



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:15 PM UTC

PDB ID : 4Y5Z / pdb_00004y5z
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

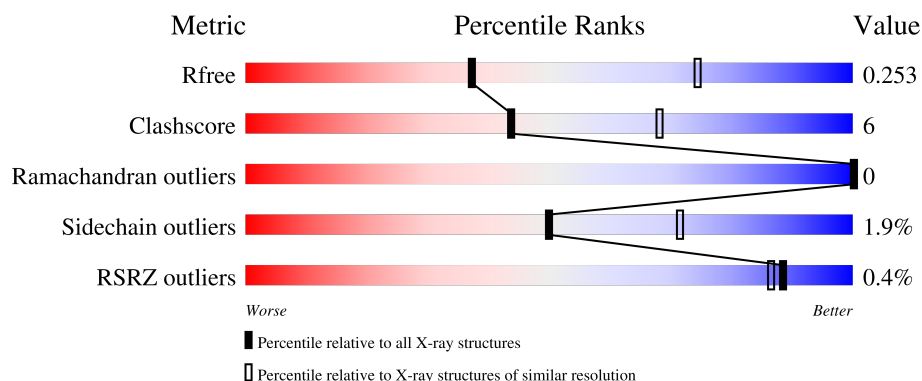
1 Overall quality at a glance

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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 57% 11% 32%
1	1	282	 57% 10% 32%
1	2	282	 59% 9% 32%
1	3	282	 55% 14% 31%
1	4	282	 60% 8% 32%

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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	 56%11%32%
1	w	282	 56%12%32%
1	x	282	 56%12%32%
1	y	282	 57%11%32%
1	z	282	 55%13%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	P	301	-	-	X	-
2	SO4	h	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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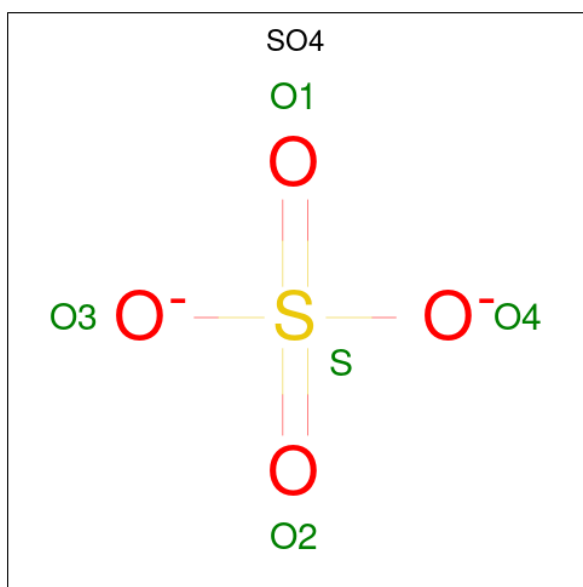
Chain	Residue	Modelled	Actual	Comment	Reference
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j	62	GLU	-	linker	UNP P02976
j	63	LEU	-	linker	UNP P02976
j	64	GLU	-	linker	UNP P02976
j	65	MET	-	linker	UNP P02976
l	-13	MET	-	expression tag	UNP P02976
l	-12	ARG	-	expression tag	UNP P02976
l	-11	GLY	-	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 (CCD ID: SO4) (formula: O₄S).



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 O 30 30	0	0
3	B	13	Total O 13 13	0	0
3	C	16	Total O 16 16	0	0
3	D	21	Total O 21 21	0	0
3	E	21	Total O 21 21	0	0
3	F	33	Total O 33 33	0	0
3	G	37	Total O 37 37	0	0
3	H	29	Total O 29 29	0	0
3	I	38	Total O 38 38	0	0
3	J	22	Total O 22 22	0	0
3	K	28	Total O 28 28	0	0
3	L	29	Total O 29 29	0	0
3	M	39	Total O 39 39	0	0
3	N	27	Total O 27 27	0	0
3	O	28	Total O 28 28	0	0
3	P	19	Total O 19 19	0	0
3	Q	16	Total O 16 16	0	0
3	R	15	Total O 15 15	0	0
3	S	16	Total O 16 16	0	0
3	T	14	Total O 14 14	0	0
3	U	30	Total O 30 30	0	0
3	V	25	Total O 25 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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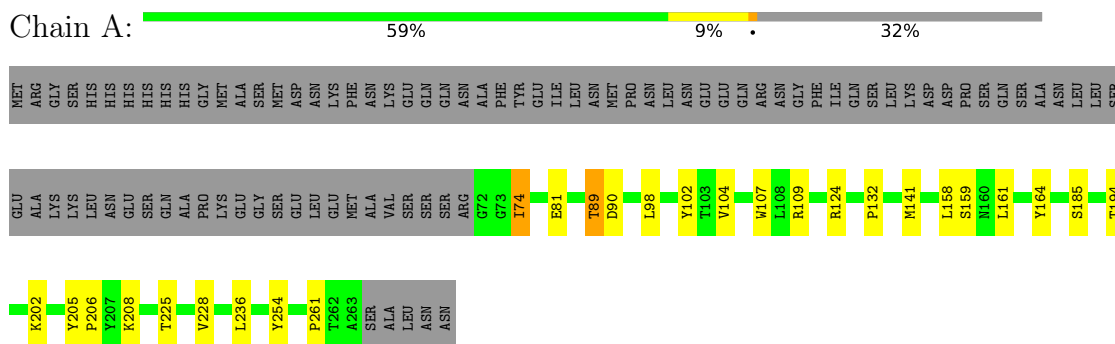
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	z	29	Total 29	O 29	0	0
3	0	23	Total 23	O 23	0	0
3	1	24	Total 24	O 24	0	0
3	2	26	Total 26	O 26	0	0
3	3	19	Total 19	O 19	0	0
3	4	16	Total 16	O 16	0	0
3	5	20	Total 20	O 20	0	0
3	6	19	Total 19	O 19	0	0
3	7	17	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

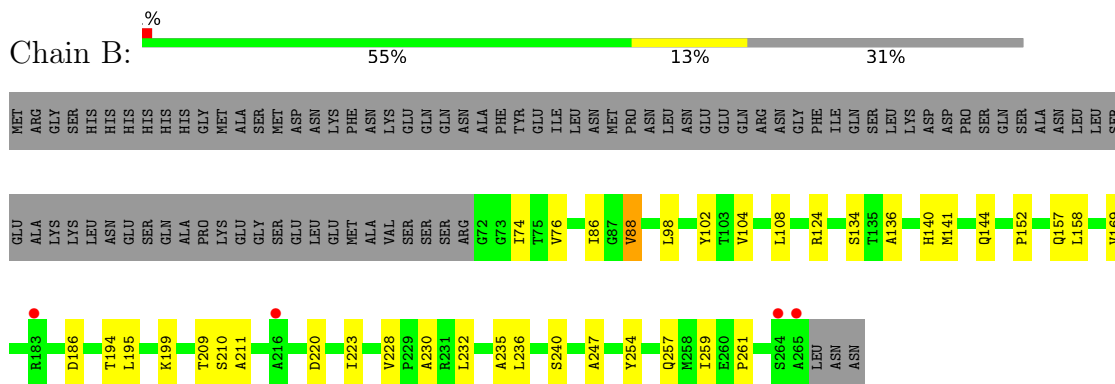
3 Residue-property plots

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

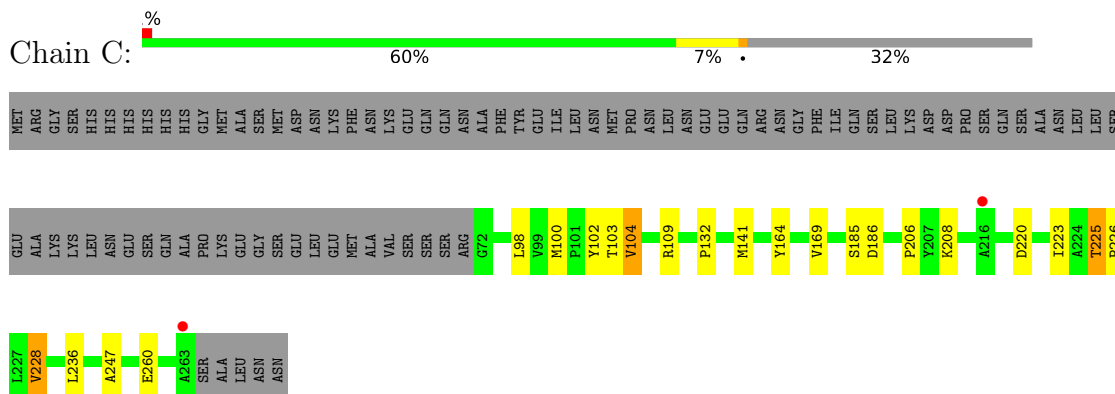
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



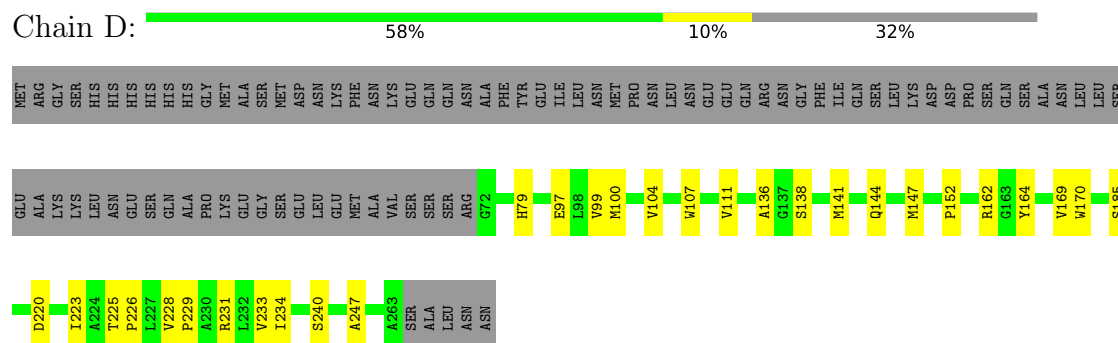
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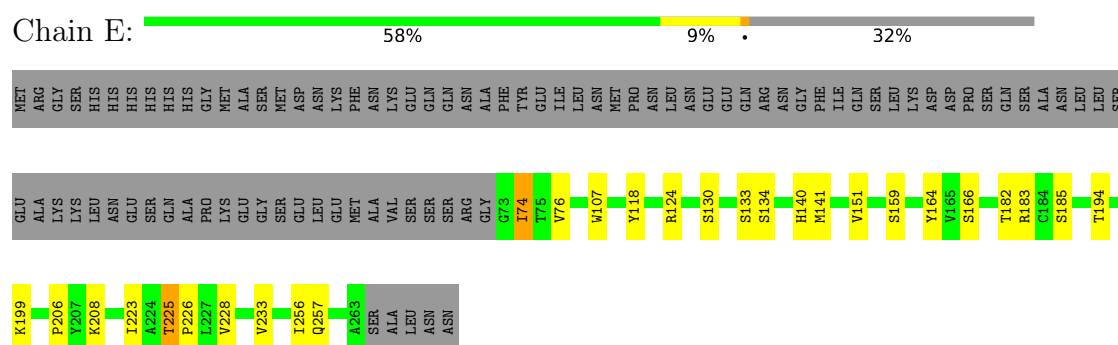
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



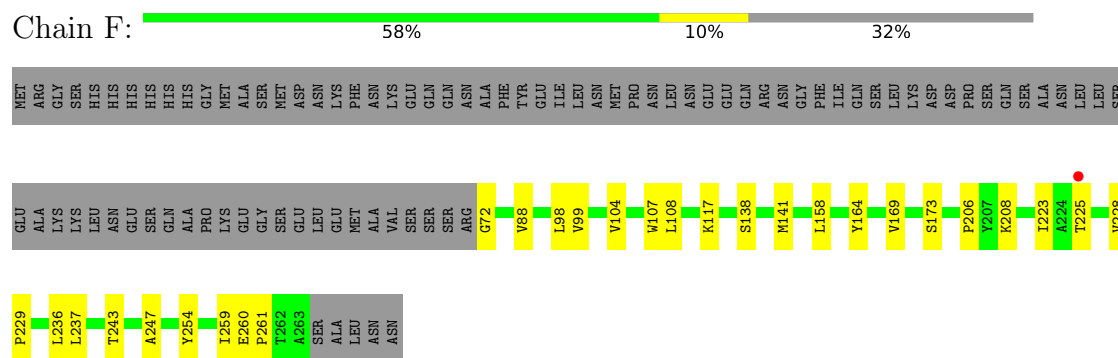
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



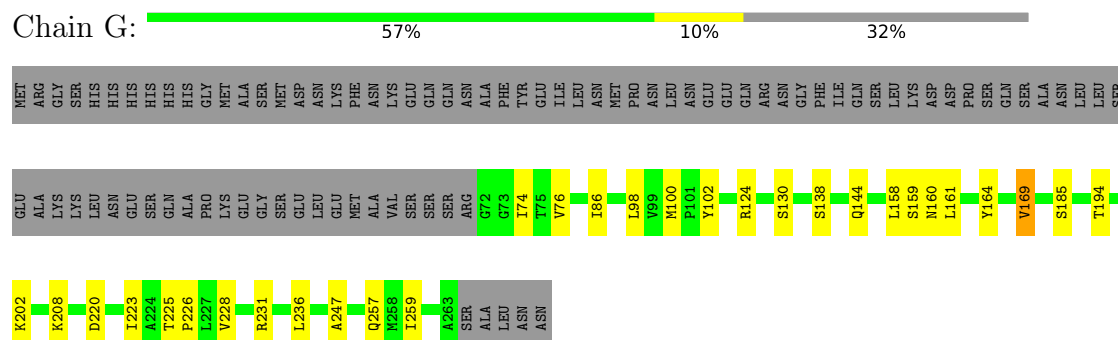
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



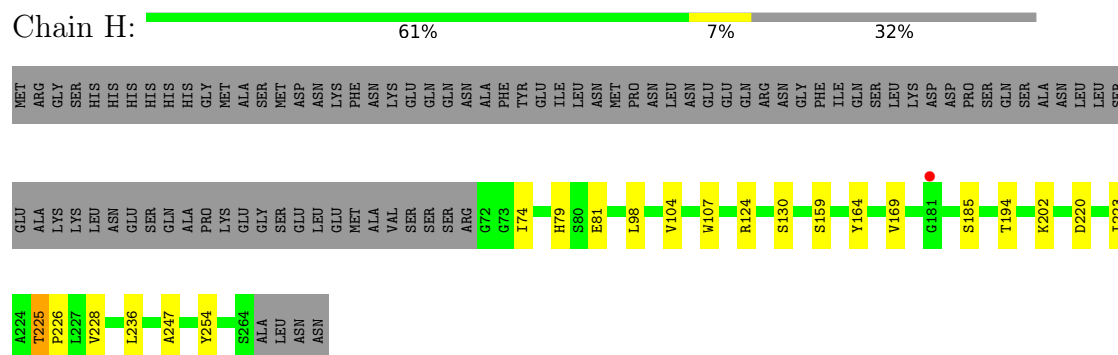
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



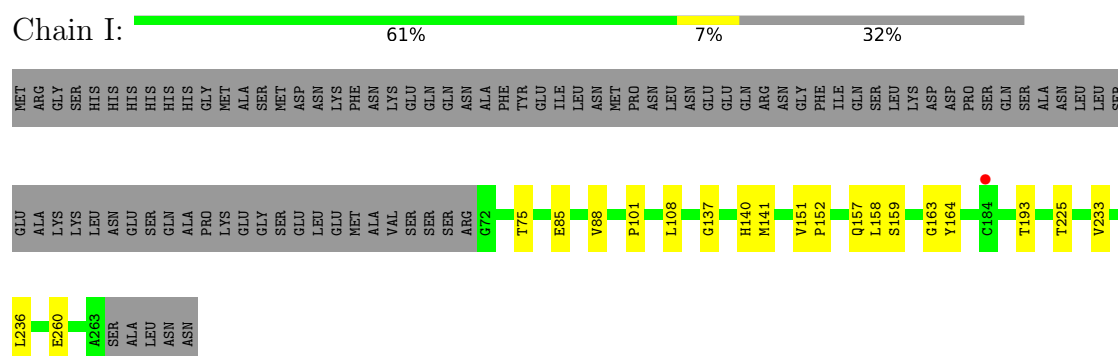
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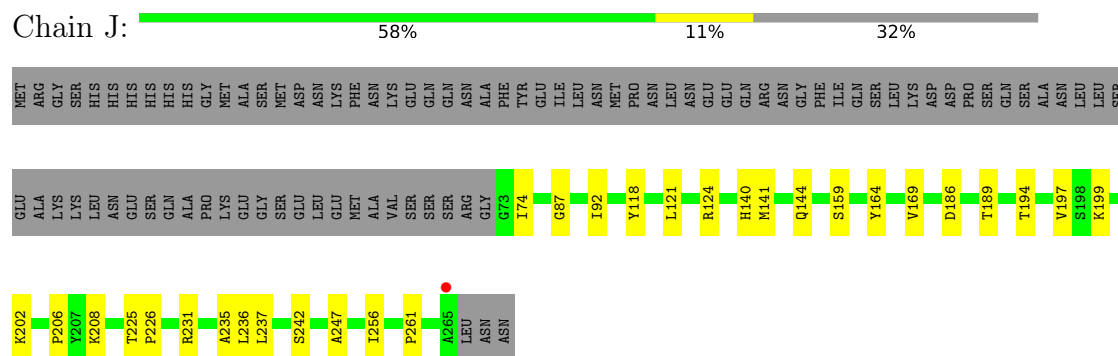
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



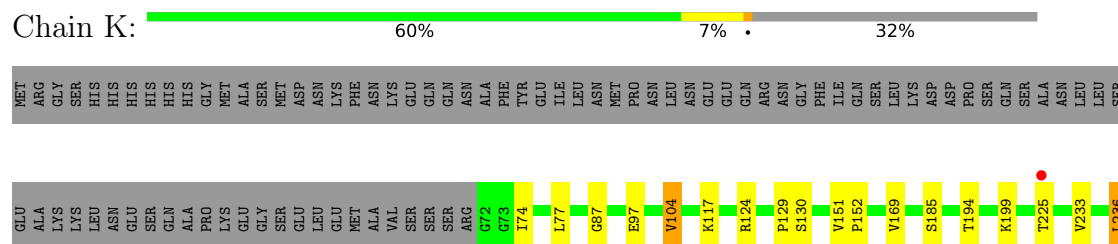
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

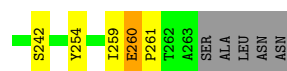


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

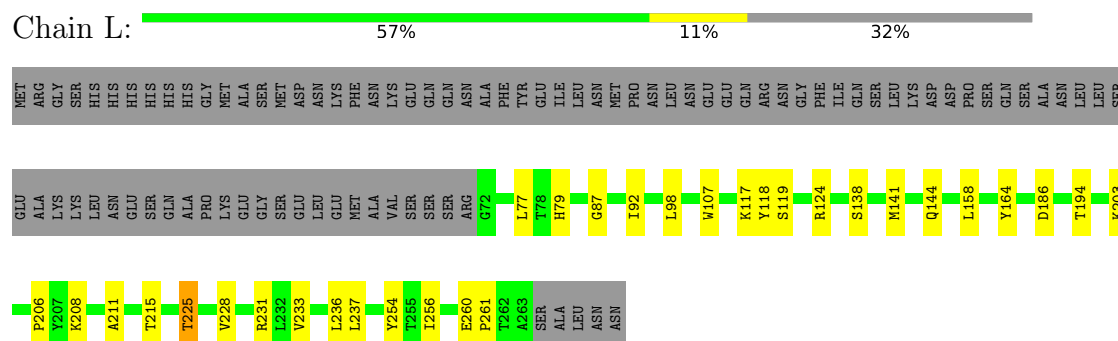


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

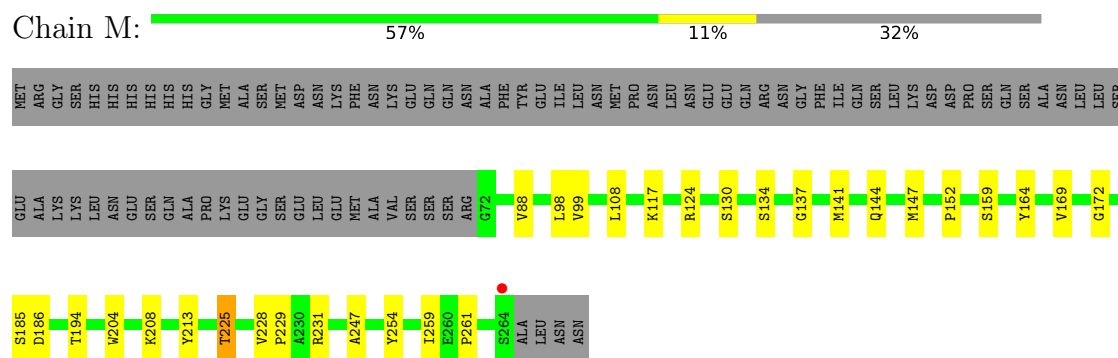




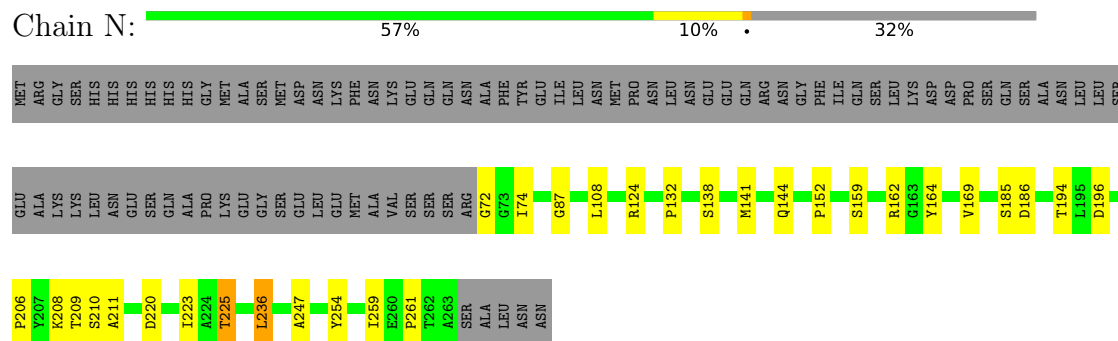
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



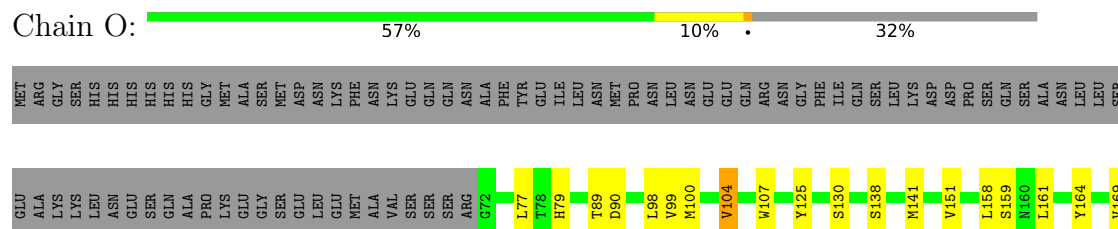
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



