



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:37 PM GMT

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

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

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (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

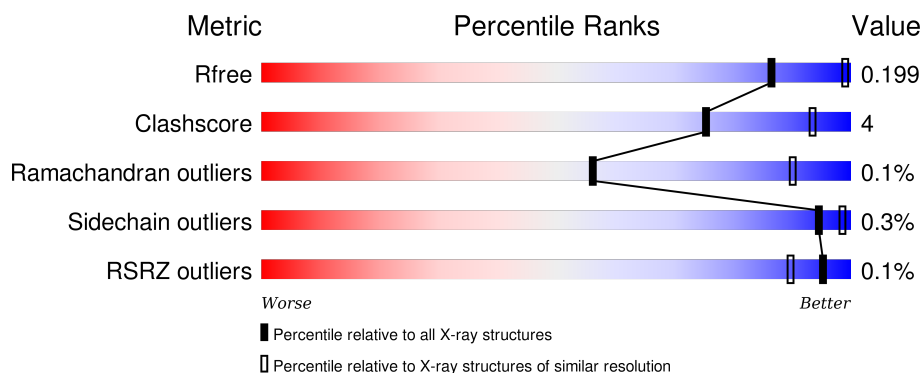
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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














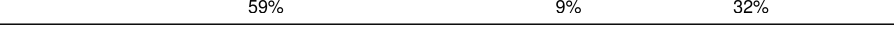







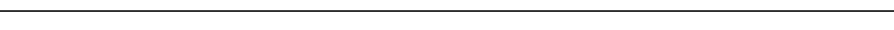

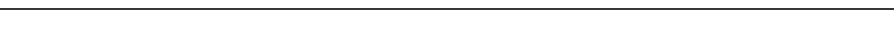
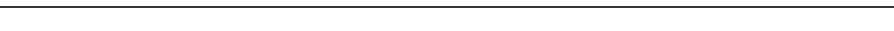


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	282	 61% 7% 32%
1	B	282	 60% 7% 32%
1	C	282	 59% 9% 32%
1	D	282	 60% 7% 32%
1	E	282	 62% 5% 32%

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

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	D	301	-	-	X	-
2	SO4	L	301	-	-	-	X
2	SO4	M	301	-	-	X	X
2	SO4	S	301	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 42805 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

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

There are 750 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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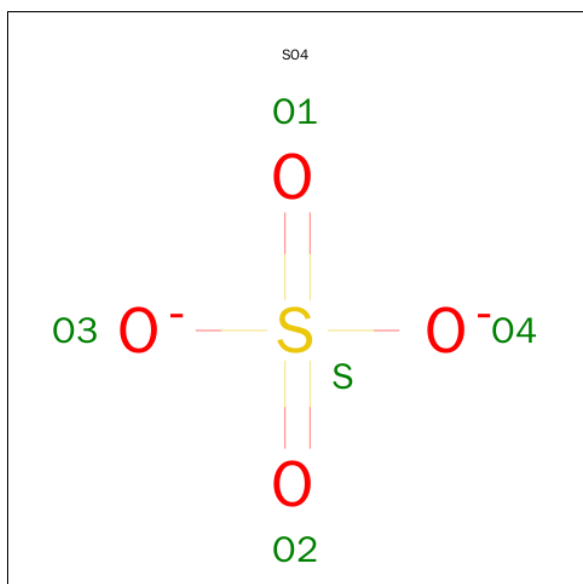
Chain	Residue	Modelled	Actual	Comment	Reference
b	-5	HIS	-	expression tag	UNP P02976
b	-4	HIS	-	expression tag	UNP P02976
b	-3	GLY	-	expression tag	UNP P02976
b	-2	MET	-	expression tag	UNP P02976
b	-1	ALA	-	expression tag	UNP P02976
b	0	SER	-	expression tag	UNP P02976
b	1	MET	-	expression tag	UNP P02976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

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

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	14	Total O 14 14	0	0
3	C	22	Total O 22 22	0	0
3	D	15	Total O 15 15	0	0
3	E	16	Total O 16 16	0	0
3	F	6	Total O 6 6	0	0
3	G	14	Total O 14 14	0	0
3	H	10	Total O 10 10	0	0
3	I	18	Total O 18 18	0	0
3	J	14	Total O 14 14	0	0
3	K	15	Total O 15 15	0	0
3	L	21	Total O 21 21	0	0
3	M	16	Total O 16 16	0	0
3	N	16	Total O 16 16	0	0

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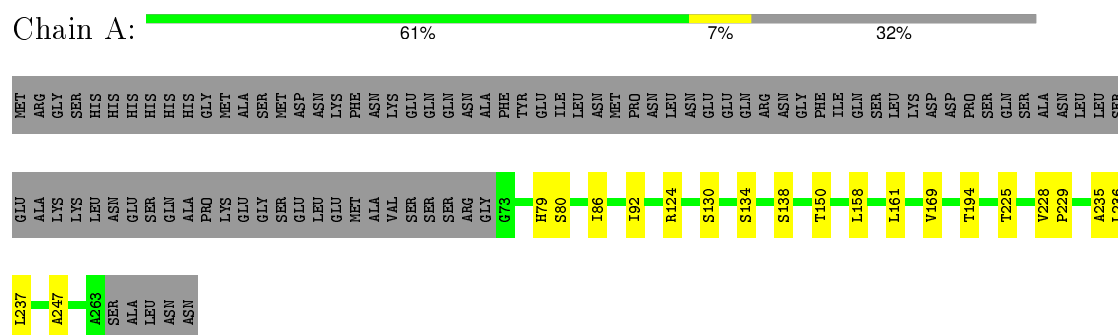
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	15	Total 15	O 15	0	0
3	P	12	Total 12	O 12	0	0
3	Q	16	Total 16	O 16	0	0
3	R	9	Total 9	O 9	0	0
3	S	11	Total 11	O 11	0	0
3	T	14	Total 14	O 14	0	0
3	U	12	Total 12	O 12	0	0
3	V	18	Total 18	O 18	0	0
3	W	8	Total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

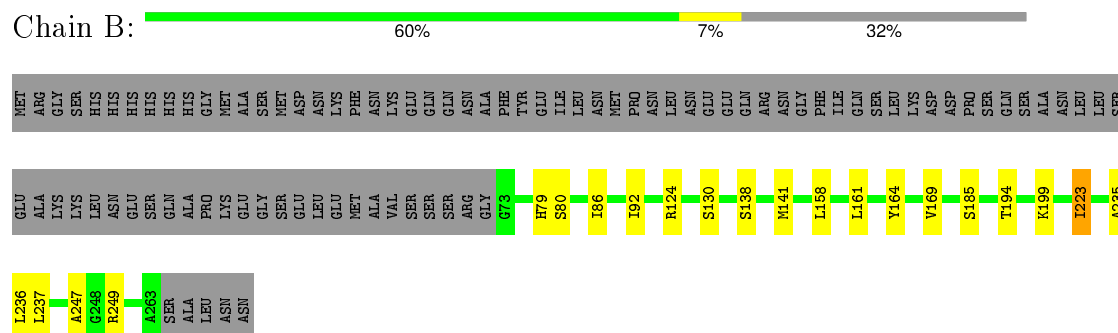
3 Residue-property plots [i](#)

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.

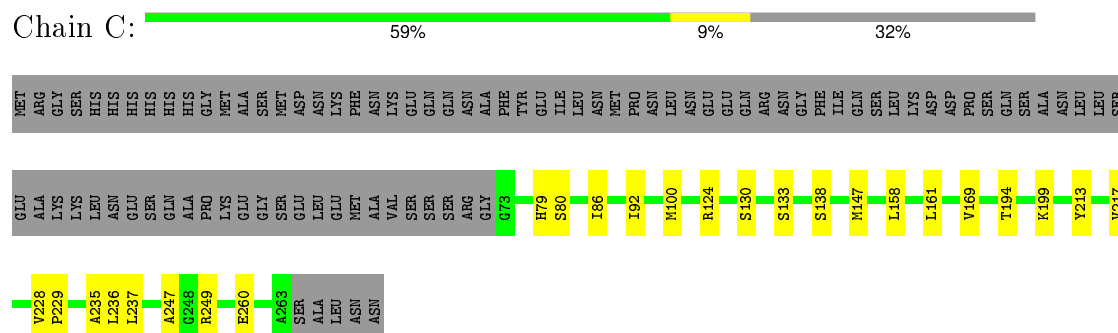
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



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

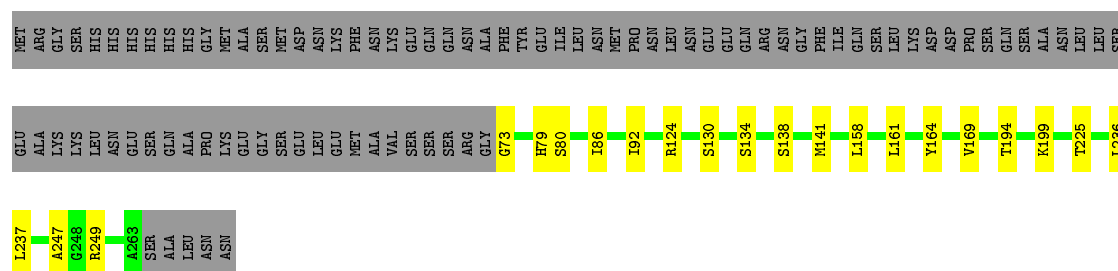


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



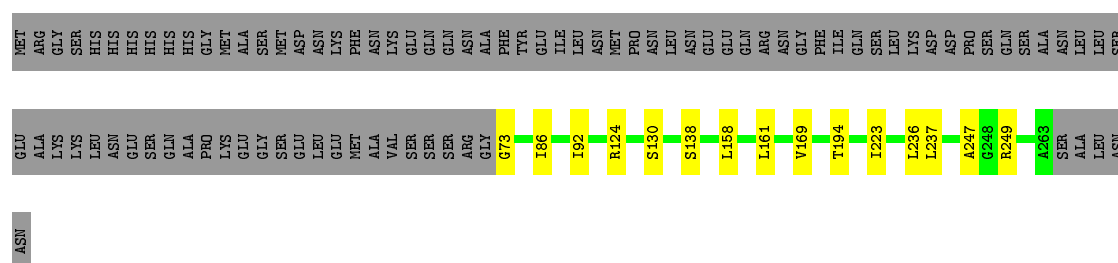
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain D:  60% 7% 32%



