

# Full wwPDB X-ray Structure Validation Report (i)

### Oct 30, 2023 - 07:20 PM JST

PDB ID	:	4Y4Y
Title	:	T=1 capsid structure of SeMV Ndel65CP fused with B-domain of S. aureus
		protein SpA at the N-terminus (C2 crystal form)
Authors	:	Gulati, A.; Murthy, M.R.N.
Deposited on	:	2015-02-11
Resolution	:	3.00  Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	282	67%	•	32%
1	В	282	67%	•	32%
1	С	282	68%		32%
1	D	282	67%	•	32%
1	Е	282	67%	•	32%
1	F	282	67%	•	32%
1	G	282	67%	•	32%



Mol	Chain	Length	Quality of chain	
1	Н	282	68%	32%
1	Ι	282	67%	32%
1	J	282	67%	32%
1	K	282	67%	32%
1	L	282	67%	32%
1	M	282	66%	32%
1	N	202	670	220/
	11	202	67%	32%
1	0	282	67%	32%
1	Р	282	68%	32%
1	Q	282	67%	32%
1	R	282	67%	32%
1	S	282	67%	32%
1	Т	282	% 67%	32%
1	I	282	670/	270/
		202	0770	JZ /0
1	V	282	67% •	32%
1	W	282	68%	32%
1	Х	282	67%	32%
1	Y	282	67%	32%
1	Z	282	67%	32%
1	a	282	68%	32%
1	b	282	67%	32%
1	с	282	66%	32%
1		000		
	a	282	67%	32%



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 42805 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	101	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	11	151	1413	901	228	276	8	0	0	0
1	В	101	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	D	151	1416	902	229	277	8	0	0	0
1	C	101	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	U	151	1416	902	229	277	8	0	0	0
1	П	191	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
		151	1418	903	229	278	8	0	0	0
1	E	191	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
		151	1399	892	227	272	8	0	0	0
1	F	101	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
1	1	151	1376	877	224	267	8	0	0	0
1	G	101	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	ŭ	151	1418	903	229	278	8	0	0	0
1	н	101	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
1	11	151	1409	898	228	275	8	0	0	0
1	т	101	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
	L	131	1418	903	229	278	8	0	0	0
1	Т	101	Total	С	Ν	0	$\mathbf{S}$	0	0	0
1	0	151	1416	902	229	277	8	0	0	0
1	K	101	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	11	151	1416	902	228	278	8	0	0	0
1	T.	101	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1		151	1416	902	229	277	8	0	0	0
1	М	101	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
	111	151	1417	902	229	278	8	0	0	0
1	N	101	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	11	151	1414	902	228	276	8	0	0	0
1	0	101	Total	$\mathbf{C}$	Ν	Ο	S		0	0
		131	1416	902	229	277	8			0
1	Р	101	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	1	131	1416	902	229	277	8			U

• Molecule 1 is a protein called Immunoglobulin G-binding protein A,Coat protein.



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	0	101	Total	С	Ν	0	S	0	0	0
	Q	191	1378	879	227	264	8	0	0	0
1	D	101	Total	С	Ν	0	S	0	0	0
	n	191	1406	895	228	275	8	0	0	0
1	C	101	Total	С	Ν	0	S	0	0	0
	G	191	1405	894	228	275	8	0	0	0
1	Т	101	Total	С	Ν	0	S	0	0	0
1	1	191	1415	902	229	276	8	0	0	0
1	TT	101	Total	С	Ν	0	S	0	0	0
1	U	191	1412	900	228	276	8	0	0	0
1	V	101	Total	С	Ν	0	S	0	0	0
1	v	191	1416	902	229	277	8	0	0	0
1	W	101	Total	С	Ν	0	S	0	0	0
	vv	191	1416	902	229	277	8	0	0	0
1	v	101	Total	С	Ν	0	S	0	0	0
1	Λ	191	1414	900	229	277	8	0	0	0
1	v	101	Total	С	Ν	0	S	0	0	0
1	1	191	1411	900	228	275	8	0	0	0
1	7	101	Total	С	Ν	0	S	0	0	0
1		191	1411	900	228	275	8	0	0	0
1	0	101	Total	С	Ν	0	S	0	0	0
1	a	191	1413	901	229	275	8	0	0	0
1	h	101	Total	С	Ν	0	S	0	0	0
	D	191	1416	902	229	277	8	0	0	0
1	0	101	Total	С	Ν	0	S	0	0	0
	U	191	1418	903	229	278	8	0	U	0
1	d	101	Total	С	Ν	0	S	0	0	0
	u	191	1415	902	229	276	8			U

There are 750 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-13	MET	-	expression tag	UNP P02976
А	-12	ARG	-	expression tag	UNP P02976
A	-11	GLY	-	expression tag	UNP P02976
А	-10	SER	-	expression tag	UNP P02976
А	-9	HIS	-	expression tag	UNP P02976
А	-8	HIS	-	expression tag	UNP P02976
А	-7	HIS	-	expression tag	UNP P02976
А	-6	HIS	-	expression tag	UNP P02976
А	-5	HIS	-	expression tag	UNP P02976
А	-4	HIS	-	expression tag	UNP P02976
А	-3	GLY	-	expression tag	UNP P02976



pression tag	0111 1 02010
pression tag	UNP P02976
linker	UNP P02976

Chain	Residue	Modelled	Actual	Comment	Reference
А	-2	MET	-	expression tag	UNP P02976
А	-1	ALA	-	expression tag	UNP P02976
А	0	SER	-	expression tag	UNP P02976
А	1	MET	-	expression tag	UNP P02976
А	2	ASP	-	expression tag	UNP P02976
А	3	ASN	-	expression tag	UNP P02976
А	4	LYS	_	expression tag	UNP P02976
А	59	GLU	-	linker	UNP P02976
А	60	GLY	-	linker	UNP P02976
А	61	SER	-	linker	UNP P02976
А	62	GLU	-	linker	UNP P02976
А	63	LEU	-	linker	UNP P02976
А	64	GLU	-	linker	UNP P02976
А	65	MET	-	linker	UNP P02976
В	-13	MET	-	expression tag	UNP P02976
В	-12	ARG	-	expression tag	UNP P02976
В	-11	GLY	-	expression tag	UNP P02976
В	-10	SER	-	expression tag	UNP P02976
В	-9	HIS	_	expression tag	UNP P02976
В	-8	HIS	-	expression tag	UNP P02976
В	-7	HIS	-	expression tag	UNP P02976
В	-6	HIS	-	expression tag	UNP P02976
В	-5	HIS	-	expression tag	UNP P02976
В	-4	HIS	-	expression tag	UNP P02976
В	-3	GLY	-	expression tag	UNP P02976
В	-2	MET	-	expression tag	UNP P02976
В	-1	ALA	-	expression tag	UNP P02976
В	0	SER	-	expression tag	UNP P02976
В	1	MET	-	expression tag	UNP P02976
В	2	ASP	-	expression tag	UNP P02976
В	3	ASN	-	expression tag	UNP P02976
В	4	LYS	-	expression tag	UNP P02976
В	59	GLU	-	linker	UNP P02976
В	60	GLY	-	linker	UNP P02976
В	61	SER	-	linker	UNP P02976
В	62	GLU	-	linker	UNP P02976
В	63	LEU	-	linker	UNP P02976
В	64	GLU	-	linker	UNP P02976
В	65	MET	-	linker	UNP P02976
С	-13	MET	-	expression tag	UNP P02976
С	-12	ARG	-	expression tag	UNP P02976
С	-11	GLY	-	expression tag	UNP P02976



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Chain	Residue	Modelled	Actual	Comment	Reference
С	-10	SER	-	expression tag	UNP P02976
С	-9	HIS	-	expression tag	UNP P02976
С	-8	HIS	-	expression tag	UNP P02976
С	-7	HIS	-	expression tag	UNP P02976
С	-6	HIS	-	expression tag	UNP P02976
С	-5	HIS	-	expression tag	UNP P02976
С	-4	HIS	-	expression tag	UNP P02976
С	-3	GLY	-	expression tag	UNP P02976
С	-2	MET	-	expression tag	UNP P02976
С	-1	ALA	-	expression tag	UNP P02976
С	0	SER	-	expression tag	UNP P02976
С	1	MET	-	expression tag	UNP P02976
С	2	ASP	-	expression tag	UNP P02976
С	3	ASN	-	expression tag	UNP P02976
С	4	LYS	-	expression tag	UNP P02976
С	59	GLU	-	linker	UNP P02976
С	60	GLY	-	linker	UNP P02976
С	61	SER	-	linker	UNP P02976
С	62	GLU	-	linker	UNP P02976
С	63	LEU	-	linker	UNP P02976
С	64	GLU	-	linker	UNP P02976
С	65	MET	-	linker	UNP P02976
D	-13	MET	-	expression tag	UNP P02976
D	-12	ARG	-	expression tag	UNP P02976
D	-11	GLY	-	expression tag	UNP P02976
D	-10	SER	-	expression tag	UNP P02976
D	-9	HIS	-	expression tag	UNP P02976
D	-8	HIS	-	expression tag	UNP P02976
D	-7	HIS	-	expression tag	UNP P02976
D	-6	HIS	-	expression tag	UNP P02976
D	-5	HIS	-	expression tag	UNP P02976
D	-4	HIS	-	expression tag	UNP P02976
D	-3	GLY	-	expression tag	UNP P02976
D	-2	MET	-	expression tag	UNP P02976
D	-1	ALA	-	expression tag	UNP P02976
D	0	SER	-	expression tag	UNP P02976
D	1	MET	-	expression tag	UNP P02976
D	2	ASP	-	expression tag	UNP P02976
D	3	ASN	-	expression tag	UNP P02976
D	4	LYS	-	expression tag	UNP P02976
D	59	GLU	-	linker	UNP P02976
D	60	GLY	-	linker	UNP P02976
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Chain	Residue	Modelled	Actual	Comment	Reference	
D	61	SER	-	linker	UNP P02976	
D	62	GLU	-	linker	UNP P02976	
D	63	LEU	-	linker	UNP P02976	
D	64	GLU	-	linker	UNP P02976	
D	65	MET	-	linker	UNP P02976	
Е	-13	MET	-	expression tag	UNP P02976	
Е	-12	ARG	-	expression tag	UNP P02976	
Е	-11	GLY	-	expression tag	UNP P02976	
Е	-10	SER	-	expression tag	UNP P02976	
Е	-9	HIS	-	expression tag	UNP P02976	
Е	-8	HIS	-	expression tag	UNP P02976	
Е	-7	HIS	-	expression tag	UNP P02976	
Е	-6	HIS	-	expression tag	UNP P02976	
Е	-5	HIS	-	expression tag	UNP P02976	
Е	-4	HIS	-	expression tag	UNP P02976	
Е	-3	GLY	-	expression tag	UNP P02976	
Е	-2	MET	-	expression tag	UNP P02976	
Е	-1	ALA	-	expression tag	UNP P02976	
Е	0	SER	-	expression tag	UNP P02976	
Е	1	MET	-	expression tag	UNP P02976	
Е	2	ASP	-	expression tag	UNP P02976	
Е	3	ASN	-	expression tag	UNP P02976	
Е	4	LYS	-	expression tag	UNP P02976	
Е	59	GLU	-	linker	UNP P02976	
Е	60	GLY	-	linker	UNP P02976	
Е	61	SER	-	linker	UNP P02976	
Е	62	GLU	-	linker	UNP P02976	
Е	63	LEU	-	linker	UNP P02976	
Е	64	GLU	-	linker	UNP P02976	
Е	65	MET	-	linker	UNP P02976	
F	-13	MET	-	expression tag	UNP P02976	
F	-12	ARG	-	expression tag	UNP P02976	
F	-11	GLY	-	expression tag	UNP P02976	
F	-10	SER	-	expression tag	UNP P02976	
F	-9	HIS	-	expression tag	UNP P02976	
F	-8	HIS	-	expression tag	UNP P02976	
F	-7	HIS	-	expression tag	UNP P02976	
F	-6	HIS	-	expression tag	UNP P02976	
F	-5	HIS	-	expression tag	UNP P02976	
F	-4	HIS	-	expression tag	UNP P02976	
F	-3	GLY	-	expression tag	UNP P02976	
F	-2	MET	-	expression tag	UNP P02976	

