



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 10:14 AM BST

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 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

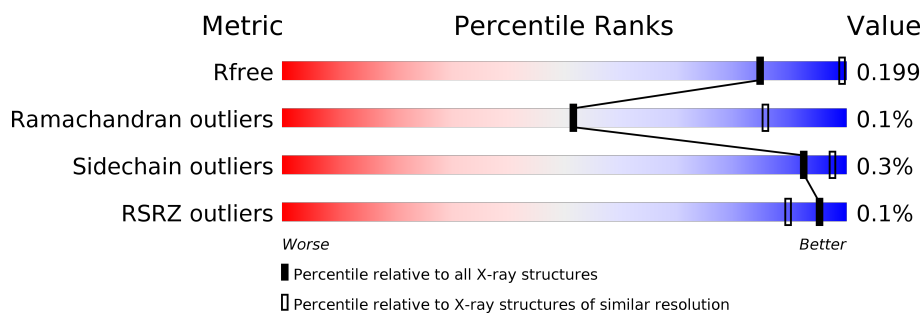
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	282	
1	B	282	
1	C	282	
1	D	282	
1	E	282	
1	F	282	
1	G	282	

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Mol	Chain	Length	Quality of chain
1	H	282	
1	I	282	
1	J	282	
1	K	282	
1	L	282	
1	M	282	
1	N	282	
1	O	282	
1	P	282	
1	Q	282	
1	R	282	
1	S	282	
1	T	282	
1	U	282	
1	V	282	
1	W	282	
1	X	282	
1	Y	282	
1	Z	282	
1	a	282	
1	b	282	
1	c	282	
1	d	282	

## 2 Entry composition

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.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1413	901	228	276	8			
1	B	191	Total	C	N	O	S	0	0	0
			1416	902	229	277	8			
1	C	191	Total	C	N	O	S	0	0	0
			1416	902	229	277	8			
1	D	191	Total	C	N	O	S	0	0	0
			1418	903	229	278	8			
1	E	191	Total	C	N	O	S	0	0	0
			1399	892	227	272	8			
1	F	191	Total	C	N	O	S	0	0	0
			1376	877	224	267	8			
1	G	191	Total	C	N	O	S	0	0	0
			1418	903	229	278	8			
1	H	191	Total	C	N	O	S	0	0	0
			1409	898	228	275	8			
1	I	191	Total	C	N	O	S	0	0	0
			1418	903	229	278	8			
1	J	191	Total	C	N	O	S	0	0	0
			1416	902	229	277	8			
1	K	191	Total	C	N	O	S	0	0	0
			1416	902	228	278	8			
1	L	191	Total	C	N	O	S	0	0	0
			1416	902	229	277	8			
1	M	191	Total	C	N	O	S	0	0	0
			1417	902	229	278	8			
1	N	191	Total	C	N	O	S	0	0	0
			1414	902	228	276	8			
1	O	191	Total	C	N	O	S	0	0	0
			1416	902	229	277	8			
1	P	191	Total	C	N	O	S	0	0	0
			1416	902	229	277	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	191	Total	C	N	O	S	0	0	0
			1378	879	227	264	8			
1	R	191	Total	C	N	O	S	0	0	0
			1406	895	228	275	8			
1	S	191	Total	C	N	O	S	0	0	0
			1405	894	228	275	8			
1	T	191	Total	C	N	O	S	0	0	0
			1415	902	229	276	8			
1	U	191	Total	C	N	O	S	0	0	0
			1412	900	228	276	8			
1	V	191	Total	C	N	O	S	0	0	0
			1416	902	229	277	8			
1	W	191	Total	C	N	O	S	0	0	0
			1416	902	229	277	8			
1	X	191	Total	C	N	O	S	0	0	0
			1414	900	229	277	8			
1	Y	191	Total	C	N	O	S	0	0	0
			1411	900	228	275	8			
1	Z	191	Total	C	N	O	S	0	0	0
			1411	900	228	275	8			
1	a	191	Total	C	N	O	S	0	0	0
			1413	901	229	275	8			
1	b	191	Total	C	N	O	S	0	0	0
			1416	902	229	277	8			
1	c	191	Total	C	N	O	S	0	0	0
			1418	903	229	278	8			
1	d	191	Total	C	N	O	S	0	0	0
			1415	902	229	276	8			