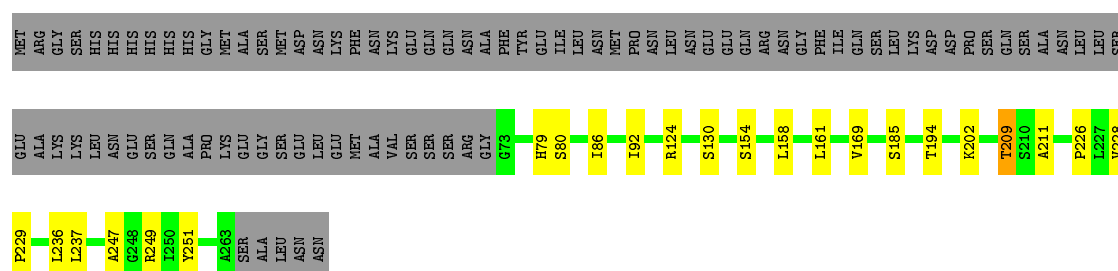
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain E:  62% 5% 32%



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

Chain F:  60% 8% 32%



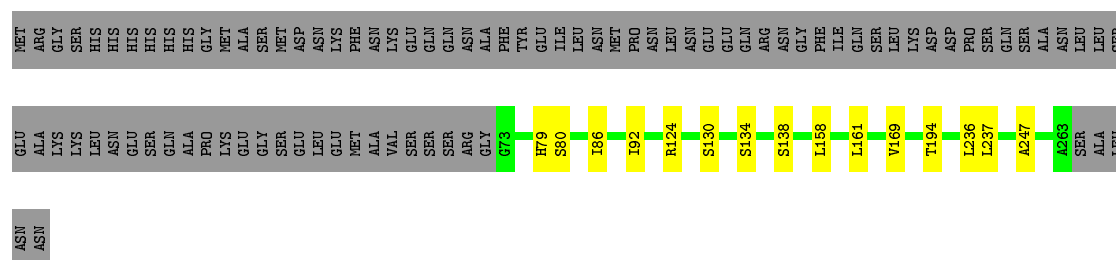
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain G:  60% 7% 32%



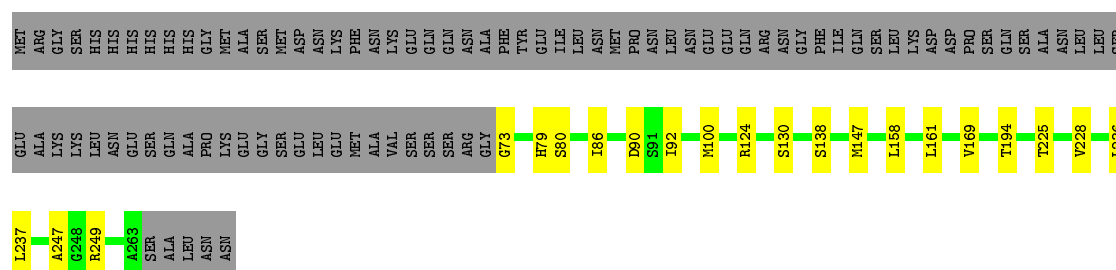
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain H:  62% 5% 32%



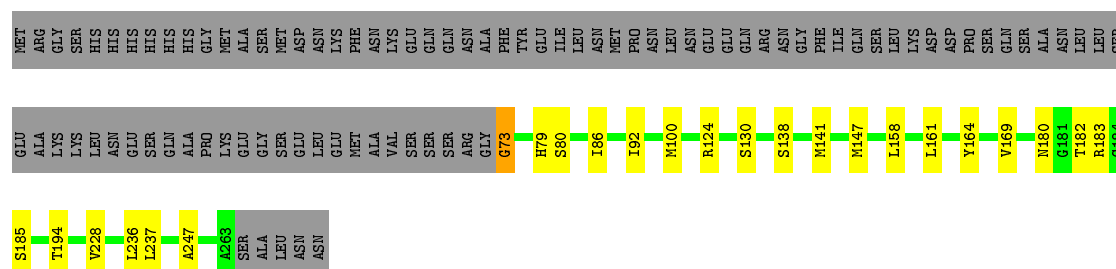
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain I:  60% 7% 32%



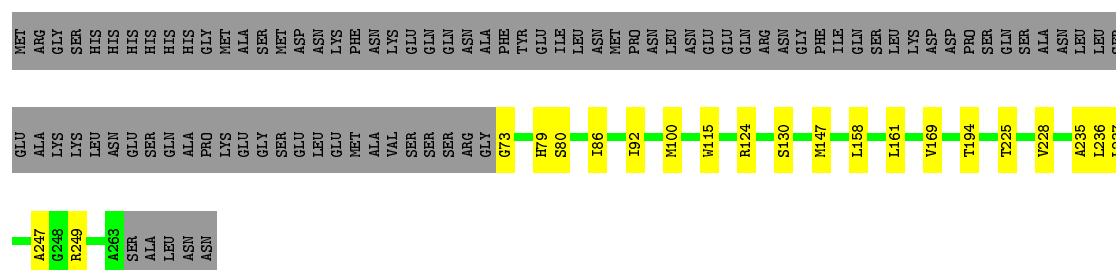
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain J:  59% 8% 32%



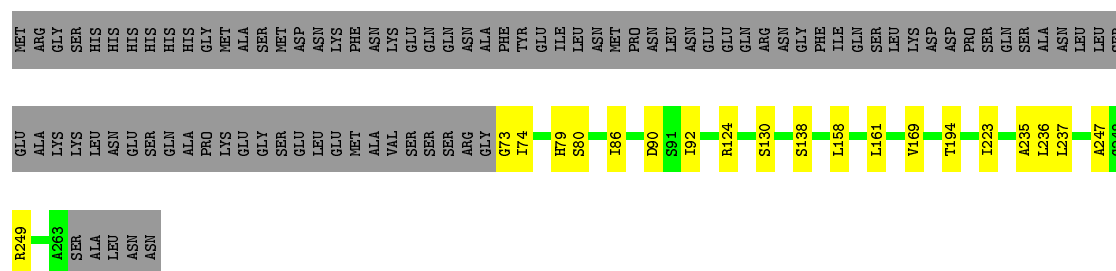
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain K:  60% 7% 32%



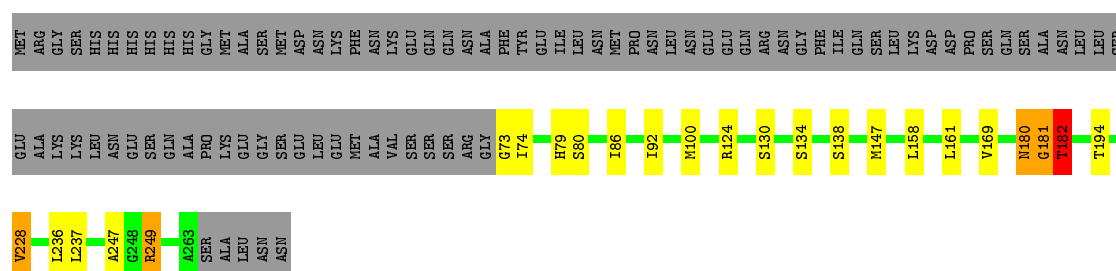
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain L:  61% 7% 32%



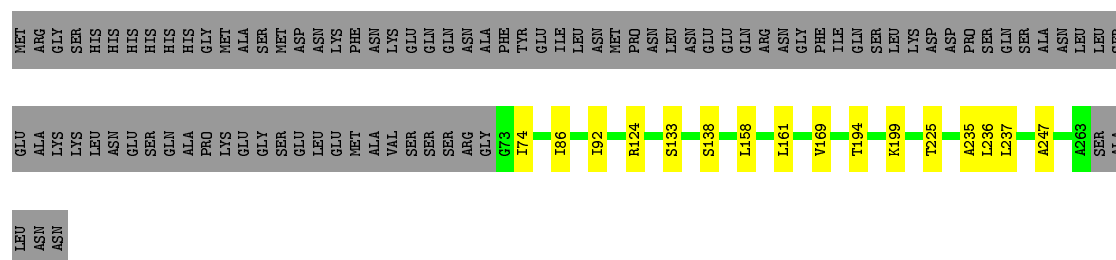
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain M:  59% 7% 32%



