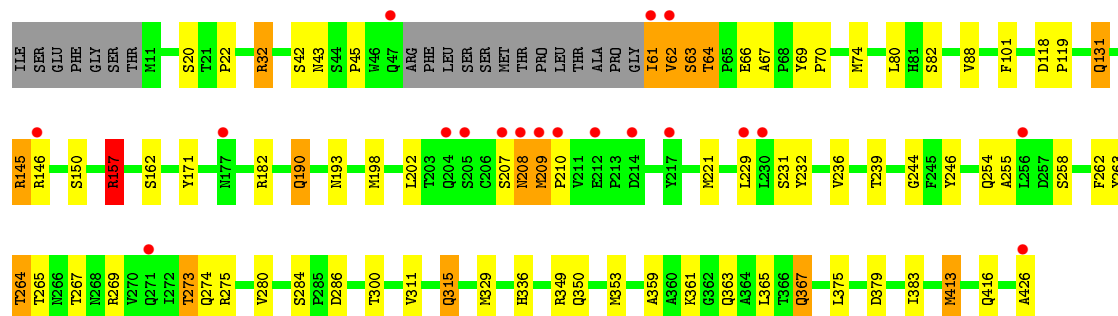
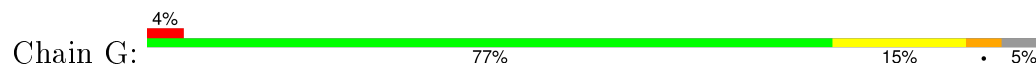


• Molecule 1: SIGMA A

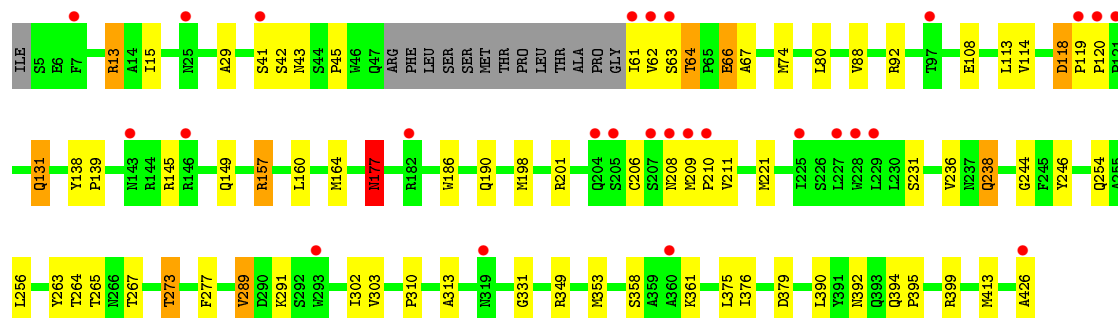
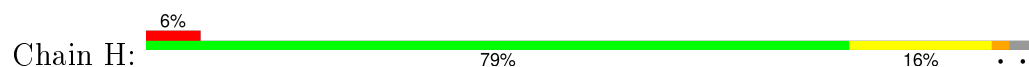




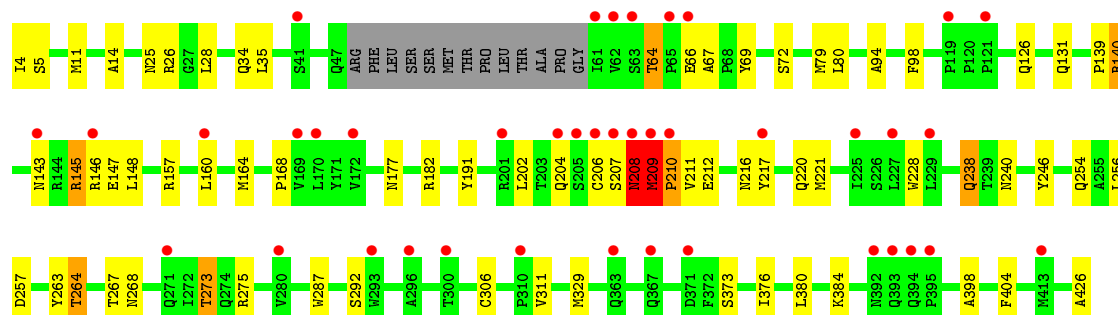
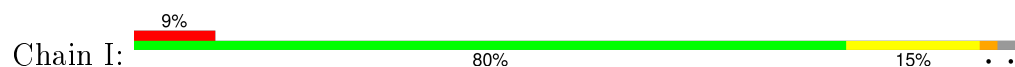
• Molecule 1: SIGMA A