There are 750 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
C	-13	MET	-	expression tag	UNP P02976
C	-12	ARG	-	expression tag	UNP P02976
C	-11	GLY	-	expression tag	UNP P02976

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
I	62	GLU	-	linker	UNP P02976
I	63	LEU	-	linker	UNP P02976
I	64	GLU	-	linker	UNP P02976
I	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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-8	HIS	-	expression tag	UNP P02976
M	-7	HIS	-	expression tag	UNP P02976
M	-6	HIS	-	expression tag	UNP P02976
M	-5	HIS	-	expression tag	UNP P02976
M	-4	HIS	-	expression tag	UNP P02976
M	-3	GLY	-	expression tag	UNP P02976
M	-2	MET	-	expression tag	UNP P02976
M	-1	ALA	-	expression tag	UNP P02976
M	0	SER	-	expression tag	UNP P02976
M	1	MET	-	expression tag	UNP P02976
M	2	ASP	-	expression tag	UNP P02976
M	3	ASN	-	expression tag	UNP P02976
M	4	LYS	-	expression tag	UNP P02976
M	59	GLU	-	linker	UNP P02976
M	60	GLY	-	linker	UNP P02976
M	61	SER	-	linker	UNP P02976
M	62	GLU	-	linker	UNP P02976
M	63	LEU	-	linker	UNP P02976
M	64	GLU	-	linker	UNP P02976
M	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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
P	1	MET	-	expression tag	UNP P02976
P	2	ASP	-	expression tag	UNP P02976
P	3	ASN	-	expression tag	UNP P02976
P	4	LYS	-	expression tag	UNP P02976
P	59	GLU	-	linker	UNP P02976
P	60	GLY	-	linker	UNP P02976
P	61	SER	-	linker	UNP P02976
P	62	GLU	-	linker	UNP P02976
P	63	LEU	-	linker	UNP P02976
P	64	GLU	-	linker	UNP P02976
P	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

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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

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

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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

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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
X	-13	MET	-	expression tag	UNP P02976
X	-12	ARG	-	expression tag	UNP P02976
X	-11	GLY	-	expression tag	UNP P02976
X	-10	SER	-	expression tag	UNP P02976
X	-9	HIS	-	expression tag	UNP P02976
X	-8	HIS	-	expression tag	UNP P02976
X	-7	HIS	-	expression tag	UNP P02976
X	-6	HIS	-	expression tag	UNP P02976
X	-5	HIS	-	expression tag	UNP P02976
X	-4	HIS	-	expression tag	UNP P02976
X	-3	GLY	-	expression tag	UNP P02976
X	-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
X	2	ASP	-	expression tag	UNP P02976
X	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
X	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
Z	-13	MET	-	expression tag	UNP P02976
Z	-12	ARG	-	expression tag	UNP P02976
Z	-11	GLY	-	expression tag	UNP P02976
Z	-10	SER	-	expression tag	UNP P02976
Z	-9	HIS	-	expression tag	UNP P02976
Z	-8	HIS	-	expression tag	UNP P02976
Z	-7	HIS	-	expression tag	UNP P02976
Z	-6	HIS	-	expression tag	UNP P02976
Z	-5	HIS	-	expression tag	UNP P02976
Z	-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

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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
Z	64	GLU	-	linker	UNP P02976
Z	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