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Comment

Actual

Reference	
UNP P02976	

Continued from previous page... Chain Residue Modelled

- 15						
	F	-1	ALA	-	expression tag	UNP P02976
	F	0	SER	-	expression tag	UNP P02976
	F	1	MET	-	expression tag	UNP P02976
	F	2	ASP	-	expression tag	UNP P02976
	F	3	ASN	-	expression tag	UNP P02976
	F	4	LYS	-	expression tag	UNP P02976
	F	59	GLU	-	linker	UNP P02976
	F	60	GLY	-	linker	UNP P02976
	F	61	SER	-	linker	UNP P02976
	F	62	GLU	-	linker	UNP P02976
	F	63	LEU	-	linker	UNP P02976
	F	64	GLU	-	linker	UNP P02976
	F	65	MET	-	linker	UNP P02976
	G	-13	MET	-	expression tag	UNP P02976
	G	-12	ARG	-	expression tag	UNP P02976
	G	-11	GLY	-	expression tag	UNP P02976
	G	-10	SER	-	expression tag	UNP P02976
	G	-9	HIS	-	expression tag	UNP P02976
	G	-8	HIS	-	expression tag	UNP P02976
	G	-7	HIS	-	expression tag	UNP P02976
	G	-6	HIS	-	expression tag	UNP P02976
	G	-5	HIS	-	expression tag	UNP P02976
	G	-4	HIS	-	expression tag	UNP P02976
	G	-3	GLY	-	expression tag	UNP P02976
	G	-2	MET	-	expression tag	UNP P02976
	G	-1	ALA	-	expression tag	UNP P02976
	G	0	SER	-	expression tag	UNP P02976
	G	1	MET	-	expression tag	UNP P02976
	G	2	ASP	-	expression tag	UNP P02976
	G	3	ASN	-	expression tag	UNP P02976
	G	4	LYS	-	expression tag	UNP P02976
	G	59	GLU	-	linker	UNP P02976
	G	60	GLY	-	linker	UNP P02976
	G	61	SER	-	linker	UNP P02976
	G	62	GLU	-	linker	UNP P02976
	G	63	LEU	-	linker	UNP P02976
	G	64	GLU	-	linker	UNP P02976
	G	65	MET	-	linker	UNP P02976
	Н	-13	MET	-	expression tag	UNP P02976
	Н	-12	ARG	-	expression tag	UNP P02976
	Н	-11	GLY	-	expression tag	UNP P02976
	Н	-10	SER	-	expression tag	UNP P02976
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Chain	Residue	Modelled	Actual	Comment	Reference
Н	-9	HIS	-	expression tag	UNP P02976
Н	-8	HIS	-	expression tag	UNP P02976
Н	-7	HIS	-	expression tag	UNP P02976
Н	-6	HIS	-	expression tag	UNP P02976
Н	-5	HIS	-	expression tag	UNP P02976
Н	-4	HIS	-	expression tag	UNP P02976
Н	-3	GLY	-	expression tag	UNP P02976
Н	-2	MET	-	expression tag	UNP P02976
Н	-1	ALA	-	expression tag	UNP P02976
Н	0	SER	-	expression tag	UNP P02976
Н	1	MET	-	expression tag	UNP P02976
Н	2	ASP	-	expression tag	UNP P02976
Н	3	ASN	-	expression tag	UNP P02976
Н	4	LYS	-	expression tag	UNP P02976
Н	59	GLU	-	linker	UNP P02976
Н	60	GLY	-	linker	UNP P02976
Н	61	SER	-	linker	UNP P02976
Н	62	GLU	-	linker	UNP P02976
Н	63	LEU	-	linker	UNP P02976
Н	64	GLU	-	linker	UNP P02976
Н	65	MET	-	linker	UNP P02976
Ι	-13	MET	-	expression tag	UNP P02976
Ι	-12	ARG	-	expression tag	UNP P02976
Ι	-11	GLY	-	expression tag	UNP P02976
Ι	-10	SER	-	expression tag	UNP P02976
Ι	-9	HIS	-	expression tag	UNP P02976
Ι	-8	HIS	-	expression tag	UNP P02976
Ι	-7	HIS	-	expression tag	UNP P02976
Ι	-6	HIS	-	expression tag	UNP P02976
Ι	-5	HIS	-	expression tag	UNP P02976
Ι	-4	HIS	-	expression tag	UNP P02976
Ι	-3	GLY	-	expression tag	UNP P02976
Ι	-2	MET	-	expression tag	UNP P02976
Ι	-1	ALA	-	expression tag	UNP P02976
Ι	0	SER	-	expression tag	UNP P02976
Ι	1	MET	-	expression tag	UNP P02976
Ι	2	ASP	-	expression tag	UNP P02976
Ι	3	ASN	-	expression tag	UNP P02976
Ι	4	LYS	-	expression tag	UNP P02976
Ι	59	GLU	-	linker	UNP P02976
Ι	60	GLY	-	linker	UNP P02976
Ι	61	SER	-	linker	UNP P02976



Chain	Residue	Modelled	Actual	Comment	Reference
Ι	62	GLU	-	linker	UNP P02976
Ι	63	LEU	-	linker	UNP P02976
Ι	64	GLU	-	linker	UNP P02976
Ι	65	MET	-	linker	UNP P02976
J	-13	MET	-	expression tag	UNP P02976
J	-12	ARG	-	expression tag	UNP P02976
J	-11	GLY	-	expression tag	UNP P02976
J	-10	SER	-	expression tag	UNP P02976
J	-9	HIS	-	expression tag	UNP P02976
J	-8	HIS	-	expression tag	UNP P02976
J	-7	HIS	-	expression tag	UNP P02976
J	-6	HIS	-	expression tag	UNP P02976
J	-5	HIS	-	expression tag	UNP P02976
J	-4	HIS	-	expression tag	UNP P02976
J	-3	GLY	-	expression tag	UNP P02976
J	-2	MET	-	expression tag	UNP P02976
J	-1	ALA	-	expression tag	UNP P02976
J	0	SER	-	expression tag	UNP P02976
J	1	MET	-	expression tag	UNP P02976
J	2	ASP	-	expression tag	UNP P02976
J	3	ASN	-	expression tag	UNP P02976
J	4	LYS	-	expression tag	UNP P02976
J	59	GLU	-	linker	UNP P02976
J	60	GLY	-	linker	UNP P02976
J	61	SER	-	linker	UNP P02976
J	62	GLU	-	linker	UNP P02976
J	63	LEU	-	linker	UNP P02976
J	64	GLU	-	linker	UNP P02976
J	65	MET	-	linker	UNP P02976
K	-13	MET	-	expression tag	UNP P02976
K	-12	ARG	-	expression tag	UNP P02976
K	-11	GLY	-	expression tag	UNP P02976
K	-10	SER	-	expression tag	UNP P02976
K	-9	HIS	-	expression tag	UNP P02976
K	-8	HIS	-	expression tag	UNP P02976
K	-7	HIS	-	expression tag	UNP P02976
K	-6	HIS	-	expression tag	UNP P02976
K	-5	HIS	-	expression tag	UNP P02976
K	-4	HIS		expression tag	UNP P02976
K	-3	GLY	-	expression tag	UNP P02976
K	-2	MET	-	expression tag	UNP P02976
K	-1	ALA	-	expression tag	UNP P02976



Continu	ea from pre	evious page			
Chain	Residue	Modelled	Actual	Comment	Reference
Κ	0	SER	-	expression tag	UNP P02976
К	1	MET	-	expression tag	UNP P02976
Κ	2	ASP	-	expression tag	UNP P02976
Κ	3	ASN	-	expression tag	UNP P02976
Κ	4	LYS	-	expression tag	UNP P02976
Κ	59	GLU	-	linker	UNP P02976
Κ	60	GLY	-	linker	UNP P02976
Κ	61	SER	-	linker	UNP P02976
К	62	GLU	-	linker	UNP P02976
Κ	63	LEU	-	linker	UNP P02976
Κ	64	GLU	-	linker	UNP P02976
Κ	65	MET	-	linker	UNP P02976
L	-13	MET	-	expression tag	UNP P02976
L	-12	ARG	-	expression tag	UNP P02976
L	-11	GLY	-	expression tag	UNP P02976
L	-10	SER	-	expression tag	UNP P02976
L	-9	HIS	-	expression tag	UNP P02976
L	-8	HIS	-	expression tag	UNP P02976
L	-7	HIS	-	expression tag	UNP P02976
L	-6	HIS	-	expression tag	UNP P02976
L	-5	HIS	-	expression tag	UNP P02976
L	-4	HIS	-	expression tag	UNP P02976
L	-3	GLY	-	expression tag	UNP P02976
L	-2	MET	-	expression tag	UNP P02976
L	-1	ALA	-	expression tag	UNP P02976
L	0	SER	-	expression tag	UNP P02976
L	1	MET	-	expression tag	UNP P02976
L	2	ASP	-	expression tag	UNP P02976
L	3	ASN	-	expression tag	UNP P02976
L	4	LYS	-	expression tag	UNP P02976
L	59	GLU	-	linker	UNP P02976
L	60	GLY	-	linker	UNP P02976
L	61	SER	-	linker	UNP P02976
L	62	GLU	-	linker	UNP P02976
L	63	LEU	-	linker	UNP P02976
L	64	GLU	-	linker	UNP P02976
L	65	MET	-	linker	UNP P02976
М	-13	MET	-	expression tag	UNP P02976
М	-12	ARG	-	expression tag	UNP P02976
М	-11	GLY	-	expression tag	UNP P02976
М	-10	SER	_	expression tag	UNP P02976