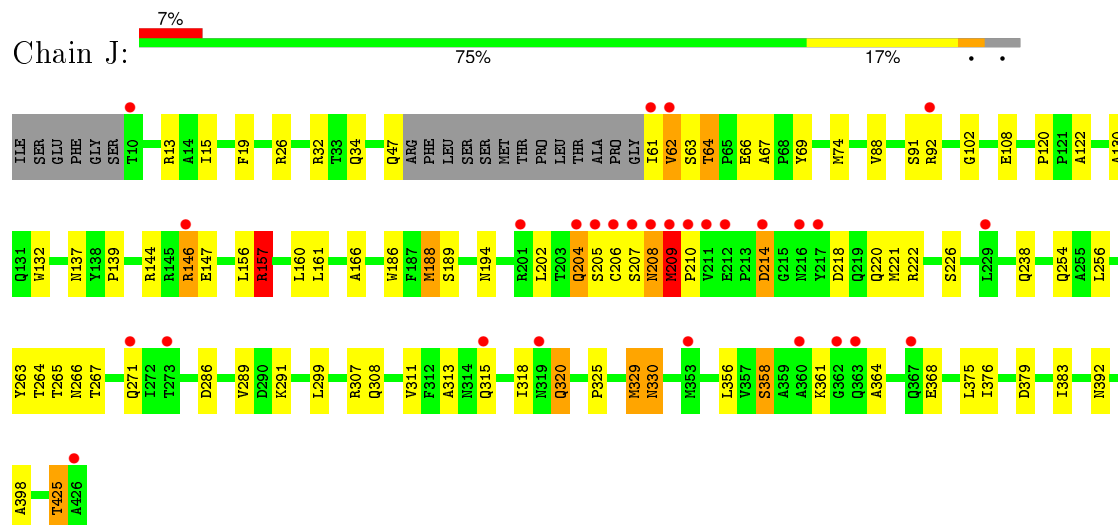
• Molecule 1: SIGMA A



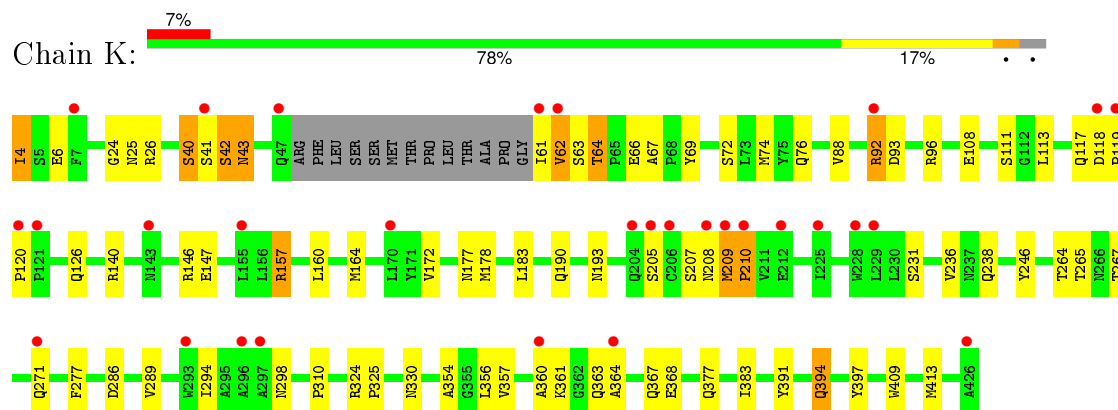
• Molecule 1: SIGMA A



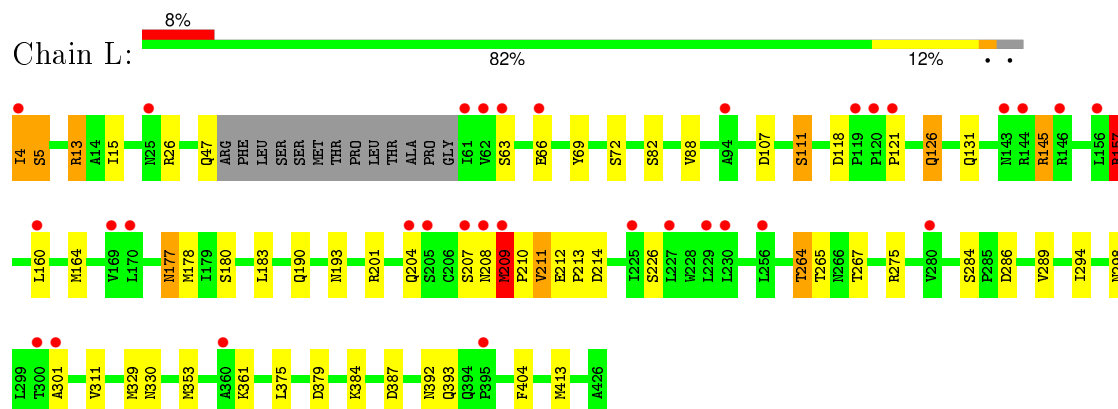
- Molecule 1: SIGMA A



- Molecule 1: SIGMA A



- Molecule 1: SIGMA A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.21Å 129.91Å 144.04Å 93.81° 105.05° 98.16°	Depositor
Resolution (Å)	29.85 – 2.34 29.85 – 2.34	Depositor EDS
% Data completeness (in resolution range)	94.4 (29.85-2.34) 92.3 (29.85-2.34)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.3.0027	Depositor
R, R_{free}	0.210 , 0.271 0.211 , 0.270	Depositor DCC
R_{free} test set	1383 reflections (0.49%)	DCC
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 61.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	0 of 282059 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41224	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 44.61 % 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 1.4877e-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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.69	0/3282	0.65	0/4478
1	B	0.62	0/3274	0.62	0/4467
1	C	0.64	0/3237	0.63	0/4418
1	D	0.63	0/3274	0.64	2/4467 (0.0%)
1	E	0.67	0/3274	0.66	0/4467
1	F	0.73	0/3237	0.70	0/4418
1	G	0.76	0/3230	0.72	3/4408 (0.1%)
1	H	0.71	0/3274	0.69	1/4467 (0.0%)
1	I	0.68	0/3282	0.65	1/4478 (0.0%)
1	J	0.67	0/3237	0.67	2/4418 (0.0%)
1	K	0.69	0/3282	0.69	1/4478 (0.0%)
1	L	0.79	0/3282	0.72	2/4478 (0.0%)
All	All	0.69	0/39165	0.67	12/53442 (0.0%)

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	1
1	D	0	3
1	E	0	1
1	F	0	1
1	G	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	2
All	All	0	12