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

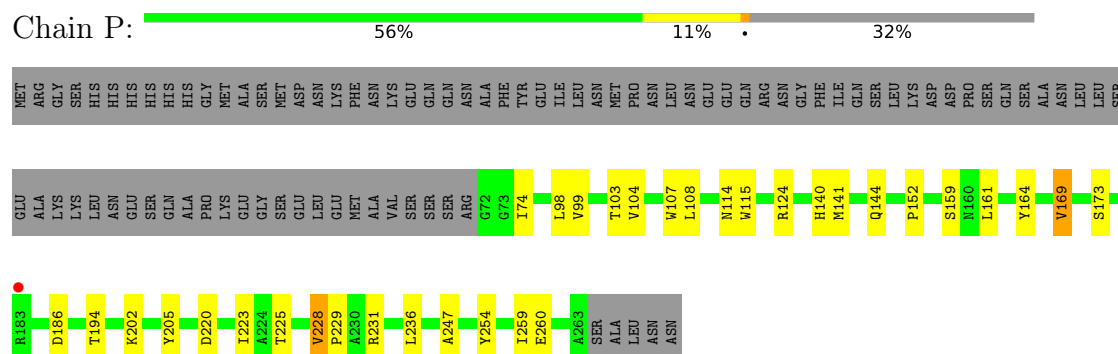


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

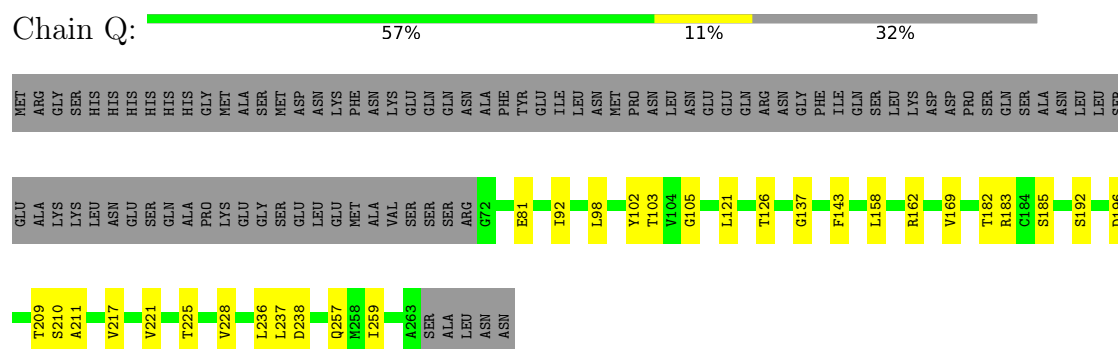




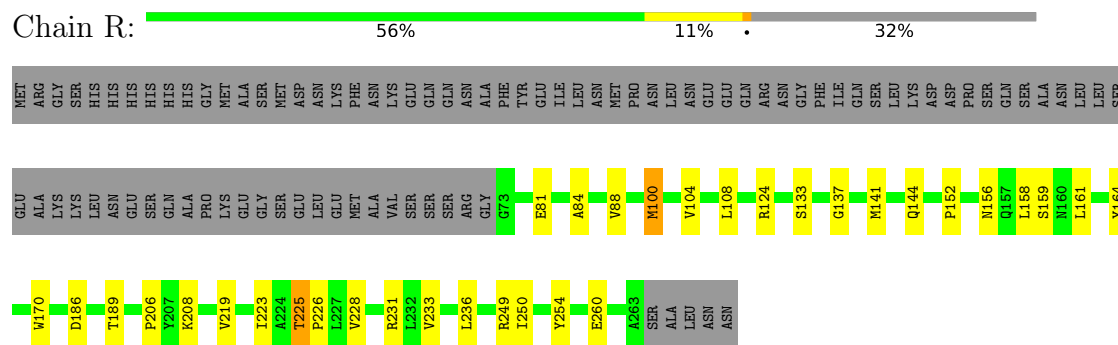
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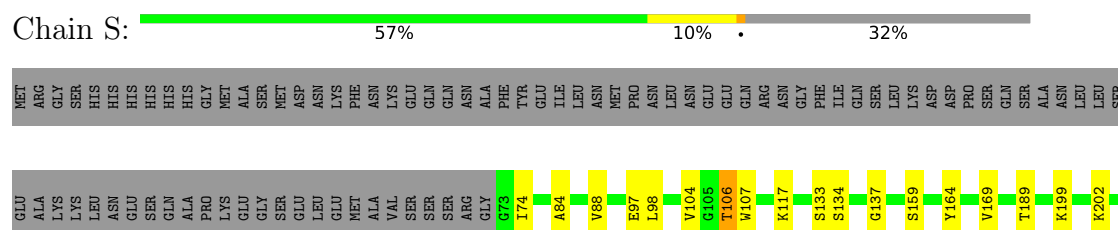
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- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



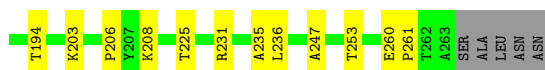
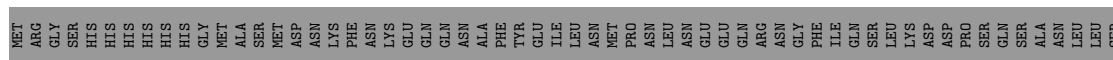
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein





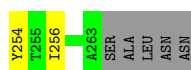
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain T: 58% 10% 32%



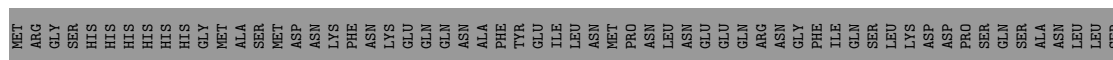
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain U: 61% 6% 32%



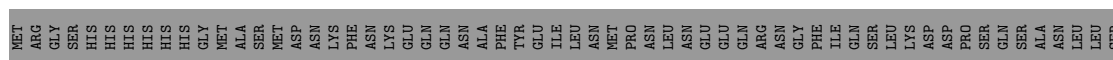
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

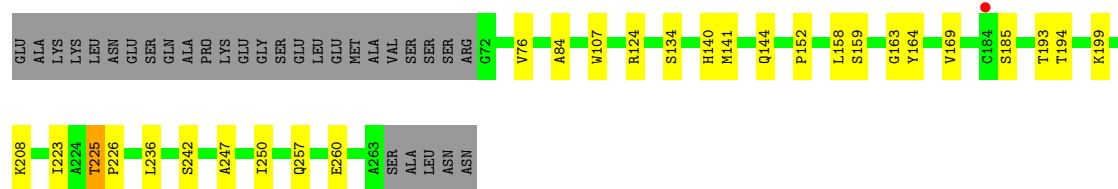
Chain V: 58% 9% 32%



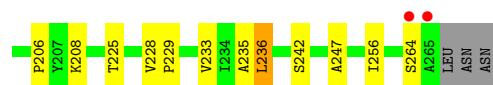
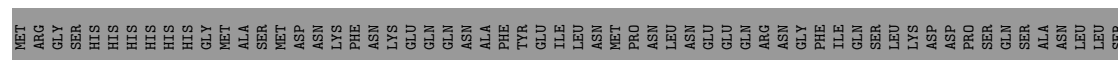
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain W: 58% 10% 32%

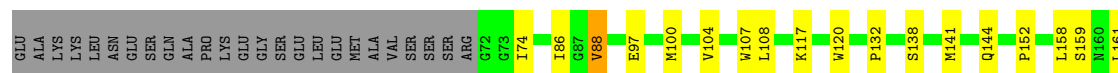
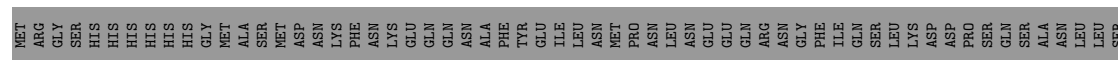




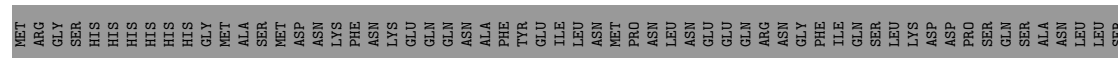
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



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

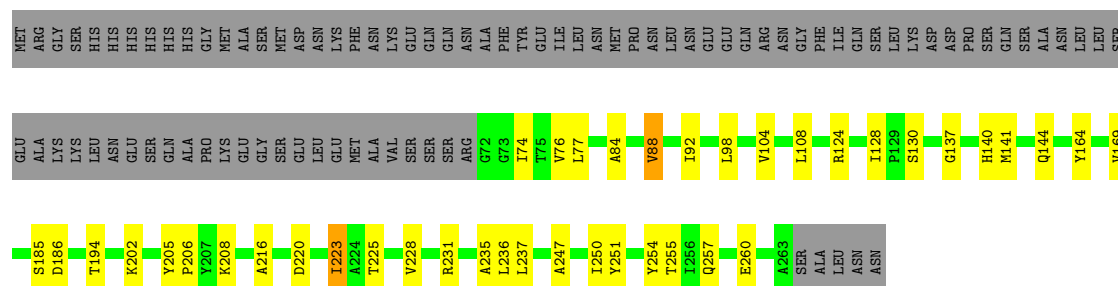


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



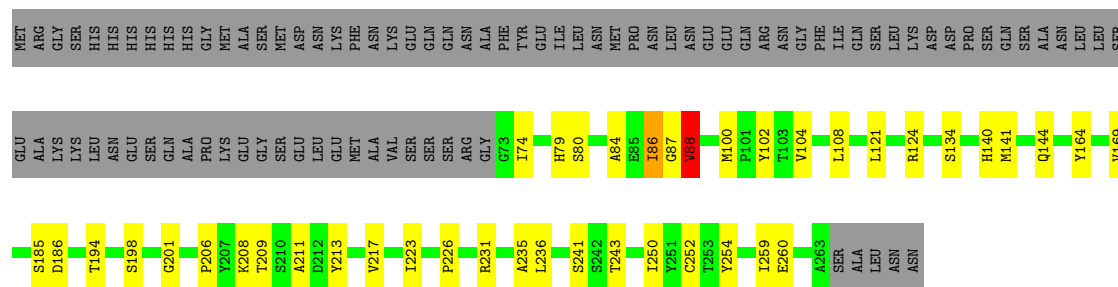
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein





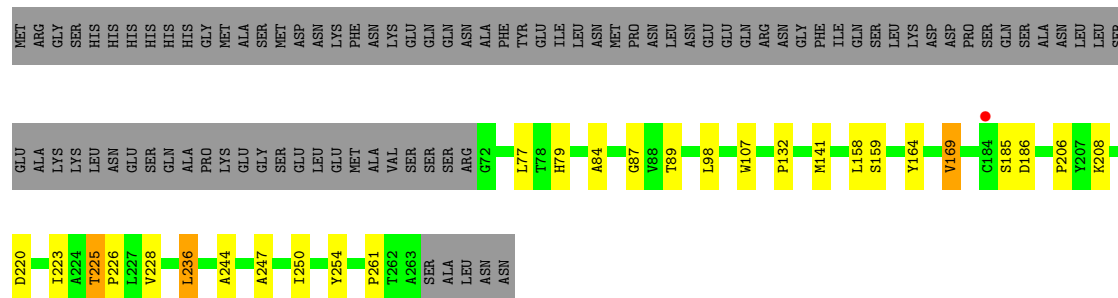
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain c: 53% 14% 32%



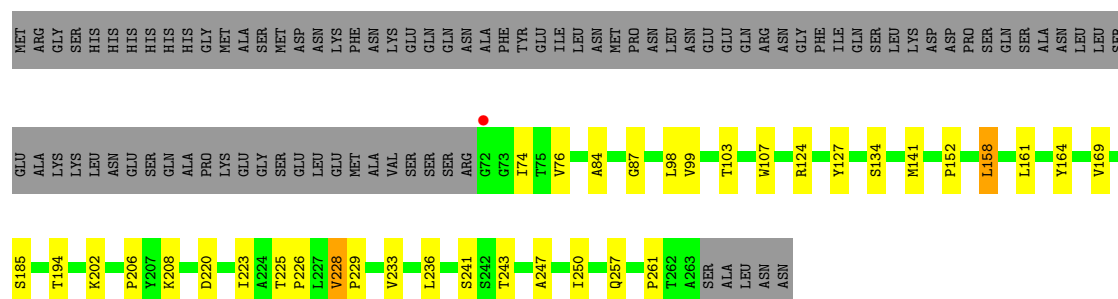
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain e: 58% 9% 32%



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

Chain g: 55% 12% 32%



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

Response	Percentage
Yes	59%
No	9%
Don't know	32%



Response	Percentage
Yes	56%
No	12%
Don't know	32%

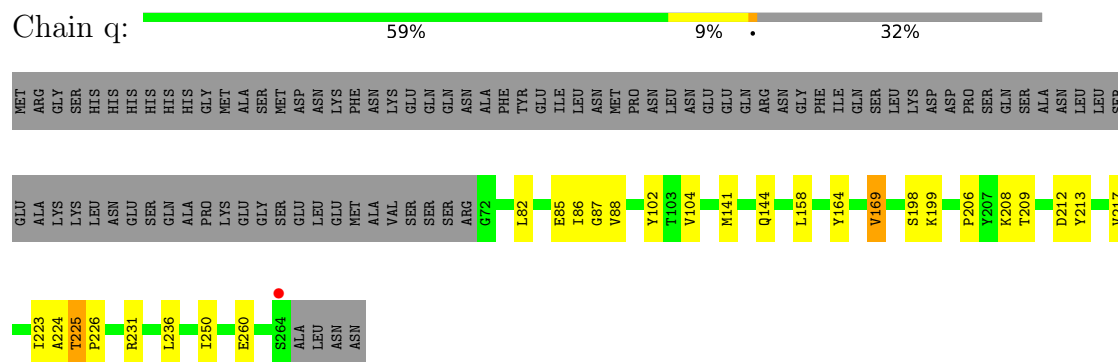


59% 9% 32%

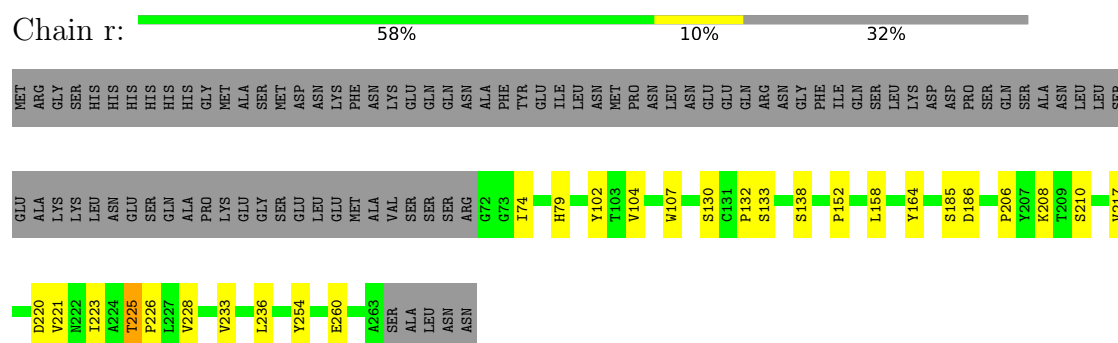


59% 9% . 32%

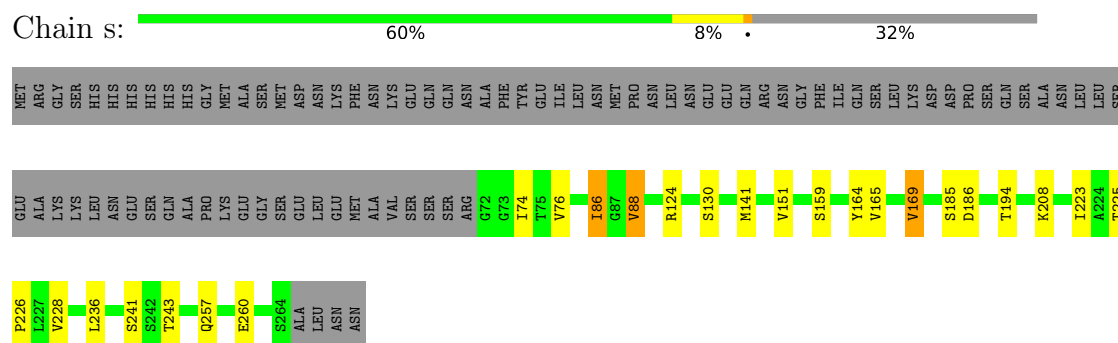
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



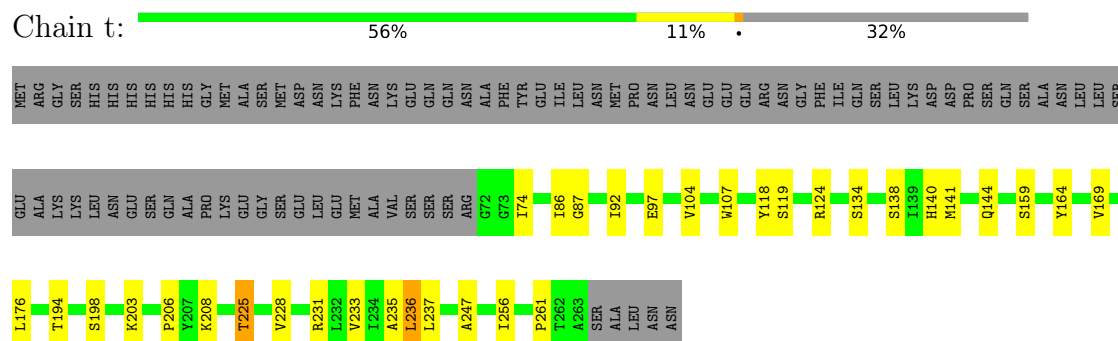
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



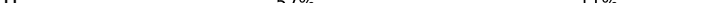
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

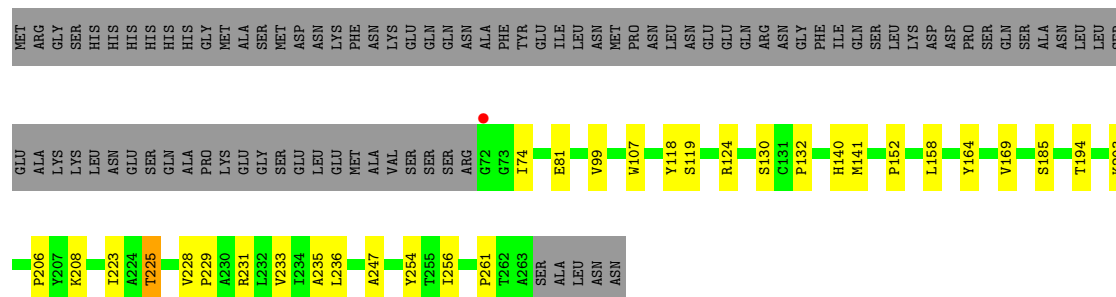


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



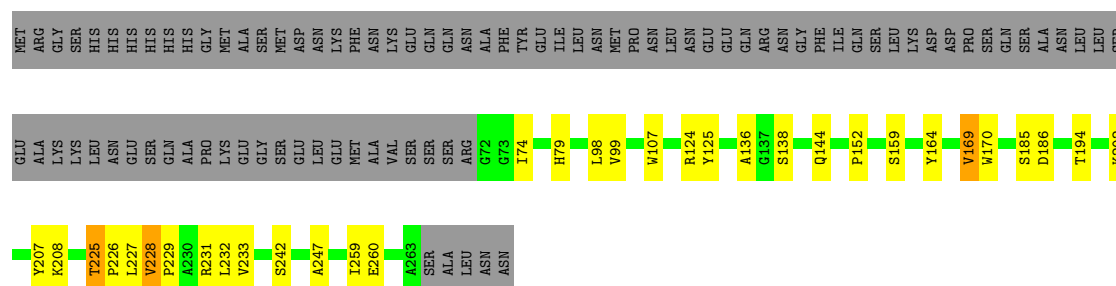
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain u:  57% 11% 32%

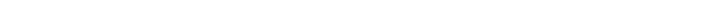


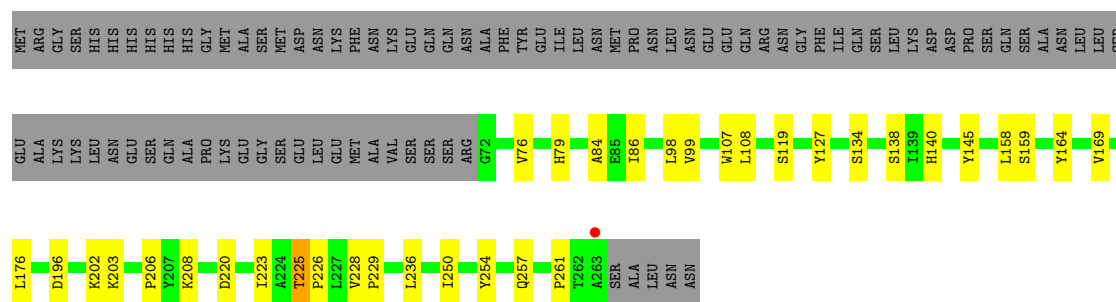
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain v: 56% 11% 32%

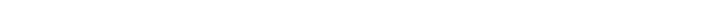


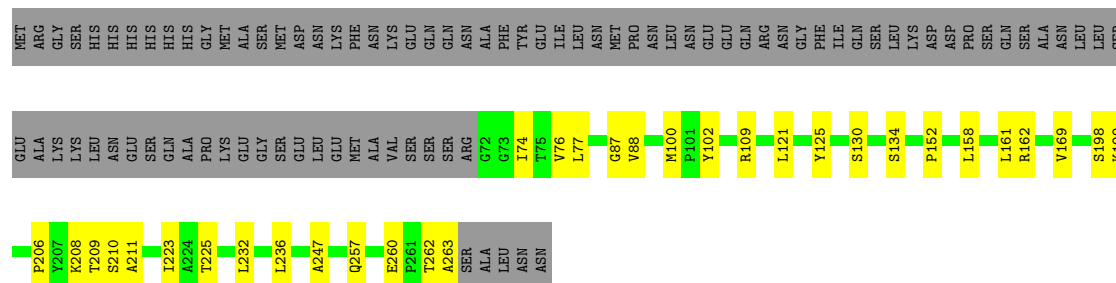
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain w:  56% 12% 32%

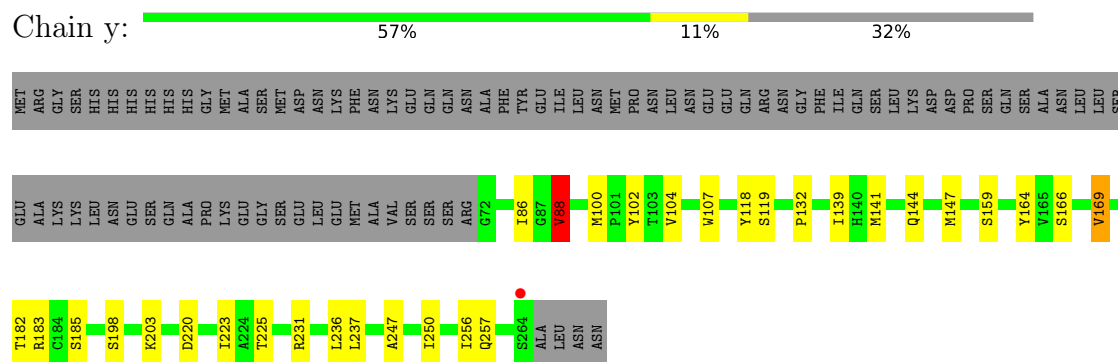


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

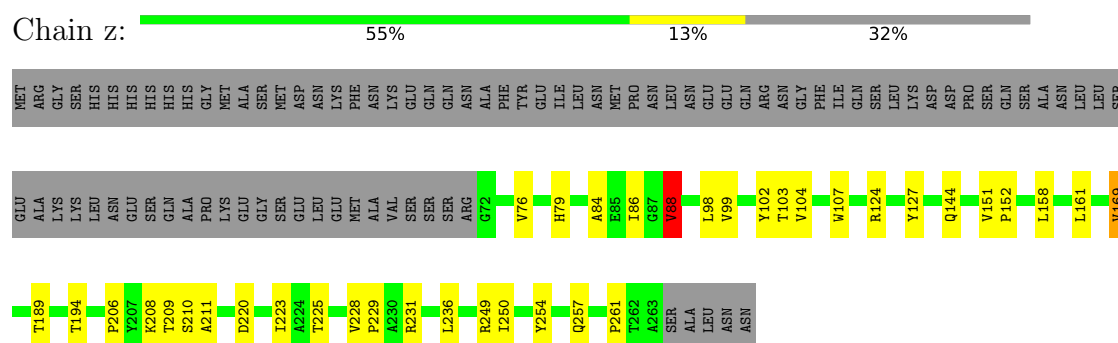
Chain x:  56% 12% 32%



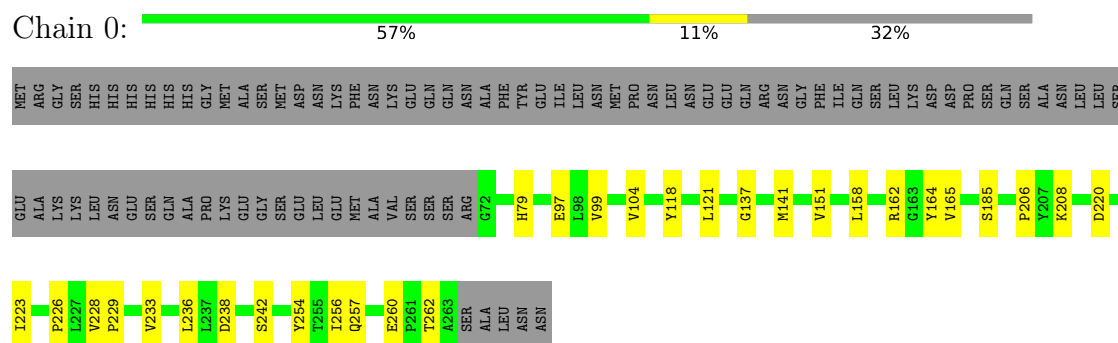
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



