



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 2, 2025 – 10:23 AM EDT

PDB ID : 9DJW / pdb_00009djw
Title : X-ray crystal structure of TNFa-VNAR D1 complex
Authors : Ubah, O.C.; Shi, K.; Aihara, H.; Barelle, C.J.; LeBeau, A.M.
Deposited on : 2024-09-06
Resolution : 3.31 Å(reported)

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

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

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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

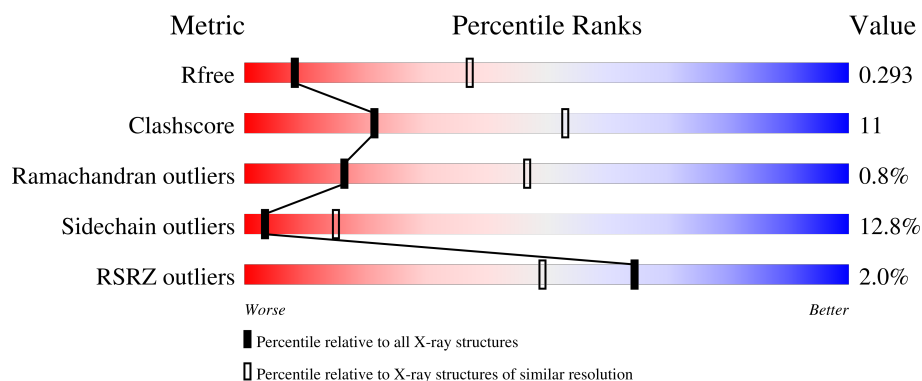
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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}	164625	1066 (3.34-3.30)
Clashscore	180529	1111 (3.34-3.30)
Ramachandran outliers	177936	1109 (3.34-3.30)
Sidechain outliers	177891	1108 (3.34-3.30)
RSRZ outliers	164620	1066 (3.34-3.30)

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	129	<div> <div>2%</div> <div>49% 29% 5% 17%</div> </div>
1	1	129	<div> <div>2%</div> <div>48% 29% 19%</div> </div>
1	5	129	<div> <div>53% 26% 5% 16%</div> </div>
1	6	129	<div> <div>47% 29% 7% 17%</div> </div>
1	7	129	<div> <div>2%</div> <div>43% 32% 8% 17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	D	129	
1	E	129	
1	F	129	
1	J	129	
1	K	129	
1	L	129	
1	P	129	
1	Q	129	
1	R	129	
1	V	129	
1	W	129	
1	X	129	
1	b	129	
1	c	129	
1	d	129	
1	h	129	
1	i	129	
1	j	129	
1	n	129	
1	o	129	
1	p	129	
1	t	129	
1	u	129	
1	v	129	
1	z	129	

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Mol	Chain	Length	Quality of chain
2	2	156	
2	3	156	
2	4	156	
2	A	156	
2	B	156	
2	C	156	
2	G	156	
2	H	156	
2	I	156	
2	M	156	
2	N	156	
2	O	156	
2	S	156	
2	T	156	
2	U	156	
2	Y	156	
2	Z	156	
2	a	156	
2	e	156	
2	f	156	
2	g	156	
2	k	156	
2	l	156	
2	m	156	
2	q	156	

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Mol	Chain	Length	Quality of chain
2	r	156	<div><div><div>%</div><div><div></div><div>75%</div><div>21%</div><div></div></div><div><div></div><div></div><div>• •</div></div></div></div>
2	s	156	<div><div><div>%</div><div><div></div><div>68%</div><div>27%</div><div></div></div><div><div></div><div></div><div>• •</div></div></div></div>
2	w	156	<div><div><div>%</div><div><div></div><div>72%</div><div>24%</div><div></div></div><div><div></div><div></div><div>•</div></div></div></div>
2	x	156	<div><div><div>3%</div><div><div></div><div>75%</div><div>22%</div><div></div></div><div><div></div><div></div><div>• •</div></div></div></div>
2	y	156	<div><div><div>%</div><div><div></div><div>69%</div><div>26%</div><div></div></div><div><div></div><div></div><div>• •</div></div></div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 60848 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 Antigen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	107	Total	C	N	O	S	0	0	0
			815	495	141	175	4			
1	1	104	Total	C	N	O	S	0	0	0
			797	485	137	171	4			
1	5	108	Total	C	N	O	S	0	0	0
			820	498	142	176	4			
1	6	107	Total	C	N	O	S	0	0	0
			815	495	141	175	4			
1	7	107	Total	C	N	O	S	0	0	0
			815	495	141	175	4			
1	D	106	Total	C	N	O	S	0	0	0
			810	492	140	174	4			
1	E	108	Total	C	N	O	S	0	0	0
			820	498	142	176	4			
1	F	106	Total	C	N	O	S	0	0	0
			810	492	140	174	4			
1	J	108	Total	C	N	O	S	0	0	0
			820	498	142	176	4			
1	K	106	Total	C	N	O	S	0	0	0
			810	492	140	174	4			
1	L	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	P	107	Total	C	N	O	S	0	0	0
			815	495	141	175	4			
1	Q	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	R	107	Total	C	N	O	S	0	0	0
			815	495	141	175	4			
1	V	106	Total	C	N	O	S	0	1	0
			821	498	144	175	4			
1	W	106	Total	C	N	O	S	0	0	0
			810	492	140	174	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	107	Total	C	N	O	S	0	0	0
			815	495	141	175	4			
1	b	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	c	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	d	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	h	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	i	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	j	105	Total	C	N	O	S	0	0	0
			802	488	138	172	4			
1	n	109	Total	C	N	O	S	0	0	0
			825	501	143	177	4			
1	o	104	Total	C	N	O	S	0	0	0
			797	485	137	171	4			
1	p	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	t	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	u	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			
1	v	105	Total	C	N	O	S	0	0	0
			802	488	138	172	4			
1	z	112	Total	C	N	O	S	0	0	0
			855	519	152	180	4			