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	J	157	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	J	157	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	D	157	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	G	157	ARG	NE-CZ-NH1	5.58	123.09	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	209	MET	Peptide
1	D	208	ASN	Peptide
1	D	209	MET	Peptide
1	D	61	ILE	Peptide
1	E	209	MET	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	3198	0	3093	34	0
1	B	3190	0	3082	61	0
1	C	3154	0	3054	64	0
1	D	3190	0	3082	54	0
1	E	3190	0	3082	44	0
1	F	3154	0	3054	37	0
1	G	3147	0	3047	53	0
1	H	3190	0	3082	65	0
1	I	3198	0	3093	57	0
1	J	3154	0	3054	69	0
1	K	3198	0	3093	59	0
1	L	3198	0	3093	34	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
2	G	5	0	0	1	0
2	H	5	0	0	2	0
2	I	5	0	0	0	0
2	J	5	0	0	3	0
2	K	5	0	0	0	0
2	L	5	0	0	1	0
3	A	262	0	0	3	0
3	B	180	0	0	6	0
3	C	186	0	0	10	0
3	D	160	0	0	5	0
3	E	223	0	0	7	0
3	F	314	0	0	5	0
3	G	305	0	0	7	0
3	H	272	0	0	4	0
3	I	226	0	0	4	0
3	J	247	0	0	9	0
3	K	301	0	0	15	0
3	L	327	0	0	10	0
All	All	41224	0	36909	614	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 8.

The worst 5 of 614 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:H:264:THR:HG21	1:H:267:THR:OG1	1.50	1.10
1:K:157:ARG:HG2	1:K:157:ARG:HH11	1.11	1.07
1:G:157:ARG:HG2	1:G:157:ARG:HH11	1.19	1.07
1:B:64:THR:HG22	1:B:67:ALA:H	1.20	1.07
1:I:140:ARG:HH11	1:I:140:ARG:HG2	1.06	1.06

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	406/423 (96%)	392 (97%)	12 (3%)	2 (0%)	34	37
1	B	405/423 (96%)	376 (93%)	26 (6%)	3 (1%)	26	28
1	C	400/423 (95%)	379 (95%)	17 (4%)	4 (1%)	19	18
1	D	405/423 (96%)	376 (93%)	21 (5%)	8 (2%)	9	6
1	E	405/423 (96%)	382 (94%)	19 (5%)	4 (1%)	19	18
1	F	400/423 (95%)	385 (96%)	13 (3%)	2 (0%)	34	37
1	G	399/423 (94%)	383 (96%)	13 (3%)	3 (1%)	24	25
1	H	405/423 (96%)	386 (95%)	17 (4%)	2 (0%)	34	37
1	I	406/423 (96%)	385 (95%)	18 (4%)	3 (1%)	26	28
1	J	400/423 (95%)	376 (94%)	18 (4%)	6 (2%)	13	10
1	K	406/423 (96%)	385 (95%)	16 (4%)	5 (1%)	16	14
1	L	406/423 (96%)	389 (96%)	13 (3%)	4 (1%)	19	18
All	All	4843/5076 (95%)	4594 (95%)	203 (4%)	46 (1%)	21	21

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	PRO
1	C	210	PRO
1	D	210	PRO
1	E	214	ASP
1	I	208	ASN

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	340/352 (97%)	323 (95%)	17 (5%)	30	37
1	B	339/352 (96%)	317 (94%)	22 (6%)	21	24
1	C	335/352 (95%)	320 (96%)	15 (4%)	34	42
1	D	339/352 (96%)	317 (94%)	22 (6%)	21	24
1	E	339/352 (96%)	323 (95%)	16 (5%)	32	40
1	F	335/352 (95%)	316 (94%)	19 (6%)	25	30
1	G	334/352 (95%)	312 (93%)	22 (7%)	21	23
1	H	339/352 (96%)	321 (95%)	18 (5%)	28	34
1	I	340/352 (97%)	326 (96%)	14 (4%)	37	47
1	J	335/352 (95%)	316 (94%)	19 (6%)	25	30
1	K	340/352 (97%)	325 (96%)	15 (4%)	35	44
1	L	340/352 (97%)	317 (93%)	23 (7%)	20	22
All	All	4055/4224 (96%)	3833 (94%)	222 (6%)	27	32

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	150	SER
1	G	239	THR
1	L	111	SER
1	F	182	ARG
1	G	61	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	25	ASN
1	G	131	GLN
1	K	43	ASN
1	F	276	HIS
1	F	336	HIS