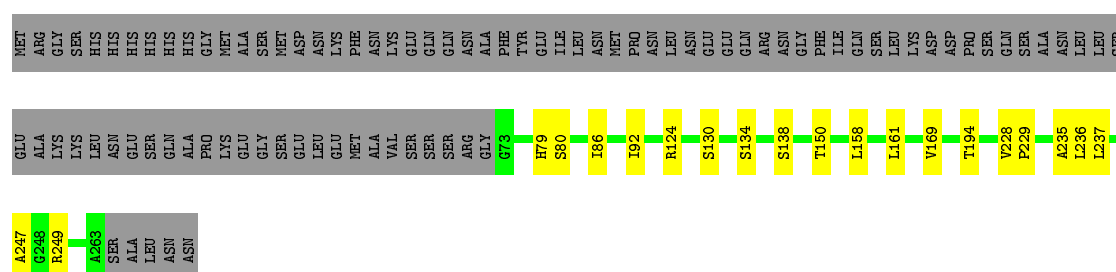
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain N:  62% 6% 32%



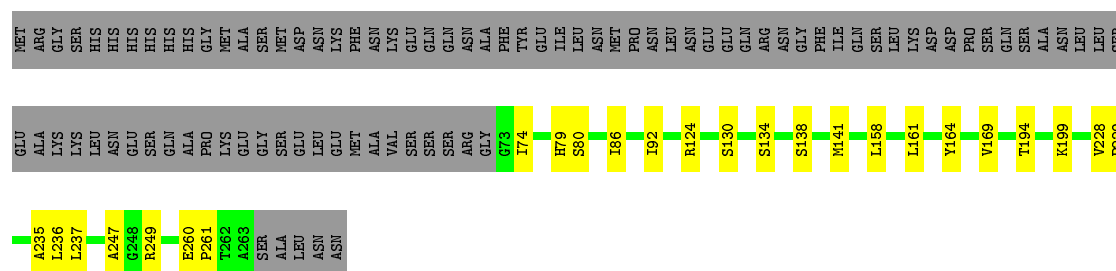
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain O:  61% 7% 32%



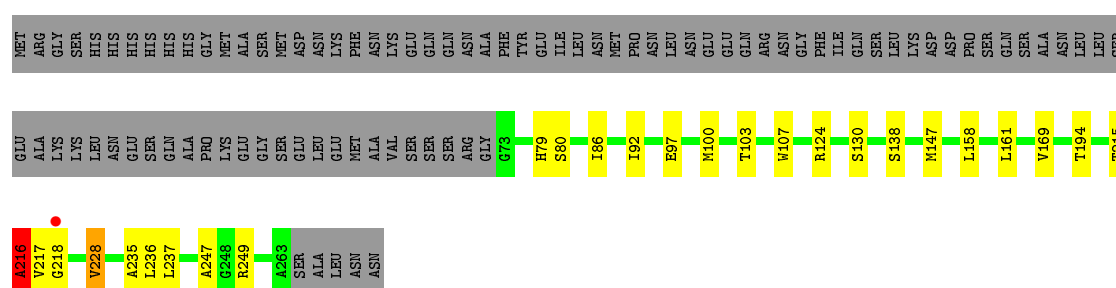
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain P:  59% 9% 32%



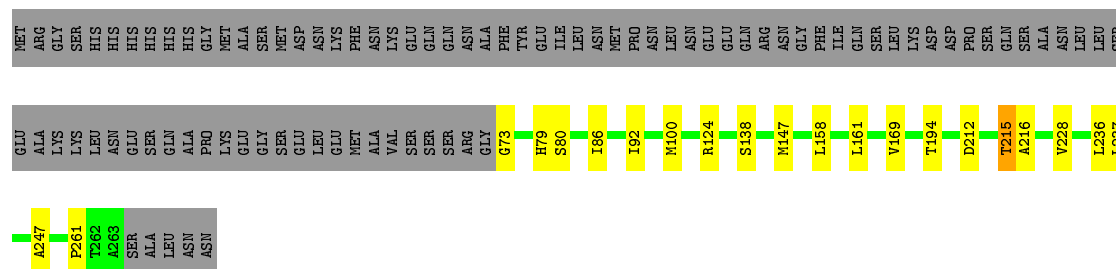
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain Q:  59% 9% 32%



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

Chain R:  60% 7% 32%

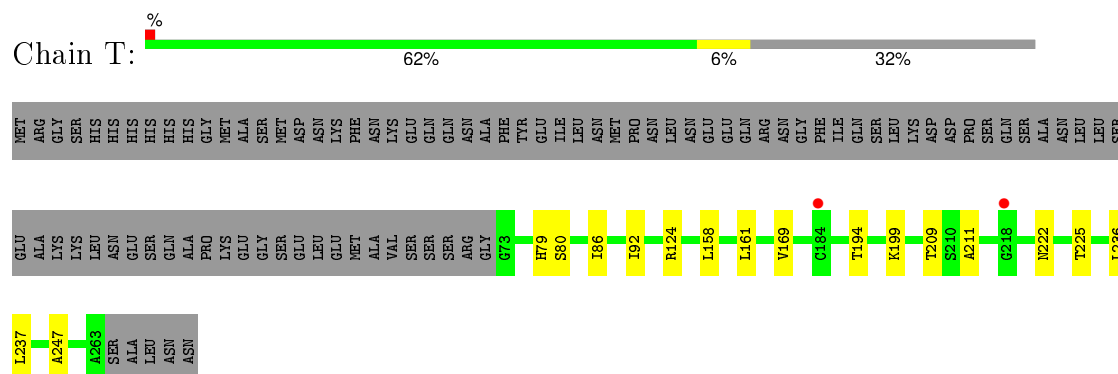


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

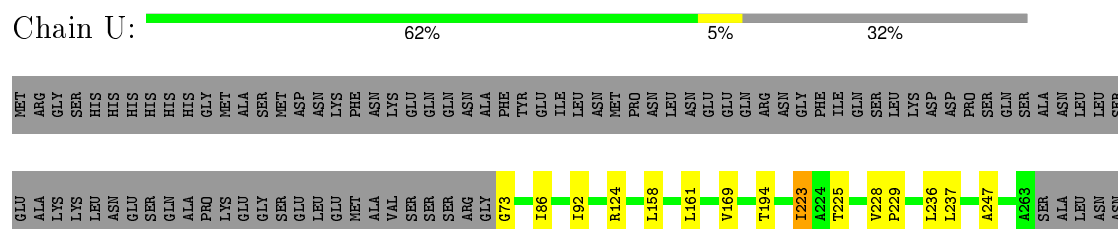
Chain S:  61% 7% 32%



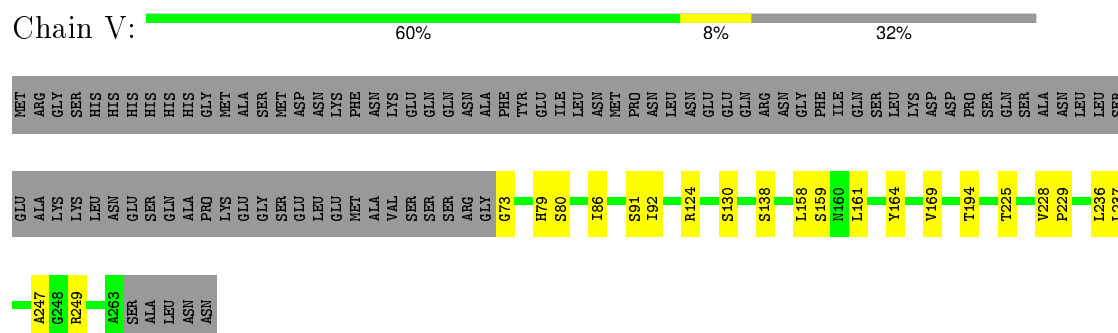
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



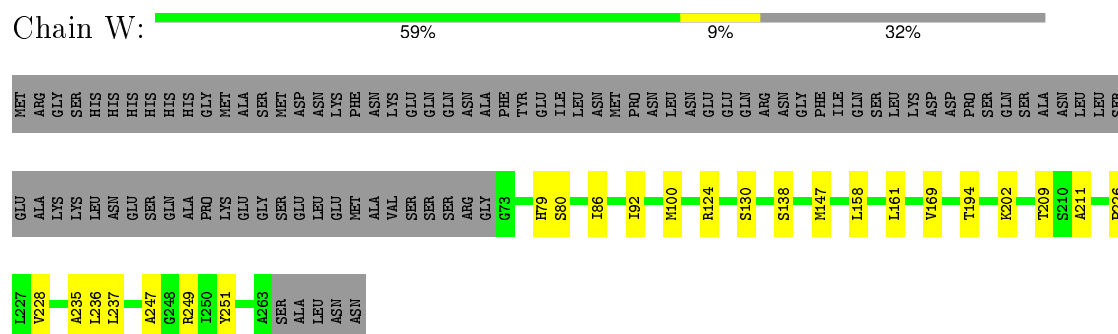
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