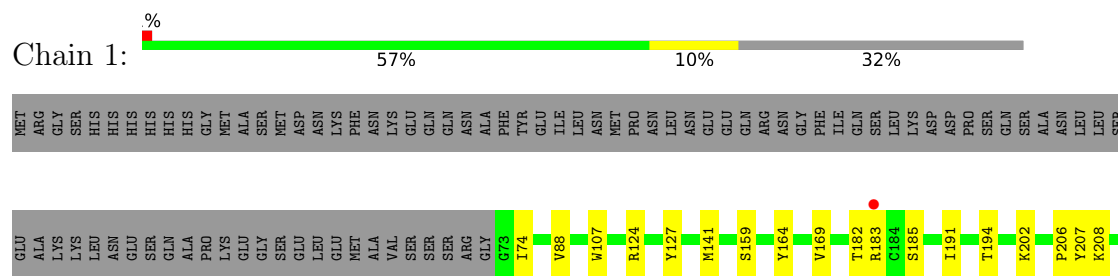
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



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



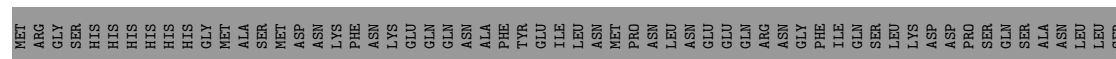
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein





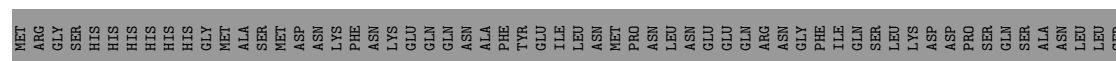
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain 2: 59% 9% 32%



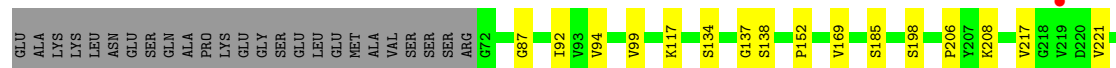
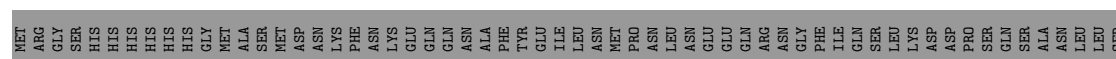
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain 3: 55% 14% 31%



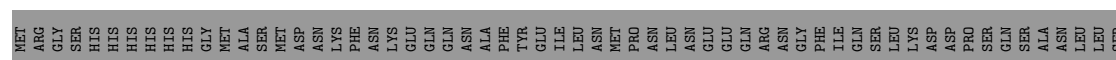
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

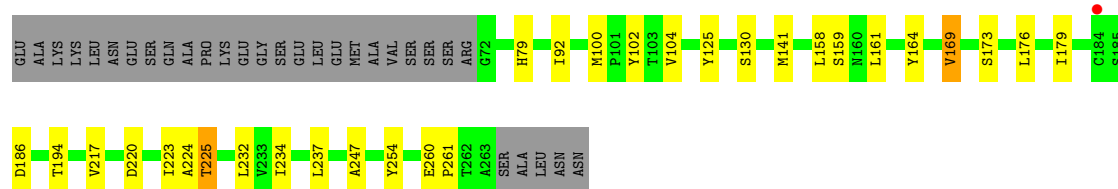
Chain 4: 60% 8% 32%



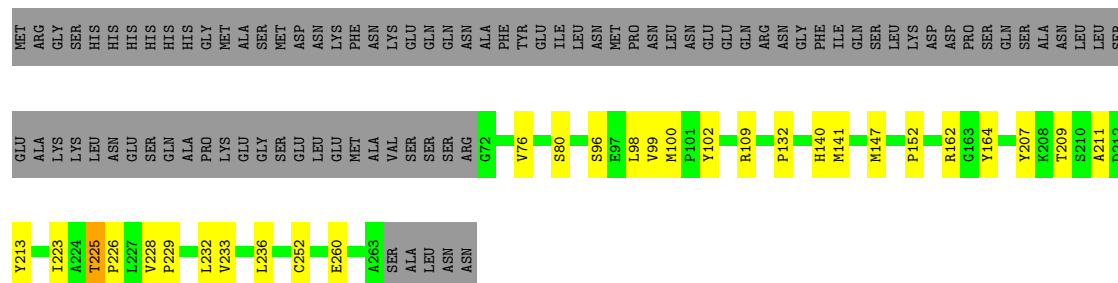
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain 5: 57% 10% 32%

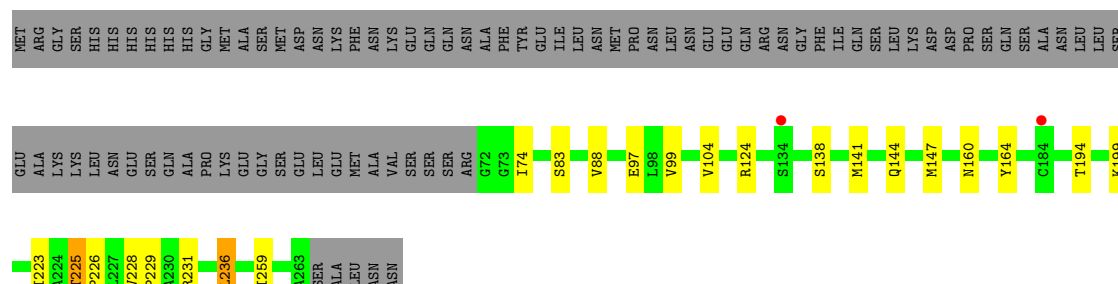




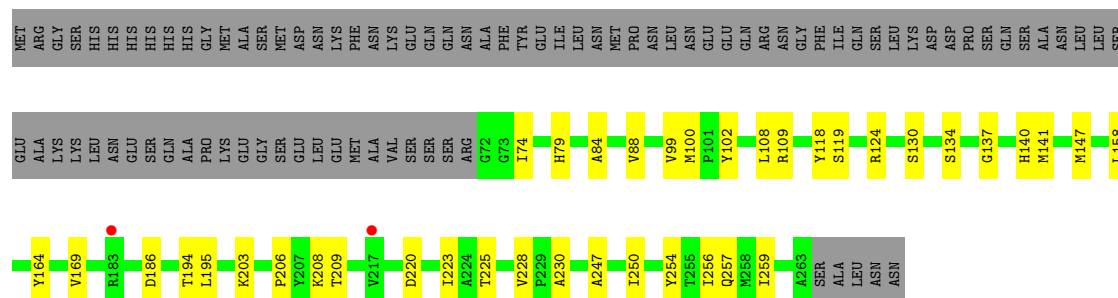
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



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

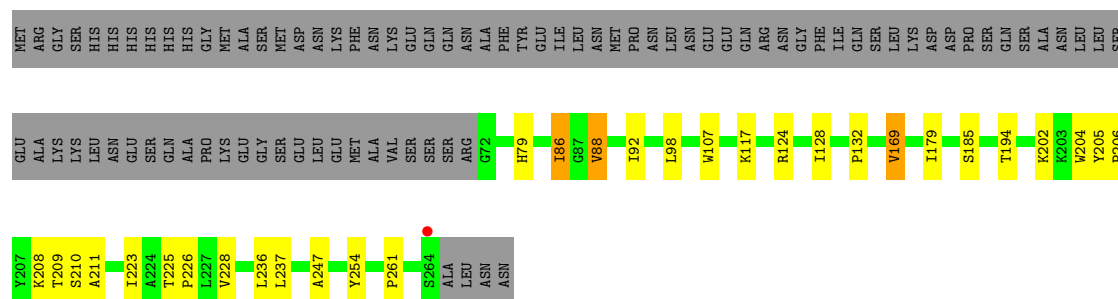


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



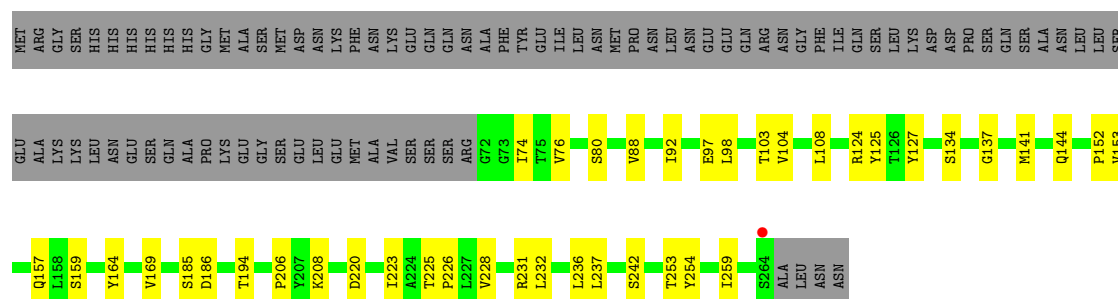
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein





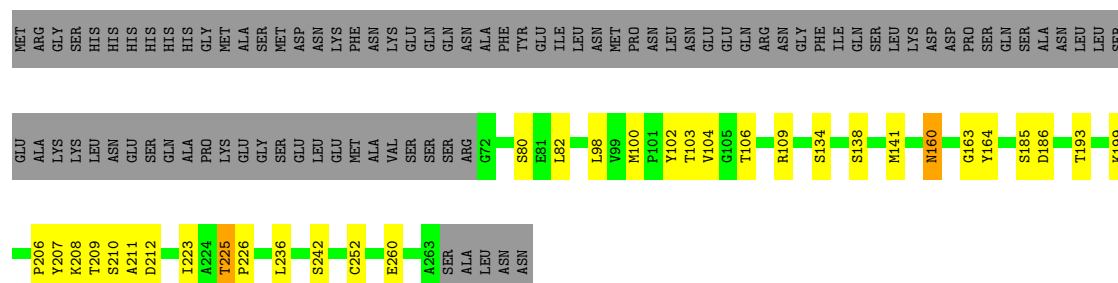
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain f: 54% 15% 32%



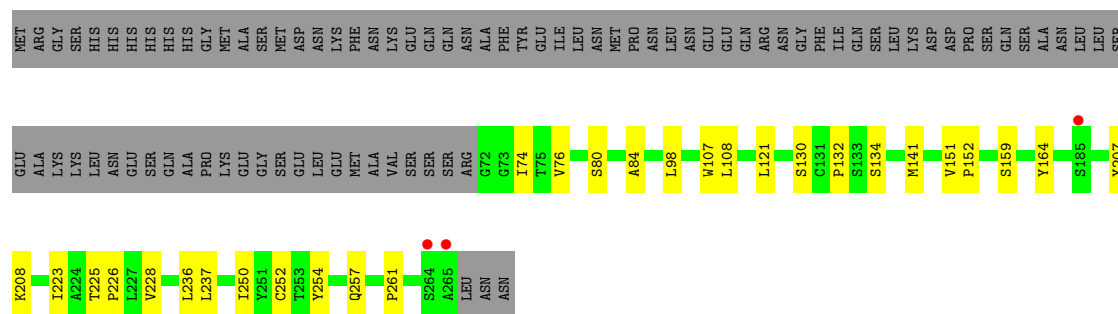
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

Chain h: 56% 11% 32%

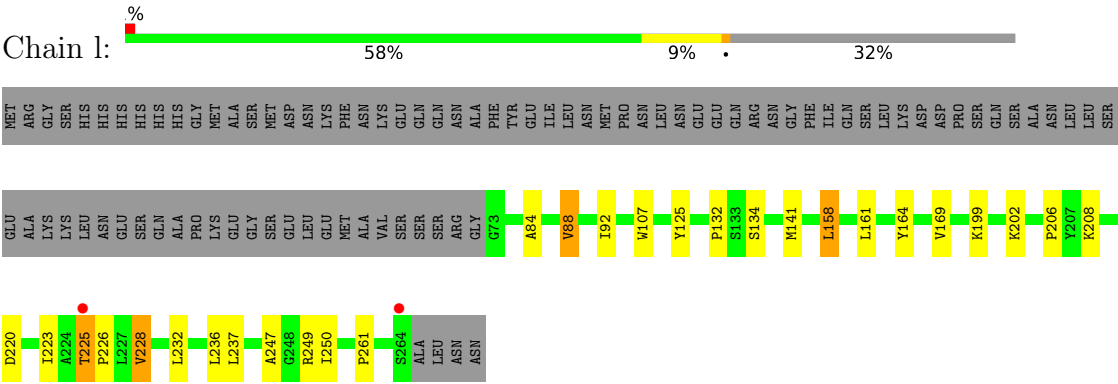


- Molecule 1: Immunoglobulin G-binding protein A, Coat protein

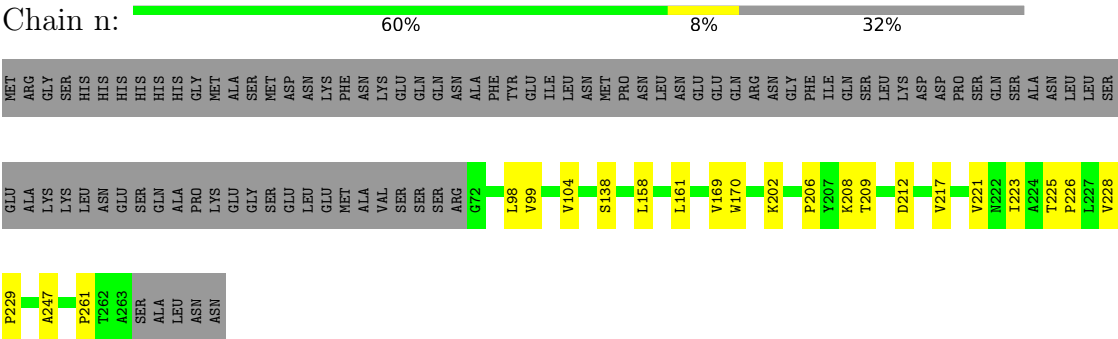
Chain j: 59% 10% 31%



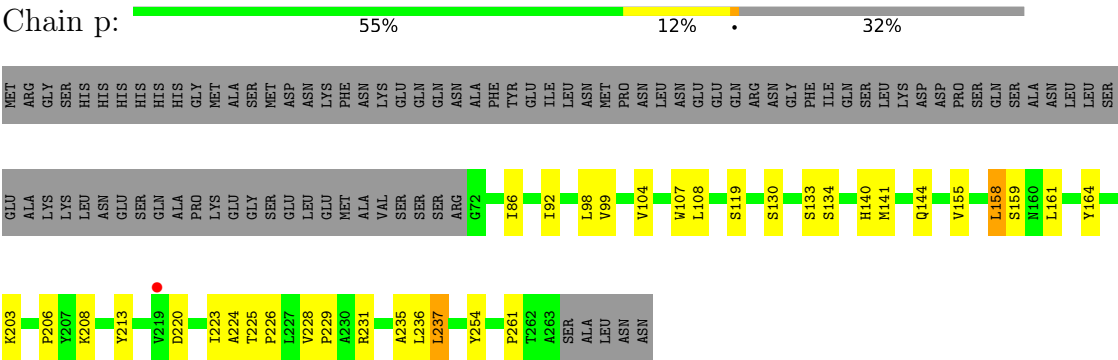
- Molecule 1: Immunoglobulin G-binding protein A, Coat protein



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 89.3 (41.92-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.9-1692	Depositor
R, R_{free}	0.196 , 0.249 0.203 , 0.253	Depositor DCC
R_{free} test set	18386 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage

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¹Intensities estimated from amplitudes.

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

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Property	Value	Source
Estimated twinning fraction	0.014 for k,l,h-k+l 0.014 for h-k+l,h,k 0.015 for k-l,-h+k-l,-h+k 0.015 for h-k,h-k+l,-k+l 0.015 for l,-h+k,-h 0.015 for -l,k-l,h 0.034 for -h+k-l,-h+k,k 0.034 for -k+l,l,-h+k 0.014 for k,k-l,-h+k-l 0.014 for k-l,h,h-k 0.014 for -h+k,-h,-k+l 0.014 for -k,h-k,h-k+l 0.015 for h-k+l,-k+l,-k 0.015 for h-k,-l,k-l 0.168 for h,h-k,-l 0.015 for -h+k,k,k-l 0.016 for -h,-k+l,l 0.015 for -k,-h,-h+k-l 0.015 for l,h-k+l,h 0.015 for -l,-k,-h 0.033 for -h+k-l,-l,-k 0.075 for -k+l,-k,h-k 0.016 for -h,-h+k-l,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	86922	wwPDB-VP
Average B, all atoms ($\text{\AA}^2$)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.59	0/1456	0.98	6/1996 (0.3%)
1	1	0.64	0/1457	0.98	2/1998 (0.1%)
1	2	0.62	0/1454	1.02	7/1994 (0.4%)
1	3	0.66	0/1466	0.99	2/2010 (0.1%)
1	4	0.61	0/1451	0.96	1/1989 (0.1%)
1	5	0.62	0/1456	0.94	4/1996 (0.2%)
1	6	0.62	0/1454	0.98	5/1993 (0.3%)
1	7	0.59	0/1454	0.90	2/1994 (0.1%)
1	A	0.62	0/1455	0.95	3/1995 (0.2%)
1	B	0.62	0/1461	0.93	1/2003 (0.0%)
1	C	0.59	0/1452	0.95	4/1990 (0.2%)
1	D	0.60	0/1452	0.93	0/1991
1	E	0.59	0/1453	0.96	5/1991 (0.3%)
1	F	0.69	0/1453	0.99	2/1992 (0.1%)
1	G	0.67	0/1459	0.96	3/1999 (0.2%)
1	H	0.65	0/1461	0.94	2/2003 (0.1%)
1	I	0.67	1/1456 (0.1%)	0.98	2/1996 (0.1%)
1	J	0.72	0/1462	0.98	3/2005 (0.1%)
1	K	0.67	0/1456	1.00	5/1996 (0.3%)
1	L	0.69	0/1459	0.96	2/1999 (0.1%)
1	M	0.70	0/1461	1.01	2/2003 (0.1%)
1	N	0.66	0/1456	0.94	2/1996 (0.1%)
1	O	0.66	0/1456	0.93	6/1996 (0.3%)
1	P	0.59	0/1456	0.95	4/1996 (0.2%)
1	Q	0.57	0/1454	0.91	4/1994 (0.2%)
1	R	0.59	0/1453	0.95	6/1992 (0.3%)
1	S	0.61	0/1449	0.98	5/1987 (0.3%)
1	T	0.60	0/1453	0.99	9/1992 (0.5%)
1	U	0.66	0/1456	0.97	2/1996 (0.1%)
1	V	0.67	0/1456	0.96	4/1996 (0.2%)
1	W	0.65	0/1456	0.99	5/1996 (0.3%)
1	X	0.69	0/1466	0.99	3/2010 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Y	0.67	0/1456	0.97	3/1996 (0.2%)
1	Z	0.63	0/1456	0.98	4/1996 (0.2%)
1	a	0.67	0/1452	0.97	5/1992 (0.3%)
1	b	0.65	0/1452	0.98	2/1990 (0.1%)
1	c	0.60	0/1450	0.93	4/1988 (0.2%)
1	d	0.65	0/1461	0.95	4/2003 (0.2%)
1	e	0.64	0/1459	0.92	2/1999 (0.1%)
1	f	0.64	0/1455	1.00	2/1997 (0.1%)
1	g	0.60	0/1452	0.95	3/1991 (0.2%)
1	h	0.64	0/1451	1.02	5/1991 (0.3%)
1	i	0.64	0/1456	0.94	2/1996 (0.1%)
1	j	0.62	0/1466	0.96	4/2010 (0.2%)
1	k	0.64	0/1459	0.96	2/2000 (0.1%)
1	l	0.63	0/1457	0.96	5/1998 (0.3%)
1	m	0.62	0/1461	0.92	2/2003 (0.1%)
1	n	0.63	0/1455	0.91	2/1995 (0.1%)
1	o	0.61	0/1447	0.91	0/1986
1	p	0.61	0/1446	0.95	2/1982 (0.1%)
1	q	0.62	0/1457	0.96	4/1999 (0.2%)
1	r	0.64	0/1456	0.91	4/1996 (0.2%)
1	s	0.68	0/1461	0.98	8/2003 (0.4%)
1	t	0.66	0/1456	0.97	2/1996 (0.1%)
1	u	0.68	0/1456	0.97	2/1996 (0.1%)
1	v	0.67	0/1456	0.99	8/1996 (0.4%)
1	w	0.61	0/1438	0.99	3/1974 (0.2%)
1	x	0.60	0/1446	0.95	4/1983 (0.2%)
1	y	0.67	0/1461	0.98	4/2003 (0.2%)
1	z	0.60	0/1454	0.99	4/1993 (0.2%)
All	All	0.64	1/87331 (0.0%)	0.96	209/119736 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	225	THR	CA-CB	5.31	1.60	1.53