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expression tag UNP P02976



HIS

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М

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Chain	Residue	Modelled	Actual	Comment	Reference
М	-8	HIS	-	expression tag	UNP P02976
М	-7	HIS	-	expression tag	UNP P02976
М	-6	HIS	-	expression tag	UNP P02976
М	-5	HIS	-	expression tag	UNP P02976
М	-4	HIS	-	expression tag	UNP P02976
М	-3	GLY	-	expression tag	UNP P02976
М	-2	MET	_	expression tag	UNP P02976
М	-1	ALA	-	expression tag	UNP P02976
М	0	SER	-	expression tag	UNP P02976
М	1	MET	-	expression tag	UNP P02976
М	2	ASP	-	expression tag	UNP P02976
М	3	ASN	-	expression tag	UNP P02976
М	4	LYS	-	expression tag	UNP P02976
М	59	GLU	-	linker	UNP P02976
М	60	GLY	-	linker	UNP P02976
М	61	SER	-	linker	UNP P02976
М	62	GLU	-	linker	UNP P02976
М	63	LEU	-	linker	UNP P02976
М	64	GLU	-	linker	UNP P02976
М	65	MET	-	linker	UNP P02976
N	-13	MET	-	expression tag	UNP P02976
N	-12	ARG	-	expression tag	UNP P02976
N	-11	GLY	-	expression tag	UNP P02976
N	-10	SER	-	expression tag	UNP P02976
N	-9	HIS	-	expression tag	UNP P02976
N	-8	HIS	-	expression tag	UNP P02976
N	-7	HIS	-	expression tag	UNP P02976
N	-6	HIS	-	expression tag	UNP P02976
N	-5	HIS	-	expression tag	UNP P02976
N	-4	HIS	-	expression tag	UNP P02976
N	-3	GLY	-	expression tag	UNP P02976
N	-2	MET	-	expression tag	UNP P02976
N	-1	ALA	-	expression tag	UNP P02976
N	0	SER	-	expression tag	UNP P02976
N	1	MET	-	expression tag	UNP P02976
N	2	ASP	-	expression tag	UNP P02976
N	3	ASN	-	expression tag	UNP P02976
N	4	LYS	-	expression tag	UNP P02976
N	59	GLU	-	linker	UNP P02976
N	60	GLY	-	linker	UNP P02976
N	61	SER	-	linker	UNP P02976
N	62	GLU	-	linker	UNP P02976



Chain	Residue	Modelled	Actual	Comment	Reference
N	63	LEU	-	linker	UNP P02976
N	64	GLU	-	linker	UNP P02976
N	65	MET	-	linker	UNP P02976
0	-13	MET	-	expression tag	UNP P02976
0	-12	ARG	-	expression tag	UNP P02976
0	-11	GLY	-	expression tag	UNP P02976
0	-10	SER	-	expression tag	UNP P02976
0	-9	HIS	-	expression tag	UNP P02976
0	-8	HIS	-	expression tag	UNP P02976
0	-7	HIS	-	expression tag	UNP P02976
0	-6	HIS	-	expression tag	UNP P02976
0	-5	HIS	-	expression tag	UNP P02976
0	-4	HIS	-	expression tag	UNP P02976
0	-3	GLY	-	expression tag	UNP P02976
0	-2	MET	-	expression tag	UNP P02976
0	-1	ALA	-	expression tag	UNP P02976
0	0	SER	-	expression tag	UNP P02976
0	1	MET	-	expression tag	UNP P02976
0	2	ASP	-	expression tag	UNP P02976
0	3	ASN	-	expression tag	UNP P02976
0	4	LYS	-	expression tag	UNP P02976
0	59	GLU	-	linker	UNP P02976
0	60	GLY	-	linker	UNP P02976
0	61	SER	-	linker	UNP P02976
0	62	GLU	-	linker	UNP P02976
0	63	LEU	-	linker	UNP P02976
0	64	GLU	-	linker	UNP P02976
0	65	MET	-	linker	UNP P02976
Р	-13	MET	-	expression tag	UNP P02976
Р	-12	ARG	-	expression tag	UNP P02976
Р	-11	GLY	-	expression tag	UNP P02976
Р	-10	SER	-	expression tag	UNP P02976
Р	-9	HIS	-	expression tag	UNP P02976
Р	-8	HIS	-	expression tag	UNP P02976
Р	-7	HIS	-	expression tag	UNP P02976
Р	-6	HIS	-	expression tag	UNP P02976
Р	-5	HIS	-	expression tag	UNP P02976
Р	-4	HIS	-	expression tag	UNP P02976
Р	-3	GLY	-	expression tag	UNP P02976
P	-2	MET	-	expression tag	UNP P02976
Р	-1	ALA	-	expression tag	UNP P02976
P	0	SER	-	expression tag	UNP P02976



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Chain	Residue	Modelled	Actual	Comment	Reference	
Р	1	MET	-	expression tag	UNP P02976	
Р	2	ASP	-	expression tag	UNP P02976	
Р	3	ASN	-	expression tag	UNP P02976	
Р	4	LYS	-	expression tag	UNP P02976	
Р	59	GLU	-	linker	UNP P02976	
Р	60	GLY	-	linker	UNP P02976	
Р	61	SER	-	linker	UNP P02976	
Р	62	GLU	-	linker	UNP P02976	
Р	63	LEU	-	linker	UNP P02976	
Р	64	GLU	-	linker	UNP P02976	
Р	65	MET	-	linker	UNP P02976	
Q	-13	MET	-	expression tag	UNP P02976	
Q	-12	ARG	-	expression tag	UNP P02976	
Q	-11	GLY	-	expression tag	UNP P02976	
Q	-10	SER	-	expression tag	UNP P02976	
Q	-9	HIS	-	expression tag	UNP P02976	
Q	-8	HIS	-	expression tag	UNP P02976	
Q	-7	HIS	-	expression tag	UNP P02976	
Q	-6	HIS	-	expression tag	UNP P02976	
Q	-5	HIS	-	expression tag	UNP P02976	
Q	-4	HIS	-	expression tag	UNP P02976	
Q	-3	GLY	-	expression tag	UNP P02976	
Q	-2	MET	-	expression tag	UNP P02976	
Q	-1	ALA	-	expression tag	UNP P02976	
Q	0	SER	-	expression tag	UNP P02976	
Q	1	MET	-	expression tag	UNP P02976	
Q	2	ASP	-	expression tag	UNP P02976	
Q	3	ASN	-	expression tag	UNP P02976	
Q	4	LYS	-	expression tag	UNP P02976	
Q	59	GLU	-	linker	UNP P02976	
Q	60	GLY	-	linker	UNP P02976	
Q	61	SER	-	linker	UNP P02976	
Q	62	GLU	-	linker	UNP P02976	
Q	63	LEU	-	linker	UNP P02976	
Q	64	GLU	-	linker	UNP P02976	
Q	65	MET	-	linker	UNP P02976	
R	-13	MET	-	expression tag	UNP P02976	
R	-12	ARG	-	expression tag	UNP P02976	
R	-11	GLY	-	expression tag	UNP P02976	
R	-10	SER	-	expression tag	UNP P02976	
R	-9	HIS	-	expression tag	UNP P02976	
R	-8	HIS	-	expression tag	UNP P02976	



Chain	Residue	Modelled	Actual	Comment	Reference
R	-7	HIS	-	expression tag	UNP P02976
R	-6	HIS	-	expression tag	UNP P02976
R	-5	HIS	-	expression tag	UNP P02976
R	-4	HIS	-	expression tag	UNP P02976
R	-3	GLY	-	expression tag	UNP P02976
R	-2	MET	-	expression tag	UNP P02976
R	-1	ALA	-	expression tag	UNP P02976
R	0	SER	-	expression tag	UNP P02976
R	1	MET	-	expression tag	UNP P02976
R	2	ASP	-	expression tag	UNP P02976
R	3	ASN	-	expression tag	UNP P02976
R	4	LYS	-	expression tag	UNP P02976
R	59	GLU	-	linker	UNP P02976
R	60	GLY	-	linker	UNP P02976
R	61	SER	-	linker	UNP P02976
R	62	GLU	-	linker	UNP P02976
R	63	LEU	-	linker	UNP P02976
R	64	GLU	-	linker	UNP P02976
R	65	MET	-	linker	UNP P02976
S	-13	MET	-	expression tag	UNP P02976
S	-12	ARG	-	expression tag	UNP P02976
S	-11	GLY	-	expression tag	UNP P02976
S	-10	SER	-	expression tag	UNP P02976
S	-9	HIS	-	expression tag	UNP P02976
S	-8	HIS	-	expression tag	UNP P02976
S	-7	HIS	-	expression tag	UNP P02976
S	-6	HIS	-	expression tag	UNP P02976
S	-5	HIS	-	expression tag	UNP P02976
S	-4	HIS	-	expression tag	UNP P02976
S	-3	GLY	-	expression tag	UNP P02976
S	-2	MET	-	expression tag	UNP P02976
S	-1	ALA	-	expression tag	UNP P02976
S	0	SER	-	expression tag	UNP P02976
S	1	MET	-	expression tag	UNP P02976
S	2	ASP	-	expression tag	UNP P02976
S	3	ASN	-	expression tag	UNP P02976
S	4	LYS	-	expression tag	UNP P02976
S	59	GLU	-	linker	UNP P02976
S	60	GLY	-	linker	UNP P02976
S	61	SER	-	linker	UNP P02976
S	62	GLU	-	linker	UNP P02976
S	63	LEU	-	linker	UNP P02976