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

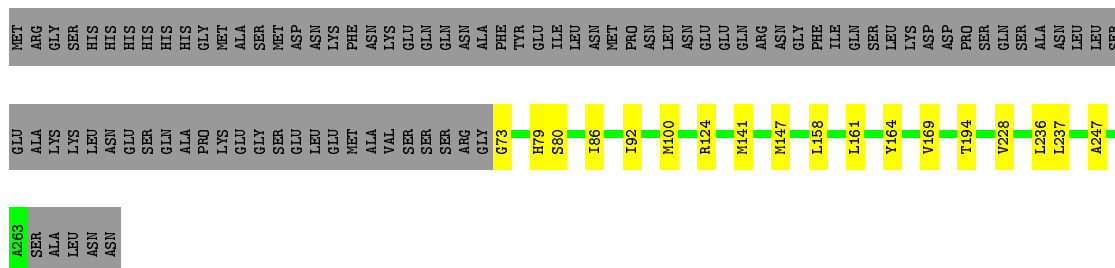


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



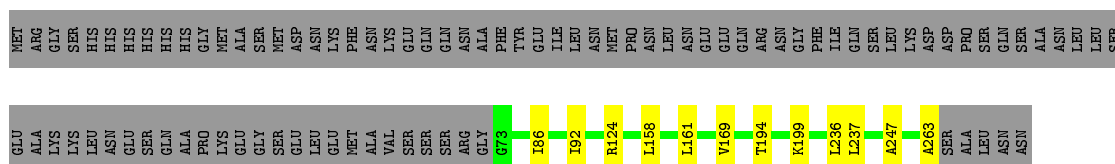
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein





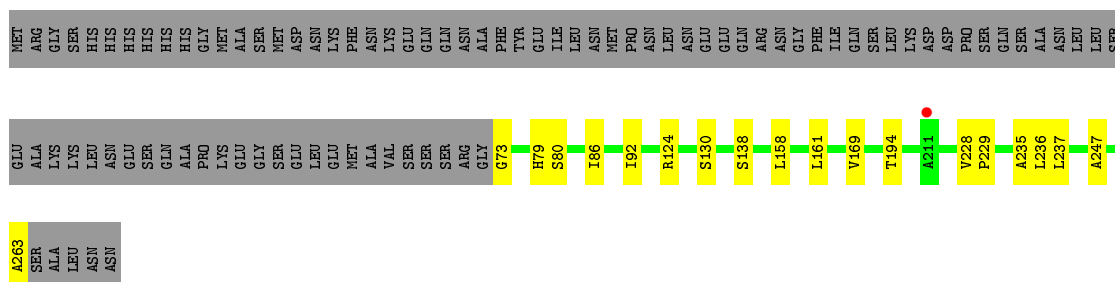
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain Y: 63% 32%



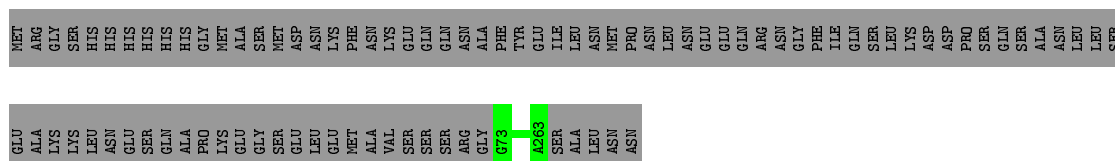
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain Z: 61% 7% 32%



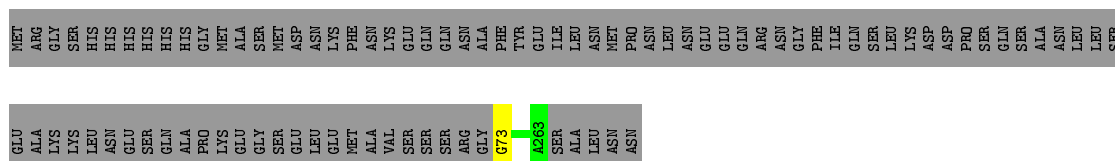
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain a: 68% 32%



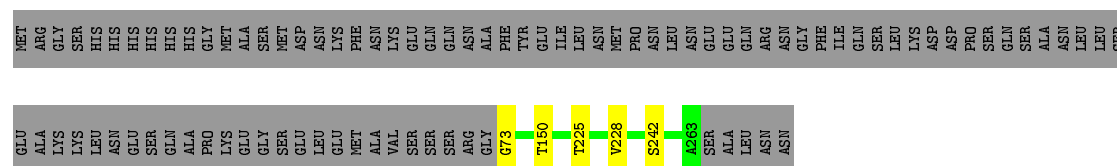
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain b: 67% 32%



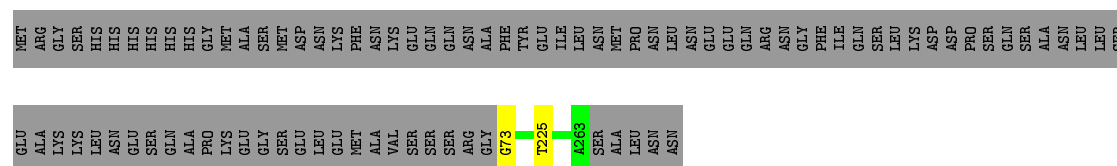
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain c:  66% . 32%



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

Chain d:  67% 32%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	288.18Å 193.04Å 189.19Å 90.00° 124.37° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 45.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-3.00) 99.7 (45.82-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.179 , 0.200 0.182 , 0.199	Depositor DCC
R_{free} test set	8494 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 169159 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	42805	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.77	0/1445	0.82	1/1983 (0.1%)
1	B	0.81	1/1448 (0.1%)	0.83	2/1986 (0.1%)
1	C	0.80	0/1448	0.84	0/1986
1	D	0.78	1/1450 (0.1%)	0.81	0/1989
1	E	0.77	1/1431 (0.1%)	0.84	1/1964 (0.1%)
1	F	0.79	0/1408	0.84	2/1935 (0.1%)
1	G	0.75	0/1450	0.82	2/1989 (0.1%)
1	H	0.76	0/1441	0.83	0/1977
1	I	0.77	1/1450 (0.1%)	0.82	0/1989
1	J	0.78	3/1448 (0.2%)	0.85	0/1986
1	K	0.79	1/1448 (0.1%)	0.83	0/1987
1	L	0.79	1/1448 (0.1%)	0.82	0/1986
1	M	0.83	1/1449 (0.1%)	0.86	3/1987 (0.2%)
1	N	0.79	0/1446	0.83	1/1984 (0.1%)
1	O	0.76	0/1448	0.81	1/1986 (0.1%)
1	P	0.75	0/1448	0.81	0/1986
1	Q	0.79	0/1409	0.89	2/1935 (0.1%)
1	R	0.78	1/1438 (0.1%)	0.87	1/1974 (0.1%)
1	S	0.77	0/1437	0.86	2/1972 (0.1%)
1	T	0.80	1/1447 (0.1%)	0.86	3/1985 (0.2%)
1	U	0.77	1/1444 (0.1%)	0.82	1/1981 (0.1%)
1	V	0.77	1/1448 (0.1%)	0.82	1/1986 (0.1%)
1	W	0.77	0/1448	0.84	0/1986
1	X	0.78	1/1446 (0.1%)	0.83	0/1983
1	Y	0.77	0/1443	0.82	1/1980 (0.1%)
1	Z	0.76	1/1443 (0.1%)	0.81	0/1980
1	a	0.74	0/1445	0.80	0/1982
1	b	0.82	1/1448 (0.1%)	0.83	0/1986
1	c	0.83	1/1450 (0.1%)	0.85	2/1989 (0.1%)
1	d	0.76	1/1447 (0.1%)	0.81	0/1985
All	All	0.78	19/43299 (0.0%)	0.83	26/59404 (0.0%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	73	GLY	N-CA	6.86	1.56	1.46
1	B	185	SER	CA-CB	6.21	1.62	1.52
1	J	185	SER	CA-CB	6.10	1.62	1.52
1	L	73	GLY	N-CA	5.99	1.55	1.46
1	T	222	ASN	CG-OD1	-5.95	1.10	1.24
1	c	73	GLY	N-CA	5.64	1.54	1.46
1	b	73	GLY	N-CA	5.48	1.54	1.46
1	E	73	GLY	N-CA	5.33	1.54	1.46
1	J	185	SER	CB-OG	5.28	1.49	1.42
1	K	73	GLY	N-CA	5.20	1.53	1.46
1	U	73	GLY	N-CA	5.19	1.53	1.46
1	V	73	GLY	N-CA	5.12	1.53	1.46
1	M	73	GLY	N-CA	5.11	1.53	1.46
1	R	73	GLY	N-CA	5.10	1.53	1.46
1	Z	73	GLY	N-CA	5.07	1.53	1.46
1	X	73	GLY	N-CA	5.04	1.53	1.46
1	d	73	GLY	N-CA	5.01	1.53	1.46
1	I	73	GLY	N-CA	5.01	1.53	1.46
1	J	73	GLY	N-CA	5.01	1.53	1.46