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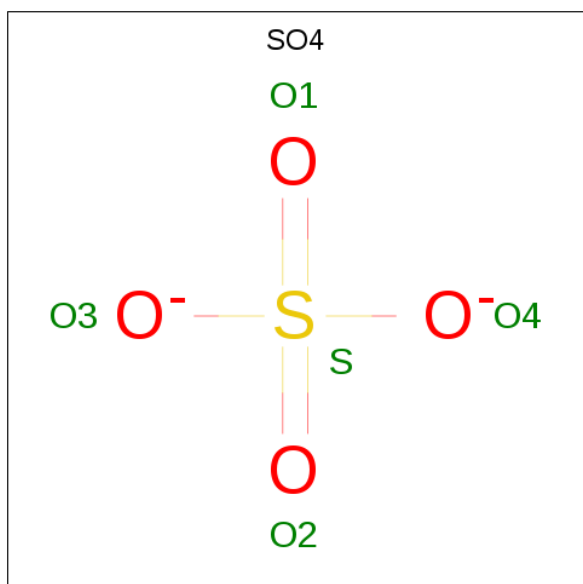
Chain	Residue	Modelled	Actual	Comment	Reference
b	-5	HIS	-	expression tag	UNP P02976
b	-4	HIS	-	expression tag	UNP P02976
b	-3	GLY	-	expression tag	UNP P02976
b	-2	MET	-	expression tag	UNP P02976
b	-1	ALA	-	expression tag	UNP P02976
b	0	SER	-	expression tag	UNP P02976
b	1	MET	-	expression tag	UNP P02976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

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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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	M	1	Total O S 5 4 1	0	0
2	S	1	Total O S 5 4 1	0	0
2	V	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	14	Total O 14 14	0	0
3	C	22	Total O 22 22	0	0
3	D	15	Total O 15 15	0	0
3	E	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	H	10	Total O 10 10	0	0
3	I	18	Total O 18 18	0	0
3	J	14	Total O 14 14	0	0
3	K	15	Total O 15 15	0	0
3	L	21	Total O 21 21	0	0
3	M	16	Total O 16 16	0	0
3	N	16	Total O 16 16	0	0

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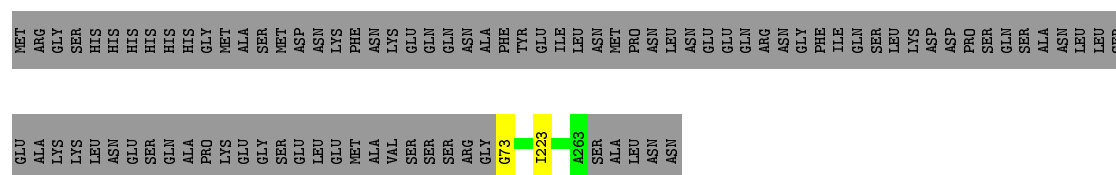


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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	15	Total 15	O 15	0	0
3	P	12	Total 12	O 12	0	0
3	Q	16	Total 16	O 16	0	0
3	R	9	Total 9	O 9	0	0
3	S	11	Total 11	O 11	0	0
3	T	14	Total 14	O 14	0	0
3	U	12	Total 12	O 12	0	0
3	V	18	Total 18	O 18	0	0
3	W	8	Total 8	O 8	0	0
3	X	17	Total 17	O 17	0	0
3	Y	11	Total 11	O 11	0	0
3	Z	13	Total 13	O 13	0	0
3	a	12	Total 12	O 12	0	0
3	b	20	Total 20	O 20	0	0
3	c	24	Total 24	O 24	0	0
3	d	16	Total 16	O 16	0	0

