



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:16 PM GMT

PDB ID : 4Y5Z  
Title : T=1 capsid structure of SeMV Ndel65CP fused with B-domain of S. aureus protein SpA at the N-terminus (P1 crystal form)  
Authors : Gulati, A.; Murthy, M.R.N.  
Deposited on : 2015-02-12  
Resolution : 2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

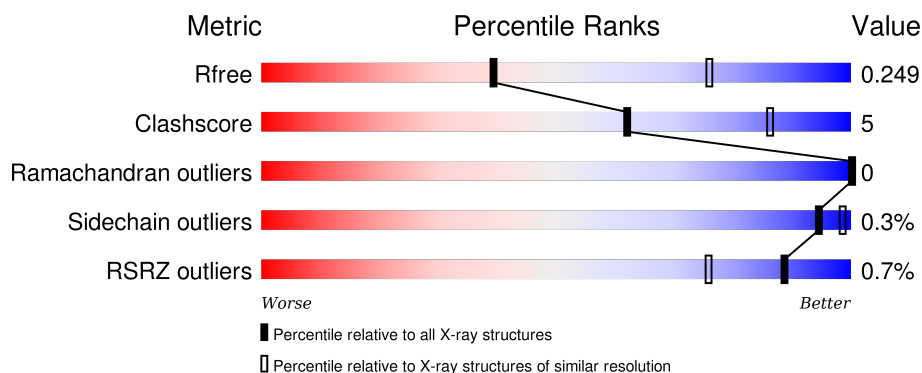
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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

Mol	Chain	Length	Quality of chain
1	0	282	<div> <div></div> <div>60% 8% 32%</div> </div>
1	1	282	<div> <div></div> <div>%</div> <div>59% 10% 32%</div> </div>
1	2	282	<div> <div></div> <div>60% 9% 32%</div> </div>
1	3	282	<div> <div></div> <div>57% 12% 31%</div> </div>
1	4	282	<div> <div></div> <div>61% 7% 32%</div> </div>












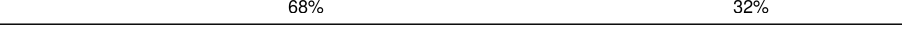







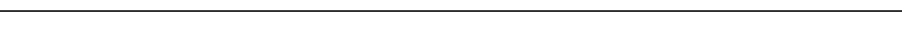

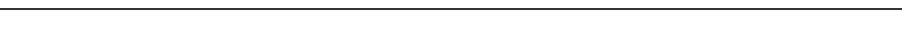
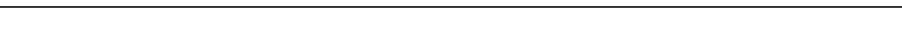


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Mol	Chain	Length	Quality of chain
1	5	282	
1	6	282	
1	7	282	
1	A	282	
1	B	282	
1	C	282	
1	D	282	
1	E	282	
1	F	282	
1	G	282	
1	H	282	
1	I	282	
1	J	282	
1	K	282	
1	L	282	
1	M	282	
1	N	282	
1	O	282	
1	P	282	
1	Q	282	
1	R	282	
1	S	282	
1	T	282	
1	U	282	
1	V	282	





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Mol	Chain	Length	Quality of chain
1	W	282	
1	X	282	
1	Y	282	
1	Z	282	
1	a	282	
1	b	282	
1	c	282	
1	d	282	
1	e	282	
1	f	282	
1	g	282	
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	

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Mol	Chain	Length	Quality of chain
1	v	282	 68%32%
1	w	282	 %68%32%
1	x	282	 68%32%
1	y	282	 %68%32%
1	z	282	 68%32%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	4	301	-	-	X	-
2	SO4	H	301	-	-	X	-
2	SO4	P	301	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 86922 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	192	Total	C	N	O	S	0	0	0
			1423	905	230	280	8			
1	B	194	Total	C	N	O	S	0	0	0
			1429	909	232	280	8			
1	C	192	Total	C	N	O	S	0	0	0
			1420	901	230	281	8			
1	D	192	Total	C	N	O	S	0	0	0
			1420	903	229	280	8			
1	E	191	Total	C	N	O	S	0	0	0
			1421	903	230	280	8			
1	F	192	Total	C	N	O	S	0	0	0
			1421	904	230	279	8			
1	G	192	Total	C	N	O	S	0	0	0
			1427	907	231	281	8			
1	H	193	Total	C	N	O	S	0	0	0
			1429	908	231	282	8			
1	I	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	J	193	Total	C	N	O	S	0	0	0
			1430	909	231	282	8			
1	K	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	L	192	Total	C	N	O	S	0	0	0
			1427	907	231	281	8			
1	M	193	Total	C	N	O	S	0	0	0
			1429	908	231	282	8			
1	N	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	O	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	P	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	192	Total	C	N	O	S	0	0	0
			1422	904	229	281	8			
1	R	191	Total	C	N	O	S	0	0	0
			1421	905	229	279	8			
1	S	191	Total	C	N	O	S	0	0	0
			1417	902	229	278	8			
1	T	192	Total	C	N	O	S	0	0	0
			1421	904	230	279	8			
1	U	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	V	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	W	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	X	194	Total	C	N	O	S	0	0	0
			1434	911	232	283	8			
1	Y	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	Z	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	a	192	Total	C	N	O	S	0	0	0
			1420	902	229	281	8			
1	c	191	Total	C	N	O	S	0	0	0
			1418	902	229	279	8			
1	e	192	Total	C	N	O	S	0	0	0
			1427	907	231	281	8			
1	g	192	Total	C	N	O	S	0	0	0
			1420	903	229	280	8			
1	i	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	k	193	Total	C	N	O	S	0	0	0
			1427	907	231	281	8			
1	m	193	Total	C	N	O	S	0	0	0
			1429	908	231	282	8			
1	o	192	Total	C	N	O	S	0	0	0
			1415	900	227	280	8			
1	q	193	Total	C	N	O	S	0	0	0
			1425	905	230	282	8			
1	r	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	s	193	Total	C	N	O	S	0	0	0
			1429	908	231	282	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	t	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	u	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	v	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	w	192	Total	C	N	O	S	0	0	0
			1406	895	226	277	8			
1	x	192	Total	C	N	O	S	0	0	0
			1414	899	229	278	8			
1	y	193	Total	C	N	O	S	0	0	0
			1429	908	231	282	8			
1	z	192	Total	C	N	O	S	0	0	0
			1422	904	230	280	8			
1	0	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	1	192	Total	C	N	O	S	0	0	0
			1425	906	230	281	8			
1	2	192	Total	C	N	O	S	0	0	0
			1422	904	229	281	8			
1	3	194	Total	C	N	O	S	0	0	0
			1434	911	232	283	8			
1	4	192	Total	C	N	O	S	0	0	0
			1419	902	230	279	8			
1	5	192	Total	C	N	O	S	0	0	0
			1424	905	230	281	8			
1	6	192	Total	C	N	O	S	0	0	0
			1422	903	230	281	8			
1	7	192	Total	C	N	O	S	0	0	0
			1422	904	229	281	8			
1	b	192	Total	C	N	O	S	0	0	0
			1420	902	230	280	8			
1	d	193	Total	C	N	O	S	0	0	0
			1429	908	231	282	8			
1	f	193	Total	C	N	O	S	0	0	0
			1423	904	229	282	8			
1	h	192	Total	C	N	O	S	0	0	0
			1419	902	229	280	8			
1	j	194	Total	C	N	O	S	0	0	0
			1434	911	232	283	8			
1	l	192	Total	C	N	O	S	0	0	0
			1425	906	230	281	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	n	192	Total	C	N	O	S	0	0	0
			1423	904	230	281	8			
1	p	192	Total	C	N	O	S	0	0	0
			1414	899	230	277	8			

There are 1500 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
D	-13	MET	-	expression tag	UNP P02976

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
g	64	GLU	-	linker	UNP P02976
g	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
i	62	GLU	-	linker	UNP P02976
i	63	LEU	-	linker	UNP P02976
i	64	GLU	-	linker	UNP P02976
i	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
k	0	SER	-	expression tag	UNP P02976
k	1	MET	-	expression tag	UNP P02976

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
1	-13	MET	-	expression tag	UNP P02976

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

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

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
7	60	GLY	-	linker	UNP P02976
7	61	SER	-	linker	UNP P02976
7	62	GLU	-	linker	UNP P02976
7	63	LEU	-	linker	UNP P02976
7	64	GLU	-	linker	UNP P02976
7	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
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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
h	-10	SER	-	expression tag	UNP P02976
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	X	1	Total	O	S	0	0
			5	4	1		
2	Z	1	Total	O	S	0	0
			5	4	1		
2	o	1	Total	O	S	0	0
			5	4	1		
2	s	1	Total	O	S	0	0
			5	4	1		
2	w	1	Total	O	S	0	0
			5	4	1		
2	4	1	Total	O	S	0	0
			5	4	1		
2	7	1	Total	O	S	0	0
			5	4	1		
2	h	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	B	13	Total 13	O 13	0	0
3	C	16	Total 16	O 16	0	0
3	D	21	Total 21	O 21	0	0
3	E	21	Total 21	O 21	0	0
3	F	33	Total 33	O 33	0	0
3	G	37	Total 37	O 37	0	0
3	H	29	Total 29	O 29	0	0
3	I	38	Total 38	O 38	0	0
3	J	22	Total 22	O 22	0	0
3	K	28	Total 28	O 28	0	0
3	L	29	Total 29	O 29	0	0
3	M	39	Total 39	O 39	0	0
3	N	27	Total 27	O 27	0	0
3	O	28	Total 28	O 28	0	0
3	P	19	Total 19	O 19	0	0
3	Q	16	Total 16	O 16	0	0
3	R	15	Total 15	O 15	0	0
3	S	16	Total 16	O 16	0	0
3	T	14	Total 14	O 14	0	0
3	U	30	Total 30	O 30	0	0
3	V	25	Total 25	O 25	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	W	34	Total O 34 34	0	0
3	X	28	Total O 28 28	0	0
3	Y	36	Total O 36 36	0	0
3	Z	28	Total O 28 28	0	0
3	a	18	Total O 18 18	0	0
3	c	18	Total O 18 18	0	0
3	e	16	Total O 16 16	0	0
3	g	25	Total O 25 25	0	0
3	i	17	Total O 17 17	0	0
3	k	20	Total O 20 20	0	0
3	m	23	Total O 23 23	0	0
3	o	16	Total O 16 16	0	0
3	q	25	Total O 25 25	0	0
3	r	28	Total O 28 28	0	0
3	s	29	Total O 29 29	0	0
3	t	28	Total O 28 28	0	0
3	u	37	Total O 37 37	0	0
3	v	32	Total O 32 32	0	0
3	w	16	Total O 16 16	0	0
3	x	20	Total O 20 20	0	0
3	y	20	Total O 20 20	0	0