All (26) bond angle outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	209	THR	CA-CB-OG1	-5.14	98.21	109.00
1	M	181	GLY	N-CA-C	-5.13	100.27	113.10
1	M	228	VAL	CA-CB-CG1	5.13	118.60	110.90
1	c	228	VAL	CA-CB-CG1	5.07	118.51	110.90
1	B	185	SER	CA-CB-OG	5.05	124.83	111.20
1	G	228	VAL	CA-CB-CG1	5.04	118.47	110.90
1	Q	228	VAL	CA-CB-CG1	5.01	118.42	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1413	0	1386	16	0
1	B	1416	0	1390	21	0
1	C	1416	0	1390	22	0
1	D	1418	0	1395	18	0
1	E	1399	0	1357	9	0
1	F	1376	0	1300	14	1
1	G	1418	0	1395	14	0
1	H	1409	0	1374	10	0
1	I	1418	0	1395	12	1
1	J	1416	0	1390	17	0
1	K	1416	0	1388	13	0
1	L	1416	0	1390	15	1
1	M	1417	0	1393	19	0
1	N	1414	0	1388	11	0
1	O	1416	0	1390	14	0
1	P	1416	0	1390	20	0
1	Q	1378	0	1327	20	0
1	R	1406	0	1368	18	0
1	S	1405	0	1363	14	0
1	T	1415	0	1393	8	0
1	U	1412	0	1381	9	0
1	V	1416	0	1396	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	1416	0	1390	18	0
1	X	1414	0	1383	11	0
1	Y	1411	0	1381	7	0
1	Z	1411	0	1381	12	0
1	a	1413	0	1388	0	0
1	b	1416	0	1390	0	0
1	c	1418	0	1395	0	1
1	d	1415	0	1393	0	0
2	D	5	0	0	3	0
2	H	5	0	0	1	0
2	L	5	0	0	0	0
2	M	5	0	0	2	0
2	S	5	0	0	3	0
2	V	5	0	0	0	0
3	A	10	0	0	0	0
3	B	14	0	0	1	0
3	C	22	0	0	1	0
3	D	15	0	0	0	0
3	E	16	0	0	0	0
3	F	6	0	0	0	0
3	G	14	0	0	0	0
3	H	10	0	0	0	0
3	I	18	0	0	0	0
3	J	14	0	0	1	0
3	K	15	0	0	1	0
3	L	21	0	0	0	0
3	M	16	0	0	1	0
3	N	16	0	0	0	0
3	O	15	0	0	0	0
3	P	12	0	0	0	0
3	Q	16	0	0	0	0
3	R	9	0	0	0	0
3	S	11	0	0	0	0
3	T	14	0	0	0	0
3	U	12	0	0	0	0
3	V	18	0	0	0	0
3	W	8	0	0	0	0
3	X	17	0	0	0	0
3	Y	11	0	0	1	0
3	Z	13	0	0	1	0
3	a	12	0	0	0	0
3	b	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	24	0	0	0	0
3	d	16	0	0	0	0
All	All	42805	0	41440	325	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 4.