There are 990 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	28	HIS	ASN	conflict	UNP Q8JGJ1
0	31	THR	LEU	conflict	UNP Q8JGJ1
0	?	-	ASN	deletion	UNP Q8JGJ1
0	?	-	VAL	deletion	UNP Q8JGJ1
0	84	ALA	TYR	conflict	UNP Q8JGJ1
0	86	GLU	TRP	conflict	UNP Q8JGJ1
0	87	CYS	TYR	conflict	UNP Q8JGJ1
0	88	GLN	GLY	conflict	UNP Q8JGJ1
0	90	GLY	ASP	conflict	UNP Q8JGJ1
0	91	LEU	CYS	conflict	UNP Q8JGJ1
0	94	TYR	LEU	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
0	107	ALA	-	expression tag	UNP Q8JGJ1
0	108	ALA	-	expression tag	UNP Q8JGJ1
0	109	ALA	-	expression tag	UNP Q8JGJ1
0	110	HIS	-	expression tag	UNP Q8JGJ1
0	111	HIS	-	expression tag	UNP Q8JGJ1
0	112	HIS	-	expression tag	UNP Q8JGJ1
0	113	HIS	-	expression tag	UNP Q8JGJ1
0	114	HIS	-	expression tag	UNP Q8JGJ1
0	115	HIS	-	expression tag	UNP Q8JGJ1
0	116	GLY	-	expression tag	UNP Q8JGJ1
0	117	ALA	-	expression tag	UNP Q8JGJ1
0	118	ALA	-	expression tag	UNP Q8JGJ1
0	119	GLU	-	expression tag	UNP Q8JGJ1
0	120	SER	-	expression tag	UNP Q8JGJ1
0	121	LYS	-	expression tag	UNP Q8JGJ1
0	122	LEU	-	expression tag	UNP Q8JGJ1
0	123	ILE	-	expression tag	UNP Q8JGJ1
0	124	SER	-	expression tag	UNP Q8JGJ1
0	125	GLU	-	expression tag	UNP Q8JGJ1
0	126	GLU	-	expression tag	UNP Q8JGJ1
0	127	ASP	-	expression tag	UNP Q8JGJ1
0	128	LEU	-	expression tag	UNP Q8JGJ1
1	28	HIS	ASN	conflict	UNP Q8JGJ1
1	31	THR	LEU	conflict	UNP Q8JGJ1
1	?	-	ASN	deletion	UNP Q8JGJ1
1	?	-	VAL	deletion	UNP Q8JGJ1
1	84	ALA	TYR	conflict	UNP Q8JGJ1
1	86	GLU	TRP	conflict	UNP Q8JGJ1
1	87	CYS	TYR	conflict	UNP Q8JGJ1
1	88	GLN	GLY	conflict	UNP Q8JGJ1
1	90	GLY	ASP	conflict	UNP Q8JGJ1
1	91	LEU	CYS	conflict	UNP Q8JGJ1
1	94	TYR	LEU	conflict	UNP Q8JGJ1
1	107	ALA	-	expression tag	UNP Q8JGJ1
1	108	ALA	-	expression tag	UNP Q8JGJ1
1	109	ALA	-	expression tag	UNP Q8JGJ1
1	110	HIS	-	expression tag	UNP Q8JGJ1
1	111	HIS	-	expression tag	UNP Q8JGJ1
1	112	HIS	-	expression tag	UNP Q8JGJ1
1	113	HIS	-	expression tag	UNP Q8JGJ1
1	114	HIS	-	expression tag	UNP Q8JGJ1
1	115	HIS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
1	116	GLY	-	expression tag	UNP Q8JGJ1
1	117	ALA	-	expression tag	UNP Q8JGJ1
1	118	ALA	-	expression tag	UNP Q8JGJ1
1	119	GLU	-	expression tag	UNP Q8JGJ1
1	120	SER	-	expression tag	UNP Q8JGJ1
1	121	LYS	-	expression tag	UNP Q8JGJ1
1	122	LEU	-	expression tag	UNP Q8JGJ1
1	123	ILE	-	expression tag	UNP Q8JGJ1
1	124	SER	-	expression tag	UNP Q8JGJ1
1	125	GLU	-	expression tag	UNP Q8JGJ1
1	126	GLU	-	expression tag	UNP Q8JGJ1
1	127	ASP	-	expression tag	UNP Q8JGJ1
1	128	LEU	-	expression tag	UNP Q8JGJ1
5	28	HIS	ASN	conflict	UNP Q8JGJ1
5	31	THR	LEU	conflict	UNP Q8JGJ1
5	?	-	ASN	deletion	UNP Q8JGJ1
5	?	-	VAL	deletion	UNP Q8JGJ1
5	84	ALA	TYR	conflict	UNP Q8JGJ1
5	86	GLU	TRP	conflict	UNP Q8JGJ1
5	87	CYS	TYR	conflict	UNP Q8JGJ1
5	88	GLN	GLY	conflict	UNP Q8JGJ1
5	90	GLY	ASP	conflict	UNP Q8JGJ1
5	91	LEU	CYS	conflict	UNP Q8JGJ1
5	94	TYR	LEU	conflict	UNP Q8JGJ1
5	107	ALA	-	expression tag	UNP Q8JGJ1
5	108	ALA	-	expression tag	UNP Q8JGJ1
5	109	ALA	-	expression tag	UNP Q8JGJ1
5	110	HIS	-	expression tag	UNP Q8JGJ1
5	111	HIS	-	expression tag	UNP Q8JGJ1
5	112	HIS	-	expression tag	UNP Q8JGJ1
5	113	HIS	-	expression tag	UNP Q8JGJ1
5	114	HIS	-	expression tag	UNP Q8JGJ1
5	115	HIS	-	expression tag	UNP Q8JGJ1
5	116	GLY	-	expression tag	UNP Q8JGJ1
5	117	ALA	-	expression tag	UNP Q8JGJ1
5	118	ALA	-	expression tag	UNP Q8JGJ1
5	119	GLU	-	expression tag	UNP Q8JGJ1
5	120	SER	-	expression tag	UNP Q8JGJ1
5	121	LYS	-	expression tag	UNP Q8JGJ1
5	122	LEU	-	expression tag	UNP Q8JGJ1
5	123	ILE	-	expression tag	UNP Q8JGJ1
5	124	SER	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
5	125	GLU	-	expression tag	UNP Q8JGJ1
5	126	GLU	-	expression tag	UNP Q8JGJ1
5	127	ASP	-	expression tag	UNP Q8JGJ1
5	128	LEU	-	expression tag	UNP Q8JGJ1
6	28	HIS	ASN	conflict	UNP Q8JGJ1
6	31	THR	LEU	conflict	UNP Q8JGJ1
6	?	-	ASN	deletion	UNP Q8JGJ1
6	?	-	VAL	deletion	UNP Q8JGJ1
6	84	ALA	TYR	conflict	UNP Q8JGJ1
6	86	GLU	TRP	conflict	UNP Q8JGJ1
6	87	CYS	TYR	conflict	UNP Q8JGJ1
6	88	GLN	GLY	conflict	UNP Q8JGJ1
6	90	GLY	ASP	conflict	UNP Q8JGJ1
6	91	LEU	CYS	conflict	UNP Q8JGJ1
6	94	TYR	LEU	conflict	UNP Q8JGJ1
6	107	ALA	-	expression tag	UNP Q8JGJ1
6	108	ALA	-	expression tag	UNP Q8JGJ1
6	109	ALA	-	expression tag	UNP Q8JGJ1
6	110	HIS	-	expression tag	UNP Q8JGJ1
6	111	HIS	-	expression tag	UNP Q8JGJ1
6	112	HIS	-	expression tag	UNP Q8JGJ1
6	113	HIS	-	expression tag	UNP Q8JGJ1
6	114	HIS	-	expression tag	UNP Q8JGJ1
6	115	HIS	-	expression tag	UNP Q8JGJ1
6	116	GLY	-	expression tag	UNP Q8JGJ1
6	117	ALA	-	expression tag	UNP Q8JGJ1
6	118	ALA	-	expression tag	UNP Q8JGJ1
6	119	GLU	-	expression tag	UNP Q8JGJ1
6	120	SER	-	expression tag	UNP Q8JGJ1
6	121	LYS	-	expression tag	UNP Q8JGJ1
6	122	LEU	-	expression tag	UNP Q8JGJ1
6	123	ILE	-	expression tag	UNP Q8JGJ1
6	124	SER	-	expression tag	UNP Q8JGJ1
6	125	GLU	-	expression tag	UNP Q8JGJ1
6	126	GLU	-	expression tag	UNP Q8JGJ1
6	127	ASP	-	expression tag	UNP Q8JGJ1
6	128	LEU	-	expression tag	UNP Q8JGJ1
7	28	HIS	ASN	conflict	UNP Q8JGJ1
7	31	THR	LEU	conflict	UNP Q8JGJ1
7	?	-	ASN	deletion	UNP Q8JGJ1
7	?	-	VAL	deletion	UNP Q8JGJ1
7	84	ALA	TYR	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
7	86	GLU	TRP	conflict	UNP Q8JGJ1
7	87	CYS	TYR	conflict	UNP Q8JGJ1
7	88	GLN	GLY	conflict	UNP Q8JGJ1
7	90	GLY	ASP	conflict	UNP Q8JGJ1
7	91	LEU	CYS	conflict	UNP Q8JGJ1
7	94	TYR	LEU	conflict	UNP Q8JGJ1
7	107	ALA	-	expression tag	UNP Q8JGJ1
7	108	ALA	-	expression tag	UNP Q8JGJ1
7	109	ALA	-	expression tag	UNP Q8JGJ1
7	110	HIS	-	expression tag	UNP Q8JGJ1
7	111	HIS	-	expression tag	UNP Q8JGJ1
7	112	HIS	-	expression tag	UNP Q8JGJ1
7	113	HIS	-	expression tag	UNP Q8JGJ1
7	114	HIS	-	expression tag	UNP Q8JGJ1
7	115	HIS	-	expression tag	UNP Q8JGJ1
7	116	GLY	-	expression tag	UNP Q8JGJ1
7	117	ALA	-	expression tag	UNP Q8JGJ1
7	118	ALA	-	expression tag	UNP Q8JGJ1
7	119	GLU	-	expression tag	UNP Q8JGJ1
7	120	SER	-	expression tag	UNP Q8JGJ1
7	121	LYS	-	expression tag	UNP Q8JGJ1
7	122	LEU	-	expression tag	UNP Q8JGJ1
7	123	ILE	-	expression tag	UNP Q8JGJ1
7	124	SER	-	expression tag	UNP Q8JGJ1
7	125	GLU	-	expression tag	UNP Q8JGJ1
7	126	GLU	-	expression tag	UNP Q8JGJ1
7	127	ASP	-	expression tag	UNP Q8JGJ1
7	128	LEU	-	expression tag	UNP Q8JGJ1
D	28	HIS	ASN	conflict	UNP Q8JGJ1
D	31	THR	LEU	conflict	UNP Q8JGJ1
D	?	-	ASN	deletion	UNP Q8JGJ1
D	?	-	VAL	deletion	UNP Q8JGJ1
D	84	ALA	TYR	conflict	UNP Q8JGJ1
D	86	GLU	TRP	conflict	UNP Q8JGJ1
D	87	CYS	TYR	conflict	UNP Q8JGJ1
D	88	GLN	GLY	conflict	UNP Q8JGJ1
D	90	GLY	ASP	conflict	UNP Q8JGJ1
D	91	LEU	CYS	conflict	UNP Q8JGJ1
D	94	TYR	LEU	conflict	UNP Q8JGJ1
D	107	ALA	-	expression tag	UNP Q8JGJ1
D	108	ALA	-	expression tag	UNP Q8JGJ1
D	109	ALA	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	110	HIS	-	expression tag	UNP Q8JGJ1
D	111	HIS	-	expression tag	UNP Q8JGJ1
D	112	HIS	-	expression tag	UNP Q8JGJ1
D	113	HIS	-	expression tag	UNP Q8JGJ1
D	114	HIS	-	expression tag	UNP Q8JGJ1
D	115	HIS	-	expression tag	UNP Q8JGJ1
D	116	GLY	-	expression tag	UNP Q8JGJ1
D	117	ALA	-	expression tag	UNP Q8JGJ1
D	118	ALA	-	expression tag	UNP Q8JGJ1
D	119	GLU	-	expression tag	UNP Q8JGJ1
D	120	SER	-	expression tag	UNP Q8JGJ1
D	121	LYS	-	expression tag	UNP Q8JGJ1
D	122	LEU	-	expression tag	UNP Q8JGJ1
D	123	ILE	-	expression tag	UNP Q8JGJ1
D	124	SER	-	expression tag	UNP Q8JGJ1
D	125	GLU	-	expression tag	UNP Q8JGJ1
D	126	GLU	-	expression tag	UNP Q8JGJ1
D	127	ASP	-	expression tag	UNP Q8JGJ1
D	128	LEU	-	expression tag	UNP Q8JGJ1
E	28	HIS	ASN	conflict	UNP Q8JGJ1
E	31	THR	LEU	conflict	UNP Q8JGJ1
E	?	-	ASN	deletion	UNP Q8JGJ1
E	?	-	VAL	deletion	UNP Q8JGJ1
E	84	ALA	TYR	conflict	UNP Q8JGJ1
E	86	GLU	TRP	conflict	UNP Q8JGJ1
E	87	CYS	TYR	conflict	UNP Q8JGJ1
E	88	GLN	GLY	conflict	UNP Q8JGJ1
E	90	GLY	ASP	conflict	UNP Q8JGJ1
E	91	LEU	CYS	conflict	UNP Q8JGJ1
E	94	TYR	LEU	conflict	UNP Q8JGJ1
E	107	ALA	-	expression tag	UNP Q8JGJ1
E	108	ALA	-	expression tag	UNP Q8JGJ1
E	109	ALA	-	expression tag	UNP Q8JGJ1
E	110	HIS	-	expression tag	UNP Q8JGJ1
E	111	HIS	-	expression tag	UNP Q8JGJ1
E	112	HIS	-	expression tag	UNP Q8JGJ1
E	113	HIS	-	expression tag	UNP Q8JGJ1
E	114	HIS	-	expression tag	UNP Q8JGJ1
E	115	HIS	-	expression tag	UNP Q8JGJ1
E	116	GLY	-	expression tag	UNP Q8JGJ1
E	117	ALA	-	expression tag	UNP Q8JGJ1
E	118	ALA	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	119	GLU	-	expression tag	UNP Q8JGJ1
E	120	SER	-	expression tag	UNP Q8JGJ1
E	121	LYS	-	expression tag	UNP Q8JGJ1
E	122	LEU	-	expression tag	UNP Q8JGJ1
E	123	ILE	-	expression tag	UNP Q8JGJ1
E	124	SER	-	expression tag	UNP Q8JGJ1
E	125	GLU	-	expression tag	UNP Q8JGJ1
E	126	GLU	-	expression tag	UNP Q8JGJ1
E	127	ASP	-	expression tag	UNP Q8JGJ1
E	128	LEU	-	expression tag	UNP Q8JGJ1
F	28	HIS	ASN	conflict	UNP Q8JGJ1
F	31	THR	LEU	conflict	UNP Q8JGJ1
F	?	-	ASN	deletion	UNP Q8JGJ1
F	?	-	VAL	deletion	UNP Q8JGJ1
F	84	ALA	TYR	conflict	UNP Q8JGJ1
F	86	GLU	TRP	conflict	UNP Q8JGJ1
F	87	CYS	TYR	conflict	UNP Q8JGJ1
F	88	GLN	GLY	conflict	UNP Q8JGJ1
F	90	GLY	ASP	conflict	UNP Q8JGJ1
F	91	LEU	CYS	conflict	UNP Q8JGJ1
F	94	TYR	LEU	conflict	UNP Q8JGJ1
F	107	ALA	-	expression tag	UNP Q8JGJ1
F	108	ALA	-	expression tag	UNP Q8JGJ1
F	109	ALA	-	expression tag	UNP Q8JGJ1
F	110	HIS	-	expression tag	UNP Q8JGJ1
F	111	HIS	-	expression tag	UNP Q8JGJ1
F	112	HIS	-	expression tag	UNP Q8JGJ1
F	113	HIS	-	expression tag	UNP Q8JGJ1
F	114	HIS	-	expression tag	UNP Q8JGJ1
F	115	HIS	-	expression tag	UNP Q8JGJ1
F	116	GLY	-	expression tag	UNP Q8JGJ1
F	117	ALA	-	expression tag	UNP Q8JGJ1
F	118	ALA	-	expression tag	UNP Q8JGJ1
F	119	GLU	-	expression tag	UNP Q8JGJ1
F	120	SER	-	expression tag	UNP Q8JGJ1
F	121	LYS	-	expression tag	UNP Q8JGJ1
F	122	LEU	-	expression tag	UNP Q8JGJ1
F	123	ILE	-	expression tag	UNP Q8JGJ1
F	124	SER	-	expression tag	UNP Q8JGJ1
F	125	GLU	-	expression tag	UNP Q8JGJ1
F	126	GLU	-	expression tag	UNP Q8JGJ1
F	127	ASP	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	128	LEU	-	expression tag	UNP Q8JGJ1
J	28	HIS	ASN	conflict	UNP Q8JGJ1
J	31	THR	LEU	conflict	UNP Q8JGJ1
J	?	-	ASN	deletion	UNP Q8JGJ1
J	?	-	VAL	deletion	UNP Q8JGJ1
J	84	ALA	TYR	conflict	UNP Q8JGJ1
J	86	GLU	TRP	conflict	UNP Q8JGJ1
J	87	CYS	TYR	conflict	UNP Q8JGJ1
J	88	GLN	GLY	conflict	UNP Q8JGJ1
J	90	GLY	ASP	conflict	UNP Q8JGJ1
J	91	LEU	CYS	conflict	UNP Q8JGJ1
J	94	TYR	LEU	conflict	UNP Q8JGJ1
J	107	ALA	-	expression tag	UNP Q8JGJ1
J	108	ALA	-	expression tag	UNP Q8JGJ1
J	109	ALA	-	expression tag	UNP Q8JGJ1
J	110	HIS	-	expression tag	UNP Q8JGJ1
J	111	HIS	-	expression tag	UNP Q8JGJ1
J	112	HIS	-	expression tag	UNP Q8JGJ1
J	113	HIS	-	expression tag	UNP Q8JGJ1
J	114	HIS	-	expression tag	UNP Q8JGJ1
J	115	HIS	-	expression tag	UNP Q8JGJ1
J	116	GLY	-	expression tag	UNP Q8JGJ1
J	117	ALA	-	expression tag	UNP Q8JGJ1
J	118	ALA	-	expression tag	UNP Q8JGJ1
J	119	GLU	-	expression tag	UNP Q8JGJ1
J	120	SER	-	expression tag	UNP Q8JGJ1
J	121	LYS	-	expression tag	UNP Q8JGJ1
J	122	LEU	-	expression tag	UNP Q8JGJ1
J	123	ILE	-	expression tag	UNP Q8JGJ1
J	124	SER	-	expression tag	UNP Q8JGJ1
J	125	GLU	-	expression tag	UNP Q8JGJ1
J	126	GLU	-	expression tag	UNP Q8JGJ1
J	127	ASP	-	expression tag	UNP Q8JGJ1
J	128	LEU	-	expression tag	UNP Q8JGJ1
K	28	HIS	ASN	conflict	UNP Q8JGJ1
K	31	THR	LEU	conflict	UNP Q8JGJ1
K	?	-	ASN	deletion	UNP Q8JGJ1
K	?	-	VAL	deletion	UNP Q8JGJ1
K	84	ALA	TYR	conflict	UNP Q8JGJ1
K	86	GLU	TRP	conflict	UNP Q8JGJ1
K	87	CYS	TYR	conflict	UNP Q8JGJ1
K	88	GLN	GLY	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	90	GLY	ASP	conflict	UNP Q8JGJ1
K	91	LEU	CYS	conflict	UNP Q8JGJ1
K	94	TYR	LEU	conflict	UNP Q8JGJ1
K	107	ALA	-	expression tag	UNP Q8JGJ1
K	108	ALA	-	expression tag	UNP Q8JGJ1
K	109	ALA	-	expression tag	UNP Q8JGJ1
K	110	HIS	-	expression tag	UNP Q8JGJ1
K	111	HIS	-	expression tag	UNP Q8JGJ1
K	112	HIS	-	expression tag	UNP Q8JGJ1
K	113	HIS	-	expression tag	UNP Q8JGJ1
K	114	HIS	-	expression tag	UNP Q8JGJ1
K	115	HIS	-	expression tag	UNP Q8JGJ1
K	116	GLY	-	expression tag	UNP Q8JGJ1
K	117	ALA	-	expression tag	UNP Q8JGJ1
K	118	ALA	-	expression tag	UNP Q8JGJ1
K	119	GLU	-	expression tag	UNP Q8JGJ1
K	120	SER	-	expression tag	UNP Q8JGJ1
K	121	LYS	-	expression tag	UNP Q8JGJ1
K	122	LEU	-	expression tag	UNP Q8JGJ1
K	123	ILE	-	expression tag	UNP Q8JGJ1
K	124	SER	-	expression tag	UNP Q8JGJ1
K	125	GLU	-	expression tag	UNP Q8JGJ1
K	126	GLU	-	expression tag	UNP Q8JGJ1
K	127	ASP	-	expression tag	UNP Q8JGJ1