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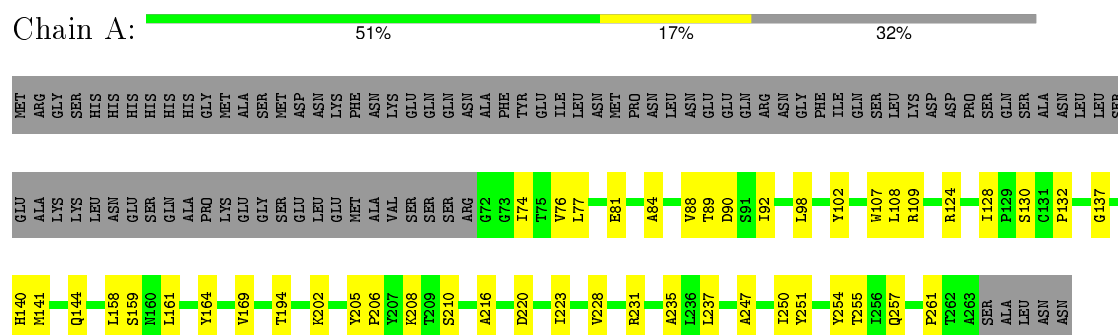
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	z	29	Total 29	O 29	0	0
3	0	23	Total 23	O 23	0	0
3	1	24	Total 24	O 24	0	0
3	2	26	Total 26	O 26	0	0
3	3	19	Total 19	O 19	0	0
3	4	16	Total 16	O 16	0	0
3	5	20	Total 20	O 20	0	0
3	6	19	Total 19	O 19	0	0
3	7	17	Total 17	O 17	0	0
3	b	23	Total 23	O 23	0	0
3	d	28	Total 28	O 28	0	0
3	f	27	Total 27	O 27	0	0
3	h	26	Total 26	O 26	0	0
3	j	16	Total 16	O 16	0	0
3	l	31	Total 31	O 31	0	0
3	n	24	Total 24	O 24	0	0
3	p	23	Total 23	O 23	0	0



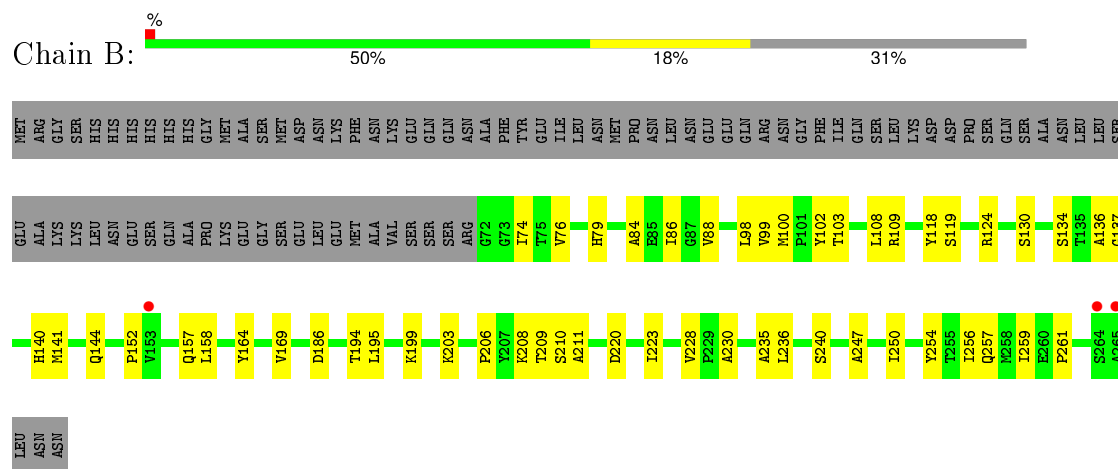
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

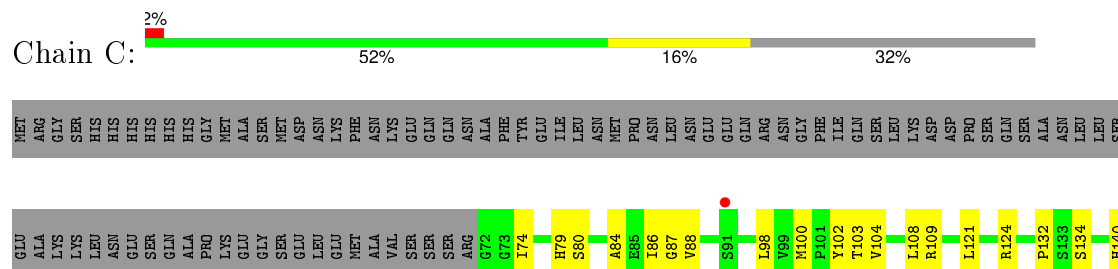
- Molecule 1: Immunoglobulin G-binding protein A,Coat protein



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

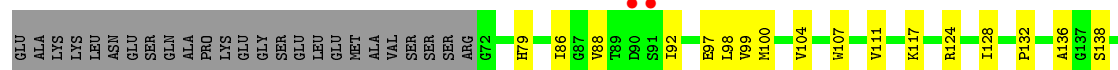
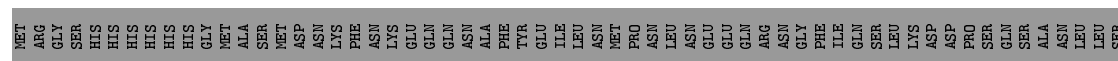


- Molecule 1: Immunoglobulin G-binding protein A,Coat protein





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



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

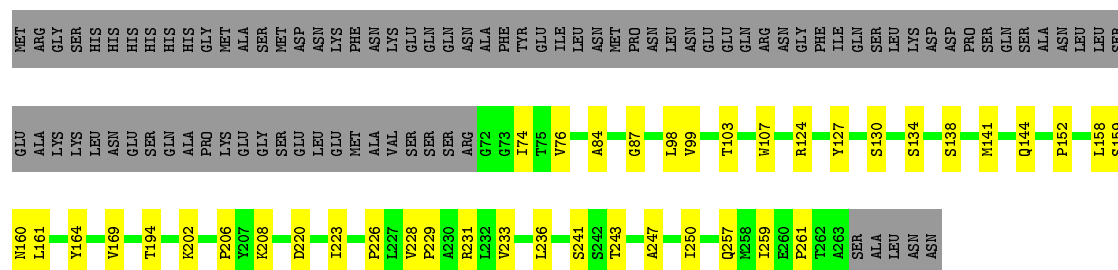


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



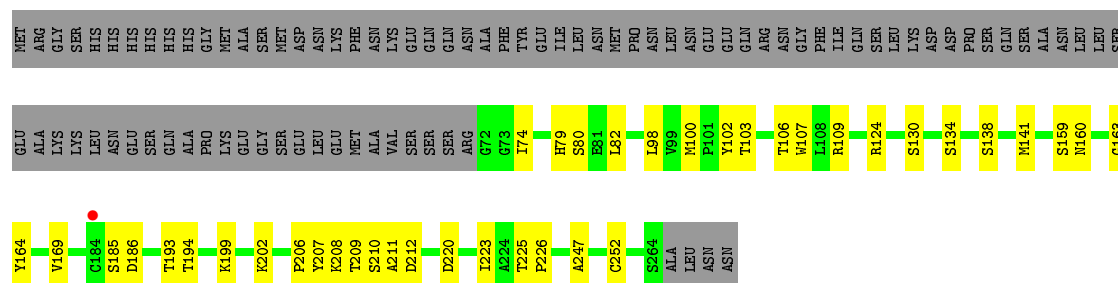
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein





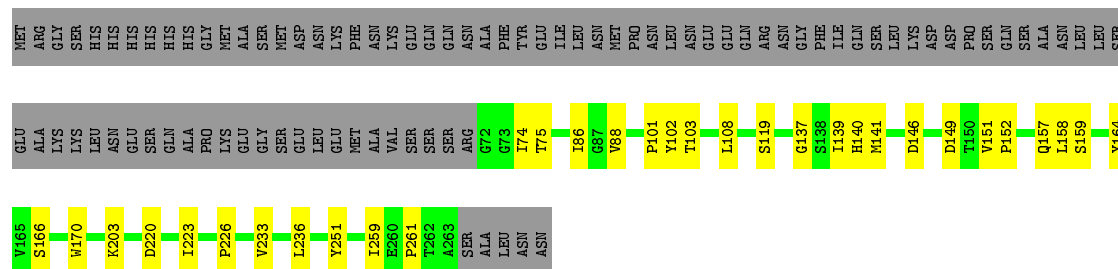
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain H: 54% 14% 32%



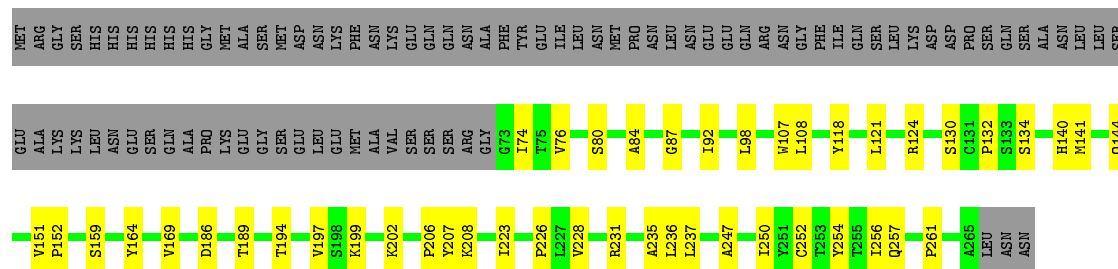
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain I: 57% 11% 32%