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	260	GLU	CA-C-N	10.02	130.64	119.92
1	0	260	GLU	C-N-CA	10.02	130.64	119.92
1	2	225	THR	CA-C-N	-9.31	110.11	120.45
1	2	225	THR	C-N-CA	-9.31	110.11	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	225	THR	CA-C-N	-9.27	111.38	120.83
1	S	225	THR	C-N-CA	-9.27	111.38	120.83
1	Y	225	THR	CA-C-N	-9.20	110.23	120.45
1	Y	225	THR	C-N-CA	-9.20	110.23	120.45
1	3	225	THR	CA-C-N	-9.08	111.57	120.83
1	3	225	THR	C-N-CA	-9.08	111.57	120.83
1	Z	225	THR	CA-C-N	-8.74	110.75	120.45
1	Z	225	THR	C-N-CA	-8.74	110.75	120.45
1	A	225	THR	CA-C-N	-8.34	111.19	120.45
1	A	225	THR	C-N-CA	-8.34	111.19	120.45
1	w	225	THR	CA-C-N	-8.30	111.24	120.45
1	w	225	THR	C-N-CA	-8.30	111.24	120.45
1	T	225	THR	CA-C-N	-8.26	111.28	120.45
1	T	225	THR	C-N-CA	-8.26	111.28	120.45
1	U	225	THR	CA-C-N	-8.18	111.37	120.45
1	U	225	THR	C-N-CA	-8.18	111.37	120.45
1	b	225	THR	CA-C-N	-7.99	111.58	120.45
1	b	225	THR	C-N-CA	-7.99	111.58	120.45
1	i	225	THR	CA-C-N	-7.93	111.64	120.45
1	i	225	THR	C-N-CA	-7.93	111.64	120.45
1	X	225	THR	CA-C-N	-7.92	112.75	120.83
1	X	225	THR	C-N-CA	-7.92	112.75	120.83
1	f	225	THR	CA-C-N	-7.77	111.49	120.12
1	f	225	THR	C-N-CA	-7.77	111.49	120.12
1	L	225	THR	CA-C-N	-7.76	111.83	120.45
1	L	225	THR	C-N-CA	-7.76	111.83	120.45
1	R	225	THR	CA-C-N	-7.75	111.85	120.45
1	R	225	THR	C-N-CA	-7.75	111.85	120.45
1	t	225	THR	CA-C-N	-7.67	111.94	120.45
1	t	225	THR	C-N-CA	-7.67	111.94	120.45
1	C	225	THR	CA-C-N	-7.65	113.03	120.83
1	C	225	THR	C-N-CA	-7.65	113.03	120.83
1	l	88	VAL	N-CA-C	7.49	119.26	108.48
1	J	225	THR	CA-C-N	-7.42	112.21	120.45
1	J	225	THR	C-N-CA	-7.42	112.21	120.45
1	k	260	GLU	CA-C-N	7.37	129.05	119.84
1	k	260	GLU	C-N-CA	7.37	129.05	119.84
1	h	225	THR	CA-C-N	-7.34	112.30	120.45
1	h	225	THR	C-N-CA	-7.34	112.30	120.45
1	C	260	GLU	CA-C-N	7.31	128.98	119.84
1	C	260	GLU	C-N-CA	7.31	128.98	119.84
1	K	225	THR	CA-C-N	-7.28	112.38	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	225	THR	C-N-CA	-7.28	112.38	120.45
1	j	225	THR	CA-C-N	-7.26	112.39	120.45
1	j	225	THR	C-N-CA	-7.26	112.39	120.45
1	V	225	THR	CA-C-N	-7.22	112.44	120.45
1	V	225	THR	C-N-CA	-7.22	112.44	120.45
1	E	225	THR	CA-C-N	-7.22	112.44	120.45
1	E	225	THR	C-N-CA	-7.22	112.44	120.45
1	6	225	THR	CA-C-N	-7.13	112.53	120.45
1	6	225	THR	C-N-CA	-7.13	112.53	120.45
1	W	260	GLU	CA-C-N	7.13	128.75	119.84
1	W	260	GLU	C-N-CA	7.13	128.75	119.84
1	y	225	THR	CA-C-N	-7.11	113.58	120.83
1	y	225	THR	C-N-CA	-7.11	113.58	120.83
1	z	86	ILE	N-CA-C	7.05	118.28	108.12
1	S	260	GLU	CA-C-N	7.03	128.63	119.84
1	S	260	GLU	C-N-CA	7.03	128.63	119.84
1	T	260	GLU	CA-C-N	7.03	128.63	119.84
1	T	260	GLU	C-N-CA	7.03	128.63	119.84
1	v	225	THR	CA-C-N	-6.98	112.70	120.45
1	v	225	THR	C-N-CA	-6.98	112.70	120.45
1	z	88	VAL	N-CA-C	6.98	118.53	108.48
1	s	88	VAL	N-CA-C	6.92	118.44	108.48
1	l	225	THR	CA-C-N	-6.81	112.89	120.45
1	l	225	THR	C-N-CA	-6.81	112.89	120.45
1	5	260	GLU	CA-C-N	6.78	128.32	119.84
1	5	260	GLU	C-N-CA	6.78	128.32	119.84
1	v	260	GLU	CA-C-N	6.70	128.21	119.84
1	v	260	GLU	C-N-CA	6.70	128.21	119.84
1	2	151	VAL	CA-C-N	6.69	127.08	119.92
1	2	151	VAL	C-N-CA	6.69	127.08	119.92
1	M	225	THR	CA-C-N	-6.53	113.21	120.45
1	M	225	THR	C-N-CA	-6.53	113.21	120.45
1	P	225	THR	CA-C-N	-6.49	113.25	120.45
1	P	225	THR	C-N-CA	-6.49	113.25	120.45
1	m	225	THR	CA-C-N	-6.47	113.27	120.45
1	m	225	THR	C-N-CA	-6.47	113.27	120.45
1	x	260	GLU	CA-C-N	6.45	126.82	119.92
1	x	260	GLU	C-N-CA	6.45	126.82	119.92
1	z	225	THR	CA-C-N	-6.42	113.33	120.45
1	z	225	THR	C-N-CA	-6.42	113.33	120.45
1	Y	88	VAL	N-CA-C	6.39	117.68	108.48
1	1	225	THR	CA-C-N	-6.38	113.37	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	225	THR	C-N-CA	-6.38	113.37	120.45
1	E	74	ILE	N-CA-C	6.32	117.90	108.23
1	R	260	GLU	CA-C-N	6.30	127.71	119.84
1	R	260	GLU	C-N-CA	6.30	127.71	119.84
1	g	225	THR	CA-C-N	-6.30	113.46	120.45
1	g	225	THR	C-N-CA	-6.30	113.46	120.45
1	I	260	GLU	CA-C-N	6.26	127.67	119.84
1	I	260	GLU	C-N-CA	6.26	127.67	119.84
1	E	151	VAL	CA-C-N	6.17	126.52	119.92
1	E	151	VAL	C-N-CA	6.17	126.52	119.92
1	7	225	THR	CA-C-N	-6.11	114.60	120.83
1	7	225	THR	C-N-CA	-6.11	114.60	120.83
1	y	88	VAL	N-CA-C	6.01	117.14	108.48
1	T	151	VAL	CA-C-N	6.00	125.96	119.78
1	T	151	VAL	C-N-CA	6.00	125.96	119.78
1	r	260	GLU	CA-C-N	5.99	127.33	119.84
1	r	260	GLU	C-N-CA	5.99	127.33	119.84
1	N	225	THR	CA-C-N	-5.97	114.74	120.83
1	N	225	THR	C-N-CA	-5.97	114.74	120.83
1	e	225	THR	CA-C-N	-5.96	113.83	120.45
1	e	225	THR	C-N-CA	-5.96	113.83	120.45
1	B	88	VAL	N-CA-C	5.95	117.05	108.48
1	q	225	THR	CA-C-N	-5.92	113.88	120.45
1	q	225	THR	C-N-CA	-5.92	113.88	120.45
1	v	242	SER	N-CA-C	-5.92	104.77	112.23
1	F	225	THR	CA-C-N	-5.92	113.88	120.45
1	F	225	THR	C-N-CA	-5.92	113.88	120.45
1	n	225	THR	CA-C-N	-5.92	114.79	120.83
1	n	225	THR	C-N-CA	-5.92	114.79	120.83
1	d	86	ILE	N-CA-C	5.85	116.55	108.12
1	O	260	GLU	CA-C-N	5.84	127.14	119.84
1	O	260	GLU	C-N-CA	5.84	127.14	119.84
1	V	260	GLU	CA-C-N	5.83	127.13	119.84
1	V	260	GLU	C-N-CA	5.83	127.13	119.84
1	2	260	GLU	CA-C-N	5.82	127.11	119.84
1	2	260	GLU	C-N-CA	5.82	127.11	119.84
1	G	225	THR	CA-C-N	-5.81	114.00	120.45
1	G	225	THR	C-N-CA	-5.81	114.00	120.45
1	W	225	THR	CA-C-N	-5.80	114.02	120.45
1	W	225	THR	C-N-CA	-5.80	114.02	120.45
1	T	86	ILE	N-CA-C	5.79	116.22	108.11
1	g	74	ILE	N-CA-C	5.78	116.75	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	225	THR	CA-C-N	-5.77	114.05	120.45
1	H	225	THR	C-N-CA	-5.77	114.05	120.45
1	6	76	VAL	N-CA-C	5.76	116.59	108.36
1	d	88	VAL	N-CA-C	5.72	116.71	108.48
1	W	242	SER	N-CA-C	-5.71	106.15	113.23
1	T	88	VAL	N-CA-C	5.68	116.66	108.48
1	a	260	GLU	CA-C-N	5.67	126.93	119.84
1	a	260	GLU	C-N-CA	5.67	126.93	119.84
1	s	225	THR	CA-C-N	-5.66	114.17	120.45
1	s	225	THR	C-N-CA	-5.66	114.17	120.45
1	q	260	GLU	CA-C-N	5.64	126.89	119.84
1	q	260	GLU	C-N-CA	5.64	126.89	119.84
1	s	86	ILE	N-CA-C	5.61	115.96	108.11
1	p	225	THR	CA-C-N	-5.60	114.24	120.45
1	p	225	THR	C-N-CA	-5.60	114.24	120.45
1	c	88	VAL	N-CA-C	5.58	116.51	108.48
1	0	151	VAL	CA-C-N	5.56	125.87	119.92
1	0	151	VAL	C-N-CA	5.56	125.87	119.92
1	4	198	SER	N-CA-C	5.52	119.11	112.38
1	2	180	ASN	N-CA-C	-5.52	106.40	113.02
1	j	74	ILE	N-CA-C	5.51	116.67	108.23
1	Q	225	THR	CA-C-N	-5.48	115.24	120.83
1	Q	225	THR	C-N-CA	-5.48	115.24	120.83
1	P	260	GLU	CA-C-N	5.47	126.68	119.84
1	P	260	GLU	C-N-CA	5.47	126.68	119.84
1	x	225	THR	CA-C-N	-5.47	114.37	120.45
1	x	225	THR	C-N-CA	-5.47	114.37	120.45
1	K	242	SER	N-CA-C	-5.44	106.60	113.18
1	a	88	VAL	N-CA-C	5.43	116.30	108.48
1	J	242	SER	N-CA-C	-5.43	106.16	112.89
1	G	86	ILE	N-CA-C	5.41	115.69	108.11
1	d	225	THR	CA-C-N	-5.40	114.46	120.45
1	d	225	THR	C-N-CA	-5.40	114.46	120.45
1	5	225	THR	CA-C-N	-5.37	114.49	120.45
1	5	225	THR	C-N-CA	-5.37	114.49	120.45
1	a	225	THR	CA-C-N	-5.36	115.36	120.83
1	a	225	THR	C-N-CA	-5.36	115.36	120.83
1	0	121	LEU	N-CA-C	-5.34	106.90	113.41
1	O	151	VAL	CA-C-N	5.33	125.62	119.92
1	O	151	VAL	C-N-CA	5.33	125.62	119.92
1	0	242	SER	N-CA-C	-5.32	106.29	112.89
1	s	151	VAL	CA-C-N	5.31	125.60	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	s	151	VAL	C-N-CA	5.31	125.60	119.92
1	l	228	VAL	CA-C-N	5.30	124.81	119.19
1	l	228	VAL	C-N-CA	5.30	124.81	119.19
1	K	260	GLU	CA-C-N	5.30	126.47	119.84
1	K	260	GLU	C-N-CA	5.30	126.47	119.84
1	T	167	GLY	N-CA-C	5.29	119.33	110.56
1	S	74	ILE	N-CA-C	5.28	116.31	108.23
1	Z	260	GLU	CA-C-N	5.28	126.44	119.84
1	Z	260	GLU	C-N-CA	5.28	126.44	119.84
1	s	260	GLU	CA-C-N	5.27	126.43	119.84
1	s	260	GLU	C-N-CA	5.27	126.43	119.84
1	v	202	LYS	N-CA-C	5.24	115.20	108.34
1	6	260	GLU	CA-C-N	5.17	126.30	119.84
1	6	260	GLU	C-N-CA	5.17	126.30	119.84
1	O	225	THR	CA-C-N	-5.17	114.72	120.45
1	O	225	THR	C-N-CA	-5.17	114.72	120.45
1	A	74	ILE	N-CA-C	5.16	116.12	108.23
1	c	260	GLU	CA-C-N	5.14	126.26	119.84
1	c	260	GLU	C-N-CA	5.14	126.26	119.84
1	h	260	GLU	CA-C-N	5.12	125.40	119.92
1	h	260	GLU	C-N-CA	5.12	125.40	119.92
1	w	86	ILE	N-CA-C	5.12	115.27	108.11
1	y	88	VAL	CB-CA-C	-5.11	103.01	110.62
1	Q	143	PHE	N-CA-C	5.11	117.81	109.59
1	u	225	THR	CA-C-N	-5.10	114.78	120.45
1	u	225	THR	C-N-CA	-5.10	114.78	120.45
1	v	227	LEU	CA-C-N	-5.09	118.90	123.33
1	v	227	LEU	C-N-CA	-5.09	118.90	123.33
1	Q	259	ILE	N-CA-C	5.09	117.35	108.95
1	X	242	SER	N-CA-C	-5.09	106.58	112.89
1	j	121	LEU	N-CA-C	-5.07	107.22	113.41
1	R	100	MET	CA-C-N	5.05	125.07	119.32
1	R	100	MET	C-N-CA	5.05	125.07	119.32
1	c	86	ILE	N-CA-C	5.03	115.36	108.12
1	r	225	THR	CA-C-N	-5.01	114.88	120.45
1	r	225	THR	C-N-CA	-5.01	114.88	120.45
1	h	242	SER	N-CA-C	-5.00	107.03	113.23

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	19	0
1	2	1422	0	1397	17	0
1	3	1434	0	1411	25	1
1	4	1419	0	1389	12	0
1	5	1424	0	1404	16	0
1	6	1422	0	1397	17	0
1	7	1422	0	1397	13	0
1	A	1423	0	1401	18	0
1	B	1429	0	1404	32	0
1	C	1420	0	1390	13	0
1	D	1420	0	1392	18	0
1	E	1421	0	1400	19	0
1	F	1421	0	1402	22	0
1	G	1427	0	1410	17	0
1	H	1429	0	1406	15	0
1	I	1424	0	1404	10	0
1	J	1430	0	1408	18	0
1	K	1424	0	1404	13	0
1	L	1427	0	1410	18	0
1	M	1429	0	1406	21	0
1	N	1424	0	1404	23	0
1	O	1424	0	1404	22	0
1	P	1424	0	1404	20	0
1	Q	1422	0	1397	15	0
1	R	1421	0	1402	22	0
1	S	1417	0	1399	19	0
1	T	1421	0	1402	18	0
1	U	1424	0	1404	11	0
1	V	1424	0	1404	19	0
1	W	1424	0	1404	17	0
1	X	1434	0	1411	18	0
1	Y	1424	0	1404	23	0
1	Z	1424	0	1404	16	0
1	a	1420	0	1393	21	0
1	b	1420	0	1392	26	0
1	c	1418	0	1396	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	1429	0	1406	21	0
1	e	1427	0	1410	16	0
1	f	1423	0	1388	28	1
1	g	1420	0	1392	23	0
1	h	1419	0	1390	23	0
1	i	1424	0	1404	15	0
1	j	1434	0	1411	19	0
1	k	1427	0	1401	25	0
1	l	1425	0	1403	19	0
1	m	1429	0	1406	18	0
1	n	1423	0	1399	17	0
1	o	1415	0	1376	17	0
1	p	1414	0	1380	21	0
1	q	1425	0	1395	18	0
1	r	1424	0	1404	18	0
1	s	1429	0	1406	15	0
1	t	1424	0	1404	21	0
1	u	1424	0	1404	20	0
1	v	1424	0	1404	19	0
1	w	1406	0	1371	23	0
1	x	1414	0	1381	26	0
1	y	1429	0	1406	21	0
1	z	1422	0	1399	27	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	0	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	2	0
2	o	5	0	0	1	0
2	s	5	0	0	0	0
2	w	5	0	0	1	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
3	4	16	0	0	0	0
3	5	20	0	0	0	0
3	6	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	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	1	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	0	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	1	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	1	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
3	m	23	0	0	1	0
3	n	24	0	0	2	0
3	o	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	p	23	0	0	0	0
3	q	25	0	0	1	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	1	0
3	v	32	0	0	0	0
3	w	16	0	0	1	0
3	x	20	0	0	1	0
3	y	20	0	0	2	0
3	z	29	0	0	0	0
All	All	86922	0	84003	1033	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 6.