Chain	Residue	Modelled	Actual Comment		Reference
S	64	GLU	-	linker	UNP P02976
S	65	MET	_	linker	UNP P02976
Т	-13	MET	-	expression tag	UNP P02976
Т	-12	ARG	-	expression tag	UNP P02976
Т	-11	GLY	-	expression tag	UNP P02976
Т	-10	SER	-	expression tag	UNP P02976
Т	-9	HIS	_	expression tag	UNP P02976
Т	-8	HIS	-	expression tag	UNP P02976
Т	-7	HIS	-	expression tag	UNP P02976
Т	-6	HIS	-	expression tag	UNP P02976
Т	-5	HIS	-	expression tag	UNP P02976
Т	-4	HIS	-	expression tag	UNP P02976
Т	-3	GLY	-	expression tag	UNP P02976
Т	-2	MET	-	expression tag	UNP P02976
Т	-1	ALA	-	expression tag	UNP P02976
Т	0	SER	-	expression tag	UNP P02976
Т	1	MET	-	expression tag	UNP P02976
Т	2	ASP	-	expression tag	UNP P02976
Т	3	ASN	_	expression tag	UNP P02976
Т	4	LYS	-	expression tag	UNP P02976
Т	59	GLU	-	linker	UNP P02976
Т	60	GLY	-	linker	UNP P02976
Т	61	SER	-	linker	UNP P02976
Т	62	GLU	-	linker	UNP P02976
Т	63	LEU	-	linker	UNP P02976
Т	64	GLU	-	linker	UNP P02976
Т	65	MET	-	linker	UNP P02976
U	-13	MET	-	expression tag	UNP P02976
U	-12	ARG	-	expression tag	UNP P02976
U	-11	GLY	-	expression tag	UNP P02976
U	-10	SER	-	expression tag	UNP P02976
U	-9	HIS	-	expression tag	UNP P02976
U	-8	HIS	-	expression tag	UNP P02976
U	-7	HIS	-	expression tag	UNP P02976
U	-6	HIS	-	expression tag	UNP P02976
U	-5	HIS	-	expression tag	UNP P02976
U	-4	HIS	-	expression tag	UNP P02976
U	-3	GLY	-	expression tag	UNP P02976
U	-2	MET	-	expression tag	UNP P02976
U	-1	ALA	-	expression tag	UNP P02976
U	0	SER	-	expression tag	UNP P02976
U	1	MET	-	expression tag	UNP P02976



Continu	Continued from previous page						
Chain	Residue	Modelled	Actual	Comment	Reference		
U	2	ASP	-	expression tag	UNP P02976		
U	3	ASN	-	expression tag	UNP P02976		
U	4	LYS	-	expression tag	UNP P02976		
U	59	GLU	-	linker	UNP P02976		
U	60	GLY	-	linker	UNP P02976		
U	61	SER	-	linker	UNP P02976		
U	62	GLU	-	linker	UNP P02976		
U	63	LEU	-	linker	UNP P02976		
U	64	GLU	-	linker	UNP P02976		
U	65	MET	-	linker	UNP P02976		
V	-13	MET	-	expression tag	UNP P02976		
V	-12	ARG	-	expression tag	UNP P02976		
V	-11	GLY	-	expression tag	UNP P02976		
V	-10	SER	-	expression tag	UNP P02976		
V	-9	HIS	-	expression tag	UNP P02976		
V	-8	HIS	-	expression tag	UNP P02976		
V	-7	HIS	-	expression tag	UNP P02976		
V	-6	HIS	-	expression tag	UNP P02976		
V	-5	HIS	-	expression tag	UNP P02976		
V	-4	HIS	-	expression tag	UNP P02976		
V	-3	GLY	-	expression tag	UNP P02976		
V	-2	MET	-	expression tag	UNP P02976		
V	-1	ALA	-	expression tag	UNP P02976		
V	0	SER	-	expression tag	UNP P02976		
V	1	MET	-	expression tag	UNP P02976		
V	2	ASP	-	expression tag	UNP P02976		
V	3	ASN	-	expression tag	UNP P02976		
V	4	LYS	-	expression tag	UNP P02976		
V	59	GLU	-	linker	UNP P02976		
V	60	GLY	-	linker	UNP P02976		
V	61	SER	-	linker	UNP P02976		
V	62	GLU	-	linker	UNP P02976		
V	63	LEU	-	linker	UNP P02976		
V	64	GLU	-	linker	UNP P02976		
V	65	MET	-	linker	UNP P02976		
W	-13	MET	-	expression tag	UNP P02976		
W	-12	ARG	-	expression tag	UNP P02976		
W	-11	GLY	-	expression tag	UNP P02976		
W	-10	SER	-	expression tag	UNP P02976		
W	-9	HIS	-	expression tag	UNP P02976		
W	-8	HIS	-	expression tag	UNP P02976		
W	-7	HIS	-	expression tag	UNP P02976		



Chain	Residue	Modelled	Actual	Comment	Reference
W	-6	HIS	-	expression tag	UNP P02976
W	-5	HIS	-	expression tag	UNP P02976
W	-4	HIS	-	expression tag	UNP P02976
W	-3	GLY	-	expression tag	UNP P02976
W	-2	MET	-	expression tag	UNP P02976
W	-1	ALA	-	expression tag	UNP P02976
W	0	SER	-	expression tag	UNP P02976
W	1	MET	-	expression tag	UNP P02976
W	2	ASP	-	expression tag	UNP P02976
W	3	ASN	-	expression tag	UNP P02976
W	4	LYS	-	expression tag	UNP P02976
W	59	GLU	-	linker	UNP P02976
W	60	GLY	-	linker	UNP P02976
W	61	SER	-	linker	UNP P02976
W	62	GLU	-	linker	UNP P02976
W	63	LEU	-	linker	UNP P02976
W	64	GLU	-	linker	UNP P02976
W	65	MET	-	linker	UNP P02976
Х	-13	MET	_	expression tag	UNP P02976
Х	-12	ARG	-	expression tag	UNP P02976
Х	-11	GLY	-	expression tag	UNP P02976
Х	-10	SER	-	expression tag	UNP P02976
Х	-9	HIS	-	expression tag	UNP P02976
Х	-8	HIS	-	expression tag	UNP P02976
Х	-7	HIS	-	expression tag	UNP P02976
Х	-6	HIS	-	expression tag	UNP P02976
Х	-5	HIS	-	expression tag	UNP P02976
Х	-4	HIS	-	expression tag	UNP P02976
Х	-3	GLY	-	expression tag	UNP P02976
Х	-2	MET	-	expression tag	UNP P02976
X	-1	ALA	-	expression tag	UNP P02976
X	0	SER	-	expression tag	UNP P02976
X	1	MET	-	expression tag	UNP P02976
Х	2	ASP	-	expression tag	UNP P02976
Х	3	ASN	-	expression tag	UNP P02976
X	4	LYS	-	expression tag	UNP P02976
X	59	GLU	-	linker	UNP P02976
X	60	GLY	-	linker	UNP P02976
X	61	SER	-	linker	UNP P02976
X	62	GLU	-	linker	UNP P02976
X	63	LEU	-	linker	UNP P02976
X	64	GLU	-	linker	UNP P02976



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Chain	Residue	Modelled	Actual	Comment	Reference
Х	65	MET	-	linker	UNP P02976
Y	-13	MET	-	expression tag	UNP P02976
Y	-12	ARG	-	expression tag	UNP P02976
Y	-11	GLY	-	expression tag	UNP P02976
Y	-10	SER	-	expression tag	UNP P02976
Y	-9	HIS	-	expression tag	UNP P02976
Y	-8	HIS	-	expression tag	UNP P02976
Y	-7	HIS	-	expression tag	UNP P02976
Y	-6	HIS	-	expression tag	UNP P02976
Y	-5	HIS	-	expression tag	UNP P02976
Y	-4	HIS	-	expression tag	UNP P02976
Y	-3	GLY	-	expression tag	UNP P02976
Y	-2	MET	-	expression tag	UNP P02976
Y	-1	ALA	-	expression tag	UNP P02976
Y	0	SER	-	expression tag	UNP P02976
Y	1	MET	-	expression tag	UNP P02976
Y	2	ASP	-	expression tag	UNP P02976
Y	3	ASN	-	expression tag	UNP P02976
Y	4	LYS	-	expression tag	UNP P02976
Y	59	GLU	-	linker	UNP P02976
Y	60	GLY	-	linker	UNP P02976
Y	61	SER	-	linker	UNP P02976
Y	62	GLU	-	linker	UNP P02976
Y	63	LEU	-	linker	UNP P02976
Y	64	GLU	-	linker	UNP P02976
Y	65	MET	-	linker	UNP P02976
Ζ	-13	MET	-	expression tag	UNP P02976
Ζ	-12	ARG	-	expression tag	UNP P02976
Ζ	-11	GLY	-	expression tag	UNP P02976
Ζ	-10	SER	-	expression tag	UNP P02976
Ζ	-9	HIS	-	expression tag	UNP P02976
Ζ	-8	HIS	-	expression tag	UNP P02976
Ζ	-7	HIS	-	expression tag	UNP P02976
Ζ	-6	HIS	-	expression tag	UNP P02976
Ζ	-5	HIS	-	expression tag	UNP P02976
Ζ	-4	HIS	-	expression tag	UNP P02976
Z	-3	GLY	-	expression tag	UNP P02976
Z	-2	MET	-	expression tag	UNP P02976
Z	-1	ALA	-	expression tag	UNP P02976
Z	0	SER	-	expression tag	UNP P02976
Z	1	MET	-	expression tag	UNP P02976
Z	2	ASP	-	expression tag	UNP P02976