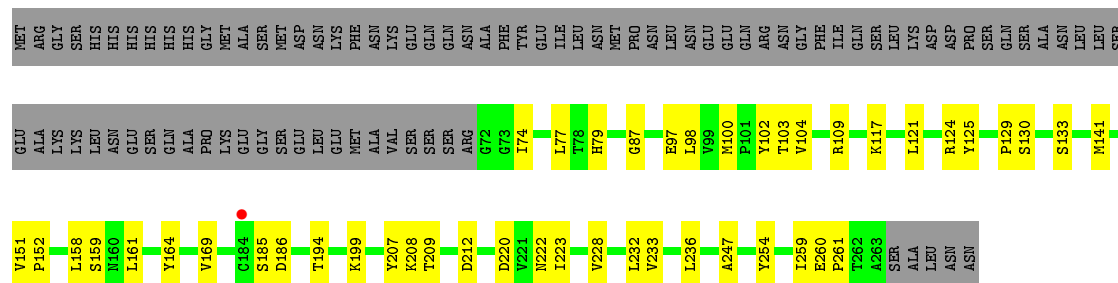
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain J: 52% 16% 32%



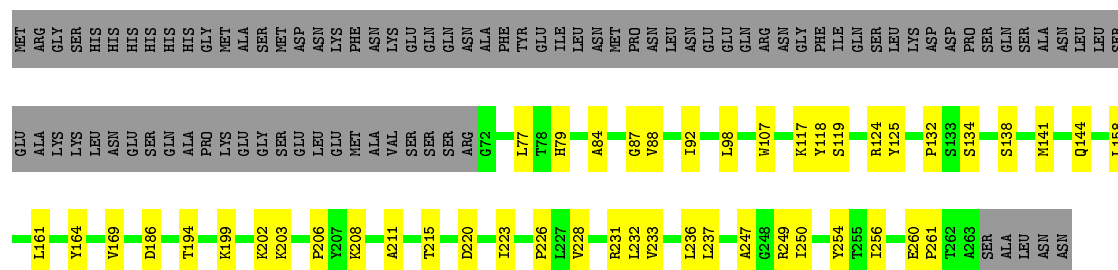
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain K: 52% 16% 32%



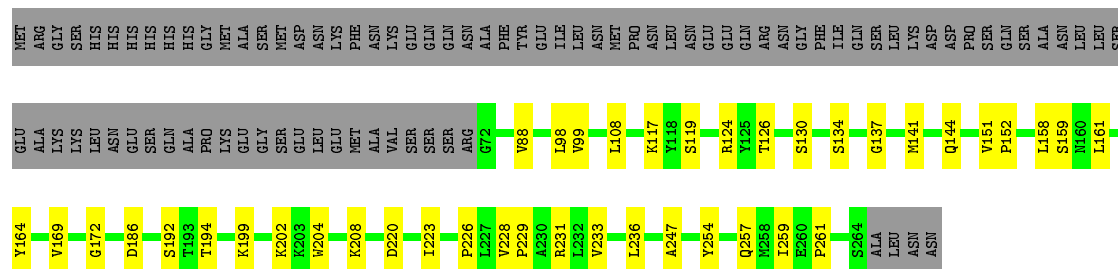
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain L: 51% 17% 32%



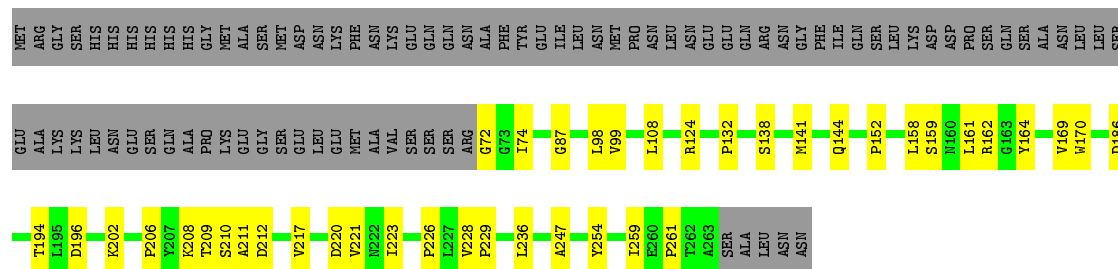
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain M: 54% 15% 32%



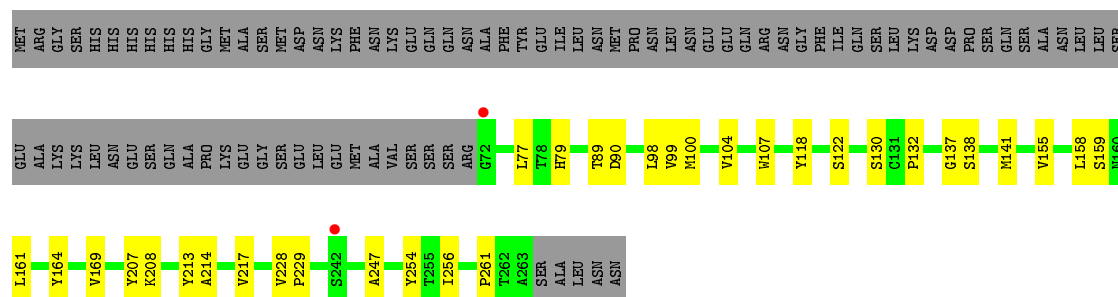
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain N: 54% 15% 32%

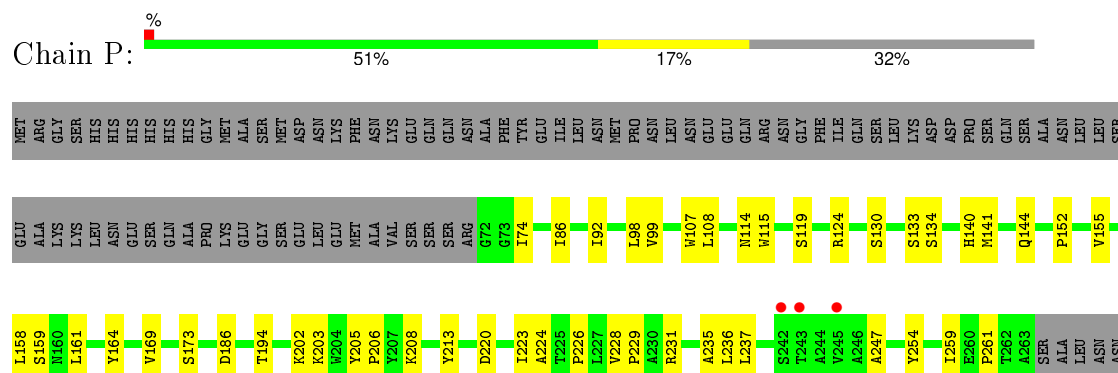


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

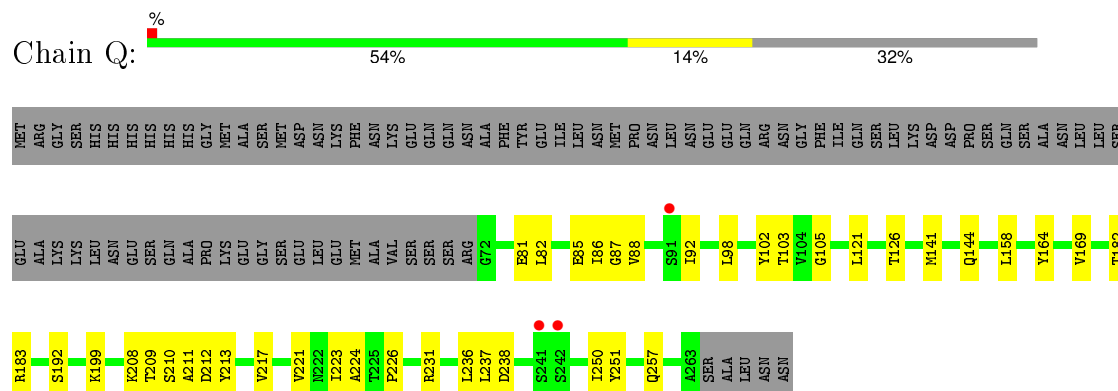
Chain O: 56% 12% 32%



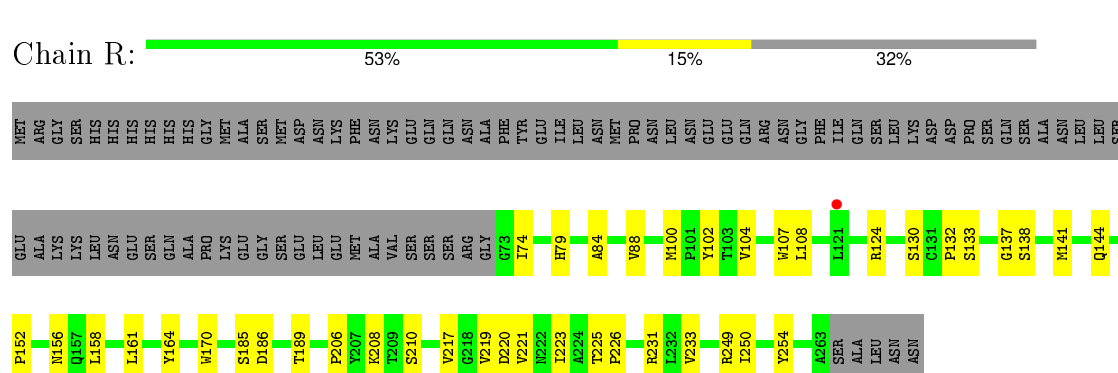
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