K	128	LEU	-	expression tag	UNP Q8JGJ1
L	28	HIS	ASN	conflict	UNP Q8JGJ1
L	31	THR	LEU	conflict	UNP Q8JGJ1
L	?	-	ASN	deletion	UNP Q8JGJ1
L	?	-	VAL	deletion	UNP Q8JGJ1
L	84	ALA	TYR	conflict	UNP Q8JGJ1
L	86	GLU	TRP	conflict	UNP Q8JGJ1
L	87	CYS	TYR	conflict	UNP Q8JGJ1
L	88	GLN	GLY	conflict	UNP Q8JGJ1
L	90	GLY	ASP	conflict	UNP Q8JGJ1
L	91	LEU	CYS	conflict	UNP Q8JGJ1
L	94	TYR	LEU	conflict	UNP Q8JGJ1
L	107	ALA	-	expression tag	UNP Q8JGJ1
L	108	ALA	-	expression tag	UNP Q8JGJ1
L	109	ALA	-	expression tag	UNP Q8JGJ1
L	110	HIS	-	expression tag	UNP Q8JGJ1
L	111	HIS	-	expression tag	UNP Q8JGJ1
L	112	HIS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
L	113	HIS	-	expression tag	UNP Q8JGJ1
L	114	HIS	-	expression tag	UNP Q8JGJ1
L	115	HIS	-	expression tag	UNP Q8JGJ1
L	116	GLY	-	expression tag	UNP Q8JGJ1
L	117	ALA	-	expression tag	UNP Q8JGJ1
L	118	ALA	-	expression tag	UNP Q8JGJ1
L	119	GLU	-	expression tag	UNP Q8JGJ1
L	120	SER	-	expression tag	UNP Q8JGJ1
L	121	LYS	-	expression tag	UNP Q8JGJ1
L	122	LEU	-	expression tag	UNP Q8JGJ1
L	123	ILE	-	expression tag	UNP Q8JGJ1
L	124	SER	-	expression tag	UNP Q8JGJ1
L	125	GLU	-	expression tag	UNP Q8JGJ1
L	126	GLU	-	expression tag	UNP Q8JGJ1
L	127	ASP	-	expression tag	UNP Q8JGJ1
L	128	LEU	-	expression tag	UNP Q8JGJ1
P	28	HIS	ASN	conflict	UNP Q8JGJ1
P	31	THR	LEU	conflict	UNP Q8JGJ1
P	?	-	ASN	deletion	UNP Q8JGJ1
P	?	-	VAL	deletion	UNP Q8JGJ1
P	84	ALA	TYR	conflict	UNP Q8JGJ1
P	86	GLU	TRP	conflict	UNP Q8JGJ1
P	87	CYS	TYR	conflict	UNP Q8JGJ1
P	88	GLN	GLY	conflict	UNP Q8JGJ1
P	90	GLY	ASP	conflict	UNP Q8JGJ1
P	91	LEU	CYS	conflict	UNP Q8JGJ1
P	94	TYR	LEU	conflict	UNP Q8JGJ1
P	107	ALA	-	expression tag	UNP Q8JGJ1
P	108	ALA	-	expression tag	UNP Q8JGJ1
P	109	ALA	-	expression tag	UNP Q8JGJ1
P	110	HIS	-	expression tag	UNP Q8JGJ1
P	111	HIS	-	expression tag	UNP Q8JGJ1
P	112	HIS	-	expression tag	UNP Q8JGJ1
P	113	HIS	-	expression tag	UNP Q8JGJ1
P	114	HIS	-	expression tag	UNP Q8JGJ1
P	115	HIS	-	expression tag	UNP Q8JGJ1
P	116	GLY	-	expression tag	UNP Q8JGJ1
P	117	ALA	-	expression tag	UNP Q8JGJ1
P	118	ALA	-	expression tag	UNP Q8JGJ1
P	119	GLU	-	expression tag	UNP Q8JGJ1
P	120	SER	-	expression tag	UNP Q8JGJ1
P	121	LYS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
P	122	LEU	-	expression tag	UNP Q8JGJ1
P	123	ILE	-	expression tag	UNP Q8JGJ1
P	124	SER	-	expression tag	UNP Q8JGJ1
P	125	GLU	-	expression tag	UNP Q8JGJ1
P	126	GLU	-	expression tag	UNP Q8JGJ1
P	127	ASP	-	expression tag	UNP Q8JGJ1
P	128	LEU	-	expression tag	UNP Q8JGJ1
Q	28	HIS	ASN	conflict	UNP Q8JGJ1
Q	31	THR	LEU	conflict	UNP Q8JGJ1
Q	?	-	ASN	deletion	UNP Q8JGJ1
Q	?	-	VAL	deletion	UNP Q8JGJ1
Q	84	ALA	TYR	conflict	UNP Q8JGJ1
Q	86	GLU	TRP	conflict	UNP Q8JGJ1
Q	87	CYS	TYR	conflict	UNP Q8JGJ1
Q	88	GLN	GLY	conflict	UNP Q8JGJ1
Q	90	GLY	ASP	conflict	UNP Q8JGJ1
Q	91	LEU	CYS	conflict	UNP Q8JGJ1
Q	94	TYR	LEU	conflict	UNP Q8JGJ1
Q	107	ALA	-	expression tag	UNP Q8JGJ1
Q	108	ALA	-	expression tag	UNP Q8JGJ1
Q	109	ALA	-	expression tag	UNP Q8JGJ1
Q	110	HIS	-	expression tag	UNP Q8JGJ1
Q	111	HIS	-	expression tag	UNP Q8JGJ1
Q	112	HIS	-	expression tag	UNP Q8JGJ1
Q	113	HIS	-	expression tag	UNP Q8JGJ1
Q	114	HIS	-	expression tag	UNP Q8JGJ1
Q	115	HIS	-	expression tag	UNP Q8JGJ1
Q	116	GLY	-	expression tag	UNP Q8JGJ1
Q	117	ALA	-	expression tag	UNP Q8JGJ1
Q	118	ALA	-	expression tag	UNP Q8JGJ1
Q	119	GLU	-	expression tag	UNP Q8JGJ1
Q	120	SER	-	expression tag	UNP Q8JGJ1
Q	121	LYS	-	expression tag	UNP Q8JGJ1
Q	122	LEU	-	expression tag	UNP Q8JGJ1
Q	123	ILE	-	expression tag	UNP Q8JGJ1
Q	124	SER	-	expression tag	UNP Q8JGJ1
Q	125	GLU	-	expression tag	UNP Q8JGJ1
Q	126	GLU	-	expression tag	UNP Q8JGJ1
Q	127	ASP	-	expression tag	UNP Q8JGJ1
Q	128	LEU	-	expression tag	UNP Q8JGJ1
R	28	HIS	ASN	conflict	UNP Q8JGJ1
R	31	THR	LEU	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	ASN	deletion	UNP Q8JGJ1
R	?	-	VAL	deletion	UNP Q8JGJ1
R	84	ALA	TYR	conflict	UNP Q8JGJ1
R	86	GLU	TRP	conflict	UNP Q8JGJ1
R	87	CYS	TYR	conflict	UNP Q8JGJ1
R	88	GLN	GLY	conflict	UNP Q8JGJ1
R	90	GLY	ASP	conflict	UNP Q8JGJ1
R	91	LEU	CYS	conflict	UNP Q8JGJ1
R	94	TYR	LEU	conflict	UNP Q8JGJ1
R	107	ALA	-	expression tag	UNP Q8JGJ1
R	108	ALA	-	expression tag	UNP Q8JGJ1
R	109	ALA	-	expression tag	UNP Q8JGJ1
R	110	HIS	-	expression tag	UNP Q8JGJ1
R	111	HIS	-	expression tag	UNP Q8JGJ1
R	112	HIS	-	expression tag	UNP Q8JGJ1
R	113	HIS	-	expression tag	UNP Q8JGJ1
R	114	HIS	-	expression tag	UNP Q8JGJ1
R	115	HIS	-	expression tag	UNP Q8JGJ1
R	116	GLY	-	expression tag	UNP Q8JGJ1
R	117	ALA	-	expression tag	UNP Q8JGJ1
R	118	ALA	-	expression tag	UNP Q8JGJ1
R	119	GLU	-	expression tag	UNP Q8JGJ1
R	120	SER	-	expression tag	UNP Q8JGJ1
R	121	LYS	-	expression tag	UNP Q8JGJ1
R	122	LEU	-	expression tag	UNP Q8JGJ1
R	123	ILE	-	expression tag	UNP Q8JGJ1
R	124	SER	-	expression tag	UNP Q8JGJ1
R	125	GLU	-	expression tag	UNP Q8JGJ1
R	126	GLU	-	expression tag	UNP Q8JGJ1
R	127	ASP	-	expression tag	UNP Q8JGJ1
R	128	LEU	-	expression tag	UNP Q8JGJ1
V	28	HIS	ASN	conflict	UNP Q8JGJ1
V	31	THR	LEU	conflict	UNP Q8JGJ1
V	?	-	ASN	deletion	UNP Q8JGJ1
V	?	-	VAL	deletion	UNP Q8JGJ1
V	84	ALA	TYR	conflict	UNP Q8JGJ1
V	86	GLU	TRP	conflict	UNP Q8JGJ1
V	87	CYS	TYR	conflict	UNP Q8JGJ1
V	88	GLN	GLY	conflict	UNP Q8JGJ1
V	90	GLY	ASP	conflict	UNP Q8JGJ1
V	91	LEU	CYS	conflict	UNP Q8JGJ1
V	94	TYR	LEU	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
V	107	ALA	-	expression tag	UNP Q8JGJ1
V	108	ALA	-	expression tag	UNP Q8JGJ1
V	109	ALA	-	expression tag	UNP Q8JGJ1
V	110	HIS	-	expression tag	UNP Q8JGJ1
V	111	HIS	-	expression tag	UNP Q8JGJ1
V	112	HIS	-	expression tag	UNP Q8JGJ1
V	113	HIS	-	expression tag	UNP Q8JGJ1
V	114	HIS	-	expression tag	UNP Q8JGJ1
V	115	HIS	-	expression tag	UNP Q8JGJ1
V	116	GLY	-	expression tag	UNP Q8JGJ1
V	117	ALA	-	expression tag	UNP Q8JGJ1
V	118	ALA	-	expression tag	UNP Q8JGJ1
V	119	GLU	-	expression tag	UNP Q8JGJ1
V	120	SER	-	expression tag	UNP Q8JGJ1
V	121	LYS	-	expression tag	UNP Q8JGJ1
V	122	LEU	-	expression tag	UNP Q8JGJ1
V	123	ILE	-	expression tag	UNP Q8JGJ1
V	124	SER	-	expression tag	UNP Q8JGJ1
V	125	GLU	-	expression tag	UNP Q8JGJ1
V	126	GLU	-	expression tag	UNP Q8JGJ1
V	127	ASP	-	expression tag	UNP Q8JGJ1
V	128	LEU	-	expression tag	UNP Q8JGJ1
W	28	HIS	ASN	conflict	UNP Q8JGJ1
W	31	THR	LEU	conflict	UNP Q8JGJ1
W	?	-	ASN	deletion	UNP Q8JGJ1
W	?	-	VAL	deletion	UNP Q8JGJ1
W	84	ALA	TYR	conflict	UNP Q8JGJ1
W	86	GLU	TRP	conflict	UNP Q8JGJ1
W	87	CYS	TYR	conflict	UNP Q8JGJ1
W	88	GLN	GLY	conflict	UNP Q8JGJ1
W	90	GLY	ASP	conflict	UNP Q8JGJ1
W	91	LEU	CYS	conflict	UNP Q8JGJ1
W	94	TYR	LEU	conflict	UNP Q8JGJ1
W	107	ALA	-	expression tag	UNP Q8JGJ1
W	108	ALA	-	expression tag	UNP Q8JGJ1
W	109	ALA	-	expression tag	UNP Q8JGJ1
W	110	HIS	-	expression tag	UNP Q8JGJ1
W	111	HIS	-	expression tag	UNP Q8JGJ1
W	112	HIS	-	expression tag	UNP Q8JGJ1
W	113	HIS	-	expression tag	UNP Q8JGJ1
W	114	HIS	-	expression tag	UNP Q8JGJ1
W	115	HIS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
W	116	GLY	-	expression tag	UNP Q8JGJ1
W	117	ALA	-	expression tag	UNP Q8JGJ1
W	118	ALA	-	expression tag	UNP Q8JGJ1
W	119	GLU	-	expression tag	UNP Q8JGJ1
W	120	SER	-	expression tag	UNP Q8JGJ1
W	121	LYS	-	expression tag	UNP Q8JGJ1
W	122	LEU	-	expression tag	UNP Q8JGJ1
W	123	ILE	-	expression tag	UNP Q8JGJ1
W	124	SER	-	expression tag	UNP Q8JGJ1
W	125	GLU	-	expression tag	UNP Q8JGJ1
W	126	GLU	-	expression tag	UNP Q8JGJ1
W	127	ASP	-	expression tag	UNP Q8JGJ1
W	128	LEU	-	expression tag	UNP Q8JGJ1
X	28	HIS	ASN	conflict	UNP Q8JGJ1
X	31	THR	LEU	conflict	UNP Q8JGJ1
X	?	-	ASN	deletion	UNP Q8JGJ1
X	?	-	VAL	deletion	UNP Q8JGJ1
X	84	ALA	TYR	conflict	UNP Q8JGJ1
X	86	GLU	TRP	conflict	UNP Q8JGJ1
X	87	CYS	TYR	conflict	UNP Q8JGJ1
X	88	GLN	GLY	conflict	UNP Q8JGJ1
X	90	GLY	ASP	conflict	UNP Q8JGJ1
X	91	LEU	CYS	conflict	UNP Q8JGJ1
X	94	TYR	LEU	conflict	UNP Q8JGJ1
X	107	ALA	-	expression tag	UNP Q8JGJ1
X	108	ALA	-	expression tag	UNP Q8JGJ1
X	109	ALA	-	expression tag	UNP Q8JGJ1
X	110	HIS	-	expression tag	UNP Q8JGJ1
X	111	HIS	-	expression tag	UNP Q8JGJ1
X	112	HIS	-	expression tag	UNP Q8JGJ1
X	113	HIS	-	expression tag	UNP Q8JGJ1
X	114	HIS	-	expression tag	UNP Q8JGJ1
X	115	HIS	-	expression tag	UNP Q8JGJ1
X	116	GLY	-	expression tag	UNP Q8JGJ1
X	117	ALA	-	expression tag	UNP Q8JGJ1
X	118	ALA	-	expression tag	UNP Q8JGJ1
X	119	GLU	-	expression tag	UNP Q8JGJ1
X	120	SER	-	expression tag	UNP Q8JGJ1
X	121	LYS	-	expression tag	UNP Q8JGJ1
X	122	LEU	-	expression tag	UNP Q8JGJ1
X	123	ILE	-	expression tag	UNP Q8JGJ1
X	124	SER	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
X	125	GLU	-	expression tag	UNP Q8JGJ1
X	126	GLU	-	expression tag	UNP Q8JGJ1
X	127	ASP	-	expression tag	UNP Q8JGJ1
X	128	LEU	-	expression tag	UNP Q8JGJ1
b	28	HIS	ASN	conflict	UNP Q8JGJ1
b	31	THR	LEU	conflict	UNP Q8JGJ1
b	?	-	ASN	deletion	UNP Q8JGJ1
b	?	-	VAL	deletion	UNP Q8JGJ1
b	84	ALA	TYR	conflict	UNP Q8JGJ1
b	86	GLU	TRP	conflict	UNP Q8JGJ1
b	87	CYS	TYR	conflict	UNP Q8JGJ1
b	88	GLN	GLY	conflict	UNP Q8JGJ1
b	90	GLY	ASP	conflict	UNP Q8JGJ1
b	91	LEU	CYS	conflict	UNP Q8JGJ1
b	94	TYR	LEU	conflict	UNP Q8JGJ1
b	107	ALA	-	expression tag	UNP Q8JGJ1
b	108	ALA	-	expression tag	UNP Q8JGJ1
b	109	ALA	-	expression tag	UNP Q8JGJ1
b	110	HIS	-	expression tag	UNP Q8JGJ1
b	111	HIS	-	expression tag	UNP Q8JGJ1
b	112	HIS	-	expression tag	UNP Q8JGJ1
b	113	HIS	-	expression tag	UNP Q8JGJ1
b	114	HIS	-	expression tag	UNP Q8JGJ1
b	115	HIS	-	expression tag	UNP Q8JGJ1
b	116	GLY	-	expression tag	UNP Q8JGJ1
b	117	ALA	-	expression tag	UNP Q8JGJ1
b	118	ALA	-	expression tag	UNP Q8JGJ1
b	119	GLU	-	expression tag	UNP Q8JGJ1
b	120	SER	-	expression tag	UNP Q8JGJ1
b	121	LYS	-	expression tag	UNP Q8JGJ1
b	122	LEU	-	expression tag	UNP Q8JGJ1
b	123	ILE	-	expression tag	UNP Q8JGJ1
b	124	SER	-	expression tag	UNP Q8JGJ1
b	125	GLU	-	expression tag	UNP Q8JGJ1
b	126	GLU	-	expression tag	UNP Q8JGJ1
b	127	ASP	-	expression tag	UNP Q8JGJ1
b	128	LEU	-	expression tag	UNP Q8JGJ1
c	28	HIS	ASN	conflict	UNP Q8JGJ1
c	31	THR	LEU	conflict	UNP Q8JGJ1
c	?	-	ASN	deletion	UNP Q8JGJ1
c	?	-	VAL	deletion	UNP Q8JGJ1
c	84	ALA	TYR	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
c	86	GLU	TRP	conflict	UNP Q8JGJ1
c	87	CYS	TYR	conflict	UNP Q8JGJ1
c	88	GLN	GLY	conflict	UNP Q8JGJ1
c	90	GLY	ASP	conflict	UNP Q8JGJ1
c	91	LEU	CYS	conflict	UNP Q8JGJ1
c	94	TYR	LEU	conflict	UNP Q8JGJ1
c	107	ALA	-	expression tag	UNP Q8JGJ1
c	108	ALA	-	expression tag	UNP Q8JGJ1
c	109	ALA	-	expression tag	UNP Q8JGJ1
c	110	HIS	-	expression tag	UNP Q8JGJ1
c	111	HIS	-	expression tag	UNP Q8JGJ1
c	112	HIS	-	expression tag	UNP Q8JGJ1
c	113	HIS	-	expression tag	UNP Q8JGJ1
c	114	HIS	-	expression tag	UNP Q8JGJ1
c	115	HIS	-	expression tag	UNP Q8JGJ1
c	116	GLY	-	expression tag	UNP Q8JGJ1
c	117	ALA	-	expression tag	UNP Q8JGJ1
c	118	ALA	-	expression tag	UNP Q8JGJ1
c	119	GLU	-	expression tag	UNP Q8JGJ1
c	120	SER	-	expression tag	UNP Q8JGJ1
c	121	LYS	-	expression tag	UNP Q8JGJ1
c	122	LEU	-	expression tag	UNP Q8JGJ1
c	123	ILE	-	expression tag	UNP Q8JGJ1
c	124	SER	-	expression tag	UNP Q8JGJ1
c	125	GLU	-	expression tag	UNP Q8JGJ1
c	126	GLU	-	expression tag	UNP Q8JGJ1
c	127	ASP	-	expression tag	UNP Q8JGJ1
c	128	LEU	-	expression tag	UNP Q8JGJ1
d	28	HIS	ASN	conflict	UNP Q8JGJ1
d	31	THR	LEU	conflict	UNP Q8JGJ1
d	?	-	ASN	deletion	UNP Q8JGJ1
d	?	-	VAL	deletion	UNP Q8JGJ1
d	84	ALA	TYR	conflict	UNP Q8JGJ1
d	86	GLU	TRP	conflict	UNP Q8JGJ1
d	87	CYS	TYR	conflict	UNP Q8JGJ1
d	88	GLN	GLY	conflict	UNP Q8JGJ1
d	90	GLY	ASP	conflict	UNP Q8JGJ1
d	91	LEU	CYS	conflict	UNP Q8JGJ1
d	94	TYR	LEU	conflict	UNP Q8JGJ1
d	107	ALA	-	expression tag	UNP Q8JGJ1
d	108	ALA	-	expression tag	UNP Q8JGJ1
d	109	ALA	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
d	110	HIS	-	expression tag	UNP Q8JGJ1
d	111	HIS	-	expression tag	UNP Q8JGJ1
d	112	HIS	-	expression tag	UNP Q8JGJ1
d	113	HIS	-	expression tag	UNP Q8JGJ1
d	114	HIS	-	expression tag	UNP Q8JGJ1
d	115	HIS	-	expression tag	UNP Q8JGJ1
d	116	GLY	-	expression tag	UNP Q8JGJ1
d	117	ALA	-	expression tag	UNP Q8JGJ1
d	118	ALA	-	expression tag	UNP Q8JGJ1
d	119	GLU	-	expression tag	UNP Q8JGJ1
d	120	SER	-	expression tag	UNP Q8JGJ1
d	121	LYS	-	expression tag	UNP Q8JGJ1
d	122	LEU	-	expression tag	UNP Q8JGJ1
d	123	ILE	-	expression tag	UNP Q8JGJ1
d	124	SER	-	expression tag	UNP Q8JGJ1
d	125	GLU	-	expression tag	UNP Q8JGJ1
d	126	GLU	-	expression tag	UNP Q8JGJ1
d	127	ASP	-	expression tag	UNP Q8JGJ1
d	128	LEU	-	expression tag	UNP Q8JGJ1