All (1033) 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	1.64	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	1.67	0.75
1:w:202:LYS:NZ	1:w:226:PRO:O	2.20	0.74
1:s:76:VAL:HG22	1:s:257:GLN:HG2	1.69	0.74
1:g:124:ARG:HB2	1:g:194:THR:HG22	1.70	0.74
1:3:98:LEU:HD22	1:3:228:VAL:HG11	1.70	0.74
1:E:206:PRO:HB2	1:E:208:LYS:HE2	1.69	0.73
1:p:86:ILE:HG23	1:p:236:LEU:HD11	1.70	0.72
1:J:202:LYS:NZ	1:J:226:PRO:O	2.21	0.72
1:N:209:THR:HG22	1:N:211:ALA:H	1.54	0.72
1:z:206:PRO:HB2	1:z:208:LYS:HE2	1.73	0.71
1:A:81:GLU:OE2	1:A:254:TYR:OH	2.05	0.71
1:X:124:ARG:HB2	1:X:194:THR:HG22	1.73	0.70
1:X:199:LYS:O	1:d:117:LYS:NZ	2.25	0.70
1:b:119:SER:OG	1:b:203:LYS:NZ	2.23	0.70
1:E:124:ARG:HB2	1:E:194:THR:HG22	1.74	0.70
1:F:98:LEU:HD22	1:F:228:VAL:HG11	1.73	0.70
1:A:89:THR:HG22	1:A:90:ASP:H	1.57	0.69
1:L:124:ARG:HB2	1:L:194:THR:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:124:ARG:HB2	1:v:194:THR:HG22	1.72	0.69
1:x:209:THR:HG22	1:x:211:ALA:H	1.56	0.69
1:Z:225:THR:HG22	1:Z:226:PRO:HD3	1.74	0.69
1:o:169:VAL:HG22	1:o:247:ALA:HB1	1.75	0.69
1:S:98:LEU:HD22	1:S:228:VAL:HG11	1.73	0.69
1:b:206:PRO:HB2	1:b:208:LYS:HE2	1.75	0.69
1:G:202:LYS:NZ	1:G:226:PRO:O	2.25	0.69
1:Y:144:GLN:OE1	1:Y:231:ARG:NH1	2.25	0.69
1:x:88:VAL:HG12	1:x:236:LEU:HD23	1.75	0.69
1:h:209:THR:HG22	1:h:211:ALA:H	1.58	0.69
1:T:124:ARG:HB2	1:T:194:THR:HG22	1.74	0.69
1:d:209:THR:HG22	1:d:211:ALA:H	1.56	0.69
1:w:220:ASP:HB3	1:w:223:ILE:HG13	1.74	0.69
1:C:100:MET:HE3	1:C:102:TYR:HB3	1.75	0.68
1:w:98:LEU:HD22	1:w:228:VAL:HG11	1.76	0.68
1:c:144:GLN:OE1	1:c:231:ARG:NH1	2.25	0.68
1:D:169:VAL:HG22	1:D:247:ALA:HB1	1.75	0.68
1:s:86:ILE:HG23	1:s:236:LEU:HD11	1.76	0.68
1:M:169:VAL:HG22	1:M:247:ALA:HB1	1.75	0.68
1:v:98:LEU:HD22	1:v:228:VAL:HG21	1.76	0.68
1:w:134:SER:HB3	2:w:301:SO4:O3	1.94	0.68
1:k:209:THR:HG23	1:k:212:ASP:H	1.60	0.67
1:2:124:ARG:HB2	1:2:194:THR:HG22	1.75	0.67
1:1:241:SER:HG	1:1:243:THR:HG1	1.42	0.67
1:B:124:ARG:HB2	1:B:194:THR:HG22	1.76	0.67
1:B:98:LEU:HD22	1:B:228:VAL:HG11	1.75	0.67
1:F:117:LYS:HE2	1:F:260:GLU:OE2	1.94	0.67
1:d:124:ARG:HB2	1:d:194:THR:HG22	1.76	0.67
1:w:127:TYR:OH	1:w:169:VAL:O	2.12	0.67
1:l:88:VAL:HG11	1:l:169:VAL:HG11	1.77	0.67
1:C:102:TYR:CE1	1:C:109:ARG:HD2	2.30	0.66
1:R:206:PRO:HB2	1:R:208:LYS:HE2	1.76	0.66
1:P:124:ARG:HB2	1:P:194:THR:HG22	1.76	0.66
1:V:74:ILE:HD11	1:x:199:LYS:HE3	1.77	0.66
1:z:124:ARG:HB2	1:z:194:THR:HG22	1.78	0.66
1:t:144:GLN:OE1	1:t:231:ARG:NH1	2.29	0.66
1:b:118:TYR:HB2	1:b:256:ILE:HD11	1.78	0.66
1:n:209:THR:HG23	1:n:212:ASP:H	1.60	0.65
1:O:98:LEU:HD22	1:O:228:VAL:HG11	1.78	0.65
1:z:88:VAL:HG11	1:z:169:VAL:HG21	1.79	0.65
1:3:209:THR:HG22	1:3:211:ALA:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:GLN:OE1	1:G:231:ARG:NH1	2.30	0.65
1:X:140:HIS:HB2	1:X:235:ALA:HB3	1.78	0.65
1:q:86:ILE:CG2	1:q:236:LEU:HD21	2.26	0.64
1:5:176:LEU:HA	1:5:179:ILE:HD12	1.78	0.64
1:Q:217:VAL:HG23	1:Q:221:VAL:HG23	1.79	0.64
1:g:202:LYS:NZ	1:g:226:PRO:O	2.30	0.64
1:L:117:LYS:HE2	1:L:260:GLU:OE1	1.98	0.64
1:5:169:VAL:HG22	1:5:247:ALA:HB1	1.80	0.63
1:J:124:ARG:HB2	1:J:194:THR:HG22	1.81	0.63
1:L:98:LEU:HD22	1:L:228:VAL:HG11	1.79	0.63
1:0:238:ASP:O	3:0:301:HOH:O	2.15	0.63
1:P:169:VAL:HG22	1:P:247:ALA:HB1	1.81	0.63
1:c:124:ARG:HB2	1:c:194:THR:HG22	1.80	0.63
1:x:88:VAL:HG11	1:x:169:VAL:HG11	1.81	0.63
1:H:220:ASP:HB3	1:H:223:ILE:HG13	1.81	0.63
1:a:220:ASP:HB3	1:a:223:ILE:HG23	1.79	0.63
1:F:141:MET:O	1:F:164:TYR:HA	1.99	0.63
1:N:72:GLY:N	3:N:301:HOH:O	2.32	0.63
1:f:144:GLN:OE1	1:f:231:ARG:NH1	2.32	0.63
1:h:98:LEU:O	1:h:103:THR:OG1	2.16	0.63
1:z:144:GLN:OE1	1:z:231:ARG:NH1	2.33	0.62
1:D:144:GLN:OE1	1:D:231:ARG:NH1	2.32	0.62
1:E:199:LYS:NZ	1:F:72:GLY:O	2.33	0.62
1:L:144:GLN:OE1	1:L:231:ARG:NH1	2.32	0.62
1:c:84:ALA:HB3	1:c:250:ILE:HB	1.80	0.62
1:R:219:VAL:HG23	1:R:223:ILE:HD12	1.82	0.61
1:g:220:ASP:HB3	1:g:223:ILE:HG13	1.81	0.61
1:R:144:GLN:OE1	1:R:231:ARG:NH1	2.34	0.61
1:e:84:ALA:HB3	1:e:250:ILE:HB	1.82	0.61
1:1:220:ASP:HB3	1:1:223:ILE:HG13	1.82	0.61
1:x:76:VAL:HG22	1:x:257:GLN:HG2	1.81	0.61
1:B:209:THR:HG22	1:B:211:ALA:H	1.64	0.61
1:V:98:LEU:HD22	1:V:228:VAL:HG21	1.82	0.61
1:i:140:HIS:ND1	1:i:164:TYR:OH	2.26	0.61
1:q:88:VAL:HG11	1:q:169:VAL:HG21	1.82	0.61
1:l:169:VAL:HB	1:l:247:ALA:HB1	1.83	0.61
1:H:124:ARG:HB2	1:H:194:THR:HG22	1.82	0.60
1:w:140:HIS:ND1	1:w:164:TYR:OH	2.31	0.60
1:3:108:LEU:HD22	1:3:254:TYR:CZ	2.36	0.60
1:S:84:ALA:HB3	1:S:250:ILE:HB	1.82	0.60
1:U:124:ARG:HB2	1:U:194:THR:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:LYS:NZ	1:H:226:PRO:O	2.34	0.60
1:h:102:TYR:CZ	1:h:209:THR:HG23	2.36	0.60
1:w:76:VAL:HG22	1:w:257:GLN:HG2	1.84	0.60
1:p:140:HIS:HB2	1:p:235:ALA:HB3	1.83	0.60
1:q:102:TYR:CE2	1:q:209:THR:HG23	2.37	0.60
1:y:182:THR:HG22	1:y:183:ARG:H	1.66	0.60
1:1:182:THR:HG22	1:1:183:ARG:H	1.67	0.60
1:T:88:VAL:HG11	1:T:169:VAL:HG11	1.83	0.60
1:a:169:VAL:HG22	1:a:247:ALA:HB1	1.82	0.60
1:F:108:LEU:HD22	1:F:254:TYR:CZ	2.36	0.60
1:0:137:GLY:N	3:0:301:HOH:O	2.33	0.60
1:X:206:PRO:HB2	1:X:208:LYS:HE2	1.83	0.60
1:x:88:VAL:CG1	1:x:236:LEU:HD23	2.31	0.59
1:3:217:VAL:HG13	1:3:221:VAL:HG12	1.83	0.59
3:q:323:HOH:O	1:3:162:ARG:HD3	2.03	0.59
1:U:118:TYR:HB2	1:U:256:ILE:HD11	1.85	0.59
1:r:220:ASP:HB3	1:r:223:ILE:HG13	1.84	0.59
1:R:84:ALA:HB3	1:R:250:ILE:HB	1.84	0.59
1:c:88:VAL:HG13	1:c:236:LEU:HD23	1.83	0.59
1:N:169:VAL:HG22	1:N:247:ALA:HB1	1.84	0.59
1:1:206:PRO:HB2	1:1:208:LYS:HD3	1.83	0.59
1:Y:88:VAL:HG11	1:Y:169:VAL:HG21	1.85	0.59
1:g:206:PRO:HB2	1:g:208:LYS:HE2	1.85	0.59
1:5:100:MET:HE3	1:5:102:TYR:HB3	1.83	0.59
1:6:209:THR:HG22	1:6:211:ALA:H	1.68	0.59
1:7:124:ARG:HB2	1:7:194:THR:HG22	1.84	0.59
1:A:206:PRO:HB2	1:A:208:LYS:HE2	1.85	0.59
1:z:220:ASP:HB3	1:z:223:ILE:HG13	1.84	0.58
1:G:98:LEU:HD22	1:G:228:VAL:HG11	1.86	0.58
1:o:191:ILE:N	3:o:402:HOH:O	2.36	0.58
1:B:88:VAL:HG12	1:B:236:LEU:HD23	1.84	0.58
1:T:206:PRO:HB2	1:T:208:LYS:HE2	1.84	0.58
1:e:169:VAL:HG22	1:e:247:ALA:HB1	1.84	0.58
1:P:98:LEU:HD22	1:P:228:VAL:HG21	1.86	0.58
1:O:89:THR:HG22	1:O:90:ASP:H	1.69	0.58
1:0:220:ASP:HB3	1:0:223:ILE:HG13	1.83	0.58
1:X:169:VAL:HG22	1:X:247:ALA:HB1	1.85	0.58
1:t:124:ARG:HB2	1:t:194:THR:HG22	1.85	0.58
1:A:124:ARG:HB2	1:A:194:THR:HG22	1.86	0.58
1:H:124:ARG:HG2	3:H:404:HOH:O	2.03	0.58
1:f:124:ARG:HB2	1:f:194:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:169:VAL:HG22	1:J:247:ALA:HB1	1.84	0.57
1:v:144:GLN:OE1	1:v:231:ARG:NH1	2.37	0.57
1:b:124:ARG:HB2	1:b:194:THR:HG22	1.86	0.57
1:R:158:LEU:HD12	1:R:161:LEU:HD12	1.85	0.57
1:a:76:VAL:HG22	1:a:257:GLN:HG2	1.85	0.57
1:Y:141:MET:O	1:Y:164:TYR:HA	2.05	0.57
1:7:160:ASN:O	1:b:79:HIS:HE1	1.87	0.57
1:J:261:PRO:HG2	1:X:79:HIS:CE1	2.38	0.57
1:y:220:ASP:HB3	1:y:223:ILE:HG12	1.86	0.57
1:z:209:THR:HG22	1:z:211:ALA:H	1.69	0.57
1:0:257:GLN:NE2	3:0:302:HOH:O	2.23	0.57
1:y:169:VAL:HG22	1:y:247:ALA:HB1	1.87	0.57
1:V:202:LYS:NZ	1:V:226:PRO:O	2.37	0.57
1:z:98:LEU:HD22	1:z:228:VAL:HG11	1.86	0.57
1:p:144:GLN:OE1	1:p:231:ARG:NH1	2.38	0.57
1:O:125:TYR:HB3	1:O:141:MET:HE1	1.87	0.57
1:y:88:VAL:HG13	1:y:236:LEU:HD23	1.86	0.57
1:B:74:ILE:HA	1:B:259:ILE:HG22	1.86	0.56
1:c:206:PRO:HB2	1:c:208:LYS:HE2	1.87	0.56
1:3:102:TYR:CE2	1:3:209:THR:HG23	2.40	0.56
1:H:169:VAL:HG22	1:H:247:ALA:HB1	1.87	0.56
1:M:141:MET:O	1:M:164:TYR:HA	2.05	0.56
1:1:207:TYR:O	1:1:208:LYS:HD2	2.05	0.56
1:h:138:SER:HB3	1:j:130:SER:HB2	1.88	0.56
1:p:206:PRO:HB2	1:p:208:LYS:HE2	1.88	0.56
1:E:223:ILE:HD13	1:m:223:ILE:HD11	1.88	0.56
1:b:84:ALA:HB3	1:b:250:ILE:HB	1.88	0.56
1:T:144:GLN:OE1	1:T:231:ARG:NH1	2.38	0.56
1:o:158:LEU:HD23	1:o:161:LEU:HD12	1.88	0.56
1:y:231:ARG:NE	3:y:302:HOH:O	2.37	0.56
1:E:182:THR:HG22	1:E:183:ARG:H	1.71	0.56
1:W:124:ARG:NH1	3:W:301:HOH:O	2.35	0.55
1:u:124:ARG:HB2	1:u:194:THR:HG22	1.88	0.55
1:N:108:LEU:HD22	1:N:254:TYR:CZ	2.42	0.55
1:W:141:MET:O	1:W:164:TYR:HA	2.06	0.55
1:q:206:PRO:HB2	1:q:208:LYS:HE2	1.89	0.55
1:b:99:VAL:HG11	1:b:195:LEU:HD22	1.88	0.55
1:N:124:ARG:HB2	1:N:194:THR:HG22	1.88	0.55
1:R:124:ARG:NH2	3:R:302:HOH:O	2.39	0.55
1:o:98:LEU:HD22	1:o:228:VAL:HG11	1.88	0.55
1:z:152:PRO:HG2	1:z:158:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:LEU:HD12	1:G:161:LEU:HD12	1.87	0.55
1:X:118:TYR:HB2	1:X:256:ILE:HD11	1.89	0.55
1:a:206:PRO:HB2	1:a:208:LYS:HE2	1.87	0.55
1:f:223:ILE:O	1:f:226:PRO:HD2	2.07	0.55
1:h:100:MET:HE3	1:h:102:TYR:HB3	1.87	0.55
1:k:100:MET:HE3	1:k:102:TYR:HB3	1.88	0.55
1:4:134:SER:HB3	2:4:301:SO4:O3	2.06	0.55
1:d:79:HIS:HB3	1:d:254:TYR:CZ	2.42	0.55
1:d:206:PRO:HB2	1:d:208:LYS:HE2	1.89	0.55
1:l:220:ASP:HB3	1:l:223:ILE:HG13	1.88	0.55
1:a:124:ARG:HB2	1:a:194:THR:HG22	1.89	0.55
1:u:169:VAL:HG22	1:u:247:ALA:HB1	1.89	0.55
1:w:140:HIS:HD1	1:w:164:TYR:HH	1.49	0.55
1:J:74:ILE:HD11	1:W:199:LYS:HE3	1.89	0.55
1:N:138:SER:HB3	1:O:130:SER:HB2	1.88	0.54
1:7:138:SER:HB3	1:b:130:SER:HB2	1.87	0.54
1:n:208:LYS:O	3:n:301:HOH:O	2.18	0.54
1:Q:182:THR:HG22	1:Q:183:ARG:H	1.71	0.54
1:Z:117:LYS:HE2	1:Z:260:GLU:OE2	2.07	0.54
1:a:216:ALA:HA	1:a:223:ILE:HD11	1.89	0.54
1:Q:257:GLN:NE2	3:Q:302:HOH:O	2.39	0.54
1:g:223:ILE:O	1:g:226:PRO:HD2	2.07	0.54
1:S:207:TYR:O	1:S:208:LYS:HD2	2.08	0.54
1:c:88:VAL:CG1	1:c:236:LEU:HD23	2.38	0.54
1:u:81:GLU:OE2	1:u:254:TYR:OH	2.21	0.54
1:5:141:MET:HG2	1:5:234:ILE:HG12	1.88	0.54
2:h:301:SO4:O4	1:l:134:SER:HB3	2.07	0.54
1:Q:237:LEU:HD12	1:Q:238:ASP:CG	2.31	0.54
1:V:169:VAL:HG22	1:V:247:ALA:HB1	1.90	0.54
1:c:102:TYR:CZ	1:c:209:THR:HG23	2.41	0.54
1:g:158:LEU:HD23	1:g:161:LEU:HD12	1.88	0.54
1:R:124:ARG:HG2	3:R:304:HOH:O	2.08	0.54
1:7:74:ILE:HA	1:7:259:ILE:HG22	1.89	0.54
1:B:76:VAL:HG22	1:B:257:GLN:HG2	1.90	0.54
1:c:209:THR:HG22	1:c:211:ALA:H	1.73	0.54
1:j:84:ALA:HB3	1:j:250:ILE:HB	1.90	0.54
1:F:169:VAL:HG22	1:F:247:ALA:HB1	1.90	0.54
1:d:169:VAL:HG22	1:d:247:ALA:HB1	1.90	0.54
1:h:160:ASN:ND2	1:j:107:TRP:HB2	2.22	0.54
1:w:261:PRO:HB3	1:1:107:TRP:CZ2	2.43	0.53
1:z:76:VAL:HG22	1:z:257:GLN:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:102:TYR:HD1	1:b:109:ARG:HG3	1.74	0.53
1:H:107:TRP:CZ2	1:j:261:PRO:HB3	2.44	0.53
1:v:169:VAL:HG22	1:v:247:ALA:HB1	1.89	0.53
1:w:107:TRP:CZ2	1:1:261:PRO:HB3	2.43	0.53
1:6:98:LEU:HD22	1:6:228:VAL:HG11	1.90	0.53
1:J:140:HIS:HB2	1:J:235:ALA:HB3	1.90	0.53
1:J:141:MET:O	1:J:164:TYR:HA	2.09	0.53
1:S:117:LYS:HE3	3:n:316:HOH:O	2.08	0.53
1:k:98:LEU:HD22	1:k:228:VAL:HG11	1.90	0.53
1:H:159:SER:HA	1:H:164:TYR:CD1	2.44	0.53
1:Y:223:ILE:HD11	1:Z:223:ILE:HD13	1.91	0.53
1:2:206:PRO:HB2	1:2:208:LYS:HE2	1.91	0.53
1:4:217:VAL:HG23	1:4:221:VAL:HG23	1.90	0.53
2:h:301:SO4:O2	1:p:134:SER:HB3	2.08	0.53
1:N:169:VAL:CG2	1:N:247:ALA:HB1	2.39	0.52
1:g:127:TYR:OH	1:g:169:VAL:O	2.18	0.52
1:w:108:LEU:HD22	1:w:254:TYR:CZ	2.44	0.52
1:e:141:MET:O	1:e:164:TYR:HA	2.09	0.52
1:0:206:PRO:HB2	1:0:208:LYS:HE2	1.92	0.52
1:E:107:TRP:CZ2	1:o:261:PRO:HB3	2.44	0.52
1:M:144:GLN:NE2	1:M:152:PRO:HD3	2.25	0.52
1:Q:92:ILE:HA	1:Q:237:LEU:HB3	1.90	0.52
1:X:159:SER:HA	1:X:164:TYR:CD1	2.45	0.52
1:R:88:VAL:HG21	1:R:137:GLY:HA3	1.91	0.52
1:m:220:ASP:O	1:m:223:ILE:HG12	2.10	0.52
1:0:97:GLU:OE2	1:0:104:VAL:HA	2.10	0.52
1:C:98:LEU:HD22	1:C:228:VAL:HG21	1.91	0.52
1:D:141:MET:O	1:D:164:TYR:HA	2.10	0.52
1:t:138:SER:HB3	1:u:130:SER:HB2	1.92	0.52
1:C:169:VAL:HG22	1:C:247:ALA:HB1	1.92	0.52
1:N:220:ASP:HB3	1:N:223:ILE:HG13	1.91	0.52
1:w:145:TYR:HH	1:w:196:ASP:H	1.53	0.52
1:f:98:LEU:HD22	1:f:228:VAL:HG11	1.91	0.52
1:p:141:MET:O	1:p:164:TYR:HA	2.10	0.52
1:z:99:VAL:O	1:z:229:PRO:HG2	2.11	0.51
1:1:124:ARG:HB2	1:1:194:THR:HG22	1.93	0.51
1:1:159:SER:HA	1:1:164:TYR:CD1	2.46	0.51
1:B:220:ASP:HB3	1:B:223:ILE:HG12	1.91	0.51
1:o:100:MET:HE3	1:o:102:TYR:HB3	1.92	0.51
1:I:140:HIS:ND1	1:I:164:TYR:OH	2.36	0.51
1:Y:261:PRO:HB3	1:d:107:TRP:CZ2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:144:GLN:OE1	1:a:231:ARG:NH1	2.44	0.51
1:e:98:LEU:HD22	1:e:228:VAL:HG11	1.92	0.51
1:v:74:ILE:HD11	1:l:199:LYS:HE3	1.92	0.51
1:w:119:SER:OG	1:w:203:LYS:NZ	2.44	0.51
1:h:223:ILE:O	1:h:226:PRO:HD2	2.10	0.51
1:b:74:ILE:HG12	1:b:259:ILE:CG2	2.40	0.51
1:f:220:ASP:HB3	1:f:223:ILE:HG13	1.92	0.51
1:L:186:ASP:OD1	1:L:186:ASP:N	2.40	0.51
1:Q:209:THR:HG22	1:Q:211:ALA:H	1.75	0.51
1:k:209:THR:HG22	1:k:212:ASP:CG	2.36	0.51
1:t:169:VAL:HG22	1:t:247:ALA:HB1	1.92	0.51
1:f:74:ILE:HA	1:f:259:ILE:HG22	1.92	0.51
1:H:225:THR:OG1	1:H:226:PRO:HD3	2.11	0.51
1:M:108:LEU:HD22	1:M:254:TYR:CZ	2.46	0.51
1:x:100:MET:HE3	1:x:102:TYR:HB3	1.93	0.51
1:B:186:ASP:OD1	1:B:186:ASP:N	2.34	0.51
1:Z:138:SER:HB3	1:a:130:SER:HB2	1.93	0.51
1:h:207:TYR:O	1:h:208:LYS:HD2	2.11	0.51
1:C:102:TYR:O	1:C:109:ARG:HD3	2.10	0.51
1:M:134:SER:HA	1:N:132:PRO:HB3	1.93	0.51
1:T:119:SER:OG	1:T:203:LYS:NZ	2.42	0.51
1:c:88:VAL:HG11	1:c:169:VAL:HG11	1.93	0.51
1:g:223:ILE:HD13	1:y:223:ILE:HD11	1.93	0.51
1:q:199:LYS:HE3	1:r:74:ILE:HD11	1.92	0.51
1:r:206:PRO:HB2	1:r:208:LYS:HE2	1.93	0.51
1:l:84:ALA:HB3	1:l:250:ILE:HB	1.92	0.51
1:K:87:GLY:O	1:K:236:LEU:HD22	2.11	0.51
1:s:159:SER:HA	1:s:164:TYR:CD1	2.46	0.51
1:K:117:LYS:HE2	1:K:260:GLU:OE2	2.11	0.51
1:U:138:SER:HB3	1:V:130:SER:HB2	1.92	0.51
1:u:231:ARG:NH2	3:u:302:HOH:O	2.32	0.51
1:6:147:MET:H	1:6:225:THR:HG22	1.76	0.51
1:B:88:VAL:CG1	1:B:236:LEU:HD23	2.41	0.50
1:S:169:VAL:HG22	1:S:247:ALA:HB1	1.93	0.50
1:s:124:ARG:HB2	1:s:194:THR:HG22	1.94	0.50
1:7:141:MET:O	1:7:164:TYR:HA	2.11	0.50
1:j:98:LEU:HD22	1:j:228:VAL:HG11	1.93	0.50
1:I:151:VAL:N	3:I:303:HOH:O	2.42	0.50
1:R:81:GLU:OE2	1:R:254:TYR:OH	2.25	0.50
1:g:152:PRO:HD2	1:g:233:VAL:HG11	1.93	0.50
1:4:117:LYS:HE2	1:4:260:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:156:ASN:HD21	1:S:106:THR:HG21	1.75	0.50
1:c:134:SER:HA	1:e:132:PRO:HB3	1.94	0.50
1:x:102:TYR:HD1	1:x:109:ARG:HG3	1.77	0.50
1:g:99:VAL:O	1:g:229:PRO:HG2	2.12	0.50
1:z:88:VAL:CG1	1:z:236:LEU:HD23	2.42	0.50
1:3:98:LEU:O	1:3:103:THR:OG1	2.26	0.50
1:G:220:ASP:HB3	1:G:223:ILE:HG13	1.93	0.50
1:6:99:VAL:O	1:6:229:PRO:HG2	2.12	0.50
1:b:102:TYR:CD2	1:b:209:THR:HA	2.45	0.50
1:3:186:ASP:OD1	1:3:186:ASP:N	2.42	0.50
1:P:186:ASP:OD1	1:P:186:ASP:N	2.36	0.50
1:w:206:PRO:HB2	1:w:208:LYS:HE2	1.93	0.50
1:7:83:SER:OG	1:7:97:GLU:OE1	2.29	0.50
1:S:220:ASP:HB3	1:S:223:ILE:HG13	1.93	0.50
1:X:87:GLY:O	1:X:236:LEU:HD22	2.11	0.50
1:k:102:TYR:HD1	1:k:109:ARG:HG3	1.77	0.50
1:6:132:PRO:HB3	1:f:134:SER:HA	1.94	0.50
1:B:223:ILE:HD11	1:x:223:ILE:HD13	1.94	0.50
1:C:225:THR:HB	1:C:226:PRO:HD3	1.93	0.50
1:J:159:SER:HA	1:J:164:TYR:CD1	2.47	0.50
1:6:98:LEU:HD11	1:6:213:TYR:CD2	2.46	0.50
1:f:108:LEU:HD22	1:f:254:TYR:CZ	2.47	0.50
1:l:158:LEU:HD23	1:l:161:LEU:HD12	1.94	0.50
1:n:206:PRO:HB2	1:n:208:LYS:HE2	1.94	0.50
1:c:79:HIS:HB3	1:c:254:TYR:CE1	2.47	0.49
1:u:141:MET:O	1:u:164:TYR:HA	2.11	0.49
1:6:225:THR:OG1	1:6:226:PRO:HD3	2.12	0.49
1:M:98:LEU:HD22	1:M:228:VAL:HG11	1.94	0.49
1:x:134:SER:HA	1:y:132:PRO:HB3	1.94	0.49
1:f:141:MET:O	1:f:164:TYR:HA	2.12	0.49
1:V:144:GLN:OE1	1:V:231:ARG:NH1	2.45	0.49
1:x:206:PRO:HB2	1:x:208:LYS:HE2	1.93	0.49
1:p:99:VAL:O	1:p:229:PRO:HG2	2.13	0.49
1:a:74:ILE:HD11	1:7:199:LYS:HE3	1.94	0.49
1:y:88:VAL:CG1	1:y:236:LEU:HD23	2.43	0.49
1:z:88:VAL:HG13	1:z:236:LEU:HD23	1.93	0.49
1:1:169:VAL:CG2	1:1:247:ALA:HB1	2.43	0.49
1:d:88:VAL:HG12	1:d:236:LEU:HD23	1.94	0.49
1:D:223:ILE:O	1:D:226:PRO:HD2	2.11	0.49
1:F:88:VAL:CG1	1:F:236:LEU:HD12	2.41	0.49
1:I:157:GLN:HE21	1:X:264:SER:C	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:223:ILE:O	1:e:226:PRO:HD2	2.13	0.49
1:f:159:SER:HA	1:f:164:TYR:CD1	2.48	0.49
1:l:206:PRO:HB2	1:l:208:LYS:HE2	1.93	0.49
1:C:141:MET:O	1:C:164:TYR:HA	2.13	0.49
1:H:223:ILE:O	1:H:226:PRO:HD2	2.12	0.49
1:P:141:MET:O	1:P:164:TYR:HA	2.12	0.49
1:c:80:SER:HA	1:c:252:CYS:O	2.12	0.49
1:o:213:TYR:O	1:o:217:VAL:HG13	2.12	0.49
1:3:144:GLN:OE1	1:3:231:ARG:NH1	2.45	0.49
1:7:88:VAL:HB	1:7:236:LEU:HD23	1.94	0.49
1:b:134:SER:HA	1:d:132:PRO:HB3	1.94	0.49
1:S:223:ILE:HD13	1:n:223:ILE:HD11	1.95	0.49
1:t:134:SER:HA	1:u:132:PRO:HB3	1.95	0.49
1:P:144:GLN:NE2	1:P:152:PRO:HD3	2.27	0.49
1:X:141:MET:O	1:X:164:TYR:HA	2.13	0.49
1:c:108:LEU:HD22	1:c:254:TYR:CE2	2.48	0.49
1:x:158:LEU:HD12	1:x:161:LEU:HD12	1.95	0.49
1:5:159:SER:HA	1:5:164:TYR:CD1	2.47	0.49
1:b:100:MET:HE3	1:b:102:TYR:HB3	1.94	0.49
1:d:86:ILE:CG2	1:d:236:LEU:HD21	2.42	0.49
1:l:202:LYS:NZ	1:l:226:PRO:O	2.41	0.49
1:A:132:PRO:HB3	1:E:134:SER:HA	1.95	0.49
1:L:141:MET:O	1:L:164:TYR:HA	2.12	0.49
1:O:141:MET:HE3	1:O:232:LEU:HD21	1.93	0.49
1:O:158:LEU:HD12	1:O:161:LEU:HD12	1.95	0.49
1:W:134:SER:HB3	2:X:301:SO4:O3	2.13	0.49
1:Y:97:GLU:OE2	1:Y:104:VAL:HA	2.13	0.49
1:f:125:TYR:CG	1:f:232:LEU:HD22	2.48	0.49
1:J:87:GLY:O	1:J:236:LEU:HD22	2.14	0.48
1:k:102:TYR:CD1	1:k:109:ARG:HG3	2.48	0.48
1:7:99:VAL:O	1:7:229:PRO:HG2	2.13	0.48
1:n:209:THR:HG22	1:n:212:ASP:CG	2.38	0.48
1:B:102:TYR:CZ	1:B:209:THR:HG23	2.48	0.48
2:7:301:SO4:O2	1:f:134:SER:HB3	2.14	0.48
1:N:209:THR:HG22	1:N:210:SER:N	2.28	0.48
1:o:122:SER:O	1:o:254:TYR:HA	2.13	0.48
1:v:186:ASP:OD1	1:v:186:ASP:N	2.41	0.48
1:A:98:LEU:HD22	1:A:228:VAL:HG11	1.94	0.48
1:v:169:VAL:CG2	1:v:247:ALA:HB1	2.44	0.48
1:w:159:SER:HA	1:w:164:TYR:CD1	2.48	0.48
1:y:147:MET:O	1:y:231:ARG:NH2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:87:GLY:O	1:2:236:LEU:HD22	2.13	0.48
1:G:100:MET:HE3	1:G:102:TYR:HB3	1.94	0.48
1:S:169:VAL:CG2	1:S:247:ALA:HB1	2.44	0.48
1:c:223:ILE:O	1:c:226:PRO:HD2	2.13	0.48
1:d:128:ILE:CD1	1:d:179:ILE:HD11	2.44	0.48
1:f:88:VAL:HG21	1:f:137:GLY:HA3	1.95	0.48
1:f:108:LEU:HB2	1:f:254:TYR:OH	2.13	0.48
1:A:159:SER:HA	1:A:164:TYR:CD2	2.49	0.48
1:D:220:ASP:HB3	1:D:223:ILE:HG13	1.95	0.48
1:E:74:ILE:HD11	1:m:199:LYS:HE3	1.95	0.48
1:P:144:GLN:OE1	1:P:231:ARG:NH1	2.47	0.48
2:P:301:SO4:O3	1:S:134:SER:HB3	2.14	0.48
1:Z:220:ASP:HB3	1:Z:223:ILE:HG13	1.95	0.48
1:e:77:LEU:HD21	1:e:107:TRP:HZ3	1.78	0.48
1:k:169:VAL:HB	1:k:247:ALA:HB1	1.95	0.48
1:k:261:PRO:HB3	1:l:107:TRP:CZ2	2.48	0.48
1:q:86:ILE:CD1	1:q:250:ILE:HG13	2.44	0.48
1:p:92:ILE:HG13	1:p:237:LEU:HD23	1.96	0.48
1:O:158:LEU:HD12	1:O:158:LEU:HA	1.66	0.48
1:W:76:VAL:HG22	1:W:257:GLN:HG2	1.96	0.48
1:5:158:LEU:HD23	1:5:161:LEU:HD12	1.96	0.48
1:h:160:ASN:HD21	1:j:107:TRP:HB2	1.79	0.48
1:B:134:SER:HA	1:C:132:PRO:HB3	1.95	0.48
1:B:144:GLN:NE2	1:B:152:PRO:HD3	2.28	0.48
1:K:124:ARG:HB2	1:K:194:THR:HG22	1.95	0.48
1:V:119:SER:OG	1:V:203:LYS:NZ	2.37	0.48
1:Y:74:ILE:HA	1:Y:259:ILE:HG22	1.95	0.48
1:t:87:GLY:O	1:t:236:LEU:HD22	2.13	0.48
1:v:74:ILE:HG12	1:v:259:ILE:CG2	2.43	0.48
1:C:220:ASP:HB3	1:C:223:ILE:HG13	1.96	0.47
1:S:107:TRP:CZ2	1:p:261:PRO:HB3	2.49	0.47
1:Y:159:SER:HA	1:Y:164:TYR:CD1	2.49	0.47
1:e:220:ASP:HB3	1:e:223:ILE:HG13	1.96	0.47
1:i:119:SER:OG	1:i:203:LYS:NZ	2.45	0.47
1:q:85:GLU:C	1:q:86:ILE:HD12	2.39	0.47
1:3:102:TYR:O	1:3:109:ARG:HD3	2.13	0.47
1:B:140:HIS:HB2	1:B:235:ALA:HB3	1.96	0.47
1:F:99:VAL:O	1:F:229:PRO:HG2	2.13	0.47
1:N:162:ARG:HH21	1:N:196:ASP:CG	2.22	0.47
1:V:147:MET:HE3	1:V:228:VAL:HG13	1.95	0.47
1:a:84:ALA:HB3	1:a:250:ILE:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:z:158:LEU:HA	1:z:161:LEU:HD13	1.95	0.47
1:4:137:GLY:C	1:4:169:VAL:HG13	2.40	0.47
1:f:92:ILE:HA	1:f:237:LEU:HB3	1.95	0.47
1:G:159:SER:HA	1:G:164:TYR:CD1	2.50	0.47
1:G:160:ASN:OD1	1:H:79:HIS:HE1	1.96	0.47
1:W:84:ALA:HB3	1:W:250:ILE:HB	1.95	0.47
1:Z:132:PRO:HB3	1:g:134:SER:HA	1.96	0.47
1:w:79:HIS:HB3	1:w:254:TYR:CZ	2.49	0.47
1:6:141:MET:O	1:6:164:TYR:HA	2.13	0.47
1:i:141:MET:O	1:i:164:TYR:HA	2.14	0.47
1:n:217:VAL:HG23	1:n:221:VAL:HG23	1.96	0.47
1:m:119:SER:HB3	1:m:257:GLN:HB2	1.96	0.47
1:j:134:SER:HA	1:l:132:PRO:HB3	1.95	0.47
1:G:74:ILE:HD11	1:k:199:LYS:HE3	1.95	0.47
1:O:207:TYR:O	1:O:208:LYS:HD2	2.14	0.47
1:c:86:ILE:CG2	1:c:236:LEU:HD21	2.44	0.47
1:e:87:GLY:O	1:e:236:LEU:HD22	2.14	0.47
1:u:118:TYR:HB2	1:u:256:ILE:HD11	1.97	0.47
1:d:88:VAL:CG1	1:d:236:LEU:HD23	2.45	0.47
1:p:108:LEU:HD22	1:p:254:TYR:CZ	2.49	0.47
1:M:99:VAL:O	1:M:229:PRO:HG2	2.14	0.47
1:N:87:GLY:O	1:N:236:LEU:HD22	2.15	0.47
1:R:141:MET:O	1:R:164:TYR:HA	2.14	0.47
1:Y:223:ILE:O	1:Y:226:PRO:HD2	2.15	0.47
1:s:165:VAL:HB	1:t:176:LEU:HD21	1.96	0.47
1:f:98:LEU:O	1:f:103:THR:OG1	2.33	0.47
1:j:141:MET:O	1:j:164:TYR:HA	2.14	0.47
1:F:117:LYS:HE3	1:F:259:ILE:HD11	1.96	0.47
1:I:152:PRO:HD2	1:I:233:VAL:HG11	1.96	0.47
1:W:124:ARG:HB2	1:W:194:THR:HG22	1.96	0.47
1:i:223:ILE:O	1:i:226:PRO:HD2	2.14	0.47
1:m:191:ILE:N	3:m:303:HOH:O	2.48	0.47
1:q:208:LYS:HB3	1:q:212:ASP:HB2	1.95	0.47
1:u:140:HIS:HB2	1:u:235:ALA:HB3	1.97	0.47
1:z:98:LEU:O	1:z:103:THR:OG1	2.32	0.47
1:2:141:MET:O	1:2:164:TYR:HA	2.15	0.47
1:P:220:ASP:HB3	1:P:223:ILE:HG13	1.97	0.47
1:S:261:PRO:HB3	1:p:107:TRP:CZ2	2.50	0.47
1:Y:144:GLN:NE2	1:Y:152:PRO:HD3	2.30	0.47
1:F:72:GLY:HA3	3:F:328:HOH:O	2.14	0.47
1:T:80:SER:OG	1:T:253:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:213:TYR:O	1:V:217:VAL:HG13	2.15	0.47
1:g:169:VAL:HB	1:g:247:ALA:HB1	1.97	0.47
1:G:124:ARG:HB2	1:G:194:THR:HG22	1.97	0.46
1:J:206:PRO:HB2	1:J:208:LYS:HE2	1.98	0.46
1:M:117:LYS:HE2	1:M:259:ILE:HD11	1.97	0.46
1:M:117:LYS:HE3	1:M:204:TRP:HB3	1.96	0.46
1:g:84:ALA:HB3	1:g:250:ILE:HB	1.97	0.46
1:m:141:MET:O	1:m:164:TYR:HA	2.16	0.46
1:u:99:VAL:O	1:u:229:PRO:HG2	2.14	0.46
1:1:74:ILE:HA	1:1:259:ILE:HG22	1.97	0.46
1:3:141:MET:O	1:3:164:TYR:HA	2.13	0.46
1:D:97:GLU:OE2	1:D:104:VAL:HA	2.15	0.46
1:R:152:PRO:HD2	1:R:233:VAL:HG11	1.96	0.46
1:c:141:MET:O	1:c:164:TYR:HA	2.15	0.46
1:k:125:TYR:CG	1:k:232:LEU:HD22	2.51	0.46
1:3:164:TYR:HH	1:4:251:TYR:HH	1.60	0.46
1:4:94:VAL:HA	1:4:234:ILE:O	2.15	0.46
1:j:80:SER:HA	1:j:252:CYS:O	2.15	0.46
1:j:223:ILE:O	1:j:226:PRO:HD2	2.15	0.46
1:l:88:VAL:CG1	1:l:236:LEU:HD12	2.45	0.46
1:S:88:VAL:HG21	1:S:137:GLY:HA3	1.97	0.46
1:T:140:HIS:HB2	1:T:235:ALA:HB3	1.97	0.46
1:U:130:SER:HB2	1:Y:138:SER:HB3	1.97	0.46
1:z:102:TYR:CE2	1:z:209:THR:HG23	2.50	0.46
1:f:80:SER:OG	1:f:253:THR:HG23	2.16	0.46
1:L:138:SER:HB3	1:M:130:SER:HB2	1.97	0.46
1:g:98:LEU:O	1:g:103:THR:OG1	2.31	0.46
1:s:88:VAL:HG11	1:s:169:VAL:HG21	1.96	0.46
1:E:182:THR:HG22	1:E:183:ARG:N	2.30	0.46
1:I:141:MET:O	1:I:164:TYR:HA	2.16	0.46
1:L:119:SER:OG	1:L:203:LYS:NZ	2.45	0.46
1:R:170:TRP:CZ2	1:S:133:SER:HB3	2.50	0.46
1:Z:141:MET:O	1:Z:164:TYR:HA	2.15	0.46
1:i:261:PRO:HB3	1:r:107:TRP:CZ2	2.50	0.46
1:t:159:SER:HA	1:t:164:TYR:CD1	2.51	0.46
1:x:121:LEU:HD23	1:x:121:LEU:HA	1.69	0.46
1:z:79:HIS:HB3	1:z:254:TYR:CZ	2.51	0.46
1:6:152:PRO:HD2	1:6:233:VAL:HG11	1.96	0.46
1:h:134:SER:C	1:j:132:PRO:HB3	2.41	0.46
1:D:107:TRP:CH2	1:D:111:VAL:HG21	2.51	0.46
1:E:223:ILE:O	1:E:226:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:144:GLN:NE2	1:N:152:PRO:HD3	2.31	0.46
1:q:223:ILE:O	1:q:226:PRO:HD2	2.15	0.46
1:B:169:VAL:CG2	1:B:247:ALA:HB1	2.46	0.46
1:B:209:THR:HG22	1:B:210:SER:N	2.30	0.46
1:N:206:PRO:HB2	1:N:208:LYS:HE2	1.96	0.46
1:R:223:ILE:O	1:R:226:PRO:HD2	2.15	0.46
1:u:119:SER:OG	1:u:203:LYS:NZ	2.41	0.46
1:v:225:THR:OG1	1:v:226:PRO:HD3	2.16	0.46
1:x:102:TYR:CD1	1:x:109:ARG:HG3	2.50	0.46
1:f:186:ASP:OD1	1:f:186:ASP:N	2.34	0.46
1:B:223:ILE:HD11	1:x:223:ILE:CD1	2.46	0.46