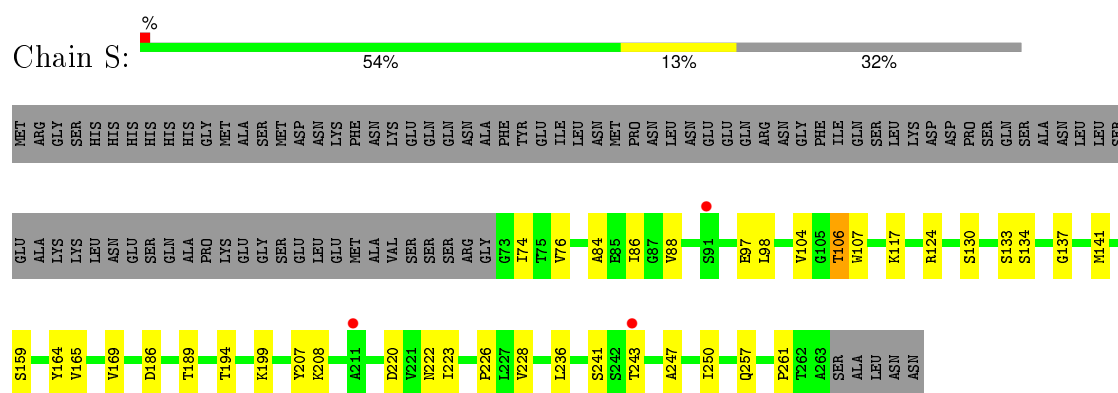
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



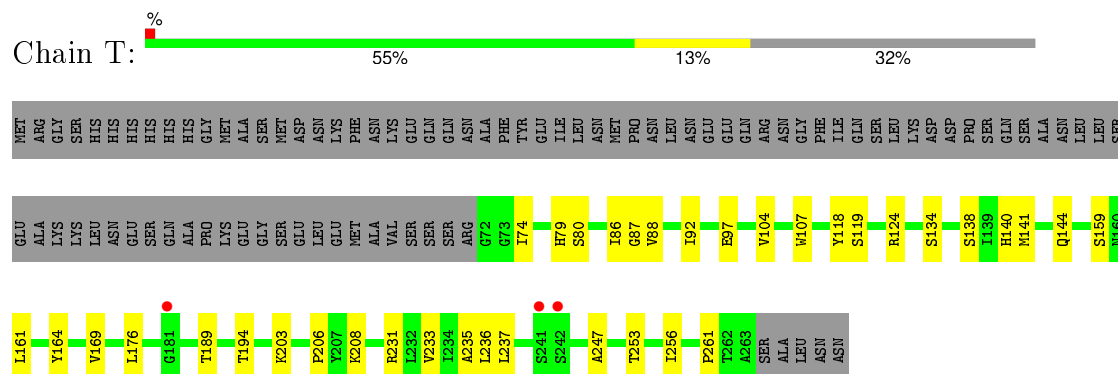
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



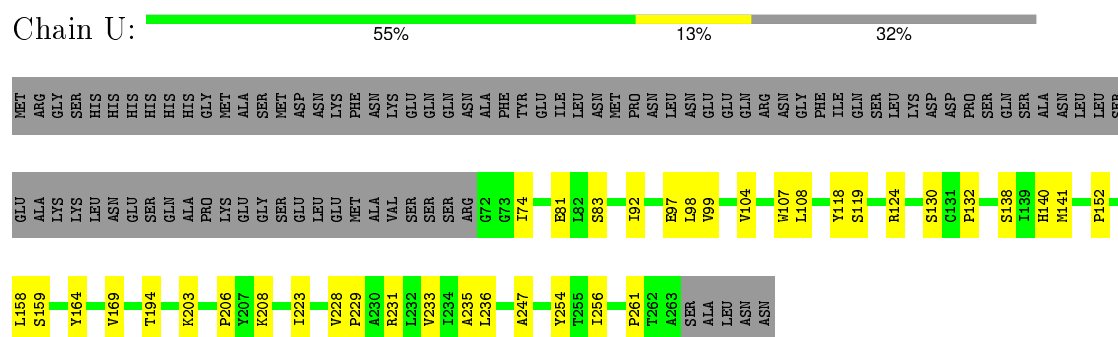
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



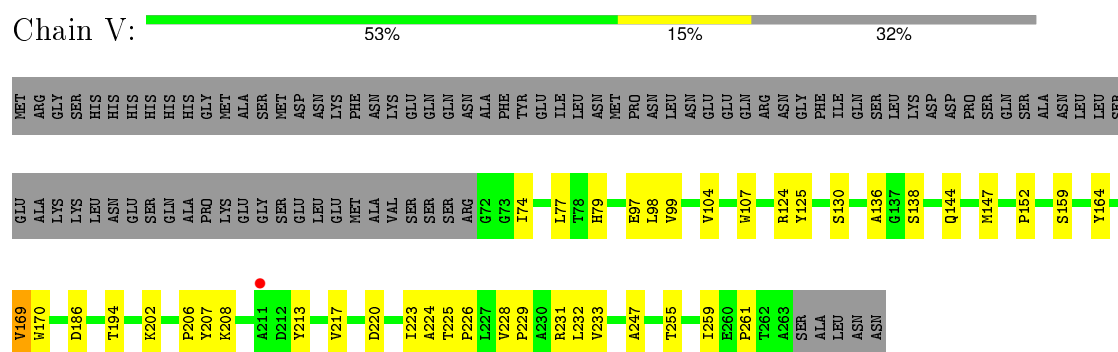
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



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

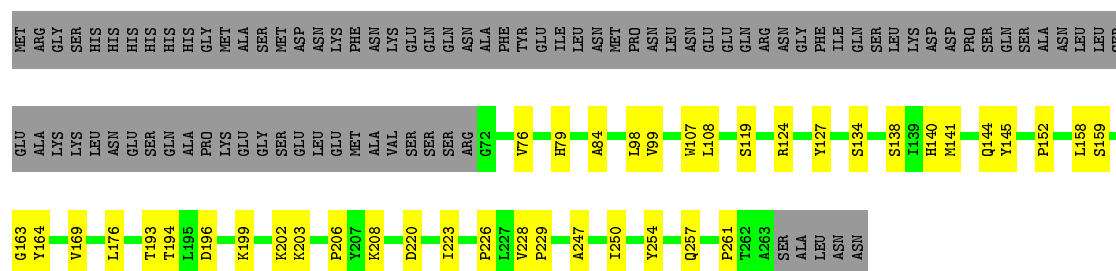


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



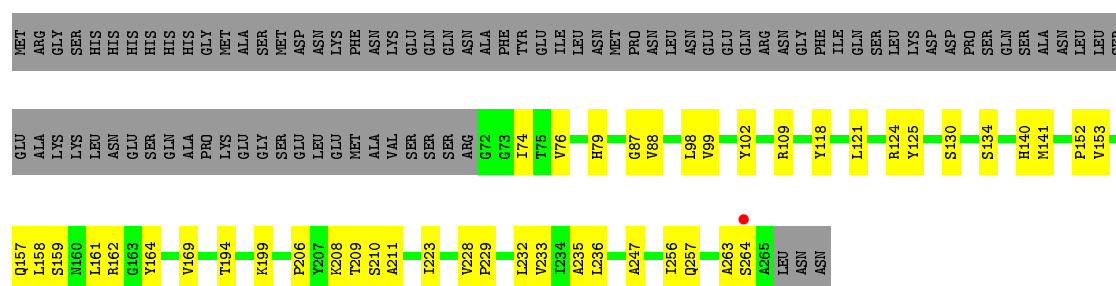
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain W:  54% 15% 32%



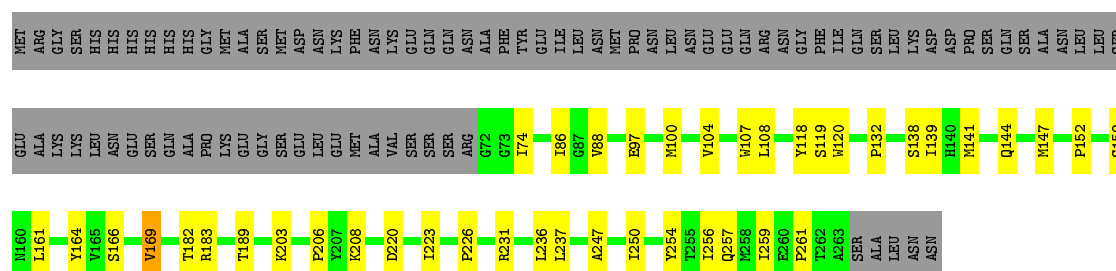
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain X:  53% 16% 31%



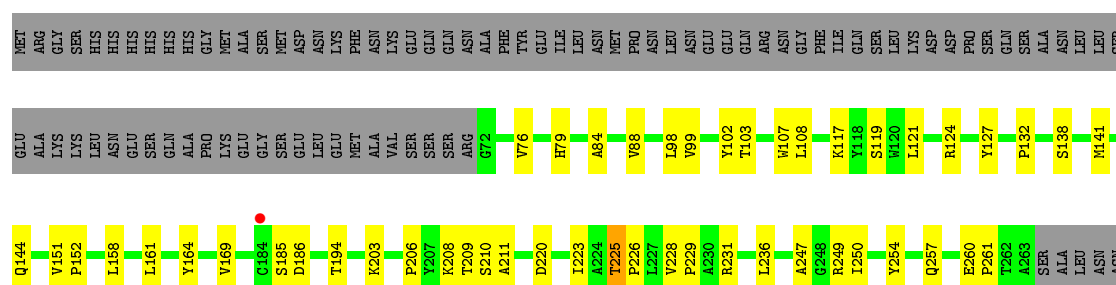
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain Y:  53% 15% 32%

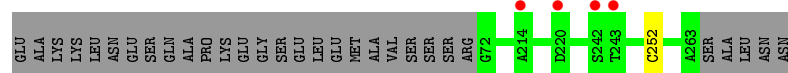


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

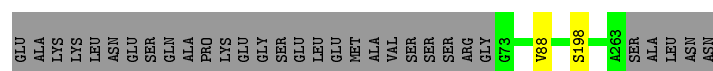
Chain Z:  51% 17% 32%



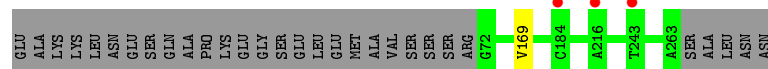
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