All (325) 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:Q:215:THR:O	1:Q:216:ALA:O	1.71	1.09
1:Q:97:GLU:OE2	1:Q:103:THR:O	1.73	1.06
1:Q:215:THR:C	1:Q:216:ALA:O	1.92	1.00
1:M:134:SER:HB3	2:M:301:SO4:O3	1.72	0.89
1:S:134:SER:HB3	2:S:301:SO4:O2	1.74	0.86
1:H:134:SER:HB3	2:H:301:SO4:O2	1.79	0.82
1:M:181:GLY:O	1:M:182:THR:O	1.99	0.79
1:R:212:ASP:O	1:R:215:THR:HG22	1.86	0.75
1:A:134:SER:HB3	2:D:301:SO4:O2	1.88	0.74
1:B:223:ILE:HD11	1:L:223:ILE:HD13	1.70	0.73
1:B:223:ILE:HD11	1:L:223:ILE:CD1	2.18	0.72
1:R:215:THR:HG23	1:R:216:ALA:N	2.03	0.71
1:M:181:GLY:O	3:M:415:HOH:O	2.09	0.70
1:Q:216:ALA:O	1:Q:218:GLY:N	2.28	0.67
1:B:138:SER:HB3	1:L:130:SER:HB2	58.68	0.66
1:C:260:GLU:OE2	3:C:319:HOH:O	2.15	0.63
1:K:92:ILE:HA	1:K:237:LEU:HB3	1.81	0.63
1:P:134:SER:HB3	2:S:301:SO4:O4	1.99	0.62
1:X:92:ILE:HA	1:X:237:LEU:HB3	1.82	0.62
1:H:92:ILE:HA	1:H:237:LEU:HB3	1.82	0.62
1:I:92:ILE:HA	1:I:237:LEU:HB3	1.82	0.61
1:T:92:ILE:HA	1:T:237:LEU:HB3	1.82	0.61
1:J:92:ILE:HA	1:J:237:LEU:HB3	1.82	0.61
1:S:92:ILE:HA	1:S:237:LEU:HB3	1.83	0.61
1:Y:92:ILE:HA	1:Y:237:LEU:HB3	1.83	0.61
1:A:92:ILE:HA	1:A:237:LEU:HB3	1.84	0.61
1:E:92:ILE:HA	1:E:237:LEU:HB3	1.83	0.61
1:D:138:SER:HB3	1:S:130:SER:HB2	84.64	0.60
1:Q:86:ILE:CG2	1:Q:236:LEU:HD21	2.31	0.60
1:U:92:ILE:HA	1:U:237:LEU:HB3	1.83	0.60
1:M:92:ILE:HA	1:M:237:LEU:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ILE:HA	1:B:237:LEU:HB3	1.86	0.60
1:N:92:ILE:HA	1:N:237:LEU:HB3	1.83	0.60
1:V:92:ILE:HA	1:V:237:LEU:HB3	1.83	0.60
1:S:86:ILE:CG2	1:S:236:LEU:HD21	2.32	0.60
1:F:92:ILE:HA	1:F:237:LEU:HB3	1.82	0.60
1:L:92:ILE:HA	1:L:237:LEU:HB3	1.83	0.60
1:R:92:ILE:HA	1:R:237:LEU:HB3	1.83	0.60
1:D:92:ILE:HA	1:D:237:LEU:HB3	1.84	0.59
1:U:86:ILE:CG2	1:U:236:LEU:HD21	2.32	0.59
1:P:92:ILE:HA	1:P:237:LEU:HB3	1.82	0.59
1:W:92:ILE:HA	1:W:237:LEU:HB3	1.83	0.59
1:W:86:ILE:CG2	1:W:236:LEU:HD21	2.33	0.59
1:M:86:ILE:CG2	1:M:236:LEU:HD21	2.32	0.59
1:G:86:ILE:CG2	1:G:236:LEU:HD21	2.33	0.59
1:Q:92:ILE:HA	1:Q:237:LEU:HB3	1.83	0.59
1:O:92:ILE:HA	1:O:237:LEU:HB3	1.83	0.59
1:Z:92:ILE:HA	1:Z:237:LEU:HB3	1.83	0.59
1:C:92:ILE:HA	1:C:237:LEU:HB3	1.85	0.59
1:Z:86:ILE:CG2	1:Z:236:LEU:HD21	2.32	0.59
1:V:138:SER:HB3	1:W:130:SER:HB2	1.85	0.58
1:D:86:ILE:CG2	1:D:236:LEU:HD21	2.34	0.58
1:G:92:ILE:HA	1:G:237:LEU:HB3	1.84	0.58
1:C:86:ILE:CG2	1:C:236:LEU:HD21	2.34	0.58
1:A:86:ILE:CG2	1:A:236:LEU:HD21	2.33	0.58
1:N:86:ILE:CG2	1:N:236:LEU:HD21	2.33	0.58
1:E:86:ILE:CG2	1:E:236:LEU:HD21	2.34	0.58
1:Y:86:ILE:CG2	1:Y:236:LEU:HD21	2.33	0.58
1:R:86:ILE:CG2	1:R:236:LEU:HD21	2.34	0.58
1:L:86:ILE:CG2	1:L:236:LEU:HD21	2.34	0.58
1:D:134:SER:HB3	2:D:301:SO4:O4	2.04	0.58
1:J:86:ILE:CG2	1:J:236:LEU:HD21	2.34	0.58
1:K:86:ILE:CG2	1:K:236:LEU:HD21	2.34	0.57
1:B:158:LEU:HD12	1:B:161:LEU:HD12	1.87	0.57
1:F:130:SER:HB2	1:G:138:SER:HB3	1.86	0.57
1:I:86:ILE:CG2	1:I:236:LEU:HD21	2.34	0.57
1:F:86:ILE:CG2	1:F:236:LEU:HD21	2.34	0.57
1:V:86:ILE:CG2	1:V:236:LEU:HD21	2.34	0.57
1:M:130:SER:HB2	1:N:138:SER:HB3	1.85	0.57
1:O:134:SER:HB3	2:S:301:SO4:O3	2.04	0.57
1:T:86:ILE:CG2	1:T:236:LEU:HD21	2.35	0.57
1:H:86:ILE:CG2	1:H:236:LEU:HD21	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ILE:CG2	1:B:236:LEU:HD21	2.34	0.57
1:O:86:ILE:CG2	1:O:236:LEU:HD21	2.34	0.57
1:X:158:LEU:HD12	1:X:161:LEU:HD12	1.87	0.57
1:W:202:LYS:NZ	1:W:226:PRO:O	2.38	0.56
1:W:158:LEU:HD12	1:W:161:LEU:HD12	1.86	0.56
1:X:86:ILE:CG2	1:X:236:LEU:HD21	2.35	0.56
1:E:158:LEU:HD12	1:E:161:LEU:HD12	1.88	0.56
1:Q:158:LEU:HD12	1:Q:161:LEU:HD12	1.87	0.56
1:N:158:LEU:HD12	1:N:161:LEU:HD12	1.88	0.56
1:J:158:LEU:HD12	1:J:161:LEU:HD12	1.87	0.56
1:F:158:LEU:HD12	1:F:161:LEU:HD12	1.87	0.56
1:S:158:LEU:HD12	1:S:161:LEU:HD12	1.87	0.56
1:A:158:LEU:HD12	1:A:161:LEU:HD12	1.86	0.56
1:B:237:LEU:HB2	3:B:305:HOH:O	41.09	0.56
1:D:158:LEU:HD12	1:D:161:LEU:HD12	1.88	0.56
1:P:86:ILE:CG2	1:P:236:LEU:HD21	2.35	0.55
1:K:158:LEU:HD12	1:K:161:LEU:HD12	1.87	0.55
1:I:130:SER:HB2	1:J:138:SER:HB3	1.88	0.55
1:U:158:LEU:HD12	1:U:161:LEU:HD12	1.88	0.55
1:C:158:LEU:HD12	1:C:161:LEU:HD12	1.88	0.55
1:C:237:LEU:HD12	1:C:237:LEU:C	2.26	0.55
1:O:158:LEU:HD12	1:O:161:LEU:HD12	1.87	0.55
1:V:158:LEU:HD12	1:V:161:LEU:HD12	1.88	0.55
1:T:158:LEU:HD12	1:T:161:LEU:HD12	1.87	0.55
1:H:158:LEU:HD12	1:H:161:LEU:HD12	1.88	0.55
1:Z:158:LEU:HD12	1:Z:161:LEU:HD12	1.88	0.55
1:P:158:LEU:HD12	1:P:161:LEU:HD12	1.88	0.55
1:R:158:LEU:HD12	1:R:161:LEU:HD12	1.88	0.54
1:Y:158:LEU:HD12	1:Y:161:LEU:HD12	1.88	0.54
1:F:249:ARG:HH22	1:G:237:LEU:HD11	1.73	0.54
1:G:158:LEU:HD12	1:G:161:LEU:HD12	1.89	0.54
1:M:158:LEU:HD12	1:M:161:LEU:HD12	1.88	0.54
1:B:237:LEU:HD11	1:L:249:ARG:HH22	52.42	0.54
1:L:158:LEU:HD12	1:L:161:LEU:HD12	1.89	0.53
1:Z:237:LEU:HD12	1:Z:237:LEU:C	2.29	0.53
1:I:158:LEU:HD12	1:I:161:LEU:HD12	1.89	0.53
1:C:130:SER:HB2	1:M:138:SER:HB3	74.66	0.53
1:K:237:LEU:C	1:K:237:LEU:HD12	2.29	0.53
1:Q:237:LEU:C	1:Q:237:LEU:HD12	2.29	0.53
1:M:180:ASN:ND2	1:M:182:THR:HG23	2.24	0.53
1:I:237:LEU:HD12	1:I:237:LEU:C	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:215:THR:CG2	1:R:216:ALA:N	2.70	0.52
1:Q:124:ARG:HB2	1:Q:194:THR:OG1	2.10	0.52
1:C:237:LEU:HD11	1:D:249:ARG:HH22	1.74	0.51
1:C:249:ARG:HH22	1:M:237:LEU:HD11	73.40	0.51
1:D:237:LEU:C	1:D:237:LEU:HD12	2.34	0.51
1:K:249:ARG:HH22	1:L:237:LEU:HD11	1.76	0.51
1:Q:130:SER:HB2	1:S:138:SER:HB3	1.92	0.51
1:I:100:MET:SD	1:I:228:VAL:HG12	2.51	0.51
1:W:237:LEU:HD12	1:W:237:LEU:C	2.32	0.51
1:G:100:MET:SD	1:G:228:VAL:HG12	2.51	0.51
1:Q:100:MET:SD	1:Q:228:VAL:HG12	2.50	0.50
1:W:100:MET:SD	1:W:228:VAL:HG12	2.51	0.50
1:H:237:LEU:HD12	1:H:237:LEU:C	2.32	0.50
1:C:100:MET:SD	1:C:228:VAL:HG12	2.51	0.50
1:V:164:TYR:HH	1:W:251:TYR:HH	1.59	0.50
1:B:237:LEU:C	1:B:237:LEU:HD12	2.32	0.50
1:X:100:MET:SD	1:X:228:VAL:HG12	2.51	0.50
1:J:100:MET:SD	1:J:228:VAL:HG12	2.51	0.50
1:F:202:LYS:NZ	1:F:226:PRO:O	2.39	0.50
1:X:237:LEU:C	1:X:237:LEU:HD12	2.32	0.50
1:A:138:SER:HB3	1:B:130:SER:HB2	1.94	0.50
1:R:212:ASP:O	1:R:215:THR:CG2	2.58	0.50
1:R:100:MET:SD	1:R:228:VAL:HG12	2.51	0.50
1:G:237:LEU:C	1:G:237:LEU:HD12	2.32	0.49
1:K:130:SER:HB2	1:L:138:SER:HB3	1.93	0.49
1:A:237:LEU:HD12	1:A:237:LEU:C	2.34	0.49
1:M:237:LEU:HD12	1:M:237:LEU:C	2.32	0.49
1:U:237:LEU:HD12	1:U:237:LEU:C	2.33	0.49
1:N:237:LEU:HD12	1:N:237:LEU:C	2.32	0.49
1:P:237:LEU:HD12	1:P:237:LEU:C	2.33	0.49
1:M:100:MET:SD	1:M:228:VAL:HG12	2.52	0.49
1:K:100:MET:SD	1:K:228:VAL:HG12	2.52	0.49
1:V:237:LEU:C	1:V:237:LEU:HD12	2.33	0.49
1:P:249:ARG:HH22	1:Q:237:LEU:HD11	1.77	0.49
1:C:138:SER:HB3	1:D:130:SER:HB2	1.96	0.48
1:B:138:SER:HB3	1:C:130:SER:HB2	1.94	0.48
1:M:249:ARG:HH22	1:N:237:LEU:HD11	1.78	0.48
1:H:138:SER:HB3	1:Z:130:SER:HB2	1.96	0.48
1:D:138:SER:HB3	1:E:130:SER:HB2	1.95	0.48
1:R:237:LEU:HD12	1:R:237:LEU:C	2.35	0.48
1:U:228:VAL:HG23	1:U:229:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:237:LEU:C	1:T:237:LEU:HD12	2.34	0.47
1:I:249:ARG:HH22	1:J:237:LEU:HD11	1.79	0.47
1:Y:237:LEU:C	1:Y:237:LEU:HD12	2.35	0.47
1:V:79:HIS:CG	1:V:80:SER:N	2.83	0.47
1:L:237:LEU:C	1:L:237:LEU:HD12	2.35	0.47
1:J:182:THR:HG22	1:J:183:ARG:N	2.30	0.47