Continued from previous page						
Chain	Residue	Modelled	Actual	Comment	Reference	
Z	3	ASN	-	expression tag	UNP P02976	
Z	4	LYS	-	expression tag	UNP P02976	
Z	59	GLU	-	linker	UNP P02976	
Z	60	GLY	-	linker	UNP P02976	
Z	61	SER	-	linker	UNP P02976	
Z	62	GLU	-	linker	UNP P02976	
Z	63	LEU	-	linker	UNP P02976	
Ζ	64	GLU	-	linker	UNP P02976	
Ζ	65	MET	-	linker	UNP P02976	
a	-13	MET	-	expression tag	UNP P02976	
a	-12	ARG	-	expression tag	UNP P02976	
a	-11	GLY	-	expression tag	UNP P02976	
a	-10	SER	-	expression tag	UNP P02976	
a	-9	HIS	-	expression tag	UNP P02976	
a	-8	HIS	-	expression tag	UNP P02976	
a	-7	HIS	-	expression tag	UNP P02976	
a	-6	HIS	-	expression tag	UNP P02976	
a	-5	HIS	-	expression tag	UNP P02976	
a	-4	HIS	-	expression tag	UNP P02976	
a	-3	GLY	-	expression tag	UNP P02976	
a	-2	MET	-	expression tag	UNP P02976	
a	-1	ALA	-	expression tag	UNP P02976	
a	0	SER	-	expression tag	UNP P02976	
a	1	MET	-	expression tag	UNP P02976	
a	2	ASP	-	expression tag	UNP P02976	
a	3	ASN	-	expression tag	UNP P02976	
a	4	LYS	-	expression tag	UNP P02976	
a	59	GLU	-	linker	UNP P02976	
a	60	GLY	-	linker	UNP P02976	
a	61	SER	-	linker	UNP P02976	
a	62	GLU	-	linker	UNP P02976	
a	63	LEU	-	linker	UNP P02976	
a	64	GLU	-	linker	UNP P02976	
a	65	MET	-	linker	UNP P02976	
b	-13	MET	-	expression tag	UNP P02976	
b	-12	ARG	-	expression tag	UNP P02976	
b	-11	GLY	-	expression tag	UNP P02976	
b	-10	SER	-	expression tag	UNP P02976	
b	-9	HIS	-	expression tag	UNP P02976	
b	-8	HIS	-	expression tag	UNP P02976	
b	-7	HIS	-	expression tag	UNP P02976	
b	-6	HIS	-	expression tag	UNP P02976	



Chain	Residue	Modelled	Actual Comment		Reference
b	-5	HIS	-	expression tag	UNP P02976
b	-4	HIS	_	expression tag	UNP P02976
b	-3	GLY	-	expression tag	UNP P02976
b	-2	MET	-	expression tag	UNP P02976
b	-1	ALA	-	expression tag	UNP P02976
b	0	SER	-	expression tag	UNP P02976
b	1	MET	-	expression tag	UNP P02976
b	2	ASP	-	expression tag	UNP P02976
b	3	ASN	-	expression tag	UNP P02976
b	4	LYS	-	expression tag	UNP P02976
b	59	GLU	-	linker	UNP P02976
b	60	GLY	-	linker	UNP P02976
b	61	SER	-	linker	UNP P02976
b	62	GLU	-	linker	UNP P02976
b	63	LEU	-	linker	UNP P02976
b	64	GLU	-	linker	UNP P02976
b	65	MET	-	linker	UNP P02976
с	-13	MET	-	expression tag	UNP P02976
с	-12	ARG	_	expression tag	UNP P02976
с	-11	GLY	-	expression tag	UNP P02976
с	-10	SER	-	expression tag	UNP P02976
с	-9	HIS	-	expression tag	UNP P02976
с	-8	HIS	-	expression tag	UNP P02976
с	-7	HIS	-	expression tag	UNP P02976
с	-6	HIS	-	expression tag	UNP P02976
с	-5	HIS	-	expression tag	UNP P02976
с	-4	HIS	-	expression tag	UNP P02976
с	-3	GLY	-	expression tag	UNP P02976
с	-2	MET	-	expression tag	UNP P02976
с	-1	ALA	-	expression tag	UNP P02976
с	0	SER	-	expression tag	UNP P02976
с	1	MET	-	expression tag	UNP P02976
с	2	ASP	-	expression tag	UNP P02976
с	3	ASN	-	expression tag	UNP P02976
с	4	LYS	-	expression tag	UNP P02976
с	59	GLU	-	linker	UNP P02976
с	60	GLY	-	linker	UNP P02976
с	61	SER	-	linker	UNP P02976
с	62	GLU	-	linker	UNP P02976
с	63	LEU	-	linker	UNP P02976
с	64	GLU	-	linker	UNP P02976
с	65	MET	-	linker	UNP P02976



Chain	Residue	Modelled	Actual	Comment	Reference
d	-13	MET	-	expression tag	UNP P02976
d	-12	ARG	_	expression tag	UNP P02976
d	-11	GLY	-	expression tag	UNP P02976
d	-10	SER	-	expression tag	UNP P02976
d	-9	HIS	-	expression tag	UNP P02976
d	-8	HIS	-	expression tag	UNP P02976
d	-7	HIS	-	expression tag	UNP P02976
d	-6	HIS	-	expression tag	UNP P02976
d	-5	HIS	-	expression tag	UNP P02976
d	-4	HIS	-	expression tag	UNP P02976
d	-3	GLY	-	expression tag	UNP P02976
d	-2	MET	-	expression tag	UNP P02976
d	-1	ALA	-	expression tag	UNP P02976
d	0	SER	-	expression tag	UNP P02976
d	1	MET	-	expression tag	UNP P02976
d	2	ASP	-	expression tag	UNP P02976
d	3	ASN	-	expression tag	UNP P02976
d	4	LYS	-	expression tag	UNP P02976
d	59	GLU	-	linker	UNP P02976
d	60	GLY	-	linker	UNP P02976
d	61	SER	-	linker	UNP P02976
d	62	GLU	-	linker	UNP P02976
d	63	LEU	-	linker	UNP P02976
d	64	GLU	-	linker	UNP P02976
d	65	MET	_	linker	UNP P02976





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	L	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	М	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	S	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	V	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	10	Total         O           10         10	0	0
3	В	14	Total         O           14         14	0	0
3	С	22	$\begin{array}{ccc} \text{Total} & \text{O} \\ 22 & 22 \end{array}$	0	0
3	D	15	Total O 15 15	0	0
3	Е	16	Total         O           16         16	0	0
3	F	6	Total O 6 6	0	0
3	G	14	Total         O           14         14	0	0
3	Н	10	Total O 10 10	0	0
3	Ι	18	Total O 18 18	0	0
3	J	14	Total         O           14         14	0	0
3	К	15	Total O 15 15	0	0
3	L	21	TotalO2121	0	0
3	М	16	Total         O           16         16	0	0
3	Ν	16	Total         O           16         16	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2 0	15	Total O	0	0	
3	0	10	15 15	0	0
3	P	19	Total O	0	0
0	I	12	12 12	0	0
3	0	16	Total O	0	0
	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	10	16 16		0
3	R	9	Total O	0	0
		-	9 9		
3	S	11	Total O	0	0
			11 11		_
3	Т	14	Total O	0	0
			14 14		
3	U	12	Total O	0	0
			12 $12$		
3	V	18	10tal U	0	0
			18 18 Tetal 0		
3	W	8		0	0
			Total O		
3	Х	17	10tal O	0	0
			Total O		
3	Y	11	10tar O	0	0
			Total O		
3	Z	13	13 13	0	0
			Total O		
3	a	12	12 12	0	0
			Total O		
3	b	20	20 20	0	0
-		2.4	Total O		0
3	С	24	24 24	0	0
2	1	1.0	Total O	0	0
5	a	10	16 16		U

Continued from previous page...



# 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: Immunoglobulin G-binding protein A,Coat protein

Chain A:	67% •	32%
MET ARG CLY CLY CLY CLY CLY ASP ASP ASP ASP ASP ASP CLY CLY CLY CLY CLY	GLN GLN ASN ASN ALA ALA ALA ALA ALA GLU CLU CLU CLU GLU GLU GLU GLU GLU CLU CLU CLU	GLM LEU LYS ASP ASP PRO SER GLN SER ALA ALA LEU LEU LEU SER SER
GLU LYS LYS LYS LYS LEU ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	SER SER ARG GLY C73 C73 C73 C15 C25 C25 C25 C25 C25 C25 C25 C25 C25 C2	
• Molecule 1: Immunoglobuli	n G-binding protein A,Coat prot	tein
Chain B:	67% .	32%
MET ARG CLY ARG CLY HIS HIS HIS HIS HIS HIS HIS ALA ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	GLN ASN ALA ALA ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	GLM GLM LEV LYS ASP ASP PRO SER ASP ASN LEU LEU LEU SER SER
CLU LYS LYS LYS LYS LYS CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	SER SER ARG GLY GLY CT7 CT7 CLY ARG ARG ARG ASS ASS ASN ASN	
• Molecule 1: Immunoglobuli	n G-binding protein A,Coat prot	tein
Chain C:	68%	32%
MET ARG CLY CLY CLY CLY MET ASP ASP ASP PHE ASN CLY CLY CLY CLY CLY CLY	GLN GLN ASN ASN ALA ALA ASN GLU ASN CLU CLU CLU GLU GLU GLU GLU GLU GLU GLU CLU	GLN CLEU LYS ASP ASP PRO SER GLN SER ASN LEU LEU LEU SER SER
GLU LYS LYS LYS LYS SER ASN ASN ALU GLU GLU GLU MET MET SFR SFR SFR	SER SER ARG GLY GLY GLY A263 A263 A263 A263 A263 A263 A263 A263	
• Molecule 1: Immunoglobuli	n G-binding protein A,Coat prot	cein
Chain D:	67% ·	32%
MET ARG CLY CLY HIS HIS HIS HIS HIS HIS HIS HIS ALA MET ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	GLN ASN ASN ASN ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	GLM GLM LLYS LLYS ASP ASP CLM SER ASLA ASN LEU LEU LEU SER SER
GLU ALIA LYS LYS LYS LEU ASN ASN ASN ASN GLU GLU GLU GLU GLU GLU MET AIA SVAL SVAL	SER SER ARG GLY C73 C73 C73 C17 C17 C17 C17 C17 C17 C17 C17 C17 C17	