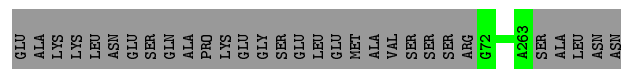
- Chain c:  67% . 32%



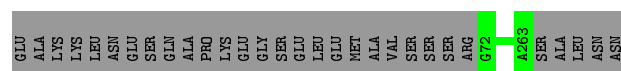
- Chain e:  68% 32%



- Chain g:  68% 32%

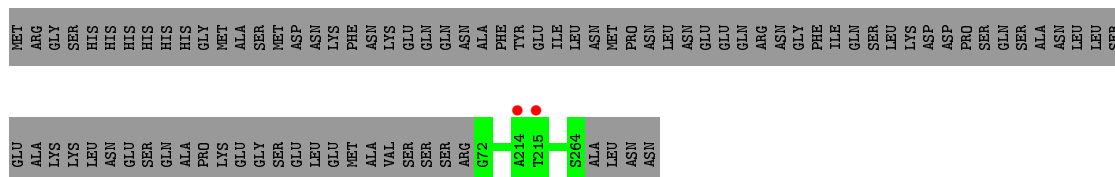


- Chain i:  68% 32%



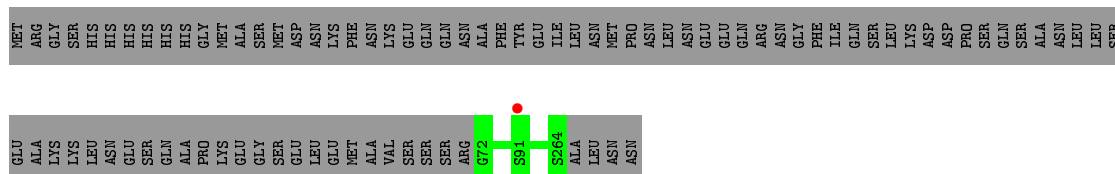
- Chain k:  %





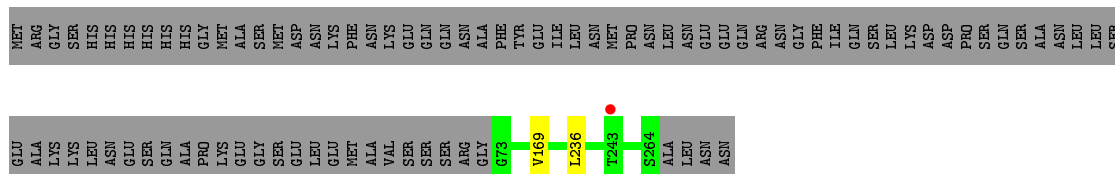
- Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain m: 68% 32%



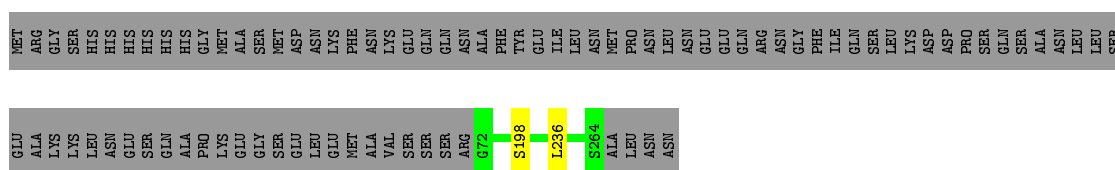
- Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain o: 67% 32%



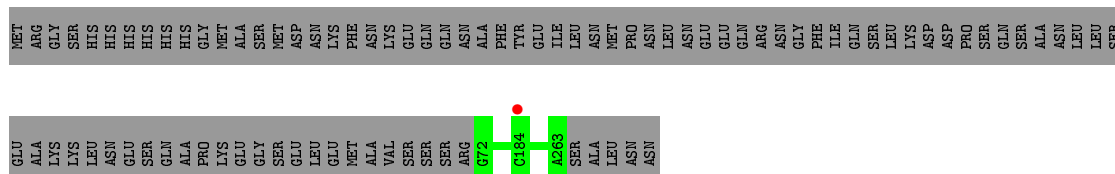
- Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain q: 68% 32%



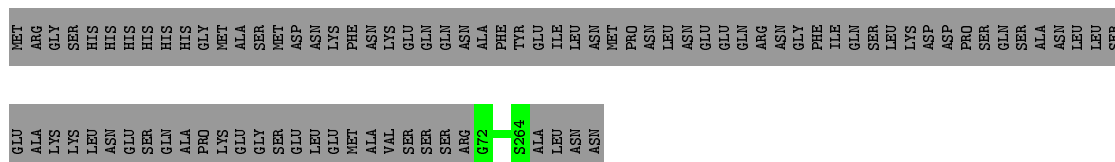
- Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain r: 68% 32%



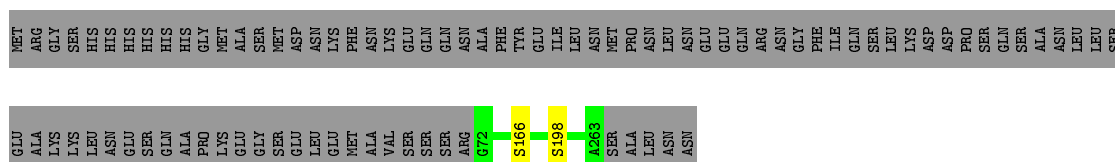
- Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain s: 68% 32%



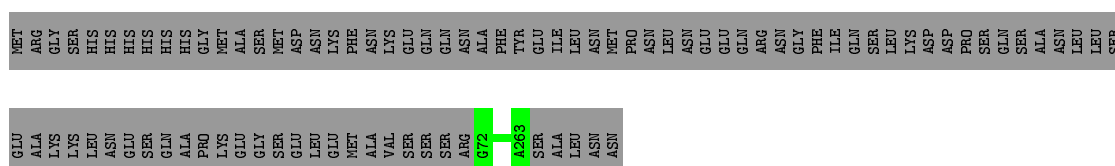
- Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain t:  67% 32%



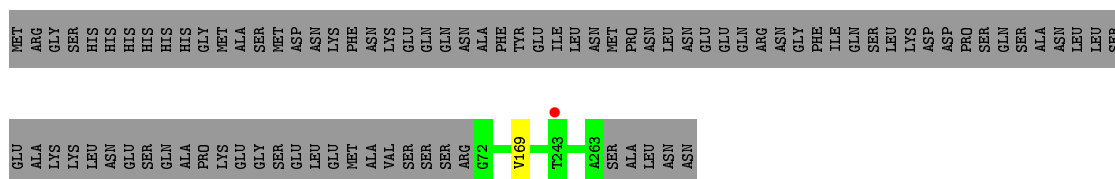
- Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain u:  68% 32%



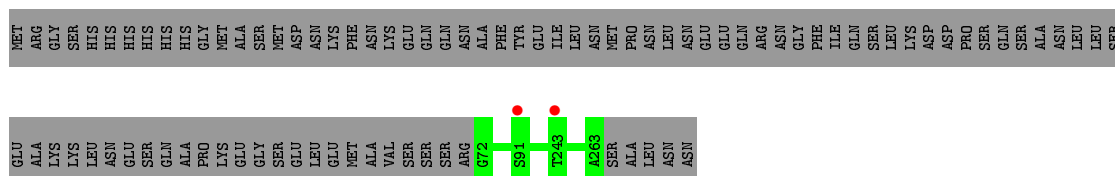
- Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain v:  68% 32%



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

Chain w:  68% 32%



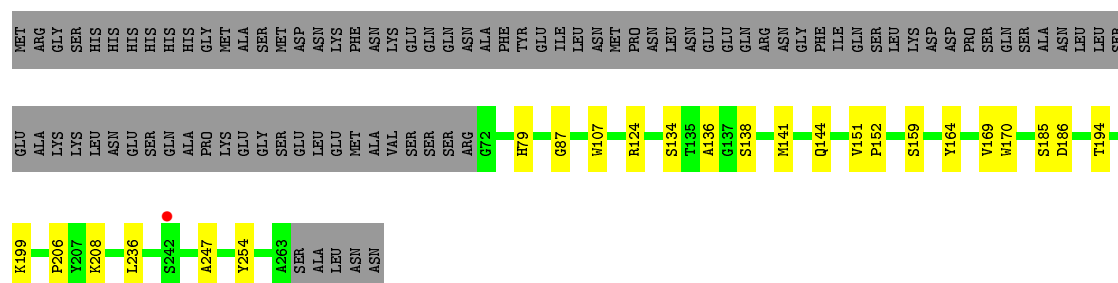
- Molecule 1: Immunoglobulin G-binding protein A,Coat protein

Chain x:  68% 32%



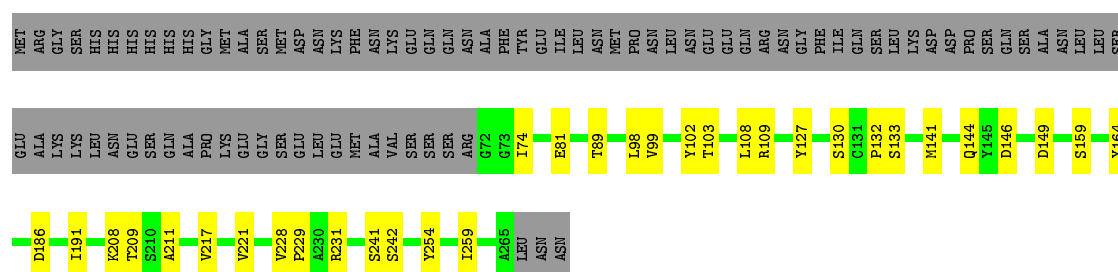


Chain 2:  60% 9% 32%



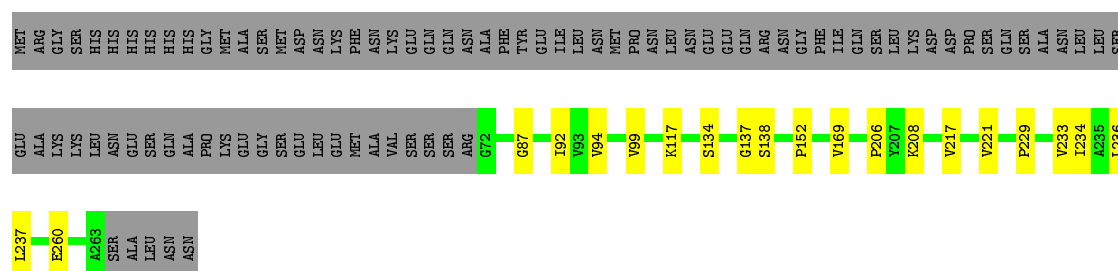
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain 3:  57% 12% 31%