1:J:237:LEU:C	1:J:237:LEU:HD12	2.34	0.47
1:S:237:LEU:HD12	1:S:237:LEU:C	2.35	0.47
1:L:79:HIS:CG	1:L:80:SER:N	2.83	0.47
1:C:79:HIS:CG	1:C:80:SER:N	2.85	0.46
1:Q:249:ARG:HH22	1:S:237:LEU:HD11	1.80	0.46
1:O:228:VAL:HG23	1:O:229:PRO:HD2	1.98	0.46
1:T:209:THR:HG22	1:T:211:ALA:H	1.81	0.46
1:W:79:HIS:CG	1:W:80:SER:N	2.84	0.46
1:L:124:ARG:HB2	1:L:194:THR:HG22	1.98	0.46
1:O:237:LEU:C	1:O:237:LEU:HD12	2.36	0.45
1:J:79:HIS:CG	1:J:80:SER:N	2.83	0.45
1:E:237:LEU:HD12	1:E:237:LEU:C	2.36	0.45
1:P:228:VAL:HG23	1:P:229:PRO:HD2	1.99	0.45
1:J:169:VAL:HB	1:J:247:ALA:HB1	1.98	0.45
1:F:228:VAL:HG23	1:F:229:PRO:HD2	1.99	0.45
1:G:130:SER:HB2	1:W:138:SER:HB3	1.99	0.45
1:P:228:VAL:HA	1:P:229:PRO:HD3	1.87	0.45
3:Y:301:HOH:O	1:Z:263:ALA:HB1	2.16	0.45
1:M:124:ARG:HB2	1:M:194:THR:HG22	1.98	0.45
1:B:79:HIS:CG	1:B:80:SER:N	2.84	0.45
1:W:209:THR:HG22	1:W:211:ALA:H	1.81	0.45
1:S:169:VAL:HB	1:S:247:ALA:HB1	1.99	0.45
1:U:228:VAL:HA	1:U:229:PRO:HD3	1.85	0.45
1:J:180:ASN:ND2	1:J:182:THR:OG1	2.50	0.45
1:F:237:LEU:HD12	1:F:237:LEU:C	2.37	0.45
1:X:79:HIS:CG	1:X:80:SER:N	2.84	0.45
1:F:251:TYR:HH	1:G:164:TYR:HH	1.63	0.45
1:D:237:LEU:HD11	1:S:249:ARG:HH22	86.71	0.45
1:F:209:THR:HG22	1:F:211:ALA:H	1.82	0.45
1:A:237:LEU:HD11	1:B:249:ARG:HH22	1.82	0.45
1:K:115:TRP:O	3:K:308:HOH:O	2.21	0.45
1:A:130:SER:HB2	1:Z:138:SER:HB3	96.59	0.45
1:V:228:VAL:HG23	1:V:229:PRO:HD2	1.99	0.44
1:R:79:HIS:CG	1:R:80:SER:N	2.85	0.44
1:A:228:VAL:HG23	1:A:229:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:73:GLY:HA2	3:J:311:HOH:O	2.17	0.44
1:G:169:VAL:HB	1:G:247:ALA:HB1	2.00	0.44
1:V:237:LEU:HD11	1:W:249:ARG:HH22	1.82	0.44
1:O:249:ARG:HH22	1:P:237:LEU:HD11	1.82	0.44
1:C:213:TYR:CZ	1:C:217:VAL:HG11	2.53	0.44
1:D:169:VAL:HB	1:D:247:ALA:HB1	2.02	0.44
1:R:169:VAL:HB	1:R:247:ALA:HB1	2.00	0.44
1:I:124:ARG:HB2	1:I:194:THR:HG22	2.00	0.44
1:J:124:ARG:HB2	1:J:194:THR:HG22	2.00	0.44
1:O:124:ARG:HB2	1:O:194:THR:HG22	1.99	0.44
1:C:124:ARG:HB2	1:C:194:THR:HG22	1.99	0.44
1:B:235:ALA:C	1:B:236:LEU:HD12	2.42	0.43
1:U:169:VAL:HB	1:U:247:ALA:HB1	2.00	0.43
1:S:79:HIS:CG	1:S:80:SER:N	2.86	0.43
1:D:124:ARG:HB2	1:D:194:THR:HG22	2.01	0.43
1:C:133:SER:OG	2:D:301:SO4:O1	2.36	0.43
1:W:124:ARG:HB2	1:W:194:THR:HG22	2.00	0.43
1:S:124:ARG:HB2	1:S:194:THR:HG22	2.00	0.43
1:T:169:VAL:HB	1:T:247:ALA:HB1	2.00	0.43
1:Q:235:ALA:C	1:Q:236:LEU:HD12	2.38	0.43
1:Q:79:HIS:CG	1:Q:80:SER:N	2.86	0.43
1:R:124:ARG:HB2	1:R:194:THR:HG22	2.01	0.43
1:Z:169:VAL:HB	1:Z:247:ALA:HB1	2.00	0.43
1:W:169:VAL:HB	1:W:247:ALA:HB1	2.00	0.43
1:M:169:VAL:HB	1:M:247:ALA:HB1	2.01	0.43
1:H:169:VAL:HB	1:H:247:ALA:HB1	1.99	0.43
1:C:169:VAL:HB	1:C:247:ALA:HB1	2.03	0.43
1:F:79:HIS:CG	1:F:80:SER:N	2.87	0.43
1:G:79:HIS:CG	1:G:80:SER:N	2.87	0.43
1:Z:228:VAL:HG23	1:Z:229:PRO:HD2	1.99	0.43
1:K:79:HIS:CG	1:K:80:SER:N	2.87	0.43
1:O:169:VAL:HB	1:O:247:ALA:HB1	1.99	0.43
1:R:138:SER:HB3	1:V:130:SER:HB2	2.01	0.43
1:N:169:VAL:HB	1:N:247:ALA:HB1	2.01	0.43
1:A:124:ARG:HB2	1:A:194:THR:HG22	2.02	0.43
1:K:124:ARG:HB2	1:K:194:THR:HG22	2.01	0.43
1:K:169:VAL:HB	1:K:247:ALA:HB1	2.01	0.43
1:N:124:ARG:HB2	1:N:194:THR:HG22	1.99	0.43
1:A:169:VAL:HB	1:A:247:ALA:HB1	2.00	0.43
1:X:169:VAL:HB	1:X:247:ALA:HB1	2.00	0.43
1:G:124:ARG:HB2	1:G:194:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:301:SO4:O2	1:N:133:SER:OG	2.36	0.42
1:K:147:MET:SD	1:K:228:VAL:HG21	2.59	0.42
1:I:169:VAL:HB	1:I:247:ALA:HB1	2.01	0.42
1:Y:124:ARG:HB2	1:Y:194:THR:HG22	2.01	0.42
1:H:124:ARG:HB2	1:H:194:THR:HG22	2.00	0.42
1:U:124:ARG:HB2	1:U:194:THR:HG22	1.99	0.42
1:C:235:ALA:C	1:C:236:LEU:HD12	2.40	0.42
1:A:235:ALA:C	1:A:236:LEU:HD12	2.40	0.42
1:D:130:SER:HB2	1:O:138:SER:HB3	90.60	0.42
1:F:124:ARG:HB2	1:F:194:THR:HG22	2.01	0.42
1:I:147:MET:SD	1:I:228:VAL:HG21	2.59	0.42
1:J:147:MET:SD	1:J:228:VAL:HG21	2.59	0.42
1:B:124:ARG:HB2	1:B:194:THR:HG22	2.02	0.42
1:D:199:LYS:HE3	1:P:74:ILE:HD11	2.01	0.42
1:R:147:MET:SD	1:R:228:VAL:HG21	2.59	0.42
1:O:228:VAL:HA	1:O:229:PRO:HD3	1.86	0.42
1:B:169:VAL:HB	1:B:247:ALA:HB1	2.02	0.42
1:I:79:HIS:CG	1:I:80:SER:N	2.88	0.42
1:Z:235:ALA:C	1:Z:236:LEU:HD12	2.40	0.42
1:V:159:SER:HA	1:V:164:TYR:CD1	2.55	0.42
1:W:79:HIS:CG	1:W:80:SER:H	2.37	0.42
1:J:79:HIS:CG	1:J:80:SER:H	2.38	0.42
1:B:199:LYS:HE3	1:L:74:ILE:HD11	2.01	0.42
1:F:169:VAL:HB	1:F:247:ALA:HB1	2.01	0.42
1:Y:169:VAL:HB	1:Y:247:ALA:HB1	2.02	0.42
1:B:237:LEU:HD11	1:C:249:ARG:HH22	1.85	0.42
1:G:249:ARG:HH22	1:W:237:LEU:HD11	1.85	0.42
1:Q:147:MET:SD	1:Q:228:VAL:HG21	2.60	0.42
1:X:124:ARG:HB2	1:X:194:THR:HG22	2.01	0.42
1:Z:79:HIS:CG	1:Z:80:SER:N	2.87	0.42
1:Y:263:ALA:HB1	3:Z:313:HOH:O	2.19	0.42
1:E:124:ARG:HB2	1:E:194:THR:HG22	2.02	0.42
1:Z:124:ARG:HB2	1:Z:194:THR:HG22	2.01	0.42
1:V:169:VAL:HB	1:V:247:ALA:HB1	2.01	0.42
1:A:79:HIS:CG	1:A:80:SER:N	2.88	0.42
1:P:130:SER:HB2	1:Q:138:SER:HB3	2.01	0.42
1:C:147:MET:SD	1:C:228:VAL:HG21	2.60	0.42
1:P:124:ARG:HB2	1:P:194:THR:HG22	2.02	0.42
1:T:79:HIS:CG	1:T:80:SER:N	2.87	0.42
1:L:169:VAL:HB	1:L:247:ALA:HB1	2.01	0.42
1:V:79:HIS:CG	1:V:80:SER:H	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:HIS:CG	1:D:80:SER:N	2.89	0.42
1:Q:169:VAL:HB	1:Q:247:ALA:HB1	2.01	0.41
1:P:169:VAL:HB	1:P:247:ALA:HB1	2.02	0.41
1:K:235:ALA:C	1:K:236:LEU:HD12	2.40	0.41
1:C:199:LYS:HE3	1:M:74:ILE:HD11	2.02	0.41
1:H:130:SER:HB2	1:I:138:SER:HB3	2.03	0.41
1:M:181:GLY:O	1:M:182:THR:C	2.58	0.41
1:W:147:MET:SD	1:W:228:VAL:HG21	2.60	0.41
1:X:147:MET:SD	1:X:228:VAL:HG21	2.60	0.41
1:M:79:HIS:CG	1:M:80:SER:N	2.88	0.41
1:O:235:ALA:C	1:O:236:LEU:HD12	2.41	0.41
1:D:237:LEU:HD11	1:E:249:ARG:HH22	1.86	0.41
1:P:249:ARG:NH2	1:Q:237:LEU:HD11	2.36	0.41
1:O:130:SER:HB2	1:P:138:SER:HB3	2.01	0.41
1:N:235:ALA:C	1:N:236:LEU:HD12	2.41	0.41
1:R:79:HIS:CG	1:R:80:SER:H	2.39	0.41
1:G:147:MET:SD	1:G:228:VAL:HG21	2.60	0.41
1:A:138:SER:HB3	1:J:130:SER:HB2	71.58	0.41
1:B:79:HIS:CG	1:B:80:SER:H	2.39	0.41
1:P:79:HIS:CG	1:P:80:SER:N	2.89	0.41
1:E:169:VAL:HB	1:E:247:ALA:HB1	2.02	0.41
1:T:124:ARG:HB2	1:T:194:THR:HG22	2.02	0.41
1:S:223:ILE:CD1	1:U:223:ILE:HD11	2.50	0.41
1:P:260:GLU:N	1:P:261:PRO:HD3	2.36	0.41
1:N:74:ILE:HD11	1:P:199:LYS:HE3	2.03	0.41
1:B:223:ILE:HG12	1:B:223:ILE:H	1.60	0.41
1:P:235:ALA:C	1:P:236:LEU:HD12	2.42	0.41
1:C:228:VAL:HA	1:C:229:PRO:HD3	1.98	0.41
1:V:124:ARG:HB2	1:V:194:THR:HG22	2.02	0.41
1:B:141:MET:O	1:B:164:TYR:HA	2.21	0.41
1:X:141:MET:O	1:X:164:TYR:HA	2.21	0.41
1:D:141:MET:O	1:D:164:TYR:HA	2.20	0.40
1:R:215:THR:HG23	1:R:216:ALA:H	1.85	0.40
1:D:134:SER:HA	1:S:132:PRO:HB3	90.73	0.40
1:F:228:VAL:HA	1:F:229:PRO:HD3	1.87	0.40
1:Q:107:TRP:CZ2	1:R:261:PRO:HB3	2.56	0.40
1:L:235:ALA:C	1:L:236:LEU:HD12	2.42	0.40
1:A:228:VAL:HA	1:A:229:PRO:HD3	1.87	0.40
1:P:141:MET:O	1:P:164:TYR:HA	2.21	0.40
1:O:79:HIS:CG	1:O:80:SER:N	2.89	0.40
1:R:237:LEU:HD11	1:V:249:ARG:HH22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:141:MET:O	1:J:164:TYR:HA	2.22	0.40
1:W:235:ALA:C	1:W:236:LEU:HD12	2.42	0.40
1:M:147:MET:SD	1:M:228:VAL:HG21	2.61	0.40
1:C:79:HIS:CG	1:C:80:SER:H	2.41	0.40
1:X:79:HIS:CG	1:X:80:SER:H	2.40	0.40
1:A:130:SER:HB2	1:E:138:SER:HB3	2.02	0.40
1:H:79:HIS:CG	1:H:80:SER:N	2.89	0.40