• Molecule 1: Immunoglobulin G-binding protein A,Coat protein

**DB** 

Chain E:	67% .	32%
MET ARG CLY SER HIS HIS HIS HIS HIS HIS HIS HIS ARG ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	CLN CLN ASN ASN ALA ASN TTR TTR TTLE TLEU ASN ASN ASN CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	SGLN SGLN LEU LEU LEU ASP ASP ALA ALA ALA ALA SER LEU LEU LEU SER
GLU ALA LIYS LIYS LIYS LIYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	SER SER ARG G1.7 C73 C73 C73 C73 C73 C73 C73 C73 C73 C7	
• Molecule 1: Immunoglobuli	n G-binding protein A,Coat prot	ein
Chain F:	67%	32%
MET ARG CLY SER HIS HIS HIS HIS HIS HIS HIS ASP ASP ASP ASP ASP ASP ASP	GLN GLN ASN ALA ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	GLN LEU LYS LYS ASP PRO SER ALA ALA ALA ALA LEU LEU SER
GLU ALA LYS LYS LYS LYS GLN GLN GLN GLU GLU GLU GLU MET MET SER SER SER SER SER SER SER SER SER SER	SER SER ARG GLY G17 G15 G15 15 6 15 6 8 18 7 209 A26 SER ALA ASN ASN	
• Molecule 1: Immunoglobuli	n G-binding protein A,Coat prot	ein
Chain G:	67% ·	32%
MET ARG GLY GLY SER HIS HIS HIS HIS AIS ASP ASP ASP ASP ASP ASP ASP CLY SER ASP	GLN GLN ASN ALA ALA ALA ALA ALA CLU CLU ASN ASN GLU GLU GLU GLU GLU GLU GLU CLU CLU CLU CLU CLU ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	SER LEU LEU ASP ASP SER ALA ASN LEU LEU LEU SER SER
GLU ALA LLYS LLYS LLYS LLYS ALN GLN GLU GLU GLU GLU GLU GLU MET MLA SER GLU MET MLA	SER SER ARG CT3 CT3 CT3 CT3 CT3 CT3 CT3 CT3 CT3 CT3	
• Molecule 1: Immunoglobuli	n G-binding protein A,Coat prot	ein
Chain H:	68%	32%
MET ARG GLY SER HIS HIS HIS HIS HIS HIS AIS MET ASR ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	GLN GLN ASN ALA ALA ALA ALA ALA ALF ASN ASN ASN GLU GLU GLU ASN ASN ASN CLI FIE CLI CLI CLI CLI CLI CLI CLI CLI ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	SER LEU LYS ASP PRO SER ALA ASN ALA ASN LEU LEU SER SER
GLU LYS LYS LYS LYS LYS CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	SER SER ARC C73 C73 C73 C73 C73 C73 C73 C73 C73 C7	
• Molecule 1: Immunoglobuli	n G-binding protein A,Coat prot	ein
Chain I:	67%	32%
MET ARG CLY SER SER HIS HIS HIS HIS HIS HIS ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	GLN GLN ASN ALA ASN TTR TTR TTR GLU ASN ASN GLU GLU GLU GLU GLU GLU GLU GLU CIU	GLM GLM LYS LYS ASP PRO SER ASP ASP ALA ASN LLEU LEU LEU SER SER
GLU ALA LYS LYS LYS LYS GLU GLU GLU GLU GLU GLU GLU MET MET MET	SER SER ARG GLY GT3 GT3 D90 D90 D90 D90 D90 A263 SER A263 SER A263 A263 SER A263 A263 A263 A263 A263 A263 A263 A263	
• Molecule 1: Immunoglobuli	n G-binding protein A,Coat prot	ein
Chain J:	67% ·	32%



### 

#### 

### • Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain K:	67%	·	32%	-

#### 

• Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain L:	67%	• 32%	
MET ARG GLY SER HIS HIS HIS HIS HIS GLY MET ALA	SER MET ASP ASP PHE PHE ASN CUU CUU CUU CUU PHE CUU CUU CUU CUU ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	MET PRO ASN ASN CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	SER GLN SER ALA ASN LEU LEU SER

#### 

• Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain M:	66%	•

32%

#### 

• Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain N.			220/
Onam N.	67%	•	32%

#### 

• Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain O:	67%	32%	
MEI ARG GLY SER HIS HIS HIS HIS HIS ALA ALA	SER MET ASP ASP LYS PHE ASN CYS GLU GLU GLU TYR CLN GLU TLE LEU ASN MET PRO	ASN ASN ASN GLU GLU GLU GLU GLN GLN CLEU LLEU LLEU LLEU LLEU ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	ALA ASN LEU LEU SER



GLU ALA LYS LYS LYS LYS GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU	ALA VAL SER SER SER ARG GLY C73 C73 C73 C73 C73 C73 C73 SER	ALA LEU ASN ASN		
• Molecule 1: Immunoglob	bulin G-binding p	rotein A,Coat pr	rotein	
Chain P:	68%		32%	
MET ARG GLY GLY HIS HIS HIS HIS HIS HIS HIS ALA ALA SER ALA SER ALA SER PHE	ASN LYS GLU GLN GLN GLN ASN ALA PHE TYR GLU ILE LEU ASN	MET PRO ASN LEU GLU GLU GLU GLN GLY GLY PHE	ILE GLN SER LEU LFU LYS ASP PRO SER GLN SER SER	ASN LEU SER
ALU ALA LYS LYS LYS ALA ASN ALA ALA ALA CLU CLU CLU CLU CLU CLU CLU	ALA VAL SER SER SER SER ARG GLY CT3 CT3 CT3 CT3 CT3 CT3 CT3 CT3 CT3 CT3	ASN		
• Molecule 1: Immunoglob	bulin G-binding p	rotein A,Coat pr	rotein	
Chain Q:	67%	·	32%	
MET ARG GLY GLY GLY HIS HIS HIS HIS HIS ALA SER ALA SER ALA SER ALA SPE CLY SER ALA	ASN LYS GLU GLN GLN ASN ALA ASN CLU TYR CLU ILE ILEU ASN	MET PRO ASN LEU ASN GLU GLU ASN GLY PHE	ILE GLN SER LEU LYS ASP ASP PRO SER SER ALA	ASN LEU LEU SER
ALU LYS LYS LYS ALA ASN ASN ASN ALA ALA ALA CLU SER SER SER CLU CLU CLU	ALA VAL SER SER SER SER ARG CIY CIY C218 C218 C218	V228 A265 SER A1.A A1.A ASN ASN		
• Molecule 1: Immunoglob	oulin G-binding p	rotein A,Coat pr	rotein	
Chain R:	67%	·	32%	
MET ARG CLY SER HIS HIS HIS HIS HIS HIS ALA ART ART ART ASN ASN LYS PHE	ASN LYS GLU GLU GLN GLN ASN ALA ASN GLU ILE LEU ASN	MET PRO ASN LEU ASN GLU GLU GLU ASN ASN ASN ASN PHE	ILE GLN SER LEU LEU LYS ASP ASP PRO SER SER ALA	ASN LEU LEU SER
GLU ALA LYS LYS LYS LYS GLU ALA ALA ALA ALA GLU CLU GLU GLU GLU GLU MET	ALA VAL SER SER SER SER ARG GLY GLY CJ3 CJ3 CJ3 CJ3 CJ3 SER SER SER	ALA LEU ASN ASN		
• Molecule 1: Immunoglob	oulin G-binding p	rotein A,Coat pr	rotein	
Chain S:	67%		32%	
MET ARG CLY CLY CLY SER HIS HIS HIS HIS ALA SER ALA SER ASN CLY SER ASN CLY SER ASN CLY SER ASN CLY SER CLY SER CLY SER CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	ASN LYS GLU GLN GLN ASN ALA ANA ALA TYR CLU TLE ILE ILEU ASN	MET PRO ASN LEU ASN GLU GLU ASN ASN GLY PHE	ILE GLN SER LEU LEU LYS ASP ASP PRO SER SER ALA	ASN LEU LEU SER
01U ALA LYS LYS LYS LYS ALA ASN ASN ALA ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU MET	ALA VAL SER SER SER SER ANG GLY C73 C73 C17 C73 C17 C17 C17 C17 C17 C17 C17 C17 C17 C17	ALA LEU ASN ASN		
• Molecule 1: Immunoglob	bulin G-binding p	rotein A,Coat pr	rotein	
Chain T:	67%	·	32%	
MET ARG CLY SER HIS HIS HIS HIS HIS HIS ALA MET ALA SER MET ASN LYS PHE	ASN LYS GLU GLU GLN GLN ALA ALA ALA TYR GLU ILE LEU ASN	MET PRO ASN ASN ASN GLU GLU GLU ASN ASN ASN ASN PHE	ILE GLN SER LEU LYS ASP ASP ASP PRO SER SER ALA	ASN LEU LEU SER



GLU ALA ALA ALA ALA ALA ALA ALA ALA GLU GLU GLU GLU GLU GLU ALA ALA ALA ALA ALA	SER SER GLY GLY G13 G13 M199 G218 M225 C184 M225 SER M225 SER M225 ASN M225 ASN ASN	
• Molecule 1: Immunoglobuli	n G-binding protein A,Coat pro	tein
Chain U:	67% .	32%
MRT ARG GLY GLY HIS HIS HIS HIS HIS HIS HIS ASR ASR ASR ASR ASR ASR ASR ASR ASR AS	GLN GLN GLN AISN AISN AISN GLN GLN AISN GLN GLN GLN GLN GLN GLN CHE CHE CHE CHE CHE CHE CHE CHE CHE CHE	GLM LEU LYS LEU LYS ASP ASP GLN SER SER ASU ASU LEU LEU LEU
GLU LYS LYS LYS LEU ALA ALA ALA ALA PRO GLU CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	SER SER GLY GLY GLY G13 1223 SER A263 SER A263 A263 A263 A263 A263 A263 A281 A281 A281 A281 A281 A281 A281 A281	
• Molecule 1: Immunoglobuli	n G-binding protein A,Coat pro	tein
Chain V:	67% ·	32%
MET ARG GLY GLY HIS HIS HIS HIS HIS HIS AIA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	GLU GLN ALA ALA ALA ALA ALA ALU CLU CLU CLU CLU CLU CLU CLU CLU CLU C	GLN SER LYS ASP ASP ASP ASP CLN SER ASN CLN SER ASN LEU LEU SER
GLU LYS LYS LYS ASN ASN ASN ASN ASN GLU CLN GLU GLU GLU GLU MET MET SER SER SER SER SER SER SER SER SER SER	SER SER ARC G17 G17 S91 S91 S91 S91 S18 S242 ASC ASC ASC ASC ASC ASC ASC ASC ASC ASC	
• Molecule 1: Immunoglobuli	n G-binding protein A,Coat pro	tein
Chain W:	68%	32%
	GLM GLM A SIN A SI	GLN CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
Chain W: Interpretent of the second state of	SER GLA SER GLA ARG ARG GLY GT3 TTR ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	32% REAL REAL REAL REAL REAL REAL REAL REAL
Chain W:	68% B 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	32%
Chain W:	68% B 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	32% M & R & & & & & & & & & & & & & & & & &
Chain W:	68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         67%         6	32% MBS SAIN SAIN SAIN SAIN SAIN SAIN SAIN SAI
Chain W:         ## 25 85 ###############################	68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         68%         67%         67%         67%         68%         68%         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         88         89         80	32%
Chain W:         ###58#################################	68%         3 3 3 3 4 4 4 5 3 1 4 5 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4	32% tein 32%
Chain W:         ####################################	68%         9 9 9 9 8 1 8 8 9 9 9 9 9 9 9 9 9 9 9 9	32%