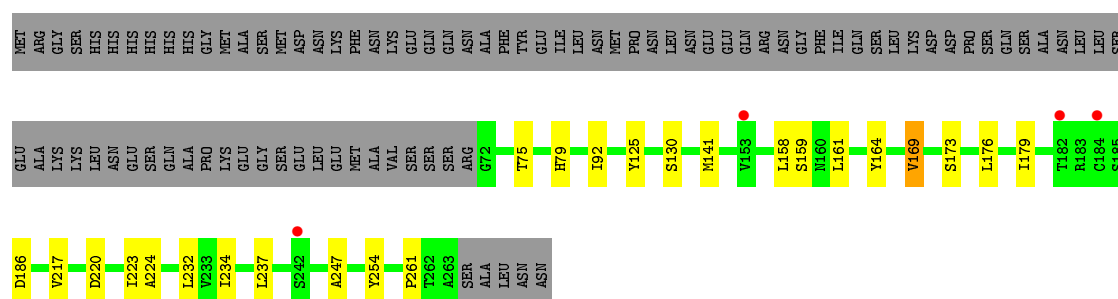
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain 4:  61% 7% 32%



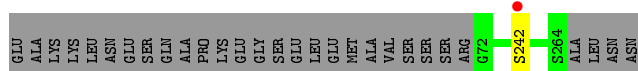
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain 5:  59% 9% 32%



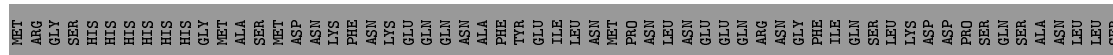
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein





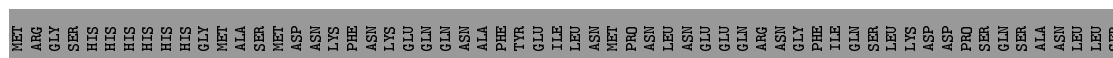
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain h: 68% 32%



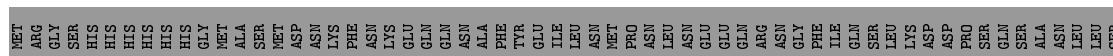
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain j: 69% 31%



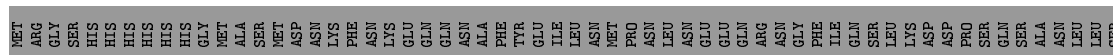
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain l: 68% 32%



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

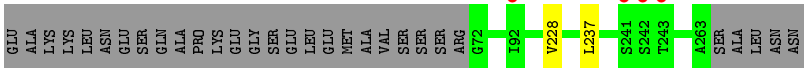
Chain n: 68% 32%



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

Chain p: 67% 32%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.48Å 187.42Å 187.93Å 61.09° 89.24° 60.20°	Depositor
Resolution (Å)	41.92 – 2.95 41.92 – 2.95	Depositor EDS
% Data completeness (in resolution range)	94.1 (41.92-2.95) 69.9 (41.92-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.196 , 0.249 0.194 , 0.249	Depositor DCC
$R_{free}$ test set	17449 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.587	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.0	EDS
Estimated twinning fraction	0.012 for k,l,h-k+l 0.012 for h-k+l,h,k 0.013 for k-l,-h+k-l,-h+k 0.013 for h-k,h-k+l,-k+l 0.012 for l,-h+k,-h 0.012 for -l,k-l,h 0.027 for -h+k-l,-h+k,k 0.027 for -k+l,l,-h+k 0.012 for k,k-l,-h+k-l 0.012 for k-l,h,h-k 0.012 for -h+k,-h,-k+l 0.012 for -k,h-k,h-k+l 0.012 for h-k+l,-k+l,-k 0.012 for h-k,-l,k-l 0.166 for h,h-k,-l 0.015 for -h+k,k,k-l 0.015 for -h,-k+l,l 0.015 for -k,-h,-h+k-l 0.013 for l,h-k+l,h 0.013 for -l,-k,-h 0.027 for -h+k-l,-l,-k 0.069 for -k+l,-k,h-k 0.014 for -h,-h+k-l,-l	Xtriage

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



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Property	Value	Source
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 365675 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	86922	wwPDB-VP
Average B, all atoms ( $\text{\AA}^2$ )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0	0.47	0/1456	0.61	0/1996
1	1	0.49	0/1457	0.64	0/1998
1	2	0.48	0/1454	0.64	0/1994
1	3	0.51	0/1466	0.66	0/2010
1	4	0.48	0/1451	0.64	0/1989
1	5	0.48	0/1456	0.61	0/1996
1	6	0.47	0/1454	0.62	0/1993
1	7	0.45	0/1454	0.62	0/1994
1	A	0.48	0/1455	0.63	0/1995
1	B	0.48	0/1461	0.63	0/2003
1	C	0.43	0/1452	0.59	0/1990
1	D	0.47	0/1452	0.60	0/1991
1	E	0.45	0/1453	0.62	0/1991
1	F	0.55	0/1453	0.67	0/1992
1	G	0.52	0/1459	0.65	0/1999
1	H	0.51	0/1461	0.64	0/2003
1	I	0.52	0/1456	0.64	0/1996
1	J	0.55	0/1462	0.68	0/2005
1	K	0.51	0/1456	0.66	0/1996
1	L	0.54	0/1459	0.65	0/1999
1	M	0.56	0/1461	0.68	0/2003
1	N	0.52	0/1456	0.63	0/1996
1	O	0.51	0/1456	0.61	0/1996
1	P	0.48	0/1456	0.62	0/1996
1	Q	0.46	0/1454	0.59	0/1994
1	R	0.44	0/1453	0.60	0/1992
1	S	0.47	0/1449	0.63	0/1987
1	T	0.48	0/1453	0.63	0/1992
1	U	0.52	0/1456	0.65	0/1996
1	V	0.54	0/1456	0.66	0/1996
1	W	0.51	0/1456	0.64	0/1996
1	X	0.54	0/1466	0.67	0/2010

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Y	0.54	0/1456	0.66	0/1996
1	Z	0.49	0/1456	0.63	0/1996
1	a	0.53	1/1452 (0.1%)	0.63	0/1992
1	b	0.51	0/1452	0.65	0/1990
1	c	0.48	0/1450	0.63	0/1988
1	d	0.51	0/1461	0.65	1/2003 (0.0%)
1	e	0.49	0/1459	0.60	0/1999
1	f	0.51	0/1455	0.67	0/1997
1	g	0.47	0/1452	0.63	0/1991
1	h	0.51	0/1451	0.67	0/1991
1	i	0.49	0/1456	0.62	0/1996
1	j	0.49	0/1466	0.62	0/2010
1	k	0.52	0/1459	0.63	0/2000
1	l	0.49	0/1457	0.63	0/1998
1	m	0.48	0/1461	0.61	0/2003
1	n	0.47	0/1455	0.61	0/1995
1	o	0.48	0/1447	0.64	0/1986
1	p	0.48	0/1446	0.62	0/1982
1	q	0.50	0/1457	0.65	1/1999 (0.1%)
1	r	0.50	0/1456	0.61	0/1996
1	s	0.53	0/1461	0.66	0/2003
1	t	0.53	0/1456	0.67	0/1996
1	u	0.55	0/1456	0.66	0/1996
1	v	0.51	0/1456	0.64	0/1996
1	w	0.47	0/1438	0.64	0/1974
1	x	0.47	0/1446	0.62	0/1983
1	y	0.52	0/1461	0.65	0/2003
1	z	0.48	0/1454	0.64	0/1993
All	All	0.50	1/87331 (0.0%)	0.64	2/119736 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	252	CYS	CB-SG	-5.53	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	236	LEU	CB-CG-CD2	-6.46	100.01	111.00
1	q	236	LEU	CB-CG-CD2	-5.47	101.70	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1424	0	1404	16	0
1	1	1425	0	1403	18	0
1	2	1422	0	1397	17	0
1	3	1434	0	1411	23	1
1	4	1419	0	1389	11	0
1	5	1424	0	1404	15	0
1	6	1422	0	1397	15	0
1	7	1422	0	1397	12	0
1	A	1423	0	1401	34	0
1	B	1429	0	1404	52	0
1	C	1420	0	1390	31	0
1	D	1420	0	1392	34	0
1	E	1421	0	1400	31	0
1	F	1421	0	1402	44	0
1	G	1427	0	1410	35	0
1	H	1429	0	1406	35	0
1	I	1424	0	1404	21	0
1	J	1430	0	1408	35	0
1	K	1424	0	1404	34	0
1	L	1427	0	1410	34	0
1	M	1429	0	1406	35	0
1	N	1424	0	1404	39	0
1	O	1424	0	1404	29	0
1	P	1424	0	1404	36	0
1	Q	1422	0	1397	31	0
1	R	1421	0	1402	35	0
1	S	1417	0	1399	32	0
1	T	1421	0	1402	32	0
1	U	1424	0	1404	28	0
1	V	1424	0	1404	32	0
1	W	1424	0	1404	32	0
1	X	1434	0	1411	37	0
1	Y	1424	0	1404	39	0
1	Z	1424	0	1404	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	1420	0	1393	0	0
1	b	1420	0	1392	0	0
1	c	1418	0	1396	0	0
1	d	1429	0	1406	0	0
1	e	1427	0	1410	0	0
1	f	1423	0	1388	0	1
1	g	1420	0	1392	0	0
1	h	1419	0	1390	0	0
1	i	1424	0	1404	0	0
1	j	1434	0	1411	0	0
1	k	1427	0	1401	0	0
1	l	1425	0	1403	0	0
1	m	1429	0	1406	0	0
1	n	1423	0	1399	0	0
1	o	1415	0	1376	0	0
1	p	1414	0	1380	0	0
1	q	1425	0	1395	0	0
1	r	1424	0	1404	0	0
1	s	1429	0	1406	0	0
1	t	1424	0	1404	0	0
1	u	1424	0	1404	0	0
1	v	1424	0	1404	0	0
1	w	1406	0	1371	0	0
1	x	1414	0	1381	0	0
1	y	1429	0	1406	0	0
1	z	1422	0	1399	0	0
2	4	5	0	0	2	0
2	7	5	0	0	1	0
2	A	5	0	0	0	0
2	H	5	0	0	2	0
2	M	5	0	0	0	0
2	P	5	0	0	2	0
2	X	5	0	0	1	0
2	Z	5	0	0	1	0
2	h	5	0	0	0	0
2	o	5	0	0	0	0
2	s	5	0	0	0	0
2	w	5	0	0	0	0
3	0	23	0	0	3	0
3	1	24	0	0	0	0
3	2	26	0	0	0	0
3	3	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4	16	0	0	0	0
3	5	20	0	0	1	0
3	6	19	0	0	0	0
3	7	17	0	0	0	0
3	A	30	0	0	1	0
3	B	13	0	0	0	0
3	C	16	0	0	0	0
3	D	21	0	0	0	0
3	E	21	0	0	0	0
3	F	33	0	0	2	0
3	G	37	0	0	0	0
3	H	29	0	0	1	0
3	I	38	0	0	1	0
3	J	22	0	0	0	0
3	K	28	0	0	1	0
3	L	29	0	0	0	0
3	M	39	0	0	1	0
3	N	27	0	0	3	0
3	O	28	0	0	0	0
3	P	19	0	0	0	0
3	Q	16	0	0	1	0
3	R	15	0	0	2	0
3	S	16	0	0	0	0
3	T	14	0	0	0	0
3	U	30	0	0	1	0
3	V	25	0	0	0	0
3	W	34	0	0	1	0
3	X	28	0	0	0	0
3	Y	36	0	0	3	1
3	Z	28	0	0	0	0
3	a	18	0	0	0	0
3	b	23	0	0	0	0
3	c	18	0	0	0	0
3	d	28	0	0	0	0
3	e	16	0	0	0	0
3	f	27	0	0	0	0
3	g	25	0	0	0	0
3	h	26	0	0	0	0
3	i	17	0	0	0	0
3	j	16	0	0	0	0
3	k	20	0	0	0	0
3	l	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	m	23	0	0	0	0
3	n	24	0	0	0	0
3	o	16	0	0	0	0
3	p	23	0	0	0	0
3	q	25	0	0	0	0
3	r	28	0	0	0	0
3	s	29	0	0	0	0
3	t	28	0	0	0	1
3	u	37	0	0	0	0
3	v	32	0	0	0	0
3	w	16	0	0	0	0
3	x	20	0	0	0	0
3	y	20	0	0	0	0
3	z	29	0	0	0	0
All	All	86922	0	84003	908	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 908 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:86:ILE:HG23	1:Y:236:LEU:HD11	1.60	0.83
1:R:217:VAL:HG13	1:R:221:VAL:HG12	7.63	0.80
1:J:144:GLN:OE1	1:J:231:ARG:NH1	2.18	0.77
1:M:144:GLN:OE1	1:M:231:ARG:NH1	2.20	0.75
1:Q:86:ILE:HG23	1:Q:236:LEU:HD21	2.74	0.75