1:D:99:VAL:O	1:D:229:PRO:HG2	2.16	0.46
1:I:88:VAL:HG21	1:I:137:GLY:HA3	1.97	0.46
1:Y:88:VAL:HG13	1:Y:236:LEU:HD22	1.97	0.46
1:a:202:LYS:O	1:a:205:TYR:HE1	1.98	0.46
1:i:74:ILE:HG12	1:i:259:ILE:CG2	2.45	0.46
1:m:126:THR:HG23	1:m:192:SER:HB2	1.97	0.46
1:z:127:TYR:OH	1:z:169:VAL:O	2.28	0.46
1:i:251:TYR:HH	1:q:164:TYR:HH	1.59	0.46
1:k:207:TYR:O	1:k:208:LYS:HD2	2.15	0.46
1:w:159:SER:HA	1:w:164:TYR:CG	2.50	0.46
1:y:139:ILE:O	1:y:166:SER:HA	2.16	0.46
1:b:186:ASP:OD1	1:b:186:ASP:N	2.44	0.46
1:h:185:SER:HB2	1:h:186:ASP:H	1.62	0.46
1:F:88:VAL:HG12	1:F:236:LEU:HD12	1.98	0.46
1:I:101:PRO:HA	1:I:108:LEU:HD23	1.98	0.46
1:K:199:LYS:HE3	1:t:74:ILE:HD11	1.97	0.46
1:M:144:GLN:HB2	1:M:231:ARG:HG2	1.98	0.46
1:v:159:SER:HA	1:v:164:TYR:CD1	2.51	0.46
1:6:109:ARG:O	1:6:207:TYR:OH	2.33	0.46
1:A:124:ARG:HG2	3:A:414:HOH:O	2.16	0.45
1:K:130:SER:HB2	1:O:138:SER:HB3	1.96	0.45
1:T:88:VAL:CG1	1:T:236:LEU:HD12	2.46	0.45
1:W:223:ILE:O	1:W:226:PRO:HD2	2.16	0.45
1:r:223:ILE:O	1:r:226:PRO:HD2	2.16	0.45
1:r:225:THR:OG1	1:r:226:PRO:HD3	2.17	0.45
1:t:119:SER:OG	1:t:203:LYS:NZ	2.49	0.45
1:u:152:PRO:HG2	1:u:158:LEU:HD13	1.98	0.45
1:2:169:VAL:HB	1:2:247:ALA:HB1	1.98	0.45
1:h:208:LYS:HB3	1:h:212:ASP:HB2	1.98	0.45
1:S:159:SER:HA	1:S:164:TYR:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:206:PRO:HB2	1:Y:208:LYS:HE2	1.98	0.45
1:a:140:HIS:HB2	1:a:235:ALA:HB3	1.98	0.45
1:o:137:GLY:C	1:o:169:VAL:HB	2.41	0.45
1:r:133:SER:HB3	1:v:170:TRP:CH2	2.51	0.45
1:t:140:HIS:HB2	1:t:235:ALA:HB3	1.98	0.45
1:5:92:ILE:HA	1:5:237:LEU:HB3	1.98	0.45
1:f:144:GLN:NE2	1:f:152:PRO:HD3	2.31	0.45
1:h:209:THR:HG22	1:h:210:SER:N	2.31	0.45
1:U:98:LEU:HD22	1:U:228:VAL:HG21	1.98	0.45
1:U:159:SER:HA	1:U:164:TYR:CD1	2.51	0.45
1:x:209:THR:HG22	1:x:210:SER:N	2.30	0.45
1:B:141:MET:HE3	1:B:232:LEU:HD21	1.97	0.45
1:Q:102:TYR:CZ	1:Q:209:THR:HG23	2.52	0.45
1:k:223:ILE:HD13	1:j:223:ILE:HD11	1.97	0.45
1:1:169:VAL:HG22	1:1:247:ALA:HB1	1.99	0.45
1:1:251:TYR:HH	1:5:164:TYR:HH	1.65	0.45
1:2:151:VAL:HA	1:2:152:PRO:HD3	1.81	0.45
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.78	0.45
1:M:261:PRO:HB3	1:2:107:TRP:CZ2	2.52	0.45
1:o:99:VAL:O	1:o:229:PRO:HG2	2.17	0.45
1:1:159:SER:HA	1:1:164:TYR:CG	2.51	0.45
1:h:102:TYR:CE2	1:h:209:THR:HG23	2.51	0.45
1:h:160:ASN:OD1	1:h:160:ASN:N	2.48	0.45
1:p:158:LEU:HD23	1:p:161:LEU:HD12	1.99	0.45
1:A:159:SER:HA	1:A:164:TYR:CG	2.51	0.45
1:M:172:GLY:O	3:M:401:HOH:O	2.20	0.45
1:T:141:MET:O	1:T:164:TYR:HA	2.16	0.45
1:r:102:TYR:HE2	1:r:210:SER:HG	1.64	0.45
1:4:152:PRO:HD2	1:4:233:VAL:HG11	1.97	0.45
1:g:87:GLY:O	1:g:236:LEU:HD22	2.16	0.45
1:3:102:TYR:CZ	1:3:209:THR:HG23	2.51	0.45
1:n:202:LYS:NZ	1:n:226:PRO:O	2.44	0.45
1:I:159:SER:HA	1:I:164:TYR:CD1	2.52	0.45
1:R:100:MET:O	1:R:104:VAL:HG13	2.16	0.45
1:a:141:MET:O	1:a:164:TYR:HA	2.17	0.45
1:z:84:ALA:HB3	1:z:250:ILE:HB	1.99	0.45
1:B:136:ALA:HB3	1:B:240:SER:HB3	1.98	0.45
1:D:147:MET:HE3	1:D:231:ARG:HH21	1.82	0.45
1:F:108:LEU:HD22	1:F:254:TYR:CE1	2.51	0.45
1:N:159:SER:HA	1:N:164:TYR:CD1	2.51	0.45
1:O:159:SER:HA	1:O:164:TYR:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:169:VAL:HB	1:O:247:ALA:HB1	1.98	0.45
1:w:145:TYR:OH	1:w:196:ASP:N	2.30	0.45
1:O:223:ILE:O	1:O:226:PRO:HD2	2.17	0.45
1:b:169:VAL:HB	1:b:247:ALA:HB1	1.99	0.45
1:B:261:PRO:HB3	1:W:107:TRP:CZ2	2.52	0.45
1:D:152:PRO:HD2	1:D:233:VAL:HG11	1.99	0.45
1:F:237:LEU:HB2	3:F:307:HOH:O	2.16	0.45
1:G:208:LYS:HE3	1:k:222:ASN:OD1	2.17	0.45
1:k:159:SER:HA	1:k:164:TYR:CD1	2.51	0.45
1:2:136:ALA:HA	1:3:132:PRO:HD3	1.99	0.45
1:4:92:ILE:HA	1:4:237:LEU:HB3	1.99	0.45
1:B:102:TYR:CE2	1:B:209:THR:HG23	2.52	0.44
1:B:108:LEU:HD22	1:B:254:TYR:CE2	2.52	0.44
1:F:88:VAL:HG11	1:F:169:VAL:HG21	1.99	0.44
1:X:141:MET:HA	1:X:233:VAL:O	2.16	0.44
1:Y:88:VAL:CG1	1:Y:236:LEU:HD22	2.47	0.44
1:a:92:ILE:HA	1:a:237:LEU:HB3	1.98	0.44
1:e:206:PRO:HB2	1:e:208:LYS:HE2	1.99	0.44
1:w:99:VAL:O	1:w:229:PRO:HG2	2.17	0.44
1:7:223:ILE:O	1:7:226:PRO:HD2	2.17	0.44
1:f:92:ILE:HB	1:f:237:LEU:HD13	1.99	0.44
1:n:98:LEU:HD22	1:n:228:VAL:HG11	1.99	0.44
1:A:107:TRP:CZ2	1:F:261:PRO:HB3	2.52	0.44
1:L:77:LEU:HD21	1:L:107:TRP:HZ3	1.82	0.44
1:V:97:GLU:OE2	1:V:104:VAL:HA	2.17	0.44
1:V:220:ASP:O	1:V:223:ILE:HG12	2.18	0.44
1:Y:107:TRP:CZ2	1:d:261:PRO:HB3	2.52	0.44
1:c:213:TYR:O	1:c:217:VAL:HG13	2.17	0.44
1:k:158:LEU:HD12	1:k:161:LEU:HD12	1.99	0.44
1:1:182:THR:HG22	1:1:183:ARG:N	2.31	0.44
1:1:202:LYS:NZ	1:1:226:PRO:HB3	2.33	0.44
1:2:79:HIS:HB3	1:2:254:TYR:CZ	2.53	0.44
1:P:140:HIS:ND1	1:P:164:TYR:OH	2.39	0.44
1:V:206:PRO:HB2	1:V:208:LYS:HE2	2.00	0.44
1:O:99:VAL:O	1:O:229:PRO:HG2	2.18	0.44
1:6:140:HIS:HB3	1:6:164:TYR:HE1	1.82	0.44
1:d:169:VAL:CG2	1:d:247:ALA:HB1	2.46	0.44
1:D:138:SER:HB3	1:E:130:SER:HB2	1.98	0.44
1:G:76:VAL:HG22	1:G:257:GLN:HG2	2.00	0.44
1:L:261:PRO:HB3	1:t:107:TRP:CZ2	2.52	0.44
1:O:107:TRP:CZ2	1:e:261:PRO:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:104:VAL:CG2	1:R:108:LEU:HD23	2.47	0.44
1:s:141:MET:O	1:s:164:TYR:HA	2.17	0.44
1:u:206:PRO:HB2	1:u:208:LYS:HE2	1.99	0.44
1:4:206:PRO:HB2	1:4:208:LYS:HE2	2.00	0.44
1:n:138:SER:HB3	1:p:130:SER:HB2	1.99	0.44
1:p:119:SER:OG	1:p:203:LYS:NZ	2.44	0.44
1:A:89:THR:HG22	1:A:90:ASP:N	2.28	0.44
1:L:206:PRO:HB2	1:L:208:LYS:HE2	1.99	0.44
1:O:100:MET:O	1:O:104:VAL:HG13	2.17	0.44
1:U:83:SER:OG	1:U:97:GLU:OE1	2.36	0.44
1:Z:169:VAL:HB	1:Z:247:ALA:HB1	2.00	0.44
1:a:88:VAL:HG21	1:a:137:GLY:HA3	1.99	0.44
1:m:108:LEU:HD22	1:m:254:TYR:CZ	2.53	0.44
1:5:125:TYR:CG	1:5:232:LEU:HD22	2.53	0.44
1:J:92:ILE:HA	1:J:237:LEU:HB3	1.99	0.44
1:U:108:LEU:HD22	1:U:254:TYR:CZ	2.52	0.44
1:g:107:TRP:CZ2	1:z:261:PRO:HB3	2.52	0.44
1:g:261:PRO:HG2	1:z:79:HIS:CE1	2.53	0.44
1:t:141:MET:HA	1:t:233:VAL:O	2.18	0.44
1:b:74:ILE:HG12	1:b:259:ILE:HG22	1.99	0.44
1:b:140:HIS:HB3	1:b:164:TYR:HE1	1.83	0.44
1:L:87:GLY:O	1:L:236:LEU:HD22	2.17	0.44
1:L:118:TYR:HB2	1:L:256:ILE:HD11	2.00	0.44
1:P:99:VAL:O	1:P:229:PRO:HG2	2.18	0.44
1:Y:108:LEU:HD22	1:Y:254:TYR:CE1	2.52	0.44
1:k:79:HIS:CE1	1:l:261:PRO:HG2	2.53	0.44
1:B:108:LEU:HB2	1:B:254:TYR:OH	2.18	0.44
1:G:169:VAL:HG13	1:G:247:ALA:HB1	2.00	0.44
1:t:92:ILE:HA	1:t:237:LEU:HB3	1.99	0.44
1:w:176:LEU:HD21	1:o:165:VAL:HB	1.99	0.44
1:1:88:VAL:HB	1:1:236:LEU:HD23	2.00	0.44
1:b:108:LEU:HD22	1:b:254:TYR:CE2	2.52	0.44
1:d:98:LEU:HD22	1:d:228:VAL:HG11	2.00	0.44
1:f:144:GLN:HB2	1:f:231:ARG:HG2	2.00	0.44
1:n:223:ILE:O	1:n:226:PRO:HD2	2.18	0.44
1:F:223:ILE:CD1	1:m:223:ILE:HD12	2.48	0.44
1:O:159:SER:HA	1:O:164:TYR:CD1	2.53	0.44
1:Q:81:GLU:OE1	1:Q:105:GLY:HA3	2.18	0.44
1:T:88:VAL:CG1	1:T:169:VAL:HG11	2.48	0.44
1:e:79:HIS:HB3	1:e:254:TYR:CZ	2.53	0.44
1:m:134:SER:HA	1:o:132:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:152:PRO:HD2	1:m:233:VAL:HG11	2.00	0.44
1:m:202:LYS:NZ	1:m:226:PRO:O	2.36	0.44
1:r:132:PRO:HD3	1:v:136:ALA:HA	1.99	0.44
1:w:138:SER:HB3	1:x:130:SER:HB2	1.99	0.44
1:6:100:MET:HE3	1:6:102:TYR:HB3	1.99	0.44
1:M:147:MET:HE2	1:M:213:TYR:CE2	2.53	0.43
1:P:161:LEU:HA	1:P:161:LEU:HD23	1.80	0.43
1:a:98:LEU:HD22	1:a:228:VAL:HG11	1.99	0.43
1:a:137:GLY:C	1:a:169:VAL:HB	2.42	0.43
1:x:77:LEU:C	1:x:77:LEU:HD23	2.43	0.43
1:d:209:THR:HG22	1:d:210:SER:N	2.32	0.43
1:j:159:SER:HA	1:j:164:TYR:CD1	2.53	0.43
1:G:74:ILE:HG12	1:G:259:ILE:CG2	2.49	0.43
1:P:169:VAL:CG2	1:P:247:ALA:HB1	2.46	0.43
1:S:220:ASP:OD2	1:S:222:ASN:HB2	2.17	0.43
1:v:207:TYR:O	1:v:208:LYS:HD2	2.18	0.43
1:4:138:SER:HB3	1:5:130:SER:HB2	2.01	0.43
1:b:220:ASP:HB3	1:b:223:ILE:HG13	2.00	0.43
1:I:75:THR:HG23	1:f:76:VAL:O	2.18	0.43
1:Q:137:GLY:C	1:Q:169:VAL:HG13	2.44	0.43
1:T:159:SER:HA	1:T:164:TYR:CG	2.52	0.43
1:W:208:LYS:HD3	1:W:208:LYS:HA	1.77	0.43
1:o:155:VAL:HG12	1:q:82:LEU:HD22	2.00	0.43
1:s:86:ILE:HG23	1:s:236:LEU:CD1	2.46	0.43
1:f:97:GLU:OE2	1:f:104:VAL:HA	2.19	0.43
1:A:102:TYR:CD1	1:A:109:ARG:HG3	2.53	0.43
1:D:79:HIS:CE1	1:5:261:PRO:HG2	2.53	0.43
1:Y:88:VAL:CG1	1:Y:169:VAL:HG21	2.47	0.43
1:Z:185:SER:HB2	1:Z:186:ASP:H	1.59	0.43
1:y:159:SER:HA	1:y:164:TYR:CD1	2.53	0.43
1:3:81:GLU:OE2	1:3:254:TYR:OH	2.21	0.43
1:d:202:LYS:O	1:d:205:TYR:HE1	2.02	0.43
1:B:169:VAL:HG22	1:B:247:ALA:HB1	2.00	0.43
1:G:208:LYS:HD3	1:G:208:LYS:HA	1.82	0.43
1:H:169:VAL:CG2	1:H:247:ALA:HB1	2.47	0.43
1:K:152:PRO:HD2	1:K:233:VAL:HG11	2.01	0.43
1:N:108:LEU:HD22	1:N:254:TYR:CE1	2.53	0.43
1:P:159:SER:HA	1:P:164:TYR:CD1	2.52	0.43
1:Z:108:LEU:HB2	1:Z:254:TYR:OH	2.18	0.43
1:s:223:ILE:O	1:s:226:PRO:HD2	2.18	0.43
1:1:127:TYR:HD2	1:1:191:ILE:HD12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:159:SER:HA	1:2:164:TYR:CG	2.54	0.43
1:3:99:VAL:O	1:3:229:PRO:HG2	2.19	0.43
1:3:127:TYR:HB3	1:3:191:ILE:HB	2.01	0.43
1:l:208:LYS:HD3	1:l:208:LYS:HA	1.86	0.43
1:2:170:TRP:CH2	1:3:133:SER:HB3	2.54	0.43
1:5:220:ASP:HB3	1:5:223:ILE:HG13	1.99	0.43
1:b:88:VAL:HG21	1:b:137:GLY:HA3	1.99	0.43
1:E:118:TYR:HB2	1:E:256:ILE:HD11	1.99	0.43
1:F:158:LEU:HD12	1:F:158:LEU:HA	1.77	0.43
1:K:261:PRO:HB3	1:P:107:TRP:CZ2	2.53	0.43
1:P:114:ASN:HB2	1:P:115:TRP:CE3	2.54	0.43
1:i:170:TRP:CH2	1:k:133:SER:HB3	2.54	0.43
1:r:138:SER:HB3	1:s:130:SER:HB2	2.00	0.43
1:v:79:HIS:CE1	1:n:261:PRO:HG2	2.54	0.43
1:z:209:THR:HG22	1:z:210:SER:N	2.34	0.43
1:h:141:MET:O	1:h:164:TYR:HA	2.18	0.43
1:l:141:MET:O	1:l:164:TYR:HA	2.19	0.43
1:B:158:LEU:HD12	1:B:158:LEU:HA	1.81	0.43
1:Z:223:ILE:O	1:Z:226:PRO:HD2	2.18	0.43
1:x:198:SER:OG	3:x:301:HOH:O	2.21	0.43
1:y:118:TYR:HB2	1:y:256:ILE:HD11	2.00	0.43
1:O:99:VAL:O	1:O:229:PRO:HG2	2.18	0.43
1:Q:237:LEU:HD11	1:R:249:ARG:HH22	1.84	0.43
1:T:159:SER:HA	1:T:164:TYR:CD1	2.54	0.43
1:Y:108:LEU:HD22	1:Y:254:TYR:CZ	2.53	0.43
1:a:108:LEU:HD22	1:a:254:TYR:CZ	2.54	0.43
1:c:121:LEU:HD23	1:c:121:LEU:HA	1.86	0.43
1:i:146:ASP:HB3	1:i:149:ASP:OD2	2.18	0.43
1:z:144:GLN:NE2	1:z:152:PRO:HD3	2.34	0.43
1:7:144:GLN:OE1	1:7:231:ARG:NH1	2.52	0.43
1:f:127:TYR:OH	1:f:169:VAL:O	2.24	0.43
1:F:138:SER:HB3	1:G:130:SER:HB2	2.01	0.43
1:J:118:TYR:HB2	1:J:256:ILE:HD11	2.01	0.43
1:S:97:GLU:OE2	1:S:104:VAL:HA	2.18	0.43
1:T:169:VAL:HB	1:T:247:ALA:HB1	2.01	0.43
1:Y:100:MET:O	1:Y:104:VAL:HG13	2.18	0.43
1:s:74:ILE:HD11	1:2:199:LYS:HE3	2.00	0.43
1:t:97:GLU:OE2	1:t:104:VAL:HA	2.18	0.43
1:4:99:VAL:O	1:4:229:PRO:HG2	2.19	0.43
1:j:207:TYR:O	1:j:208:LYS:HD2	2.19	0.43
1:B:223:ILE:HD12	1:V:223:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:209:THR:HG22	1:Q:210:SER:N	2.34	0.42
1:r:152:PRO:HD2	1:r:233:VAL:HG11	1.99	0.42
1:j:76:VAL:HG22	1:j:257:GLN:HG2	2.01	0.42
1:l:92:ILE:HA	1:l:237:LEU:HB3	2.01	0.42
1:K:129:PRO:HB3	1:K:169:VAL:O	2.20	0.42
1:N:108:LEU:HB2	1:N:254:TYR:OH	2.19	0.42
1:O:77:LEU:HD21	1:O:107:TRP:HZ3	1.84	0.42
1:W:169:VAL:HB	1:W:247:ALA:HB1	2.00	0.42
1:g:261:PRO:HB3	1:z:107:TRP:CZ2	2.54	0.42
1:t:206:PRO:HB2	1:t:208:LYS:HE2	2.01	0.42
1:y:100:MET:HE3	1:y:102:TYR:HB3	2.01	0.42
1:y:119:SER:OG	1:y:203:LYS:NZ	2.45	0.42
1:z:88:VAL:CG1	1:z:169:VAL:HG21	2.46	0.42
1:2:134:SER:HB3	2:4:301:SO4:O4	2.19	0.42
1:2:185:SER:HB2	1:2:186:ASP:H	1.61	0.42
1:6:102:TYR:CZ	1:6:209:THR:HG23	2.54	0.42
1:b:208:LYS:HA	1:b:208:LYS:HD3	1.84	0.42
1:B:86:ILE:HG22	1:B:236:LEU:HD21	2.01	0.42
1:X:153:VAL:HG22	1:X:157:GLN:OE1	2.19	0.42
1:t:208:LYS:HA	1:t:208:LYS:HD3	1.83	0.42
1:x:152:PRO:HG2	1:x:158:LEU:HD13	2.02	0.42
1:y:86:ILE:HG13	1:y:250:ILE:HG13	2.01	0.42
1:4:87:GLY:O	1:4:236:LEU:HD22	2.19	0.42
1:j:237:LEU:HD11	1:l:249:ARG:NH2	2.34	0.42
1:n:158:LEU:HD12	1:n:161:LEU:HD12	2.02	0.42
1:F:173:SER:HB2	1:J:189:THR:HG22	2.01	0.42
1:F:206:PRO:HB2	1:F:208:LYS:HE2	2.00	0.42
1:H:81:GLU:OE2	1:H:254:TYR:OH	2.28	0.42
1:M:124:ARG:HB2	1:M:194:THR:HG22	2.01	0.42
1:k:152:PRO:HG2	1:k:158:LEU:HD13	2.01	0.42
1:r:158:LEU:HD22	1:r:164:TYR:HD1	1.84	0.42
1:d:223:ILE:O	1:d:226:PRO:HD2	2.20	0.42
1:C:206:PRO:HB2	1:C:208:LYS:HE2	2.00	0.42
1:H:98:LEU:HD23	1:H:98:LEU:HA	1.84	0.42
1:I:163:GLY:O	1:I:193:THR:OG1	2.28	0.42
1:N:186:ASP:OD1	1:N:186:ASP:N	2.48	0.42
1:P:108:LEU:HD22	1:P:254:TYR:CZ	2.55	0.42
1:W:163:GLY:O	1:W:193:THR:OG1	2.17	0.42
1:Y:161:LEU:HA	1:Y:161:LEU:HD23	1.84	0.42
1:i:158:LEU:HD12	1:i:158:LEU:HA	1.70	0.42
1:o:100:MET:O	1:o:104:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:87:GLY:O	1:q:236:LEU:HD23	2.19	0.42
1:x:169:VAL:HB	1:x:247:ALA:HB1	2.02	0.42
1:b:118:TYR:CB	1:b:256:ILE:HD11	2.47	0.42
1:A:261:PRO:HB3	1:F:107:TRP:CZ2	2.54	0.42
1:B:86:ILE:CG2	1:B:236:LEU:HD21	2.49	0.42
1:B:199:LYS:HE3	1:x:74:ILE:HD11	2.02	0.42
1:O:79:HIS:HB3	1:O:254:TYR:CZ	2.54	0.42
1:Q:121:LEU:HD23	1:Q:121:LEU:HA	1.93	0.42
1:V:208:LYS:HA	1:V:208:LYS:HD3	1.87	0.42
1:c:241:SER:OG	1:c:243:THR:O	2.37	0.42
1:m:151:VAL:HA	1:m:152:PRO:HD3	1.93	0.42
1:m:158:LEU:HD12	1:m:161:LEU:HD12	2.02	0.42
1:o:214:ALA:O	1:o:217:VAL:HG22	2.20	0.42
1:u:169:VAL:CG2	1:u:247:ALA:HB1	2.50	0.42
1:v:152:PRO:HD2	1:v:233:VAL:HG11	2.02	0.42
1:y:237:LEU:HD11	1:z:249:ARG:NH2	2.34	0.42
1:d:92:ILE:HA	1:d:237:LEU:HB3	2.01	0.42
1:f:206:PRO:HB2	1:f:208:LYS:HE2	2.00	0.42
1:l:223:ILE:O	1:l:226:PRO:HD2	2.20	0.42
1:p:213:TYR:HE1	1:p:224:ALA:HB1	1.85	0.42
1:B:157:GLN:HG2	1:x:263:ALA:HB3	2.01	0.42
1:H:74:ILE:HD11	1:h:199:LYS:HE3	2.00	0.42
1:P:98:LEU:O	1:P:103:THR:OG1	2.35	0.42
1:Q:98:LEU:O	1:Q:103:THR:OG1	2.36	0.42
1:U:92:ILE:HA	1:U:236:LEU:O	2.20	0.42
1:W:158:LEU:HD12	1:W:158:LEU:HA	1.76	0.42
1:Z:119:SER:OG	1:Z:203:LYS:NZ	2.45	0.42
1:s:159:SER:HA	1:s:164:TYR:CG	2.54	0.42
1:3:89:THR:HA	1:3:241:SER:O	2.19	0.42
1:5:217:VAL:HG12	1:5:224:ALA:HB2	2.00	0.42
1:h:80:SER:HA	1:h:252:CYS:O	2.19	0.42
1:n:170:TRP:CZ2	1:p:133:SER:HB3	2.55	0.42
1:M:159:SER:HA	1:M:164:TYR:CD1	2.54	0.42
2:Z:301:SO4:O3	1:g:134:SER:HB3	2.20	0.42
1:5:186:ASP:OD1	1:5:186:ASP:N	2.41	0.42
1:d:117:LYS:HE3	1:d:204:TRP:HB3	2.01	0.42
1:l:125:TYR:CG	1:l:232:LEU:HD22	2.55	0.42
1:n:99:VAL:O	1:n:229:PRO:HG2	2.20	0.42
1:p:223:ILE:O	1:p:226:PRO:HD2	2.19	0.42
1:A:202:LYS:HG3	1:A:205:TYR:CE1	2.55	0.42
1:D:136:ALA:HB3	1:D:240:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:77:LEU:HD22	1:K:254:TYR:HE1	1.85	0.42
1:N:138:SER:HB3	1:O:130:SER:CB	2.49	0.42
1:O:125:TYR:CB	1:O:141:MET:HE1	2.49	0.42
1:R:144:GLN:NE2	1:R:152:PRO:HD3	2.35	0.42
1:X:159:SER:HA	1:X:164:TYR:CG	2.54	0.42
1:c:100:MET:HE3	1:c:102:TYR:HB3	2.02	0.42
1:g:76:VAL:HG22	1:g:257:GLN:HG2	2.02	0.42
1:i:86:ILE:HG22	1:i:236:LEU:HD21	2.02	0.42
1:r:79:HIS:HB3	1:r:254:TYR:CE1	2.54	0.42
1:t:118:TYR:HB2	1:t:256:ILE:HD11	2.01	0.42
1:0:79:HIS:HB3	1:0:254:TYR:CZ	2.55	0.42
1:2:138:SER:HB3	1:3:130:SER:HB2	2.02	0.42
1:E:159:SER:HA	1:E:164:TYR:CD1	2.55	0.42
1:F:208:LYS:NZ	3:F:305:HOH:O	2.45	0.42
1:K:97:GLU:OE2	1:K:104:VAL:HA	2.19	0.42
1:M:88:VAL:HG21	1:M:137:GLY:HA3	2.01	0.42
1:N:74:ILE:HA	1:N:259:ILE:HG22	2.02	0.42
1:N:261:PRO:HG2	1:0:79:HIS:CE1	2.55	0.42
1:O:141:MET:HE2	1:O:141:MET:HB3	1.85	0.42
1:Z:185:SER:HB2	1:Z:186:ASP:OD1	2.20	0.42
1:c:87:GLY:O	1:c:236:LEU:HD22	2.19	0.42
1:g:98:LEU:HD22	1:g:228:VAL:HG21	2.01	0.42
1:i:139:ILE:O	1:i:166:SER:HA	2.20	0.42
1:y:257:GLN:NE2	3:y:301:HOH:O	2.28	0.42
1:z:151:VAL:HA	1:z:152:PRO:HD3	1.95	0.42
1:5:159:SER:HA	1:5:164:TYR:CG	2.55	0.42
1:f:153:VAL:HG22	1:f:157:GLN:OE1	2.20	0.42
1:E:76:VAL:HG22	1:E:257:GLN:HG2	2.02	0.41
1:K:77:LEU:C	1:K:77:LEU:HD23	2.44	0.41
1:O:77:LEU:HD21	1:O:107:TRP:CZ3	2.54	0.41
1:O:207:TYR:C	1:O:208:LYS:HD2	2.45	0.41
1:W:144:GLN:NE2	1:W:152:PRO:HD3	2.35	0.41
1:Z:108:LEU:HD22	1:Z:254:TYR:CZ	2.55	0.41
1:g:141:MET:O	1:g:164:TYR:HA	2.20	0.41
1:g:241:SER:OG	1:g:243:THR:O	2.38	0.41
1:k:87:GLY:O	1:k:236:LEU:HD22	2.20	0.41
1:w:84:ALA:HB3	1:w:250:ILE:HB	2.01	0.41
1:y:144:GLN:OE1	1:y:231:ARG:NH1	2.53	0.41
1:3:146:ASP:O	1:3:149:ASP:HB2	2.20	0.41
1:7:97:GLU:OE2	1:7:104:VAL:HA	2.20	0.41
1:h:82:LEU:HD22	1:p:155:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:217:VAL:HG12	1:V:224:ALA:HB2	2.03	0.41
1:X:134:SER:HA	1:Y:132:PRO:HB3	2.01	0.41
1:o:141:MET:O	1:o:164:TYR:HA	2.20	0.41
1:s:208:LYS:HA	1:s:208:LYS:HD3	1.77	0.41
1:3:159:SER:HA	1:3:164:TYR:CD1	2.55	0.41
1:U:97:GLU:OE2	1:U:104:VAL:HA	2.20	0.41
1:a:128:ILE:HB	1:a:251:TYR:HE2	1.85	0.41
1:c:140:HIS:HB2	1:c:235:ALA:HB3	2.02	0.41
1:k:141:MET:O	1:k:164:TYR:HA	2.21	0.41
1:x:87:GLY:O	1:x:236:LEU:HD22	2.20	0.41
1:L:92:ILE:HA	1:L:237:LEU:HB3	2.01	0.41
1:N:141:MET:O	1:N:164:TYR:HA	2.20	0.41
1:V:186:ASP:OD1	1:V:186:ASP:N	2.49	0.41
1:k:185:SER:HB2	1:k:186:ASP:H	1.65	0.41
1:r:186:ASP:HB2	1:s:186:ASP:OD2	2.20	0.41
1:u:152:PRO:HD2	1:u:233:VAL:HG11	2.01	0.41
1:7:147:MET:HE1	1:7:231:ARG:HB3	2.02	0.41
1:b:118:TYR:HA	1:b:257:GLN:O	2.20	0.41
1:h:138:SER:HB3	1:j:130:SER:CB	2.50	0.41
1:j:108:LEU:HD13	1:j:254:TYR:CE1	2.55	0.41
1:N:208:LYS:HA	1:N:208:LYS:HD3	1.83	0.41
1:O:89:THR:HG22	1:O:90:ASP:N	2.33	0.41
1:R:186:ASP:OD1	1:R:186:ASP:N	2.47	0.41
1:Z:84:ALA:HB3	1:Z:250:ILE:HB	2.01	0.41
1:Z:121:LEU:HD23	1:Z:121:LEU:HA	1.85	0.41
1:q:158:LEU:HD12	1:q:158:LEU:HA	1.69	0.41
1:u:223:ILE:HG12	1:n:223:ILE:HD12	2.02	0.41
1:3:74:ILE:HA	1:3:259:ILE:HG22	2.02	0.41
1:b:141:MET:O	1:b:164:TYR:HA	2.20	0.41
1:p:220:ASP:HB3	1:p:223:ILE:HG13	2.02	0.41
1:Q:126:THR:HG23	1:Q:192:SER:HB2	2.03	0.41
1:V:147:MET:HG2	1:V:213:TYR:HE1	1.86	0.41
1:X:99:VAL:O	1:X:229:PRO:HG2	2.20	0.41
1:c:201:GLY:HA3	3:c:318:HOH:O	2.20	0.41
1:k:97:GLU:OE2	1:k:104:VAL:HA	2.20	0.41
1:m:158:LEU:HD12	1:m:158:LEU:HA	1.80	0.41
1:q:144:GLN:OE1	1:q:231:ARG:NH1	2.54	0.41
1:w:145:TYR:HD1	3:w:402:HOH:O	2.04	0.41
1:0:141:MET:O	1:0:164:TYR:HA	2.20	0.41
1:2:144:GLN:NE2	1:2:152:PRO:HD3	2.35	0.41
1:D:162:ARG:HA	1:D:162:ARG:HD2	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:79:HIS:CE1	1:t:261:PRO:HG2	2.56	0.41
1:M:108:LEU:HD22	1:M:254:TYR:CE2	2.55	0.41
1:R:156:ASN:O	1:R:159:SER:OG	2.33	0.41
1:k:151:VAL:HA	1:k:152:PRO:HD3	1.93	0.41
1:r:79:HIS:HB3	1:r:254:TYR:CZ	2.56	0.41
1:z:158:LEU:HD12	1:z:161:LEU:HD13	2.02	0.41
1:6:96:SER:HA	1:6:232:LEU:O	2.20	0.41
1:p:159:SER:HA	1:p:164:TYR:CG	2.55	0.41
1:A:74:ILE:HD11	1:J:199:LYS:HE3	2.03	0.41
1:A:141:MET:O	1:A:164:TYR:HA	2.20	0.41
1:C:186:ASP:OD1	1:C:186:ASP:N	2.51	0.41
1:G:138:SER:HB3	1:H:130:SER:HB2	2.02	0.41
1:K:151:VAL:HA	1:K:152:PRO:HD3	1.93	0.41
1:e:159:SER:HA	1:e:164:TYR:CG	2.55	0.41
1:k:121:LEU:HD23	1:k:121:LEU:HA	1.96	0.41
1:0:141:MET:HA	1:0:233:VAL:O	2.21	0.41
1:D:169:VAL:CG2	1:D:247:ALA:HB1	2.47	0.41
1:J:121:LEU:O	1:J:197:VAL:HG21	2.21	0.41
1:L:79:HIS:HB3	1:L:254:TYR:CZ	2.55	0.41
1:L:211:ALA:O	1:L:215:THR:HG23	2.21	0.41
1:S:199:LYS:HE3	1:u:74:ILE:HD11	2.03	0.41
1:T:261:PRO:HB3	1:u:107:TRP:CZ2	2.56	0.41
1:U:99:VAL:O	1:U:229:PRO:HG2	2.20	0.41
1:a:77:LEU:O	1:a:255:THR:HA	2.21	0.41
1:c:74:ILE:HA	1:c:259:ILE:HG22	2.03	0.41
1:e:89:THR:HG22	1:e:244:ALA:HA	2.03	0.41
1:k:220:ASP:OD2	1:k:222:ASN:HB2	2.21	0.41
1:o:98:LEU:HD11	1:o:213:TYR:CD2	2.56	0.41
1:r:185:SER:HB2	1:r:186:ASP:H	1.61	0.41
1:v:107:TRP:CZ2	1:n:261:PRO:HB3	2.55	0.41
1:v:125:TYR:CG	1:v:232:LEU:HD22	2.55	0.41
1:x:162:ARG:HD2	1:x:162:ARG:HA	1.86	0.41
1:y:141:MET:O	1:y:164:TYR:HA	2.20	0.41
1:0:118:TYR:HB2	1:0:256:ILE:HD11	2.03	0.41
1:3:108:LEU:HB2	1:3:254:TYR:OH	2.20	0.41
1:6:223:ILE:O	1:6:226:PRO:HD2	2.21	0.41
1:h:163:GLY:O	1:h:193:THR:OG1	2.29	0.41
1:C:98:LEU:O	1:C:103:THR:OG1	2.38	0.41
1:D:141:MET:HG2	1:D:234:ILE:HG12	2.03	0.41
1:D:170:TRP:CH2	1:E:133:SER:HB3	2.56	0.41
1:E:141:MET:HA	1:E:233:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:SER:HA	1:E:164:TYR:CG	2.56	0.41
1:W:140:HIS:ND1	1:W:164:TYR:OH	2.45	0.41
1:X:121:LEU:HD23	1:X:121:LEU:HA	1.76	0.41
1:a:186:ASP:HB2	1:c:186:ASP:CG	2.46	0.41
1:i:220:ASP:HB3	1:i:223:ILE:HG13	2.02	0.41
1:o:118:TYR:HB2	1:o:256:ILE:HD11	2.03	0.41
1:q:141:MET:O	1:q:164:TYR:HA	2.20	0.41
1:q:217:VAL:HG12	1:q:224:ALA:HB2	2.02	0.41
1:s:241:SER:OG	1:s:243:THR:O	2.38	0.41
1:x:125:TYR:CG	1:x:232:LEU:HD22	2.55	0.41
1:5:79:HIS:HD2	1:5:254:TYR:OH	2.04	0.41
1:n:169:VAL:HB	1:n:247:ALA:HB1	2.03	0.41
1:E:141:MET:O	1:E:164:TYR:HA	2.21	0.40
1:W:159:SER:HA	1:W:164:TYR:CD1	2.56	0.40
1:X:98:LEU:HD22	1:X:228:VAL:HG11	2.02	0.40
1:0:162:ARG:HA	1:0:162:ARG:HD2	1.94	0.40
1:2:159:SER:HA	1:2:164:TYR:CD1	2.56	0.40
1:6:80:SER:HA	1:6:252:CYS:O	2.22	0.40
1:6:162:ARG:HA	1:6:162:ARG:HD2	1.83	0.40
1:d:128:ILE:HD13	1:d:179:ILE:HD11	2.03	0.40
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.86	0.40
1:B:195:LEU:HD11	1:B:230:ALA:HB3	2.03	0.40
1:B:261:PRO:HB3	1:W:107:TRP:CE2	2.56	0.40
1:C:100:MET:O	1:C:104:VAL:HG13	2.21	0.40
1:L:141:MET:HA	1:L:233:VAL:O	2.21	0.40
1:T:208:LYS:HA	1:T:208:LYS:HD3	1.91	0.40
1:Y:120:TRP:O	3:Y:302:HOH:O	2.22	0.40
1:i:102:TYR:HD2	1:i:103:THR:HG23	1.85	0.40
1:1:141:MET:O	1:1:164:TYR:HA	2.21	0.40
1:f:124:ARG:HH11	1:f:124:ARG:HD2	1.75	0.40
1:j:151:VAL:HA	1:j:152:PRO:HD3	1.92	0.40
1:D:100:MET:O	1:D:104:VAL:HG13	2.22	0.40
1:P:173:SER:HB2	1:T:189:THR:HG22	2.04	0.40
1:R:104:VAL:HG21	1:R:108:LEU:HD23	2.02	0.40
1:V:261:PRO:HB3	1:y:107:TRP:CZ2	2.56	0.40
1:e:185:SER:HB2	1:e:186:ASP:H	1.71	0.40
1:i:134:SER:HB3	2:o:301:SO4:O2	2.22	0.40
1:m:169:VAL:HB	1:m:247:ALA:HB1	2.03	0.40
1:v:99:VAL:O	1:v:229:PRO:HG2	2.21	0.40
1:y:182:THR:HG22	1:y:183:ARG:N	2.35	0.40
1:f:159:SER:HA	1:f:164:TYR:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:169:VAL:CG2	1:J:247:ALA:HB1	2.50	0.40
3:K:308:HOH:O	1:T:161:LEU:HA	2.21	0.40
1:P:74:ILE:HA	1:P:259:ILE:HG22	2.03	0.40
1:P:202:LYS:HG3	1:P:205:TYR:CE1	2.57	0.40
1:S:202:LYS:NZ	1:S:226:PRO:O	2.54	0.40
1:V:77:LEU:O	1:V:255:THR:HA	2.21	0.40
1:m:108:LEU:HB2	1:m:254:TYR:OH	2.22	0.40
1:r:130:SER:HB2	1:v:138:SER:HB3	2.03	0.40
1:t:138:SER:HB3	1:u:130:SER:CB	2.51	0.40
1:b:108:LEU:HB2	1:b:254:TYR:OH	2.21	0.40
1:h:206:PRO:HB2	1:h:208:LYS:HD3	2.02	0.40
1:E:140:HIS:ND1	1:E:166:SER:HB2	2.37	0.40
1:J:186:ASP:OD1	1:J:186:ASP:N	2.45	0.40
1:K:74:ILE:HA	1:K:259:ILE:HG22	2.03	0.40
1:M:186:ASP:OD1	1:M:186:ASP:N	2.36	0.40
1:M:208:LYS:HD3	1:M:208:LYS:HA	1.74	0.40
2:P:301:SO4:O2	1:R:133:SER:OG	2.40	0.40
1:Q:162:ARG:HH21	1:Q:196:ASP:CG	2.29	0.40
1:T:79:HIS:CE1	1:u:261:PRO:HG2	2.56	0.40
1:e:77:LEU:HD21	1:e:107:TRP:CZ3	2.56	0.40
1:m:88:VAL:HB	1:m:236:LEU:HD23	2.04	0.40
1:q:213:TYR:O	1:q:217:VAL:HG13	2.21	0.40
1:t:86:ILE:HD12	1:t:86:ILE:HG23	1.83	0.40
1:3:208:LYS:HA	1:3:208:LYS:HD3	1.94	0.40
1:b:147:MET:HE1	1:b:230:ALA:HA	2.03	0.40
1:h:106:THR:O	1:h:109:ARG:HB3	2.21	0.40
1:p:98:LEU:HD11	1:p:213:TYR:CD2	2.56	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)
1:3:242: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%)	154 (98%)	4 (2%)	42	66
1	1	158/238 (66%)	155 (98%)	3 (2%)	50	71
1	2	157/238 (66%)	157 (100%)	0	100	100
1	3	158/238 (66%)	154 (98%)	4 (2%)	42	66
1	4	155/238 (65%)	153 (99%)	2 (1%)	61	78
1	5	158/238 (66%)	153 (97%)	5 (3%)	34	59
1	6	157/238 (66%)	156 (99%)	1 (1%)	78	89
1	7	157/238 (66%)	154 (98%)	3 (2%)	50	71
1	A	157/238 (66%)	153 (98%)	4 (2%)	42	66
1	B	156/238 (66%)	155 (99%)	1 (1%)	78	89
1	C	156/238 (66%)	152 (97%)	4 (3%)	40	65
1	D	156/238 (66%)	153 (98%)	3 (2%)	50	71
1	E	157/238 (66%)	154 (98%)	3 (2%)	50	71
1	F	157/238 (66%)	155 (99%)	2 (1%)	61	78
1	G	158/238 (66%)	155 (98%)	3 (2%)	50	71
1	H	158/238 (66%)	154 (98%)	4 (2%)	42	66
1	I	158/238 (66%)	155 (98%)	3 (2%)	50	71