h	28	HIS	ASN	conflict	UNP Q8JGJ1
h	31	THR	LEU	conflict	UNP Q8JGJ1
h	?	-	ASN	deletion	UNP Q8JGJ1
h	?	-	VAL	deletion	UNP Q8JGJ1
h	84	ALA	TYR	conflict	UNP Q8JGJ1
h	86	GLU	TRP	conflict	UNP Q8JGJ1
h	87	CYS	TYR	conflict	UNP Q8JGJ1
h	88	GLN	GLY	conflict	UNP Q8JGJ1
h	90	GLY	ASP	conflict	UNP Q8JGJ1
h	91	LEU	CYS	conflict	UNP Q8JGJ1
h	94	TYR	LEU	conflict	UNP Q8JGJ1
h	107	ALA	-	expression tag	UNP Q8JGJ1
h	108	ALA	-	expression tag	UNP Q8JGJ1
h	109	ALA	-	expression tag	UNP Q8JGJ1
h	110	HIS	-	expression tag	UNP Q8JGJ1
h	111	HIS	-	expression tag	UNP Q8JGJ1
h	112	HIS	-	expression tag	UNP Q8JGJ1
h	113	HIS	-	expression tag	UNP Q8JGJ1
h	114	HIS	-	expression tag	UNP Q8JGJ1
h	115	HIS	-	expression tag	UNP Q8JGJ1
h	116	GLY	-	expression tag	UNP Q8JGJ1
h	117	ALA	-	expression tag	UNP Q8JGJ1
h	118	ALA	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
h	119	GLU	-	expression tag	UNP Q8JGJ1
h	120	SER	-	expression tag	UNP Q8JGJ1
h	121	LYS	-	expression tag	UNP Q8JGJ1
h	122	LEU	-	expression tag	UNP Q8JGJ1
h	123	ILE	-	expression tag	UNP Q8JGJ1
h	124	SER	-	expression tag	UNP Q8JGJ1
h	125	GLU	-	expression tag	UNP Q8JGJ1
h	126	GLU	-	expression tag	UNP Q8JGJ1
h	127	ASP	-	expression tag	UNP Q8JGJ1
h	128	LEU	-	expression tag	UNP Q8JGJ1
i	28	HIS	ASN	conflict	UNP Q8JGJ1
i	31	THR	LEU	conflict	UNP Q8JGJ1
i	?	-	ASN	deletion	UNP Q8JGJ1
i	?	-	VAL	deletion	UNP Q8JGJ1
i	84	ALA	TYR	conflict	UNP Q8JGJ1
i	86	GLU	TRP	conflict	UNP Q8JGJ1
i	87	CYS	TYR	conflict	UNP Q8JGJ1
i	88	GLN	GLY	conflict	UNP Q8JGJ1
i	90	GLY	ASP	conflict	UNP Q8JGJ1
i	91	LEU	CYS	conflict	UNP Q8JGJ1
i	94	TYR	LEU	conflict	UNP Q8JGJ1
i	107	ALA	-	expression tag	UNP Q8JGJ1
i	108	ALA	-	expression tag	UNP Q8JGJ1
i	109	ALA	-	expression tag	UNP Q8JGJ1
i	110	HIS	-	expression tag	UNP Q8JGJ1
i	111	HIS	-	expression tag	UNP Q8JGJ1
i	112	HIS	-	expression tag	UNP Q8JGJ1
i	113	HIS	-	expression tag	UNP Q8JGJ1
i	114	HIS	-	expression tag	UNP Q8JGJ1
i	115	HIS	-	expression tag	UNP Q8JGJ1
i	116	GLY	-	expression tag	UNP Q8JGJ1
i	117	ALA	-	expression tag	UNP Q8JGJ1
i	118	ALA	-	expression tag	UNP Q8JGJ1
i	119	GLU	-	expression tag	UNP Q8JGJ1
i	120	SER	-	expression tag	UNP Q8JGJ1
i	121	LYS	-	expression tag	UNP Q8JGJ1
i	122	LEU	-	expression tag	UNP Q8JGJ1
i	123	ILE	-	expression tag	UNP Q8JGJ1
i	124	SER	-	expression tag	UNP Q8JGJ1
i	125	GLU	-	expression tag	UNP Q8JGJ1
i	126	GLU	-	expression tag	UNP Q8JGJ1
i	127	ASP	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
i	128	LEU	-	expression tag	UNP Q8JGJ1
j	28	HIS	ASN	conflict	UNP Q8JGJ1
j	31	THR	LEU	conflict	UNP Q8JGJ1
j	?	-	ASN	deletion	UNP Q8JGJ1
j	?	-	VAL	deletion	UNP Q8JGJ1
j	84	ALA	TYR	conflict	UNP Q8JGJ1
j	86	GLU	TRP	conflict	UNP Q8JGJ1
j	87	CYS	TYR	conflict	UNP Q8JGJ1
j	88	GLN	GLY	conflict	UNP Q8JGJ1
j	90	GLY	ASP	conflict	UNP Q8JGJ1
j	91	LEU	CYS	conflict	UNP Q8JGJ1
j	94	TYR	LEU	conflict	UNP Q8JGJ1
j	107	ALA	-	expression tag	UNP Q8JGJ1
j	108	ALA	-	expression tag	UNP Q8JGJ1
j	109	ALA	-	expression tag	UNP Q8JGJ1
j	110	HIS	-	expression tag	UNP Q8JGJ1
j	111	HIS	-	expression tag	UNP Q8JGJ1
j	112	HIS	-	expression tag	UNP Q8JGJ1
j	113	HIS	-	expression tag	UNP Q8JGJ1
j	114	HIS	-	expression tag	UNP Q8JGJ1
j	115	HIS	-	expression tag	UNP Q8JGJ1
j	116	GLY	-	expression tag	UNP Q8JGJ1
j	117	ALA	-	expression tag	UNP Q8JGJ1
j	118	ALA	-	expression tag	UNP Q8JGJ1
j	119	GLU	-	expression tag	UNP Q8JGJ1
j	120	SER	-	expression tag	UNP Q8JGJ1
j	121	LYS	-	expression tag	UNP Q8JGJ1
j	122	LEU	-	expression tag	UNP Q8JGJ1
j	123	ILE	-	expression tag	UNP Q8JGJ1
j	124	SER	-	expression tag	UNP Q8JGJ1
j	125	GLU	-	expression tag	UNP Q8JGJ1
j	126	GLU	-	expression tag	UNP Q8JGJ1
j	127	ASP	-	expression tag	UNP Q8JGJ1
j	128	LEU	-	expression tag	UNP Q8JGJ1
n	28	HIS	ASN	conflict	UNP Q8JGJ1
n	31	THR	LEU	conflict	UNP Q8JGJ1
n	?	-	ASN	deletion	UNP Q8JGJ1
n	?	-	VAL	deletion	UNP Q8JGJ1
n	84	ALA	TYR	conflict	UNP Q8JGJ1
n	86	GLU	TRP	conflict	UNP Q8JGJ1
n	87	CYS	TYR	conflict	UNP Q8JGJ1
n	88	GLN	GLY	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
n	90	GLY	ASP	conflict	UNP Q8JGJ1
n	91	LEU	CYS	conflict	UNP Q8JGJ1
n	94	TYR	LEU	conflict	UNP Q8JGJ1
n	107	ALA	-	expression tag	UNP Q8JGJ1
n	108	ALA	-	expression tag	UNP Q8JGJ1
n	109	ALA	-	expression tag	UNP Q8JGJ1
n	110	HIS	-	expression tag	UNP Q8JGJ1
n	111	HIS	-	expression tag	UNP Q8JGJ1
n	112	HIS	-	expression tag	UNP Q8JGJ1
n	113	HIS	-	expression tag	UNP Q8JGJ1
n	114	HIS	-	expression tag	UNP Q8JGJ1
n	115	HIS	-	expression tag	UNP Q8JGJ1
n	116	GLY	-	expression tag	UNP Q8JGJ1
n	117	ALA	-	expression tag	UNP Q8JGJ1
n	118	ALA	-	expression tag	UNP Q8JGJ1
n	119	GLU	-	expression tag	UNP Q8JGJ1
n	120	SER	-	expression tag	UNP Q8JGJ1
n	121	LYS	-	expression tag	UNP Q8JGJ1
n	122	LEU	-	expression tag	UNP Q8JGJ1
n	123	ILE	-	expression tag	UNP Q8JGJ1
n	124	SER	-	expression tag	UNP Q8JGJ1
n	125	GLU	-	expression tag	UNP Q8JGJ1
n	126	GLU	-	expression tag	UNP Q8JGJ1
n	127	ASP	-	expression tag	UNP Q8JGJ1
n	128	LEU	-	expression tag	UNP Q8JGJ1
o	28	HIS	ASN	conflict	UNP Q8JGJ1
o	31	THR	LEU	conflict	UNP Q8JGJ1
o	?	-	ASN	deletion	UNP Q8JGJ1
o	?	-	VAL	deletion	UNP Q8JGJ1
o	84	ALA	TYR	conflict	UNP Q8JGJ1
o	86	GLU	TRP	conflict	UNP Q8JGJ1
o	87	CYS	TYR	conflict	UNP Q8JGJ1
o	88	GLN	GLY	conflict	UNP Q8JGJ1
o	90	GLY	ASP	conflict	UNP Q8JGJ1
o	91	LEU	CYS	conflict	UNP Q8JGJ1
o	94	TYR	LEU	conflict	UNP Q8JGJ1
o	107	ALA	-	expression tag	UNP Q8JGJ1
o	108	ALA	-	expression tag	UNP Q8JGJ1
o	109	ALA	-	expression tag	UNP Q8JGJ1
o	110	HIS	-	expression tag	UNP Q8JGJ1
o	111	HIS	-	expression tag	UNP Q8JGJ1
o	112	HIS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
o	113	HIS	-	expression tag	UNP Q8JGJ1
o	114	HIS	-	expression tag	UNP Q8JGJ1
o	115	HIS	-	expression tag	UNP Q8JGJ1
o	116	GLY	-	expression tag	UNP Q8JGJ1
o	117	ALA	-	expression tag	UNP Q8JGJ1
o	118	ALA	-	expression tag	UNP Q8JGJ1
o	119	GLU	-	expression tag	UNP Q8JGJ1
o	120	SER	-	expression tag	UNP Q8JGJ1
o	121	LYS	-	expression tag	UNP Q8JGJ1
o	122	LEU	-	expression tag	UNP Q8JGJ1
o	123	ILE	-	expression tag	UNP Q8JGJ1
o	124	SER	-	expression tag	UNP Q8JGJ1
o	125	GLU	-	expression tag	UNP Q8JGJ1
o	126	GLU	-	expression tag	UNP Q8JGJ1
o	127	ASP	-	expression tag	UNP Q8JGJ1
o	128	LEU	-	expression tag	UNP Q8JGJ1
p	28	HIS	ASN	conflict	UNP Q8JGJ1
p	31	THR	LEU	conflict	UNP Q8JGJ1
p	?	-	ASN	deletion	UNP Q8JGJ1
p	?	-	VAL	deletion	UNP Q8JGJ1
p	84	ALA	TYR	conflict	UNP Q8JGJ1
p	86	GLU	TRP	conflict	UNP Q8JGJ1
p	87	CYS	TYR	conflict	UNP Q8JGJ1
p	88	GLN	GLY	conflict	UNP Q8JGJ1
p	90	GLY	ASP	conflict	UNP Q8JGJ1
p	91	LEU	CYS	conflict	UNP Q8JGJ1
p	94	TYR	LEU	conflict	UNP Q8JGJ1
p	107	ALA	-	expression tag	UNP Q8JGJ1
p	108	ALA	-	expression tag	UNP Q8JGJ1
p	109	ALA	-	expression tag	UNP Q8JGJ1
p	110	HIS	-	expression tag	UNP Q8JGJ1
p	111	HIS	-	expression tag	UNP Q8JGJ1
p	112	HIS	-	expression tag	UNP Q8JGJ1
p	113	HIS	-	expression tag	UNP Q8JGJ1
p	114	HIS	-	expression tag	UNP Q8JGJ1
p	115	HIS	-	expression tag	UNP Q8JGJ1
p	116	GLY	-	expression tag	UNP Q8JGJ1
p	117	ALA	-	expression tag	UNP Q8JGJ1
p	118	ALA	-	expression tag	UNP Q8JGJ1
p	119	GLU	-	expression tag	UNP Q8JGJ1
p	120	SER	-	expression tag	UNP Q8JGJ1
p	121	LYS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
p	122	LEU	-	expression tag	UNP Q8JGJ1
p	123	ILE	-	expression tag	UNP Q8JGJ1
p	124	SER	-	expression tag	UNP Q8JGJ1
p	125	GLU	-	expression tag	UNP Q8JGJ1
p	126	GLU	-	expression tag	UNP Q8JGJ1
p	127	ASP	-	expression tag	UNP Q8JGJ1
p	128	LEU	-	expression tag	UNP Q8JGJ1
t	28	HIS	ASN	conflict	UNP Q8JGJ1
t	31	THR	LEU	conflict	UNP Q8JGJ1
t	?	-	ASN	deletion	UNP Q8JGJ1
t	?	-	VAL	deletion	UNP Q8JGJ1
t	84	ALA	TYR	conflict	UNP Q8JGJ1
t	86	GLU	TRP	conflict	UNP Q8JGJ1
t	87	CYS	TYR	conflict	UNP Q8JGJ1
t	88	GLN	GLY	conflict	UNP Q8JGJ1
t	90	GLY	ASP	conflict	UNP Q8JGJ1
t	91	LEU	CYS	conflict	UNP Q8JGJ1
t	94	TYR	LEU	conflict	UNP Q8JGJ1
t	107	ALA	-	expression tag	UNP Q8JGJ1
t	108	ALA	-	expression tag	UNP Q8JGJ1
t	109	ALA	-	expression tag	UNP Q8JGJ1
t	110	HIS	-	expression tag	UNP Q8JGJ1
t	111	HIS	-	expression tag	UNP Q8JGJ1
t	112	HIS	-	expression tag	UNP Q8JGJ1
t	113	HIS	-	expression tag	UNP Q8JGJ1
t	114	HIS	-	expression tag	UNP Q8JGJ1
t	115	HIS	-	expression tag	UNP Q8JGJ1
t	116	GLY	-	expression tag	UNP Q8JGJ1
t	117	ALA	-	expression tag	UNP Q8JGJ1
t	118	ALA	-	expression tag	UNP Q8JGJ1
t	119	GLU	-	expression tag	UNP Q8JGJ1
t	120	SER	-	expression tag	UNP Q8JGJ1
t	121	LYS	-	expression tag	UNP Q8JGJ1
t	122	LEU	-	expression tag	UNP Q8JGJ1
t	123	ILE	-	expression tag	UNP Q8JGJ1
t	124	SER	-	expression tag	UNP Q8JGJ1
t	125	GLU	-	expression tag	UNP Q8JGJ1
t	126	GLU	-	expression tag	UNP Q8JGJ1
t	127	ASP	-	expression tag	UNP Q8JGJ1
t	128	LEU	-	expression tag	UNP Q8JGJ1
u	28	HIS	ASN	conflict	UNP Q8JGJ1
u	31	THR	LEU	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
u	?	-	ASN	deletion	UNP Q8JGJ1
u	?	-	VAL	deletion	UNP Q8JGJ1
u	84	ALA	TYR	conflict	UNP Q8JGJ1
u	86	GLU	TRP	conflict	UNP Q8JGJ1
u	87	CYS	TYR	conflict	UNP Q8JGJ1
u	88	GLN	GLY	conflict	UNP Q8JGJ1
u	90	GLY	ASP	conflict	UNP Q8JGJ1
u	91	LEU	CYS	conflict	UNP Q8JGJ1
u	94	TYR	LEU	conflict	UNP Q8JGJ1
u	107	ALA	-	expression tag	UNP Q8JGJ1
u	108	ALA	-	expression tag	UNP Q8JGJ1
u	109	ALA	-	expression tag	UNP Q8JGJ1
u	110	HIS	-	expression tag	UNP Q8JGJ1
u	111	HIS	-	expression tag	UNP Q8JGJ1
u	112	HIS	-	expression tag	UNP Q8JGJ1
u	113	HIS	-	expression tag	UNP Q8JGJ1
u	114	HIS	-	expression tag	UNP Q8JGJ1
u	115	HIS	-	expression tag	UNP Q8JGJ1
u	116	GLY	-	expression tag	UNP Q8JGJ1
u	117	ALA	-	expression tag	UNP Q8JGJ1
u	118	ALA	-	expression tag	UNP Q8JGJ1
u	119	GLU	-	expression tag	UNP Q8JGJ1
u	120	SER	-	expression tag	UNP Q8JGJ1
u	121	LYS	-	expression tag	UNP Q8JGJ1
u	122	LEU	-	expression tag	UNP Q8JGJ1
u	123	ILE	-	expression tag	UNP Q8JGJ1
u	124	SER	-	expression tag	UNP Q8JGJ1
u	125	GLU	-	expression tag	UNP Q8JGJ1
u	126	GLU	-	expression tag	UNP Q8JGJ1
u	127	ASP	-	expression tag	UNP Q8JGJ1
u	128	LEU	-	expression tag	UNP Q8JGJ1
v	28	HIS	ASN	conflict	UNP Q8JGJ1
v	31	THR	LEU	conflict	UNP Q8JGJ1
v	?	-	ASN	deletion	UNP Q8JGJ1
v	?	-	VAL	deletion	UNP Q8JGJ1
v	84	ALA	TYR	conflict	UNP Q8JGJ1
v	86	GLU	TRP	conflict	UNP Q8JGJ1
v	87	CYS	TYR	conflict	UNP Q8JGJ1
v	88	GLN	GLY	conflict	UNP Q8JGJ1
v	90	GLY	ASP	conflict	UNP Q8JGJ1
v	91	LEU	CYS	conflict	UNP Q8JGJ1
v	94	TYR	LEU	conflict	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
v	107	ALA	-	expression tag	UNP Q8JGJ1
v	108	ALA	-	expression tag	UNP Q8JGJ1
v	109	ALA	-	expression tag	UNP Q8JGJ1
v	110	HIS	-	expression tag	UNP Q8JGJ1
v	111	HIS	-	expression tag	UNP Q8JGJ1
v	112	HIS	-	expression tag	UNP Q8JGJ1
v	113	HIS	-	expression tag	UNP Q8JGJ1
v	114	HIS	-	expression tag	UNP Q8JGJ1
v	115	HIS	-	expression tag	UNP Q8JGJ1
v	116	GLY	-	expression tag	UNP Q8JGJ1
v	117	ALA	-	expression tag	UNP Q8JGJ1
v	118	ALA	-	expression tag	UNP Q8JGJ1
v	119	GLU	-	expression tag	UNP Q8JGJ1
v	120	SER	-	expression tag	UNP Q8JGJ1
v	121	LYS	-	expression tag	UNP Q8JGJ1
v	122	LEU	-	expression tag	UNP Q8JGJ1
v	123	ILE	-	expression tag	UNP Q8JGJ1
v	124	SER	-	expression tag	UNP Q8JGJ1
v	125	GLU	-	expression tag	UNP Q8JGJ1
v	126	GLU	-	expression tag	UNP Q8JGJ1
v	127	ASP	-	expression tag	UNP Q8JGJ1
v	128	LEU	-	expression tag	UNP Q8JGJ1
z	28	HIS	ASN	conflict	UNP Q8JGJ1
z	31	THR	LEU	conflict	UNP Q8JGJ1
z	?	-	ASN	deletion	UNP Q8JGJ1
z	?	-	VAL	deletion	UNP Q8JGJ1
z	84	ALA	TYR	conflict	UNP Q8JGJ1
z	86	GLU	TRP	conflict	UNP Q8JGJ1
z	87	CYS	TYR	conflict	UNP Q8JGJ1
z	88	GLN	GLY	conflict	UNP Q8JGJ1
z	90	GLY	ASP	conflict	UNP Q8JGJ1
z	91	LEU	CYS	conflict	UNP Q8JGJ1
z	94	TYR	LEU	conflict	UNP Q8JGJ1
z	107	ALA	-	expression tag	UNP Q8JGJ1
z	108	ALA	-	expression tag	UNP Q8JGJ1
z	109	ALA	-	expression tag	UNP Q8JGJ1
z	110	HIS	-	expression tag	UNP Q8JGJ1
z	111	HIS	-	expression tag	UNP Q8JGJ1
z	112	HIS	-	expression tag	UNP Q8JGJ1
z	113	HIS	-	expression tag	UNP Q8JGJ1
z	114	HIS	-	expression tag	UNP Q8JGJ1
z	115	HIS	-	expression tag	UNP Q8JGJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
z	116	GLY	-	expression tag	UNP Q8JGJ1
z	117	ALA	-	expression tag	UNP Q8JGJ1
z	118	ALA	-	expression tag	UNP Q8JGJ1
z	119	GLU	-	expression tag	UNP Q8JGJ1
z	120	SER	-	expression tag	UNP Q8JGJ1
z	121	LYS	-	expression tag	UNP Q8JGJ1
z	122	LEU	-	expression tag	UNP Q8JGJ1
z	123	ILE	-	expression tag	UNP Q8JGJ1
z	124	SER	-	expression tag	UNP Q8JGJ1
z	125	GLU	-	expression tag	UNP Q8JGJ1
z	126	GLU	-	expression tag	UNP Q8JGJ1
z	127	ASP	-	expression tag	UNP Q8JGJ1
z	128	LEU	-	expression tag	UNP Q8JGJ1