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:L:90:ASP:OD1	1:c:242:SER:OG[4_546]	1.99	0.21
1:F:154:SER:OG	1:I:90:ASP:OD2[4_455]	2.10	0.10

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	B	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
1	C	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
1	D	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	E	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
1	F	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	G	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	H	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	I	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
1	J	189/282 (67%)	180 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	189/282 (67%)	180 (95%)	9 (5%)	0	100	100
1	L	189/282 (67%)	180 (95%)	9 (5%)	0	100	100
1	M	189/282 (67%)	177 (94%)	11 (6%)	1 (0%)	34	76
1	N	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	O	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	P	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	Q	189/282 (67%)	179 (95%)	8 (4%)	2 (1%)	17	58
1	R	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
1	S	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	T	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
1	U	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
1	V	189/282 (67%)	180 (95%)	9 (5%)	0	100	100
1	W	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	X	189/282 (67%)	180 (95%)	9 (5%)	0	100	100
1	Y	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
1	Z	189/282 (67%)	180 (95%)	9 (5%)	0	100	100
1	a	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
1	b	189/282 (67%)	180 (95%)	9 (5%)	0	100	100
1	c	189/282 (67%)	181 (96%)	8 (4%)	0	100	100
1	d	189/282 (67%)	182 (96%)	7 (4%)	0	100	100
All	All	5670/8460 (67%)	5427 (96%)	240 (4%)	3 (0%)	56	90

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	154/238 (65%)	153 (99%)	1 (1%)	90	97
1	B	155/238 (65%)	155 (100%)	0	100	100
1	C	155/238 (65%)	155 (100%)	0	100	100
1	D	156/238 (66%)	155 (99%)	1 (1%)	90	97
1	E	149/238 (63%)	149 (100%)	0	100	100
1	F	140/238 (59%)	140 (100%)	0	100	100
1	G	156/238 (66%)	155 (99%)	1 (1%)	90	97
1	H	152/238 (64%)	152 (100%)	0	100	100
1	I	156/238 (66%)	155 (99%)	1 (1%)	90	97
1	J	155/238 (65%)	155 (100%)	0	100	100
1	K	155/238 (65%)	154 (99%)	1 (1%)	90	97
1	L	155/238 (65%)	155 (100%)	0	100	100
1	M	156/238 (66%)	154 (99%)	2 (1%)	76	93
1	N	154/238 (65%)	153 (99%)	1 (1%)	90	97
1	O	155/238 (65%)	155 (100%)	0	100	100
1	P	155/238 (65%)	155 (100%)	0	100	100
1	Q	143/238 (60%)	143 (100%)	0	100	100
1	R	152/238 (64%)	152 (100%)	0	100	100
1	S	151/238 (63%)	151 (100%)	0	100	100
1	T	155/238 (65%)	154 (99%)	1 (1%)	90	97
1	U	153/238 (64%)	152 (99%)	1 (1%)	88	96
1	V	156/238 (66%)	155 (99%)	1 (1%)	90	97
1	W	155/238 (65%)	155 (100%)	0	100	100
1	X	154/238 (65%)	154 (100%)	0	100	100
1	Y	153/238 (64%)	153 (100%)	0	100	100
1	Z	153/238 (64%)	153 (100%)	0	100	100
1	a	154/238 (65%)	154 (100%)	0	100	100
1	b	155/238 (65%)	155 (100%)	0	100	100
1	c	156/238 (66%)	155 (99%)	1 (1%)	90	97
1	d	155/238 (65%)	154 (99%)	1 (1%)	90	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4603/7140 (64%)	4590 (100%)	13 (0%)	94 98

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

Mol	Chain	Res	Type
1	A	225	THR
1	D	225	THR
1	G	225	THR
1	I	225	THR
1	K	225	THR
1	M	180	ASN
1	M	182	THR
1	N	225	THR
1	T	225	THR
1	U	225	THR
1	V	225	THR
1	c	225	THR
1	d	225	THR

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	D	301	-	4,4,4	0.32	0	6,6,6	0.07	0
2	SO4	H	301	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	L	301	-	4,4,4	0.32	0	6,6,6	0.06	0
2	SO4	M	301	-	4,4,4	0.32	0	6,6,6	0.07	0
2	SO4	S	301	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	V	301	-	4,4,4	0.32	0	6,6,6	0.07	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	D	301	-	-	0/0/0/0	0/0/0/0
2	SO4	H	301	-	-	0/0/0/0	0/0/0/0
2	SO4	L	301	-	-	0/0/0/0	0/0/0/0
2	SO4	M	301	-	-	0/0/0/0	0/0/0/0
2	SO4	S	301	-	-	0/0/0/0	0/0/0/0
2	SO4	V	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.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	SO4	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	SO4	1	0
2	M	301	SO4	2	0
2	S	301	SO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/282 (67%)	-0.59	0 100 100	25, 40, 70, 84	0
1	B	191/282 (67%)	-0.61	0 100 100	25, 36, 69, 79	0
1	C	191/282 (67%)	-0.71	0 100 100	22, 31, 55, 91	0
1	D	191/282 (67%)	-0.56	0 100 100	23, 34, 69, 77	0
1	E	191/282 (67%)	-0.64	0 100 100	26, 38, 75, 88	0
1	F	191/282 (67%)	-0.45	0 100 100	26, 43, 84, 97	0
1	G	191/282 (67%)	-0.64	0 100 100	25, 38, 65, 80	0
1	H	191/282 (67%)	-0.60	0 100 100	26, 39, 68, 83	0
1	I	191/282 (67%)	-0.72	0 100 100	23, 37, 69, 80	0
1	J	191/282 (67%)	-0.63	0 100 100	22, 35, 67, 82	0
1	K	191/282 (67%)	-0.63	0 100 100	20, 32, 65, 76	0
1	L	191/282 (67%)	-0.75	0 100 100	18, 29, 60, 79	0
1	M	191/282 (67%)	-0.69	0 100 100	19, 30, 60, 79	0
1	N	191/282 (67%)	-0.70	0 100 100	21, 34, 66, 79	0
1	O	191/282 (67%)	-0.61	0 100 100	25, 37, 67, 79	0
1	P	191/282 (67%)	-0.58	0 100 100	23, 37, 66, 81	0
1	Q	191/282 (67%)	-0.45	1 (0%) 91 76	27, 42, 101, 143	0
1	R	191/282 (67%)	-0.45	0 100 100	26, 44, 85, 113	0
1	S	191/282 (67%)	-0.61	0 100 100	24, 39, 72, 83	0
1	T	191/282 (67%)	-0.60	2 (1%) 84 60	23, 36, 66, 85	0
1	U	191/282 (67%)	-0.62	0 100 100	21, 36, 72, 86	0
1	V	191/282 (67%)	-0.62	0 100 100	25, 36, 65, 78	0
1	W	191/282 (67%)	-0.65	0 100 100	23, 37, 64, 82	0
1	X	191/282 (67%)	-0.70	0 100 100	19, 34, 66, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	191/282 (67%)	-0.63	0 100 100	21, 35, 69, 81	0
1	Z	191/282 (67%)	-0.59	1 (0%) 91 76	25, 38, 72, 87	0
1	a	191/282 (67%)	-0.51	0 100 100	25, 39, 73, 89	0
1	b	191/282 (67%)	-0.71	0 100 100	19, 30, 57, 79	0
1	c	191/282 (67%)	-0.69	0 100 100	19, 30, 64, 78	0
1	d	191/282 (67%)	-0.62	0 100 100	25, 36, 68, 75	0
All	All	5730/8460 (67%)	-0.62	4 (0%) 95 90	18, 36, 70, 143	0

All (4) RSRZ outliers are listed below:

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

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	S	301	5/5	0.99	0.19	2.95	4,4,4,4	0
2	SO4	L	301	5/5	0.99	0.17	2.45	2,2,2,2	0
2	SO4	M	301	5/5	0.99	0.19	2.08	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	D	301	5/5	0.99	0.19	1.45	6,7,7,7	0
2	SO4	H	301	5/5	0.99	0.16	0.90	8,8,9,9	0
2	SO4	V	301	5/5	0.99	0.20	-0.17	5,6,6,6	0

6.5 Other polymers [i](#)

There are no such residues in this entry.