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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%)	155 (98%)	3 (2%)	50	71
1	L	158/238 (66%)	156 (99%)	2 (1%)	61	78
1	M	158/238 (66%)	156 (99%)	2 (1%)	61	78
1	N	158/238 (66%)	155 (98%)	3 (2%)	50	71
1	O	158/238 (66%)	154 (98%)	4 (2%)	42	66
1	P	158/238 (66%)	154 (98%)	4 (2%)	42	66
1	Q	157/238 (66%)	153 (98%)	4 (2%)	42	66
1	R	157/238 (66%)	153 (98%)	4 (2%)	42	66
1	S	157/238 (66%)	153 (98%)	4 (2%)	42	66
1	T	157/238 (66%)	156 (99%)	1 (1%)	78	89
1	U	158/238 (66%)	156 (99%)	2 (1%)	61	78
1	V	158/238 (66%)	154 (98%)	4 (2%)	42	66
1	W	158/238 (66%)	155 (98%)	3 (2%)	50	71
1	X	158/238 (66%)	155 (98%)	3 (2%)	50	71
1	Y	158/238 (66%)	152 (96%)	6 (4%)	29	55
1	Z	158/238 (66%)	154 (98%)	4 (2%)	42	66
1	a	157/238 (66%)	153 (98%)	4 (2%)	42	66
1	b	156/238 (66%)	154 (99%)	2 (1%)	61	78
1	c	157/238 (66%)	153 (98%)	4 (2%)	42	66
1	d	158/238 (66%)	156 (99%)	2 (1%)	61	78
1	e	158/238 (66%)	154 (98%)	4 (2%)	42	66
1	f	156/238 (66%)	154 (99%)	2 (1%)	61	78
1	g	156/238 (66%)	153 (98%)	3 (2%)	50	71
1	h	156/238 (66%)	152 (97%)	4 (3%)	40	65
1	i	158/238 (66%)	155 (98%)	3 (2%)	50	71
1	j	158/238 (66%)	157 (99%)	1 (1%)	78	89
1	k	157/238 (66%)	156 (99%)	1 (1%)	78	89
1	l	158/238 (66%)	155 (98%)	3 (2%)	50	71
1	m	158/238 (66%)	156 (99%)	2 (1%)	61	78
1	n	157/238 (66%)	156 (99%)	1 (1%)	78	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	154/238 (65%)	151 (98%)	3 (2%)	50	71
1	p	153/238 (64%)	149 (97%)	4 (3%)	40	65
1	q	157/238 (66%)	153 (98%)	4 (2%)	42	66
1	r	158/238 (66%)	155 (98%)	3 (2%)	50	71
1	s	158/238 (66%)	155 (98%)	3 (2%)	50	71
1	t	158/238 (66%)	154 (98%)	4 (2%)	42	66
1	u	158/238 (66%)	154 (98%)	4 (2%)	42	66
1	v	158/238 (66%)	155 (98%)	3 (2%)	50	71
1	w	153/238 (64%)	150 (98%)	3 (2%)	48	71
1	x	154/238 (65%)	153 (99%)	1 (1%)	78	89
1	y	158/238 (66%)	153 (97%)	5 (3%)	34	59
1	z	157/238 (66%)	153 (98%)	4 (2%)	42	66
All	All	9429/14280 (66%)	9250 (98%)	179 (2%)	50	71