- Molecule 2 is a protein called Tumor necrosis factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	154	Total	C	N	O	S	0	0	0
			1202	764	209	227	2			
2	3	151	Total	C	N	O	S	0	0	0
			1183	754	206	221	2			
2	4	155	Total	C	N	O	S	0	0	0
			1208	767	210	229	2			
2	A	156	Total	C	N	O	S	0	0	0
			1219	773	214	230	2			
2	B	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	C	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	G	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	H	152	Total	C	N	O	S	0	0	0
			1188	757	207	222	2			
2	I	152	Total	C	N	O	S	0	0	0
			1190	758	207	223	2			
2	M	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	N	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	O	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	S	154	Total	C	N	O	S	0	0	0
			1202	764	209	227	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	156	Total	C	N	O	S	0	0	0
			1219	773	214	230	2			
2	U	150	Total	C	N	O	S	0	0	0
			1172	748	202	220	2			
2	Y	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	Z	152	Total	C	N	O	S	0	0	0
			1190	758	207	223	2			
2	a	154	Total	C	N	O	S	0	0	0
			1202	764	209	227	2			
2	e	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	f	156	Total	C	N	O	S	0	0	0
			1219	773	214	230	2			
2	g	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	k	156	Total	C	N	O	S	0	0	0
			1219	773	214	230	2			
2	l	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	m	151	Total	C	N	O	S	0	0	0
			1179	752	203	222	2			
2	q	146	Total	C	N	O	S	0	0	0
			1145	733	198	212	2			
2	r	152	Total	C	N	O	S	0	0	0
			1190	758	207	223	2			
2	s	152	Total	C	N	O	S	0	0	0
			1190	758	207	223	2			
2	w	156	Total	C	N	O	S	0	0	0
			1219	773	214	230	2			
2	x	153	Total	C	N	O	S	0	0	0
			1196	761	208	225	2			
2	y	152	Total	C	N	O	S	0	0	0
			1190	758	207	223	2			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