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:242:SER:N	1:f:242:SER:OG[1_556]	2.09	0.11
3:Y:330:HOH:O	3:t:328:HOH:O[1_645]	2.16	0.04

## 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	0	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	1	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	2	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	3	192/282 (68%)	186 (97%)	6 (3%)	0	100	100
1	4	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	5	190/282 (67%)	183 (96%)	7 (4%)	0	100	100
1	6	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	7	190/282 (67%)	185 (97%)	5 (3%)	0	100	100
1	A	190/282 (67%)	183 (96%)	7 (4%)	0	100	100
1	B	192/282 (68%)	185 (96%)	7 (4%)	0	100	100
1	C	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	D	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	E	189/282 (67%)	183 (97%)	6 (3%)	0	100	100
1	F	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	G	190/282 (67%)	186 (98%)	4 (2%)	0	100	100
1	H	191/282 (68%)	185 (97%)	6 (3%)	0	100	100
1	I	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	J	191/282 (68%)	184 (96%)	7 (4%)	0	100	100
1	K	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	L	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	M	191/282 (68%)	184 (96%)	7 (4%)	0	100	100
1	N	190/282 (67%)	185 (97%)	5 (3%)	0	100	100
1	O	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	P	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	Q	190/282 (67%)	184 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	189/282 (67%)	184 (97%)	5 (3%)	0	100	100
1	S	189/282 (67%)	183 (97%)	6 (3%)	0	100	100
1	T	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	U	190/282 (67%)	185 (97%)	5 (3%)	0	100	100
1	V	190/282 (67%)	185 (97%)	5 (3%)	0	100	100
1	W	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	X	192/282 (68%)	185 (96%)	7 (4%)	0	100	100
1	Y	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	Z	190/282 (67%)	183 (96%)	7 (4%)	0	100	100
1	a	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	b	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	c	189/282 (67%)	183 (97%)	6 (3%)	0	100	100
1	d	191/282 (68%)	185 (97%)	6 (3%)	0	100	100
1	e	190/282 (67%)	183 (96%)	7 (4%)	0	100	100
1	f	191/282 (68%)	184 (96%)	7 (4%)	0	100	100
1	g	190/282 (67%)	183 (96%)	7 (4%)	0	100	100
1	h	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	i	190/282 (67%)	183 (96%)	7 (4%)	0	100	100
1	j	192/282 (68%)	185 (96%)	7 (4%)	0	100	100
1	k	191/282 (68%)	185 (97%)	6 (3%)	0	100	100
1	l	190/282 (67%)	183 (96%)	7 (4%)	0	100	100
1	m	191/282 (68%)	185 (97%)	6 (3%)	0	100	100
1	n	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	o	190/282 (67%)	185 (97%)	5 (3%)	0	100	100
1	p	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	q	191/282 (68%)	185 (97%)	6 (3%)	0	100	100
1	r	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	s	191/282 (68%)	185 (97%)	6 (3%)	0	100	100
1	t	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	u	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	v	190/282 (67%)	184 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	x	190/282 (67%)	184 (97%)	6 (3%)	0	100	100
1	y	191/282 (68%)	185 (97%)	6 (3%)	0	100	100
1	z	190/282 (67%)	185 (97%)	5 (3%)	0	100	100
All	All	11414/16920 (68%)	11050 (97%)	364 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	0	158/238 (66%)	157 (99%)	1 (1%)	90	97
1	1	158/238 (66%)	157 (99%)	1 (1%)	90	97
1	2	157/238 (66%)	157 (100%)	0	100	100
1	3	158/238 (66%)	158 (100%)	0	100	100
1	4	155/238 (65%)	155 (100%)	0	100	100
1	5	158/238 (66%)	156 (99%)	2 (1%)	76	92
1	6	157/238 (66%)	157 (100%)	0	100	100
1	7	157/238 (66%)	157 (100%)	0	100	100
1	A	157/238 (66%)	157 (100%)	0	100	100
1	B	156/238 (66%)	156 (100%)	0	100	100
1	C	156/238 (66%)	156 (100%)	0	100	100
1	D	156/238 (66%)	156 (100%)	0	100	100
1	E	157/238 (66%)	157 (100%)	0	100	100
1	F	157/238 (66%)	156 (99%)	1 (1%)	90	97
1	G	158/238 (66%)	158 (100%)	0	100	100
1	H	158/238 (66%)	158 (100%)	0	100	100
1	I	158/238 (66%)	158 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	158/238 (66%)	158 (100%)	0	100	100
1	K	158/238 (66%)	158 (100%)	0	100	100
1	L	158/238 (66%)	158 (100%)	0	100	100
1	M	158/238 (66%)	158 (100%)	0	100	100
1	N	158/238 (66%)	158 (100%)	0	100	100
1	O	158/238 (66%)	158 (100%)	0	100	100
1	P	158/238 (66%)	158 (100%)	0	100	100
1	Q	157/238 (66%)	157 (100%)	0	100	100
1	R	157/238 (66%)	156 (99%)	1 (1%)	90	97
1	S	157/238 (66%)	155 (99%)	2 (1%)	76	92
1	T	157/238 (66%)	157 (100%)	0	100	100
1	U	158/238 (66%)	158 (100%)	0	100	100
1	V	158/238 (66%)	157 (99%)	1 (1%)	90	97
1	W	158/238 (66%)	158 (100%)	0	100	100
1	X	158/238 (66%)	158 (100%)	0	100	100
1	Y	158/238 (66%)	156 (99%)	2 (1%)	76	92
1	Z	158/238 (66%)	157 (99%)	1 (1%)	90	97
1	a	157/238 (66%)	157 (100%)	0	100	100
1	b	156/238 (66%)	155 (99%)	1 (1%)	90	97
1	c	157/238 (66%)	155 (99%)	2 (1%)	76	92
1	d	158/238 (66%)	157 (99%)	1 (1%)	90	97
1	e	158/238 (66%)	157 (99%)	1 (1%)	90	97
1	f	156/238 (66%)	156 (100%)	0	100	100
1	g	156/238 (66%)	156 (100%)	0	100	100
1	h	156/238 (66%)	155 (99%)	1 (1%)	90	97
1	i	158/238 (66%)	158 (100%)	0	100	100
1	j	158/238 (66%)	158 (100%)	0	100	100
1	k	157/238 (66%)	157 (100%)	0	100	100
1	l	158/238 (66%)	158 (100%)	0	100	100
1	m	158/238 (66%)	158 (100%)	0	100	100
1	n	157/238 (66%)	157 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	154/238 (65%)	152 (99%)	2 (1%)	76	92
1	p	153/238 (64%)	151 (99%)	2 (1%)	76	92
1	q	157/238 (66%)	156 (99%)	1 (1%)	90	97
1	r	158/238 (66%)	158 (100%)	0	100	100
1	s	158/238 (66%)	158 (100%)	0	100	100
1	t	158/238 (66%)	156 (99%)	2 (1%)	76	92
1	u	158/238 (66%)	158 (100%)	0	100	100
1	v	158/238 (66%)	157 (99%)	1 (1%)	90	97
1	w	153/238 (64%)	153 (100%)	0	100	100
1	x	154/238 (65%)	154 (100%)	0	100	100
1	y	158/238 (66%)	156 (99%)	2 (1%)	76	92
1	z	157/238 (66%)	156 (99%)	1 (1%)	90	97
All	All	9429/14280 (66%)	9400 (100%)	29 (0%)	94	98