ALA ALA LIYS LIYS LIYS CLU ASN ASN ASN ASN ALA ALA CLU CLU CLU CLU CLU CLU CLU CLU SER ALA SER ALA	SER SER ARG GLY GLY CLY CLY CLY AR ALA ALA ALA ALA ALA ALA ALA ALA ALA	
• Molecule 1: Immunoglobulir	n G-binding protein A,Coat pro	tein
Chain Z:	67%	32%
MET ARG GLY SER HIS HIS HIS HIS HIS HIS ALA SET ALA SET ASN CLY SC ASN CLY SC CLY CLY CLY CLY CLA CLA CLA CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	GLN GLN ALA ALA ALA ALA CLU TTR GLU ASN CLU ASN GLU ASN GLU ASN GLU ASN GLU ASN CLU TLEU ASN ASS CLU	GLN SER LEU LYS ASP PRO SER ASP ASN ALA ASN LEU LEU SER
	•	
GLU ALLA LYSS LYSS LIZU ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	SER SER ARG CT3 CT3 CT3 AZ SER AZ SER AZ SER AZ AZ SER AZ AZ AZ AZ AZ AZ AZ AZ AZ AZ AZ AZ AZ	
• Molecule 1: Immunoglobulir	n G-binding protein A,Coat pro	tein
Chain a:	68%	32%
MRT MRT GLY GLY GLY GLY GLY GLY MRT MRT MRT MRT MRT MRT MRT MRT MRT MRT	GLN ASN ASN ASN ASN ASN TYR ALL ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	GLN SER LYS ASP ASP ASP PRO SER ALA ASN ALA ASN LEU LEU SER
ALL ALL ALL ALL ALL ALL ALL ALL ALL ALL	SER SER SER 317 773 773 773 773 773 773 773 773 773	
• Molecule 1: Immunoglobulir	n G-binding protein A,Coat pro	tein
Chain b:	67%	32%
MET ARG GLY GLY HIS HIS HIS HIS HIS HIS AIS ASP ASP CLY CYS CLV CLY CLY CLY	GLN GLN ASN ASN TTR TTR TTR GLU ASN ASN GLU GLU GLU GLU GLU GLU GLU GLU TTR TTR	GLN SER LEU LEU LYS ASP PRO PRO PRO SER ASP ASN ASN LEU LEU SER SER
GLU LYS LYS LYS LYS CUU SER CLU CLU CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV	SER ARG CLY CLY CLY ASC SER AZC AZC ASN ASN ASN	
• Molecule 1: Immunoglobulin	n G-binding protein A,Coat pro	tein
Chain c:	66% ·	32%
MET MET GLY GLY HIS HIS HIS HIS HIS HIS HIS ALA MET ALA ASP MET ASP ASP ASN CLY SC CLU CC CLU CC CLU CC CC CLY CC CC CC CC CC CC CC CC CC CC CC CC CC	GLN ASN ASN ALA ASN TYR ALA GLU ASN ASN GLU GLU GLU GLU GLU GLU GLU GLU CILY	GLN SER LFU LFU LFU ASP PRO SER ASP ASN ALA ASN LEU LEU SER
ALU LYS LYS LYS LYS ALU ALU ALU ALU ALU ALU ALU CLU CLU CLU CLU CLU SER ALA ALA ALA SER SER SER SER SER SER SER SER SER SER	SER ARG (173 673 673 673 715 722 722 722 722 722 722 722 722 722 72	
• Molecule 1: Immunoglobulir	n G-binding protein A,Coat pro	tein
Chain d:	67% •	32%
MET MET SER GLY SER HIS HIS HIS HIS HIS MET MET ALA ASP ASP ASP PHE LYS CLU	GLN ASN ASN ALA ASN TYR GLU CLU ASN ASN GLU GLU GLU GLU GLU GLU GLU GLU TLE ILE	GLN SER LLEU LLEU LLEU ASP PRO SER ALA ASN LLEU LEU SER SER

# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	288.18Å 193.04Å 189.19Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $124.37^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	50.00 - 3.00	Depositor
Resolution (A)	45.82 - 3.00	EDS
% Data completeness	99.7 (50.00-3.00)	Depositor
(in resolution range)	99.7 (45.82 - 3.00)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$< I/\sigma(I) > 1$	$2.25 (at 3.01 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
P. P.	0.179 , $0.200$	Depositor
$n, n_{free}$	0.182 , $0.199$	DCC
$R_{free}$ test set	8494 reflections $(5.02\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	47.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35, 44.7	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	42805	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: 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).

Mal	Chain	Bo	ond lengths	Bond angles	
WIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.77	0/1445	0.82	1/1983~(0.1%)
1	В	0.81	1/1448~(0.1%)	0.83	2/1986~(0.1%)
1	С	0.80	0/1448	0.84	0/1986
1	D	0.78	1/1450~(0.1%)	0.81	0/1989
1	Е	0.77	1/1431~(0.1%)	0.84	1/1964~(0.1%)
1	F	0.79	0/1408	0.84	2/1935~(0.1%)
1	G	0.75	0/1450	0.82	2/1989~(0.1%)
1	Н	0.76	0/1441	0.83	0/1977
1	Ι	0.77	1/1450~(0.1%)	0.82	0/1989
1	J	0.78	3/1448~(0.2%)	0.85	0/1986
1	Κ	0.79	1/1448~(0.1%)	0.83	0/1987
1	L	0.79	1/1448~(0.1%)	0.82	0/1986
1	М	0.83	1/1449~(0.1%)	0.86	3/1987~(0.2%)
1	Ν	0.79	0/1446	0.83	1/1984~(0.1%)
1	0	0.76	0/1448	0.81	1/1986~(0.1%)
1	Р	0.75	0/1448	0.81	0/1986
1	Q	0.79	0/1409	0.89	2/1935~(0.1%)
1	R	0.78	1/1438~(0.1%)	0.87	1/1974~(0.1%)
1	S	0.77	0/1437	0.86	2/1972~(0.1%)
1	Т	0.80	1/1447~(0.1%)	0.86	3/1985~(0.2%)
1	U	0.77	1/1444~(0.1%)	0.82	1/1981~(0.1%)
1	V	0.77	1/1448~(0.1%)	0.82	1/1986~(0.1%)
1	W	0.77	0/1448	0.84	0/1986
1	Х	0.78	1/1446~(0.1%)	0.83	0/1983
1	Y	0.77	0/1443	0.82	1/1980~(0.1%)
1	Ζ	0.76	1/1443~(0.1%)	0.81	0/1980
1	a	0.74	0/1445	0.80	0/1982
1	b	0.82	1/1448~(0.1%)	0.83	0/1986
1	с	0.83	$1/\overline{1450}~(0.1\%)$	0.85	$2/\overline{1989}~(0.1\%)$
1	d	0.76	$1/\overline{1447}~(0.1\%)$	0.81	0/1985
All	All	0.78	19/43299~(0.0%)	0.83	26/59404~(0.0%)



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	GLY	N-CA	6.86	1.56	1.46
1	В	185	SER	CA-CB	6.21	1.62	1.52
1	J	185	SER	CA-CB	6.10	1.62	1.52
1	L	73	GLY	N-CA	5.99	1.55	1.46
1	Т	222	ASN	CG-OD1	-5.95	1.10	1.24
1	с	73	GLY	N-CA	5.64	1.54	1.46
1	b	73	GLY	N-CA	5.48	1.54	1.46
1	Ε	73	GLY	N-CA	5.33	1.54	1.46
1	J	185	SER	CB-OG	5.28	1.49	1.42
1	Κ	73	GLY	N-CA	5.20	1.53	1.46
1	U	73	GLY	N-CA	5.19	1.53	1.46
1	V	73	GLY	N-CA	5.12	1.53	1.46
1	М	73	GLY	N-CA	5.11	1.53	1.46
1	R	73	GLY	N-CA	5.10	1.53	1.46
1	Ζ	73	GLY	N-CA	5.07	1.53	1.46
1	Х	73	GLY	N-CA	5.04	1.53	1.46
1	d	73	GLY	N-CA	5.01	1.53	1.46
1	Ι	73	GLY	N-CA	5.01	1.53	1.46
1	J	73	GLY	N-CA	5.01	1.53	1.46

All (19) bond length outliers are listed below:

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	S	231	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	S	231	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	Q	216	ALA	N-CA-C	-7.50	90.76	111.00
1	Т	199	LYS	CB-CG-CD	7.10	130.05	111.60
1	R	215	THR	CA-CB-CG2	-6.95	102.67	112.40
1	Ν	199	LYS	CB-CG-CD	6.44	128.34	111.60
1	Т	222	ASN	CB-CG-OD1	-6.08	109.44	121.60
1	0	150	THR	CA-CB-CG2	5.96	120.75	112.40
1	с	150	THR	CA-CB-CG2	5.82	120.55	112.40
1	А	150	THR	CA-CB-CG2	5.80	120.52	112.40
1	М	249	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	F	185	SER	CA-CB-OG	5.78	126.79	111.20
1	V	91	SER	N-CA-CB	5.47	118.70	110.50
1	G	117	LYS	CB-CG-CD	5.45	125.78	111.60
1	Т	199	LYS	CD-CE-NZ	5.45	124.22	111.70
1	Е	223	ILE	CG1-CB-CG2	5.38	123.24	111.40
1	U	223	ILE	CG1-CB-CG2	5.36	123.20	111.40
1	В	223	ILE	CG1-CB-CG2	5.34	123.15	111.40
1	Y	199	LYS	CB-CG-CD	5.24	125.22	111.60