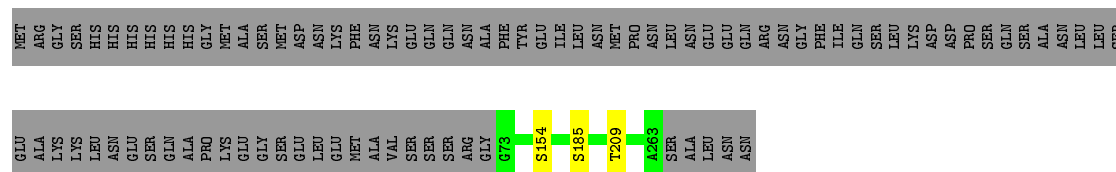


Chain E:  67% 32%



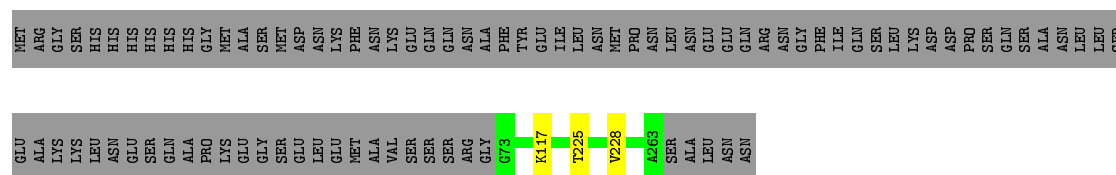
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain F:  67% 32%



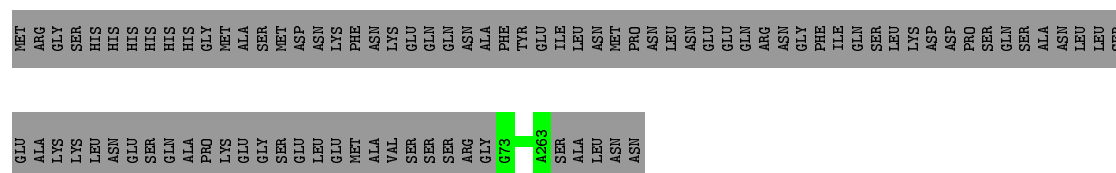
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain G:  67% 32%



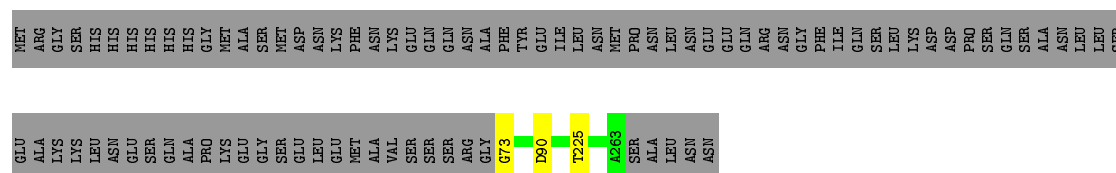
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain H:  68% 32%



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

Chain I:  67% 32%



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

Chain J:  67% 32%

MET ARG GLY SER HIS HIS HIS HIS HIS MET MET SER MET MET ASP ASN LYS PHE ASN LYS GLN GLN GLN ALA ASN ARG TYR LEU LEU ASN MET PRO ASN ASN LEU LEU GLU GLU GLN ARG ASN GLY PHE TLE GLN SER SER LEU LYS ASP ASP PRO PRO GLN SER SER ALA ASN LEU LEU SER

GLU ALA LYS LEU ASN GLU SER GLN ALA PRO GLY LYS MET GLY SER MET ASP GLU LEU MET MET ALA VAL SER SER SER ARG GLY G73 S185 A263 SER ALA LEU ASN

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

Chain K:  67% 32%

MET ARG GLY SER HIS HIS HIS HIS HIS MET MET SER MET MET ASP ASN LYS PHE ASN LYS GLN GLN GLN ALA ASN ARG TYR TLE LEU LEU ASN MET PRO ASN ASN LEU LEU GLU GLU GLN ARG ASN GLY PHE TLE GLN SER SER LEU LYS ASP ASP PRO PRO GLN SER SER ALA ASN LEU LEU SER

GLU ALA LYS LEU ASN GLU SER GLN ALA PRO GLY LYS MET GLY SER MET ASP GLU LEU MET MET ALA VAL SER SER SER ARG GLY G73 T225 A263 SER ALA LEU ASN