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	THR
1	A	104	VAL
1	A	185	SER
1	A	236	LEU
1	B	104	VAL
1	C	104	VAL
1	C	185	SER
1	C	228	VAL
1	C	236	LEU
1	D	185	SER
1	D	225	THR
1	D	228	VAL
1	E	185	SER
1	E	225	THR
1	E	228	VAL
1	F	104	VAL
1	F	243	THR
1	G	169	VAL
1	G	185	SER
1	G	236	LEU
1	H	104	VAL

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Mol	Chain	Res	Type
1	H	185	SER
1	H	228	VAL
1	H	236	LEU
1	I	85	GLU
1	I	158	LEU
1	I	236	LEU
1	K	104	VAL
1	K	185	SER
1	K	236	LEU
1	L	158	LEU
1	L	225	THR
1	M	185	SER
1	M	225	THR
1	N	185	SER
1	N	225	THR
1	N	236	LEU
1	O	104	VAL
1	O	185	SER
1	O	225	THR
1	O	236	LEU
1	P	104	VAL
1	P	169	VAL
1	P	228	VAL
1	P	236	LEU
1	Q	158	LEU
1	Q	185	SER
1	Q	228	VAL
1	Q	236	LEU
1	R	189	THR
1	R	225	THR
1	R	228	VAL
1	R	236	LEU
1	S	106	THR
1	S	189	THR
1	S	225	THR
1	S	236	LEU
1	T	185	SER
1	U	228	VAL
1	U	236	LEU
1	V	104	VAL
1	V	169	VAL
1	V	194	THR

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Mol	Chain	Res	Type
1	V	228	VAL
1	W	185	SER
1	W	225	THR
1	W	236	LEU
1	X	158	LEU
1	X	185	SER
1	X	236	LEU
1	Y	117	LYS
1	Y	158	LEU
1	Y	169	VAL
1	Y	185	SER
1	Y	189	THR
1	Y	225	THR
1	Z	104	VAL
1	Z	225	THR
1	Z	228	VAL
1	Z	236	LEU
1	a	104	VAL
1	a	185	SER
1	a	223	ILE
1	a	236	LEU
1	c	88	VAL
1	c	104	VAL
1	c	185	SER
1	c	198	SER
1	e	158	LEU
1	e	169	VAL
1	e	225	THR
1	e	236	LEU
1	g	158	LEU
1	g	185	SER
1	g	228	VAL
1	i	104	VAL
1	i	228	VAL
1	i	236	LEU
1	k	236	LEU
1	m	185	SER
1	m	236	LEU
1	o	104	VAL
1	o	169	VAL
1	o	236	LEU
1	q	104	VAL

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Mol	Chain	Res	Type
1	q	169	VAL
1	q	198	SER
1	q	225	THR
1	r	104	VAL
1	r	228	VAL
1	r	236	LEU
1	s	169	VAL
1	s	185	SER
1	s	228	VAL
1	t	198	SER
1	t	225	THR
1	t	228	VAL
1	t	236	LEU
1	u	185	SER
1	u	225	THR
1	u	228	VAL
1	u	236	LEU
1	v	169	VAL
1	v	185	SER
1	v	228	VAL
1	w	158	LEU
1	w	225	THR
1	w	236	LEU
1	x	262	THR
1	y	88	VAL
1	y	104	VAL
1	y	169	VAL
1	y	185	SER
1	y	198	SER
1	z	88	VAL
1	z	104	VAL
1	z	169	VAL
1	z	189	THR
1	0	185	SER
1	0	228	VAL
1	0	236	LEU
1	0	262	THR
1	1	185	SER
1	1	228	VAL
1	1	236	LEU
1	3	104	VAL
1	3	169	VAL

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Mol	Chain	Res	Type
1	3	185	SER
1	3	236	LEU
1	4	185	SER
1	4	236	LEU
1	5	104	VAL
1	5	169	VAL
1	5	173	SER
1	5	194	THR
1	5	225	THR
1	6	236	LEU
1	7	225	THR
1	7	228	VAL
1	7	236	LEU
1	b	158	LEU
1	b	228	VAL
1	d	169	VAL
1	d	185	SER
1	f	185	SER
1	f	236	LEU
1	h	104	VAL
1	h	160	ASN
1	h	225	THR
1	h	236	LEU
1	j	236	LEU
1	l	158	LEU
1	l	225	THR
1	l	228	VAL
1	n	104	VAL
1	p	104	VAL
1	p	158	LEU
1	p	228	VAL
1	p	237	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	257	GLN
1	K	160	ASN
1	M	257	GLN
1	R	222	ASN
1	S	168	GLN
1	Z	156	ASN

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Mol	Chain	Res	Type
1	g	156	ASN
1	i	160	ASN
1	k	79	HIS
1	k	160	ASN
1	m	79	HIS
1	u	222	ASN
1	v	156	ASN
1	z	160	ASN
1	1	168	GLN
1	2	156	ASN
1	3	168	GLN
1	6	222	ASN
1	d	168	GLN
1	f	160	ASN
1	j	79	HIS
1	l	160	ASN
1	n	160	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	o	301	-	4,4,4	0.36	0	6,6,6	0.25	0
2	SO4	s	301	-	4,4,4	0.63	0	6,6,6	0.54	0
2	SO4	M	301	-	4,4,4	0.64	0	6,6,6	0.34	0
2	SO4	7	301	-	4,4,4	0.35	0	6,6,6	0.40	0
2	SO4	w	301	-	4,4,4	0.50	0	6,6,6	0.38	0
2	SO4	A	301	-	4,4,4	0.26	0	6,6,6	0.28	0
2	SO4	X	301	-	4,4,4	0.66	0	6,6,6	0.59	0
2	SO4	H	301	-	4,4,4	0.59	0	6,6,6	0.28	0
2	SO4	h	301	-	4,4,4	0.46	0	6,6,6	0.39	0
2	SO4	Z	301	-	4,4,4	0.50	0	6,6,6	0.46	0
2	SO4	4	301	-	4,4,4	0.22	0	6,6,6	0.41	0
2	SO4	P	301	-	4,4,4	0.35	0	6,6,6	0.28	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.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	o	301	SO4	1	0
2	7	301	SO4	1	0
2	w	301	SO4	1	0
2	X	301	SO4	1	0
2	h	301	SO4	2	0
2	Z	301	SO4	1	0
2	4	301	SO4	2	0
2	P	301	SO4	2	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, 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	0	192/282 (68%)	-0.15	0 100 100	16, 26, 43, 55	0
1	1	192/282 (68%)	0.02	3 (1%) 70 63	19, 29, 47, 57	0
1	2	192/282 (68%)	-0.18	0 100 100	15, 26, 41, 51	0
1	3	194/282 (68%)	0.01	1 (0%) 87 83	17, 27, 43, 57	0
1	4	192/282 (68%)	-0.06	1 (0%) 87 83	17, 30, 53, 69	0
1	5	192/282 (68%)	-0.05	1 (0%) 87 83	20, 30, 51, 61	0
1	6	192/282 (68%)	-0.04	0 100 100	20, 30, 55, 64	0
1	7	192/282 (68%)	-0.04	2 (1%) 79 74	19, 31, 50, 57	0
1	A	192/282 (68%)	-0.13	0 100 100	15, 29, 44, 49	0
1	B	194/282 (68%)	0.02	4 (2%) 63 55	21, 31, 51, 62	0
1	C	192/282 (68%)	-0.01	2 (1%) 79 74	21, 33, 54, 71	0
1	D	192/282 (68%)	-0.06	0 100 100	19, 32, 53, 62	0
1	E	191/282 (67%)	-0.04	0 100 100	22, 30, 49, 60	0
1	F	192/282 (68%)	-0.38	1 (0%) 87 83	10, 20, 38, 48	0
1	G	192/282 (68%)	-0.39	0 100 100	12, 19, 37, 48	0
1	H	193/282 (68%)	-0.29	1 (0%) 87 83	11, 21, 42, 56	0
1	I	192/282 (68%)	-0.37	1 (0%) 87 83	11, 19, 36, 50	0
1	J	193/282 (68%)	-0.39	1 (0%) 87 83	10, 16, 34, 56	0
1	K	192/282 (68%)	-0.29	1 (0%) 87 83	10, 20, 38, 55	0
1	L	192/282 (68%)	-0.46	0 100 100	8, 17, 33, 47	0
1	M	193/282 (68%)	-0.34	1 (0%) 87 83	9, 19, 38, 51	0
1	N	192/282 (68%)	-0.36	0 100 100	11, 20, 39, 53	0
1	O	192/282 (68%)	-0.32	0 100 100	11, 20, 43, 55	0
1	P	192/282 (68%)	-0.08	1 (0%) 87 83	18, 30, 49, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Q	192/282 (68%)	-0.05	0 100 100	20, 33, 54, 62	0
1	R	191/282 (67%)	-0.07	0 100 100	19, 32, 50, 60	0
1	S	191/282 (67%)	-0.01	0 100 100	18, 31, 49, 59	0
1	T	192/282 (68%)	-0.14	1 (0%) 87 83	17, 28, 43, 52	0
1	U	192/282 (68%)	-0.39	0 100 100	11, 21, 38, 49	0
1	V	192/282 (68%)	-0.32	0 100 100	9, 22, 41, 51	0
1	W	192/282 (68%)	-0.30	1 (0%) 87 83	11, 21, 38, 47	0
1	X	194/282 (68%)	-0.33	2 (1%) 79 74	11, 18, 33, 54	0
1	Y	192/282 (68%)	-0.35	0 100 100	12, 19, 36, 42	0
1	Z	192/282 (68%)	-0.16	0 100 100	16, 27, 41, 46	0
1	a	192/282 (68%)	-0.01	0 100 100	18, 29, 56, 66	0
1	b	192/282 (68%)	0.01	2 (1%) 79 74	19, 28, 48, 60	0
1	c	191/282 (67%)	-0.17	0 100 100	18, 29, 49, 54	0
1	d	193/282 (68%)	-0.20	1 (0%) 87 83	12, 26, 41, 48	0
1	e	192/282 (68%)	-0.22	1 (0%) 87 83	14, 25, 42, 53	0
1	f	193/282 (68%)	0.00	1 (0%) 87 83	18, 28, 43, 57	0
1	g	192/282 (68%)	-0.18	1 (0%) 87 83	16, 25, 44, 53	0
1	h	192/282 (68%)	-0.08	0 100 100	17, 27, 45, 60	0
1	i	192/282 (68%)	-0.31	0 100 100	14, 25, 44, 47	0
1	j	194/282 (68%)	-0.25	3 (1%) 72 65	16, 24, 44, 74	0
1	k	193/282 (68%)	-0.15	1 (0%) 87 83	15, 25, 43, 58	0
1	l	192/282 (68%)	-0.22	2 (1%) 79 74	15, 24, 43, 63	0
1	m	193/282 (68%)	-0.15	2 (1%) 79 74	13, 26, 45, 54	0
1	n	192/282 (68%)	-0.17	0 100 100	16, 26, 44, 52	0
1	o	192/282 (68%)	0.02	1 (0%) 87 83	18, 31, 51, 69	0
1	p	192/282 (68%)	-0.01	1 (0%) 87 83	20, 30, 53, 69	0
1	q	193/282 (68%)	-0.05	1 (0%) 87 83	18, 27, 45, 59	0
1	r	192/282 (68%)	-0.31	0 100 100	10, 21, 42, 58	0
1	s	193/282 (68%)	-0.33	0 100 100	10, 20, 36, 51	0
1	t	192/282 (68%)	-0.44	0 100 100	10, 17, 33, 46	0
1	u	192/282 (68%)	-0.36	1 (0%) 87 83	9, 19, 38, 48	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	v	192/282 (68%)	-0.37	0 100 100	11, 19, 36, 45	0
1	w	192/282 (68%)	0.02	1 (0%) 87 83	17, 30, 52, 65	0
1	x	192/282 (68%)	-0.17	0 100 100	19, 28, 48, 53	0
1	y	193/282 (68%)	-0.22	1 (0%) 87 83	15, 25, 44, 51	0
1	z	192/282 (68%)	-0.17	0 100 100	16, 26, 46, 53	0
All	All	11534/16920 (68%)	-0.18	45 (0%) 88 86	8, 26, 46, 74	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	4	219	VAL	3.6
1	j	265	ALA	3.5
1	l	264	SER	3.1
1	f	264	SER	3.0
1	H	181	GLY	3.0
1	q	264	SER	3.0
1	g	72	GLY	2.9
1	b	217	VAL	2.9
1	l	225	THR	2.9
1	o	264	SER	2.7
1	e	184	CYS	2.6
1	j	185	SER	2.5
1	J	265	ALA	2.5
1	M	264	SER	2.5
1	B	183	ARG	2.5
1	T	181	GLY	2.4
1	l	212	ASP	2.4
1	d	264	SER	2.4
1	X	265	ALA	2.3
1	m	225	THR	2.3
1	u	72	GLY	2.3
1	I	184	CYS	2.2
1	j	264	SER	2.2
1	B	265	ALA	2.2
1	w	263	ALA	2.2
1	b	183	ARG	2.2
1	p	219	VAL	2.2
1	m	240	SER	2.2
1	l	183	ARG	2.2
1	F	225	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	k	87	GLY	2.1
1	1	264	SER	2.1
1	7	184	CYS	2.1
1	C	216	ALA	2.1
1	P	183	ARG	2.1
1	W	184	CYS	2.1
1	X	264	SER	2.1
1	5	184	CYS	2.1
1	7	134	SER	2.1
1	y	264	SER	2.1
1	B	264	SER	2.0
1	3	183	ARG	2.0
1	C	263	ALA	2.0
1	B	216	ALA	2.0
1	K	225	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	4	301	5/5	0.98	0.07	13,14,22,22	0
2	SO4	M	301	5/5	0.99	0.05	0,5,8,10	0
2	SO4	P	301	5/5	0.99	0.04	6,17,21,26	0
2	SO4	Z	301	5/5	0.99	0.08	0,11,15,17	0
2	SO4	o	301	5/5	0.99	0.08	7,9,15,20	0
2	SO4	s	301	5/5	0.99	0.05	0,4,7,11	0
2	SO4	w	301	5/5	0.99	0.06	0,12,16,16	0
2	SO4	A	301	5/5	0.99	0.05	8,19,20,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	7	301	5/5	0.99	0.06	5,14,20,21	0
2	SO4	h	301	5/5	0.99	0.07	0,8,13,13	0
2	SO4	X	301	5/5	1.00	0.05	0,5,8,8	0
2	SO4	H	301	5/5	1.00	0.05	0,7,10,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.