5.3.3 RNA ⓘ

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](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1427	-	4,4,4	0.33	0	6,6,6	0.23	0
2	SO4	B	1427	-	4,4,4	0.41	0	6,6,6	0.20	0
2	SO4	C	1427	-	4,4,4	0.26	0	6,6,6	0.26	0
2	SO4	D	1427	-	4,4,4	0.32	0	6,6,6	0.38	0
2	SO4	E	1427	-	4,4,4	0.56	0	6,6,6	0.17	0
2	SO4	F	1427	-	4,4,4	0.31	0	6,6,6	0.41	0
2	SO4	G	1427	-	4,4,4	0.28	0	6,6,6	0.21	0
2	SO4	H	1427	-	4,4,4	0.43	0	6,6,6	0.25	0
2	SO4	I	1427	-	4,4,4	0.30	0	6,6,6	0.37	0
2	SO4	J	1427	-	4,4,4	0.24	0	6,6,6	0.35	0
2	SO4	K	1427	-	4,4,4	0.47	0	6,6,6	0.38	0
2	SO4	L	1427	-	4,4,4	0.41	0	6,6,6	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1427	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	D	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	I	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	J	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	K	1427	-	-	0/0/0/0	0/0/0/0
2	SO4	L	1427	-	-	0/0/0/0	0/0/0/0

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.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1427	SO4	1	0
2	F	1427	SO4	1	0
2	G	1427	SO4	1	0
2	H	1427	SO4	2	0
2	J	1427	SO4	3	0
2	L	1427	SO4	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	410/423 (96%)	0.39	36 (8%) 12 19	18, 31, 52, 72	0
1	B	409/423 (96%)	0.99	74 (18%) 2 3	21, 46, 89, 102	0
1	C	404/423 (95%)	0.77	55 (13%) 4 8	25, 41, 68, 90	0
1	D	409/423 (96%)	1.21	120 (29%) 1 1	22, 47, 88, 96	0
1	E	409/423 (96%)	0.63	50 (12%) 5 9	19, 38, 66, 84	0
1	F	404/423 (95%)	0.21	17 (4%) 40 52	14, 27, 50, 81	0
1	G	403/423 (95%)	0.23	19 (4%) 35 48	12, 26, 47, 84	0
1	H	409/423 (96%)	0.36	27 (6%) 22 32	15, 30, 51, 77	0
1	I	410/423 (96%)	0.46	40 (9%) 10 16	20, 35, 55, 81	0
1	J	404/423 (95%)	0.32	29 (7%) 18 27	20, 34, 58, 90	0
1	K	410/423 (96%)	0.27	30 (7%) 18 27	15, 30, 54, 76	0
1	L	410/423 (96%)	0.32	32 (7%) 16 24	14, 27, 49, 68	0
All	All	4891/5076 (96%)	0.51	529 (10%) 8 13	12, 34, 70, 102	0

The worst 5 of 529 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	205	SER	10.6
1	B	205	SER	10.2
1	C	119	PRO	9.6
1	D	208	ASN	9.3
1	B	61	ILE	8.9

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	C	1427	5/5	0.95	0.37	2.93	85,85,85,86	0
2	SO4	F	1427	5/5	0.95	0.23	2.48	63,63,66,66	0
2	SO4	D	1427	5/5	0.94	0.26	1.51	63,66,67,68	0
2	SO4	L	1427	5/5	0.99	0.17	0.93	46,47,48,48	0
2	SO4	B	1427	5/5	0.97	0.21	0.86	63,63,64,65	0
2	SO4	J	1427	5/5	0.95	0.24	0.84	74,75,75,76	0
2	SO4	E	1427	5/5	0.99	0.18	0.75	49,50,51,52	0
2	SO4	K	1427	5/5	0.98	0.20	0.72	49,49,51,52	0
2	SO4	G	1427	5/5	0.97	0.15	0.60	67,67,68,68	0
2	SO4	A	1427	5/5	0.99	0.15	0.35	48,49,49,50	0
2	SO4	I	1427	5/5	0.97	0.17	0.19	55,56,57,58	0
2	SO4	H	1427	5/5	0.99	0.14	0.05	42,44,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.