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

Chain L:  67% 32%

MET ARG GLY SER HIS HIS HIS HIS HIS MET MET SER MET MET ASP ASN LYS PHE ASN LYS GLN GLN GLN ALA ASN ARG TYR TLE LEU LEU ASN MET PRO ASN ASN LEU LEU GLU GLU GLN ARG ASN GLY PHE TLE GLN SER SER LEU LYS ASP ASP PRO PRO GLN SER SER ALA ASN LEU LEU SER

GLU ALA LYS LEU ASN GLU SER GLN ALA PRO GLY LYS MET MET ALA VAL SER SER SER ARG GLY G73 D90 A263 SER ALA LEU ASN

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

Chain M:  66% 32%

MET ARG GLY SER HIS HIS HIS HIS HIS MET MET SER MET MET ASP ASN LYS PHE ASN LYS GLN GLN GLN ALA ASN ARG TYR TLE LEU LEU ASN MET PRO ASN ASN LEU LEU GLU GLU GLN ARG ASN GLY PHE TLE GLN SER SER LEU LYS ASP ASP PRO PRO GLN SER SER ALA ASN LEU LEU SER

GLU ALA LYS LEU ASN GLU SER GLN ALA PRO GLY LYS MET MET ALA VAL SER SER SER ARG GLY G73 M180 G181 T182 V228 R249 A263 SER ALA LEU ASN

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

Chain N:  67% 32%

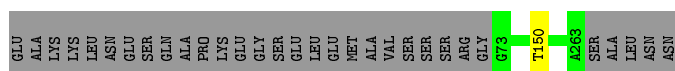
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GLU ALA LYS LEU ASN GLU SER GLN ALA PRO GLY LYS MET MET ALA VAL SER SER SER ARG GLY G73 K199 T225 A263 SER ALA LEU ASN

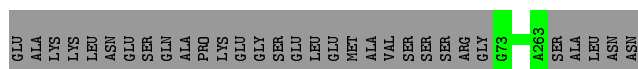
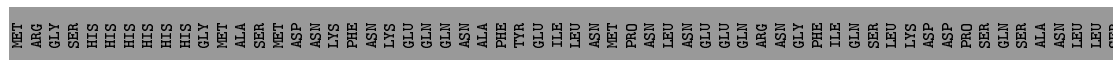
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain O:  67% 32%

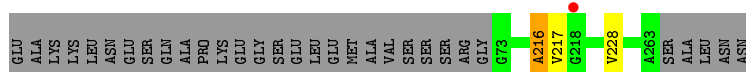
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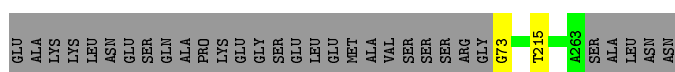
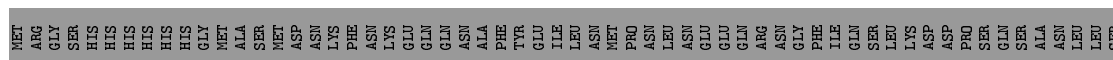
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



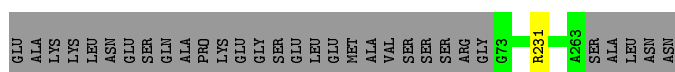
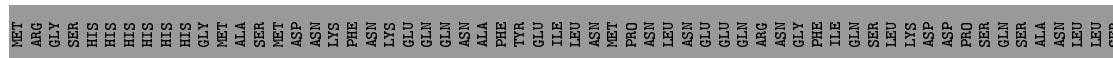
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



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

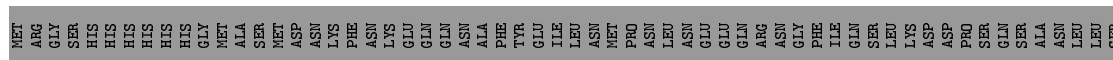


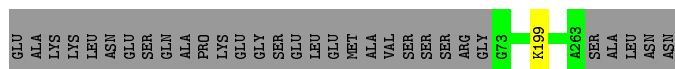
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