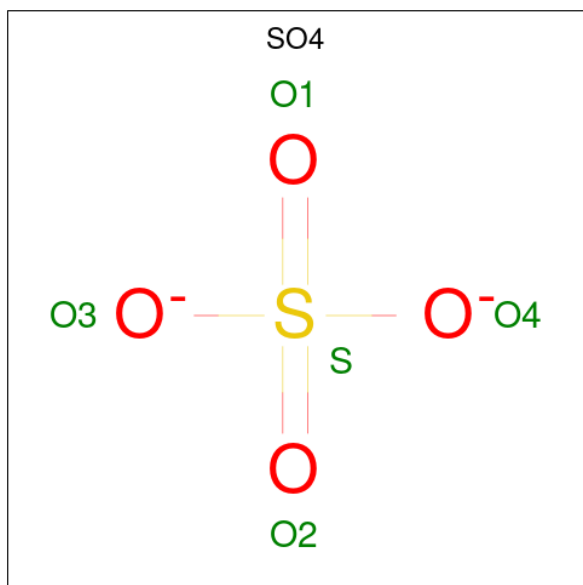
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	0	1	Total	C	O	0	0
			6	3	3		
3	1	1	Total	C	O	0	0
			6	3	3		
3	5	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		
3	V	1	Total	C	O	0	0
			6	3	3		
3	W	1	Total	C	O	0	0
			6	3	3		
3	a	1	Total	C	O	0	0
			6	3	3		
3	b	1	Total	C	O	0	0
			6	3	3		
3	b	1	Total	C	O	0	0
			6	3	3		
3	b	1	Total	C	O	0	0
			6	3	3		
3	h	1	Total	C	O	0	0
			6	3	3		
3	n	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	t	1	Total	C	O	0	0
			6	3	3		
3	t	1	Total	C	O	0	0
			6	3	3		
3	z	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	O	S	0	0
			5	4	1		
4	h	1	Total	O	S	0	0
			5	4	1		
4	t	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	S	1	Total	Cl	0	0
			1	1		