PDB EIN DATA BANK

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	F	209	THR	CA-CB-OG1	-5.14	98.21	109.00
1	М	181	GLY	N-CA-C	-5.13	100.27	113.10
1	М	228	VAL	CA-CB-CG1	5.13	118.60	110.90
1	с	228	VAL	CA-CB-CG1	5.07	118.51	110.90
1	В	185	SER	CA-CB-OG	5.05	124.83	111.20
1	G	228	VAL	CA-CB-CG1	5.04	118.47	110.90
1	Q	228	VAL	CA-CB-CG1	5.01	118.42	110.90

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

### 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	Perce	ntiles
1	А	189/282~(67%)	181 (96%)	8 (4%)	0	100	100
1	В	189/282~(67%)	182 (96%)	7 (4%)	0	100	100
1	С	189/282~(67%)	182 (96%)	7 (4%)	0	100	100
1	D	189/282~(67%)	181 (96%)	8 (4%)	0	100	100
1	Ε	189/282~(67%)	182 (96%)	7 (4%)	0	100	100
1	F	189/282~(67%)	181 (96%)	8 (4%)	0	100	100
1	G	189/282~(67%)	181 (96%)	8 (4%)	0	100	100
1	Н	189/282~(67%)	181 (96%)	8 (4%)	0	100	100
1	Ι	189/282~(67%)	182 (96%)	7 (4%)	0	100	100
1	J	189/282~(67%)	180 (95%)	9 (5%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Κ	189/282~(67%)	180 (95%)	9~(5%)	0	100 100
1	L	189/282~(67%)	180~(95%)	9~(5%)	0	100 100
1	М	189/282~(67%)	177 (94%)	11 (6%)	1 (0%)	29 68
1	Ν	189/282~(67%)	181 (96%)	8 (4%)	0	100 100
1	Ο	189/282~(67%)	181 (96%)	8 (4%)	0	100 100
1	Р	189/282~(67%)	181 (96%)	8 (4%)	0	100 100
1	Q	189/282~(67%)	179~(95%)	8 (4%)	2(1%)	14 50
1	R	189/282~(67%)	182 (96%)	7 (4%)	0	100 100
1	S	189/282~(67%)	181 (96%)	8 (4%)	0	100 100
1	Т	189/282~(67%)	182 (96%)	7 (4%)	0	100 100
1	U	189/282~(67%)	182 (96%)	7 (4%)	0	100 100
1	V	189/282~(67%)	180 (95%)	9~(5%)	0	100 100
1	W	189/282~(67%)	181 (96%)	8 (4%)	0	100 100
1	Х	189/282~(67%)	180 (95%)	9~(5%)	0	100 100
1	Y	189/282~(67%)	182 (96%)	7 (4%)	0	100 100
1	Z	189/282~(67%)	180 (95%)	9~(5%)	0	100 100
1	a	189/282~(67%)	182 (96%)	7~(4%)	0	100 100
1	b	189/282~(67%)	180 (95%)	9~(5%)	0	100 100
1	с	189/282~(67%)	181 (96%)	8 (4%)	0	100 100
1	d	189/282~(67%)	182 (96%)	7 (4%)	0	100 100
All	All	5670/8460~(67%)	5427 (96%)	240 (4%)	3~(0%)	51 85

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All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	М	182	THR
1	Q	216	ALA
1	Q	217	VAL

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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.



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	154/238~(65%)	153~(99%)	1 (1%)	86	95
1	В	155/238~(65%)	155 (100%)	0	100	100
1	С	155/238~(65%)	155 (100%)	0	100	100
1	D	156/238~(66%)	155 (99%)	1 (1%)	86	95
1	Е	149/238~(63%)	149 (100%)	0	100	100
1	F	140/238~(59%)	140 (100%)	0	100	100
1	G	156/238~(66%)	155 (99%)	1 (1%)	86	95
1	Н	152/238~(64%)	152 (100%)	0	100	100
1	Ι	156/238~(66%)	155 (99%)	1 (1%)	86	95
1	J	155/238~(65%)	155 (100%)	0	100	100
1	К	155/238~(65%)	154 (99%)	1 (1%)	86	95
1	L	155/238~(65%)	155 (100%)	0	100	100
1	М	156/238~(66%)	154 (99%)	2 (1%)	69	89
1	Ν	154/238~(65%)	153 (99%)	1 (1%)	86	95
1	О	155/238~(65%)	155 (100%)	0	100	100
1	Р	155/238~(65%)	155 (100%)	0	100	100
1	Q	143/238~(60%)	143 (100%)	0	100	100
1	R	152/238~(64%)	152 (100%)	0	100	100
1	S	151/238~(63%)	151 (100%)	0	100	100
1	Т	155/238~(65%)	154 (99%)	1 (1%)	86	95
1	U	153/238~(64%)	152 (99%)	1 (1%)	84	94
1	V	156/238~(66%)	155 (99%)	1 (1%)	86	95
1	W	155/238~(65%)	155 (100%)	0	100	100
1	Х	154/238~(65%)	154 (100%)	0	100	100
1	Y	153/238~(64%)	153 (100%)	0	100	100
1	Ζ	153/238~(64%)	153 (100%)	0	100	100
1	a	154/238~(65%)	154 (100%)	0	100	100
1	b	155/238~(65%)	155 (100%)	0	100	100
1	с	156/238~(66%)	155 (99%)	1 (1%)	86	95
1	d	155/238~(65%)	154 (99%)	1 (1%)	86	95

The Analysed column shows the number of residues for which the side chain conformation was analysed, and the total number of residues.



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4603/7140~(64%)	4590 (100%)	13 (0%)	92 97

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	225	THR
1	D	225	THR
1	G	225	THR
1	Ι	225	THR
1	Κ	225	THR
1	М	180	ASN
1	М	182	THR
1	Ν	225	THR
1	Т	225	THR
1	U	225	THR
1	V	225	THR
1	с	225	THR
1	d	225	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	160	ASN
1	J	180	ASN
1	М	180	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 monosaccharides in this entry.



## 5.6 Ligand geometry (i)

6 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	B	ond leng	$\operatorname{gths}$	Bond angles		
					Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	SO4	М	301	-	4,4,4	0.32	0	$6,\!6,\!6$	0.05	0
2	SO4	V	301	-	4,4,4	0.32	0	6,6,6	0.05	0
2	SO4	L	301	-	4,4,4	0.32	0	6,6,6	0.05	0
2	SO4	S	301	-	4,4,4	0.33	0	6,6,6	0.05	0
2	SO4	D	301	-	4,4,4	0.32	0	6,6,6	0.05	0
2	SO4	Н	301	-	4,4,4	0.33	0	6,6,6	0.05	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.

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 (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,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#	₽RSR	.Z>2	$OWAB(Å^2)$	Q < 0.9
1	А	191/282~(67%)	-0.59	0	100	100	25, 40, 70, 84	0
1	В	191/282~(67%)	-0.62	0	100	100	25, 36, 69, 79	0
1	С	191/282~(67%)	-0.71	0	100	100	22, 31, 55, 91	0
1	D	191/282~(67%)	-0.56	0	100	100	23, 34, 69, 77	0
1	Е	191/282~(67%)	-0.64	0	100	100	26, 38, 75, 88	0
1	F	191/282~(67%)	-0.45	0	100	100	26, 43, 84, 97	0
1	G	191/282~(67%)	-0.65	0	100	100	25, 38, 65, 80	0
1	Η	191/282~(67%)	-0.60	0	100	100	26, 39, 68, 83	0
1	Ι	191/282~(67%)	-0.73	0	100	100	22, 37, 69, 80	0
1	J	191/282~(67%)	-0.63	0	100	100	22, 35, 67, 82	0
1	Κ	191/282~(67%)	-0.63	0	100	100	20, 32, 65, 76	0
1	L	191/282~(67%)	-0.75	0	100	100	18, 29, 60, 79	0
1	М	191/282~(67%)	-0.69	0	100	100	19, 30, 60, 79	0
1	Ν	191/282~(67%)	-0.71	0	100	100	21, 34, 66, 79	0
1	Ο	191/282~(67%)	-0.61	0	100	100	25, 37, 67, 79	0
1	Р	191/282~(67%)	-0.58	0	100	100	23, 37, 66, 81	0
1	Q	191/282~(67%)	-0.45	1 (0	9%) 9	1 75	27, 42, 101, 143	0
1	R	191/282~(67%)	-0.45	0	100	100	26,  44,  85,  113	0
1	S	191/282~(67%)	-0.61	0	100	100	24, 39, 72, 83	0
1	Т	191/282~(67%)	-0.60	2 (1	%) 8	2 59	23, 36, 66, 85	0
1	U	191/282~(67%)	-0.62	0	100	100	21, 36, 72, 86	0
1	V	191/282~(67%)	-0.62	1 (0	9%) 9	1 75	25, 36, 65, 78	0
1	W	191/282~(67%)	-0.65	0	100	100	23, 37, 64, 82	0
1	Х	191/282~(67%)	-0.70	0	100	100	19, 34, 66, 78	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	Y	191/282~(67%)	-0.63	0 100 100	21,  35,  69,  81	0
1	Z	191/282~(67%)	-0.59	1 (0%) 91 75	25, 38, 72, 87	0
1	a	191/282~(67%)	-0.52	0 100 100	25,  39,  73,  89	0
1	b	191/282~(67%)	-0.71	0 100 100	19,30,57,79	0
1	с	191/282~(67%)	-0.70	0 100 100	19, 30, 64, 78	0
1	d	191/282~(67%)	-0.62	0 100 100	25, 36, 68, 75	0
All	All	5730/8460~(67%)	-0.62	5 (0%) 95 89	18, 36, 70, 143	0

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All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	218	GLY	3.4
1	Ζ	211	ALA	2.6
1	Т	218	GLY	2.4
1	Т	184	CYS	2.1
1	V	242	SER	2.0

## 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 monosaccharides 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. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
2	SO4	D	301	5/5	0.99	0.19	6,7,7,7	0
2	SO4	Н	301	5/5	0.99	0.16	$8,\!8,\!9,\!9$	0
2	SO4	L	301	5/5	0.99	0.17	2,2,2,2	0
2	SO4	М	301	5/5	0.99	0.19	2,2,2,2	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	SO4	S	301	5/5	0.99	0.19	$4,\!4,\!4,\!4$	0
2	SO4	V	301	5/5	0.99	0.20	$5,\!6,\!6,\!6$	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