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

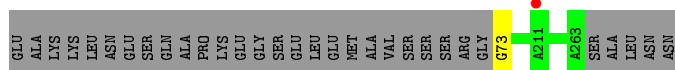
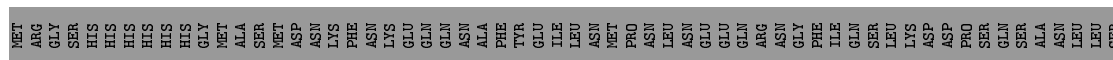






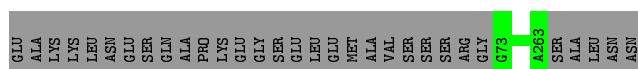
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain Z: 67% 32%



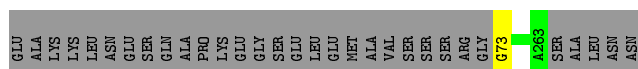
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain a: 68% 32%



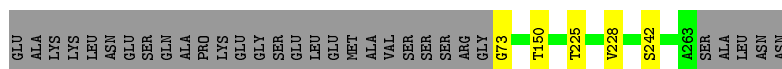
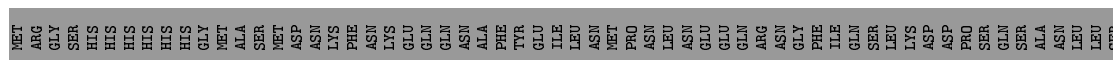
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain b: 67% 32%



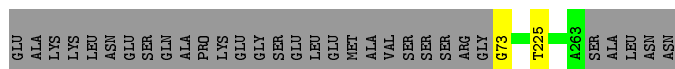
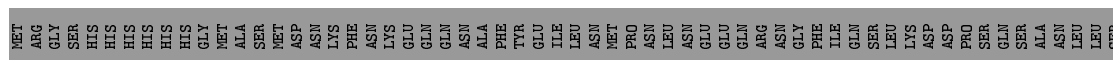
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain c: 66% 32%



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

Chain d: 67% 32%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	288.18Å 193.04Å 189.19Å 90.00° 124.37° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 45.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.00) 99.7 (45.82-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.179 , 0.200 0.182 , 0.199	Depositor DCC
$R_{free}$ test set	8494 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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>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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.77	0/1445	0.82	1/1983 (0.1%)
1	B	0.81	1/1448 (0.1%)	0.83	2/1986 (0.1%)
1	C	0.80	0/1448	0.84	0/1986
1	D	0.78	1/1450 (0.1%)	0.81	0/1989
1	E	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	H	0.76	0/1441	0.83	0/1977
1	I	0.77	1/1450 (0.1%)	0.82	0/1989
1	J	0.78	3/1448 (0.2%)	0.85	0/1986
1	K	0.79	1/1448 (0.1%)	0.83	0/1987
1	L	0.79	1/1448 (0.1%)	0.82	0/1986
1	M	0.83	1/1449 (0.1%)	0.86	3/1987 (0.2%)
1	N	0.79	0/1446	0.83	1/1984 (0.1%)
1	O	0.76	0/1448	0.81	1/1986 (0.1%)
1	P	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	T	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	X	0.78	1/1446 (0.1%)	0.83	0/1983
1	Y	0.77	0/1443	0.82	1/1980 (0.1%)
1	Z	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	c	0.83	1/1450 (0.1%)	0.85	2/1989 (0.1%)
1	d	0.76	1/1447 (0.1%)	0.81	0/1985
All	All	0.78	19/43299 (0.0%)	0.83	26/59404 (0.0%)

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	GLY	N-CA	6.86	1.56	1.46
1	B	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	T	222	ASN	CG-OD1	-5.95	1.10	1.24

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	T	199	LYS	CB-CG-CD	7.10	130.05	111.60
1	R	215	THR	CA-CB-CG2	-6.95	102.67	112.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