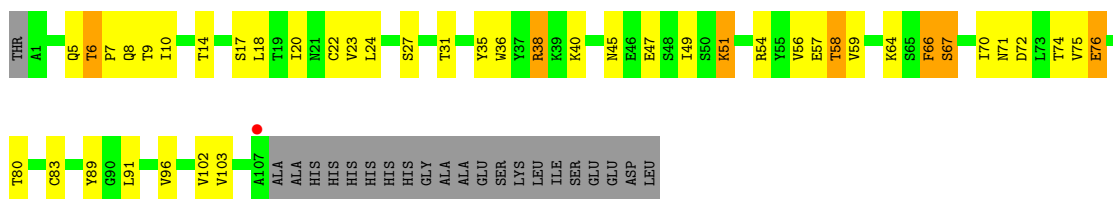
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total 2	O 2	0	0
6	I	1	Total 1	O 1	0	0
6	J	1	Total 1	O 1	0	0
6	P	1	Total 1	O 1	0	0
6	U	1	Total 1	O 1	0	0
6	V	2	Total 2	O 2	0	0
6	X	1	Total 1	O 1	0	0

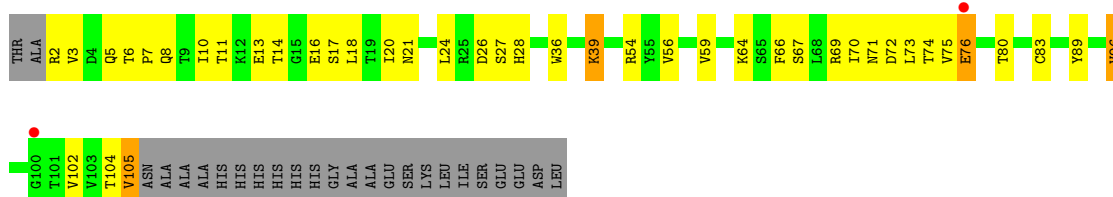
3 Residue-property plots [i](#)