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	q	198	SER
1	v	169	VAL
1	h	160	ASN
1	t	166	SER
1	y	88	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	V	160	ASN
1	f	160	ASN
1	W	79	HIS
1	H	79	HIS
1	y	160	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	4	301	-	4,4,4	0.61	0	6,6,6	0.36	0
2	SO4	7	301	-	4,4,4	0.91	0	6,6,6	0.70	0
2	SO4	A	301	-	4,4,4	0.72	0	6,6,6	0.39	0
2	SO4	H	301	-	4,4,4	1.40	0	6,6,6	0.31	0
2	SO4	M	301	-	4,4,4	1.51	0	6,6,6	0.40	0
2	SO4	P	301	-	4,4,4	0.85	0	6,6,6	0.25	0
2	SO4	X	301	-	4,4,4	1.55	0	6,6,6	0.69	0
2	SO4	Z	301	-	4,4,4	1.20	0	6,6,6	0.66	0
2	SO4	h	301	-	4,4,4	1.13	0	6,6,6	0.34	0
2	SO4	o	301	-	4,4,4	0.91	0	6,6,6	0.26	0
2	SO4	s	301	-	4,4,4	1.50	0	6,6,6	0.78	0
2	SO4	w	301	-	4,4,4	1.23	0	6,6,6	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	4	301	-	-	0/0/0/0	0/0/0/0
2	SO4	7	301	-	-	0/0/0/0	0/0/0/0
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	H	301	-	-	0/0/0/0	0/0/0/0
2	SO4	M	301	-	-	0/0/0/0	0/0/0/0
2	SO4	P	301	-	-	0/0/0/0	0/0/0/0
2	SO4	X	301	-	-	0/0/0/0	0/0/0/0
2	SO4	Z	301	-	-	0/0/0/0	0/0/0/0
2	SO4	h	301	-	-	0/0/0/0	0/0/0/0
2	SO4	o	301	-	-	0/0/0/0	0/0/0/0
2	SO4	s	301	-	-	0/0/0/0	0/0/0/0
2	SO4	w	301	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	4	301	SO4	2	0
2	7	301	SO4	1	0
2	H	301	SO4	2	0
2	P	301	SO4	2	0
2	X	301	SO4	1	0
2	Z	301	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	0	192/282 (68%)	-0.45	1 (0%) 91 81	16, 26, 43, 55	0
1	1	192/282 (68%)	-0.44	2 (1%) 84 67	19, 29, 47, 57	0
1	2	192/282 (68%)	-0.54	1 (0%) 91 81	15, 26, 41, 51	0
1	3	194/282 (68%)	-0.51	0 100 100	17, 27, 43, 57	0
1	4	192/282 (68%)	-0.46	0 100 100	17, 30, 53, 69	0
1	5	192/282 (68%)	-0.44	4 (2%) 67 46	20, 30, 51, 61	0
1	6	192/282 (68%)	-0.37	3 (1%) 74 55	20, 30, 55, 64	0
1	7	192/282 (68%)	-0.45	1 (0%) 91 81	19, 31, 50, 57	0
1	A	192/282 (68%)	-0.49	0 100 100	15, 29, 44, 49	0
1	B	194/282 (68%)	-0.43	3 (1%) 76 57	21, 31, 51, 62	0
1	C	192/282 (68%)	-0.33	5 (2%) 59 38	21, 33, 54, 71	0
1	D	192/282 (68%)	-0.28	7 (3%) 46 28	19, 32, 53, 62	0
1	E	191/282 (67%)	-0.32	4 (2%) 67 46	22, 30, 49, 60	0
1	F	192/282 (68%)	-0.67	0 100 100	10, 20, 38, 48	0
1	G	192/282 (68%)	-0.71	0 100 100	12, 19, 37, 48	0
1	H	193/282 (68%)	-0.58	1 (0%) 91 81	11, 21, 42, 56	0
1	I	192/282 (68%)	-0.68	0 100 100	11, 19, 36, 50	0
1	J	193/282 (68%)	-0.65	0 100 100	10, 16, 34, 56	0
1	K	192/282 (68%)	-0.59	1 (0%) 91 81	10, 20, 38, 55	0
1	L	192/282 (68%)	-0.74	0 100 100	8, 17, 33, 47	0
1	M	193/282 (68%)	-0.69	0 100 100	9, 19, 38, 51	0
1	N	192/282 (68%)	-0.66	0 100 100	11, 20, 39, 53	0
1	O	192/282 (68%)	-0.58	2 (1%) 84 67	11, 20, 43, 55	0
1	P	192/282 (68%)	-0.45	3 (1%) 74 55	18, 30, 49, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Q	192/282 (68%)	-0.33	3 (1%) 74 55	20, 33, 54, 62	0
1	R	191/282 (67%)	-0.37	1 (0%) 91 81	19, 32, 50, 60	0
1	S	191/282 (67%)	-0.36	3 (1%) 74 55	18, 31, 49, 59	0
1	T	192/282 (68%)	-0.46	3 (1%) 74 55	17, 28, 43, 52	0
1	U	192/282 (68%)	-0.61	0 100 100	11, 21, 38, 49	0
1	V	192/282 (68%)	-0.55	1 (0%) 91 81	9, 22, 41, 51	0
1	W	192/282 (68%)	-0.60	0 100 100	11, 21, 38, 47	0
1	X	194/282 (68%)	-0.63	1 (0%) 91 81	11, 18, 33, 54	0
1	Y	192/282 (68%)	-0.67	0 100 100	12, 19, 36, 42	0
1	Z	192/282 (68%)	-0.45	1 (0%) 91 81	16, 27, 41, 46	0
1	a	192/282 (68%)	-0.35	4 (2%) 67 46	18, 29, 56, 66	0
1	b	192/282 (68%)	-0.44	1 (0%) 91 81	19, 28, 48, 60	0
1	c	191/282 (67%)	-0.39	0 100 100	18, 29, 49, 54	0
1	d	193/282 (68%)	-0.54	0 100 100	12, 26, 41, 48	0
1	e	192/282 (68%)	-0.38	3 (1%) 74 55	14, 25, 42, 53	0
1	f	193/282 (68%)	-0.47	1 (0%) 91 81	18, 28, 43, 57	0
1	g	192/282 (68%)	-0.48	0 100 100	16, 25, 44, 53	0
1	h	192/282 (68%)	-0.43	1 (0%) 91 81	17, 27, 45, 60	0
1	i	192/282 (68%)	-0.53	0 100 100	14, 25, 44, 47	0
1	j	194/282 (68%)	-0.49	2 (1%) 84 67	16, 24, 44, 74	0
1	k	193/282 (68%)	-0.40	2 (1%) 84 67	15, 25, 43, 58	0
1	l	192/282 (68%)	-0.38	2 (1%) 84 67	15, 24, 43, 63	0
1	m	193/282 (68%)	-0.42	1 (0%) 91 81	13, 26, 45, 54	0
1	n	192/282 (68%)	-0.42	0 100 100	16, 26, 44, 52	0
1	o	192/282 (68%)	-0.39	1 (0%) 91 81	18, 31, 51, 69	0
1	p	192/282 (68%)	-0.33	4 (2%) 67 46	21, 30, 53, 69	0
1	q	193/282 (68%)	-0.43	0 100 100	18, 27, 45, 59	0
1	r	192/282 (68%)	-0.54	1 (0%) 91 81	10, 21, 42, 58	0
1	s	193/282 (68%)	-0.58	0 100 100	10, 20, 36, 51	0
1	t	192/282 (68%)	-0.69	0 100 100	10, 17, 33, 46	0
1	u	192/282 (68%)	-0.63	0 100 100	9, 19, 38, 48	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	v	192/282 (68%)	-0.65	1 (0%) 91 81	11, 19, 36, 45	0
1	w	192/282 (68%)	-0.39	2 (1%) 84 67	17, 30, 52, 65	0
1	x	192/282 (68%)	-0.45	0 100 100	19, 28, 48, 53	0
1	y	193/282 (68%)	-0.39	3 (1%) 74 55	15, 25, 44, 51	0
1	z	192/282 (68%)	-0.49	1 (0%) 91 81	16, 26, 46, 53	0
All	All	11534/16920 (68%)	-0.49	81 (0%) 89 76	8, 26, 46, 74	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	p	242	SER	4.1
1	a	242	SER	3.8
1	S	211	ALA	3.4
1	w	91	SER	3.3
1	D	91	SER	3.2

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	o	301	5/5	0.99	0.16	1.04	7,9,15,20	0
2	SO4	H	301	5/5	1.00	0.15	0.91	0,7,10,11	0
2	SO4	X	301	5/5	0.99	0.14	0.79	0,5,8,8	0
2	SO4	M	301	5/5	0.99	0.13	0.32	0,5,8,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	s	301	5/5	0.99	0.12	-0.25	0,4,7,11	0
2	SO4	w	301	5/5	0.99	0.13	-0.40	0,12,16,16	0
2	SO4	Z	301	5/5	1.00	0.13	-0.50	0,11,15,17	0
2	SO4	7	301	5/5	0.99	0.12	-0.60	5,14,20,21	0
2	SO4	4	301	5/5	0.99	0.13	-0.74	13,14,22,22	0
2	SO4	A	301	5/5	1.00	0.12	-0.95	8,19,20,21	0
2	SO4	P	301	5/5	0.99	0.10	-1.37	6,17,21,26	0
2	SO4	h	301	5/5	1.00	0.12	-1.82	0,8,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.