## 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	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	B	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
1	C	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
1	D	189/282 (67%)	181 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	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	H	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	I	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
1	J	189/282 (67%)	180 (95%)	9 (5%)	0	100	100
1	K	189/282 (67%)	180 (95%)	9 (5%)	0	100	100
1	L	189/282 (67%)	180 (95%)	9 (5%)	0	100	100
1	M	189/282 (67%)	177 (94%)	11 (6%)	1 (0%)	29	68
1	N	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	O	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	P	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	T	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	X	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	c	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

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	182	THR
1	Q	216	ALA

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Mol	Chain	Res	Type
1	Q	217	VAL

### 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	154/238 (65%)	153 (99%)	1 (1%)	86	95
1	B	155/238 (65%)	155 (100%)	0	100	100
1	C	155/238 (65%)	155 (100%)	0	100	100
1	D	156/238 (66%)	155 (99%)	1 (1%)	86	95
1	E	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	H	152/238 (64%)	152 (100%)	0	100	100
1	I	156/238 (66%)	155 (99%)	1 (1%)	86	95
1	J	155/238 (65%)	155 (100%)	0	100	100
1	K	155/238 (65%)	154 (99%)	1 (1%)	86	95
1	L	155/238 (65%)	155 (100%)	0	100	100
1	M	156/238 (66%)	154 (99%)	2 (1%)	69	89
1	N	154/238 (65%)	153 (99%)	1 (1%)	86	95
1	O	155/238 (65%)	155 (100%)	0	100	100
1	P	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	T	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	154/238 (65%)	154 (100%)	0	100	100
1	Y	153/238 (64%)	153 (100%)	0	100	100
1	Z	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	c	156/238 (66%)	155 (99%)	1 (1%)	86	95
1	d	155/238 (65%)	154 (99%)	1 (1%)	86	95
All	All	4603/7140 (64%)	4590 (100%)	13 (0%)	92	97

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	180	ASN
1	M	182	THR
1	V	225	THR
1	K	225	THR
1	U	225	THR

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

Mol	Chain	Res	Type
1	B	160	ASN
1	J	180	ASN
1	M	180	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

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	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	V	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	H	301	-	4,4,4	0.33	0	6,6,6	0.05	0
2	SO4	M	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	D	301	-	4,4,4	0.32	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 ⓘ

### 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	191/282 (67%)	-0.59	0	100	100	25, 40, 70, 84	0
1	B	191/282 (67%)	-0.62	0	100	100	25, 36, 69, 79	0
1	C	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	E	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	H	191/282 (67%)	-0.60	0	100	100	26, 39, 68, 83	0
1	I	191/282 (67%)	-0.73	0	100	100	23, 37, 69, 80	0
1	J	191/282 (67%)	-0.63	0	100	100	22, 35, 67, 82	0
1	K	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	M	191/282 (67%)	-0.69	0	100	100	19, 30, 60, 79	0
1	N	191/282 (67%)	-0.71	0	100	100	21, 34, 66, 79	0
1	O	191/282 (67%)	-0.61	0	100	100	25, 37, 67, 79	0
1	P	191/282 (67%)	-0.58	0	100	100	23, 37, 66, 81	0
1	Q	191/282 (67%)	-0.45	1 (0%)	91	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	T	191/282 (67%)	-0.60	2 (1%)	82	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%)	91	75	25, 36, 65, 78	0
1	W	191/282 (67%)	-0.65	0	100	100	23, 37, 64, 82	0
1	X	191/282 (67%)	-0.70	0	100	100	19, 34, 66, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	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	c	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

All (5) RSRZ outliers are listed below:

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

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	V	301	5/5	0.99	0.20	5,6,6,6	0
2	SO4	S	301	5/5	0.99	0.19	4,4,4,4	0
2	SO4	H	301	5/5	0.99	0.16	8,8,9,9	0
2	SO4	M	301	5/5	0.99	0.19	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	L	301	5/5	0.99	0.17	2,2,2,2	0
2	SO4	D	301	5/5	0.99	0.19	6,7,7,7	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.