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

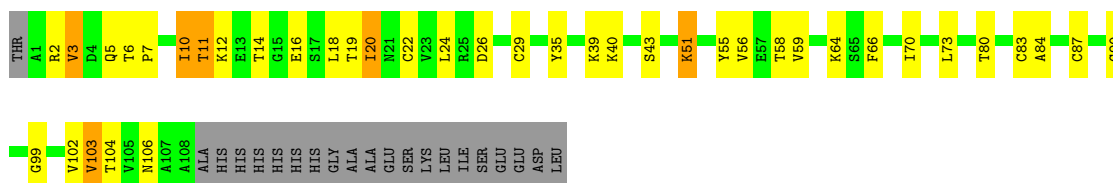
- Molecule 1: Antigen receptor



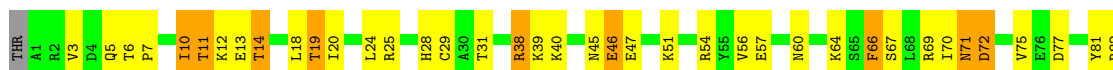
- Molecule 1: Antigen receptor

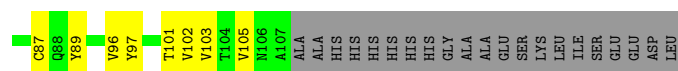


- Molecule 1: Antigen receptor

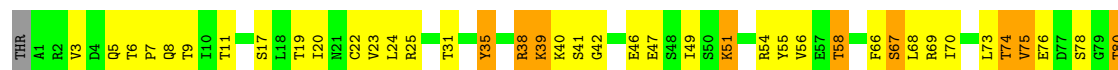


- Molecule 1: Antigen receptor

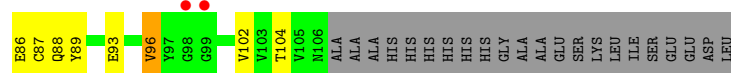




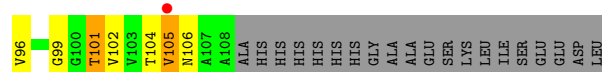
- Molecule 1: Antigen receptor



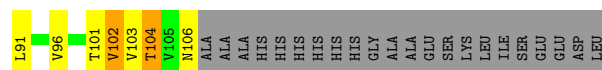
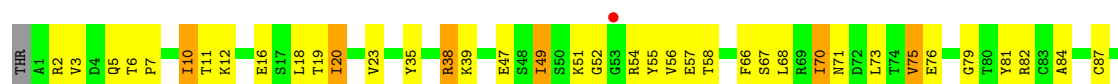
- Molecule 1: Antigen receptor



- Molecule 1: Antigen receptor

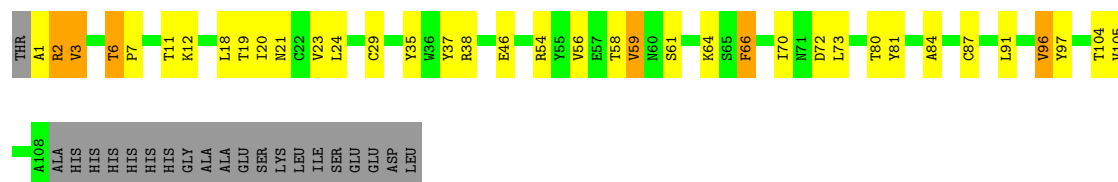


- Molecule 1: Antigen receptor



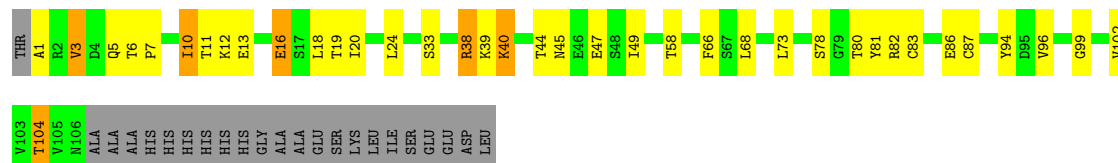
- Molecule 1: Antigen receptor





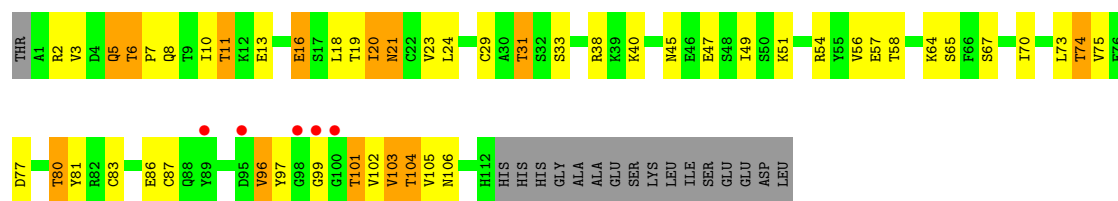
• Molecule 1: Antigen receptor

Chain K: 53% 25% 5% 18%



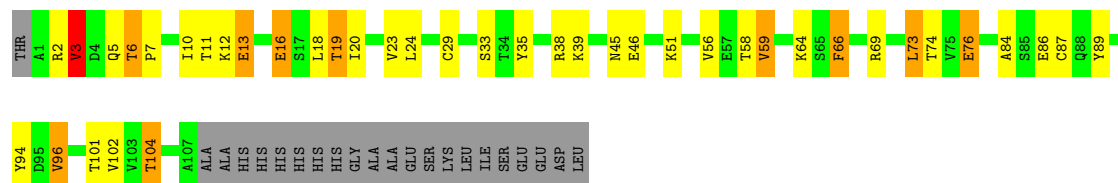
• Molecule 1: Antigen receptor

Chain L: 47% 29% 10% 13%



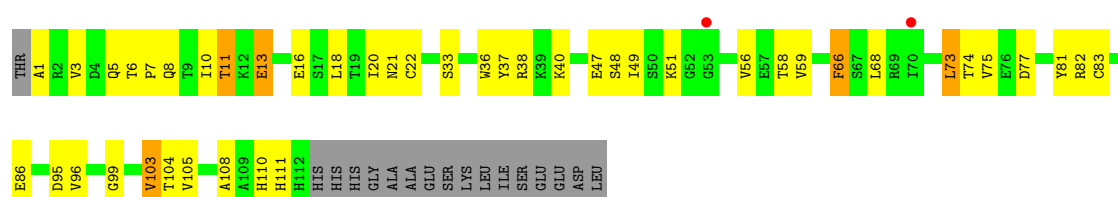
• Molecule 1: Antigen receptor

Chain P: 51% 23% 8% 17%

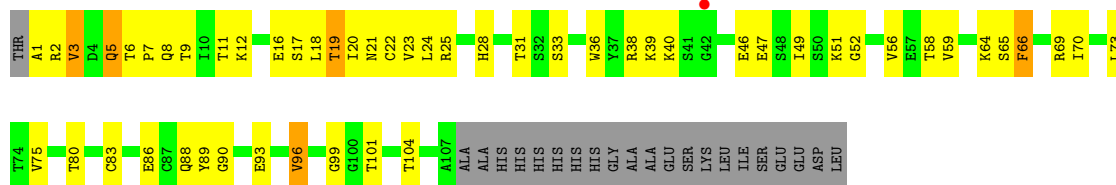


• Molecule 1: Antigen receptor

Chain Q: 52% 31% 13%



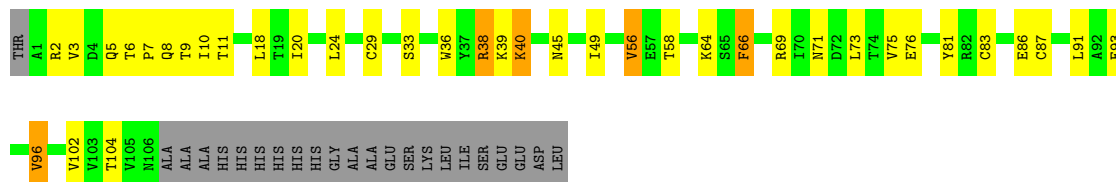
• Molecule 1: Antigen receptor



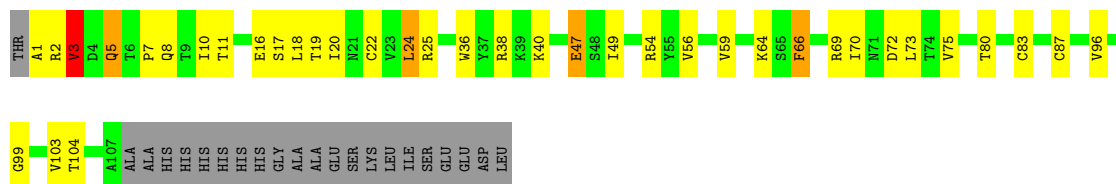
- Molecule 1: Antigen receptor



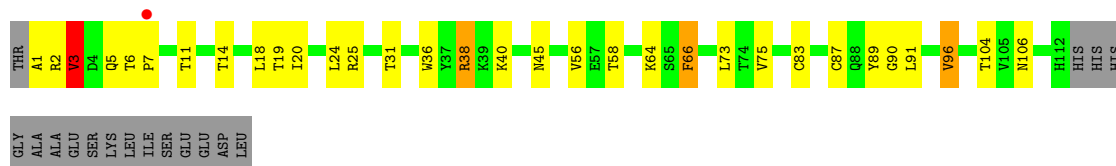
- Molecule 1: Antigen receptor



- Molecule 1: Antigen receptor

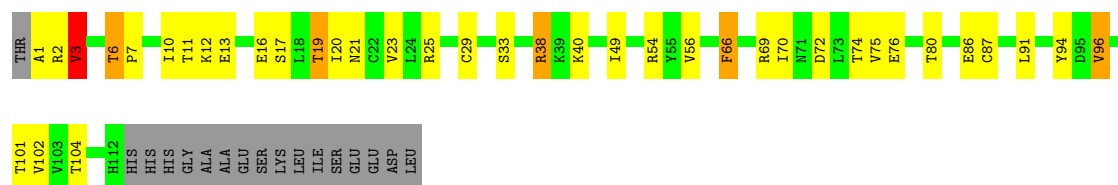


- Molecule 1: Antigen receptor



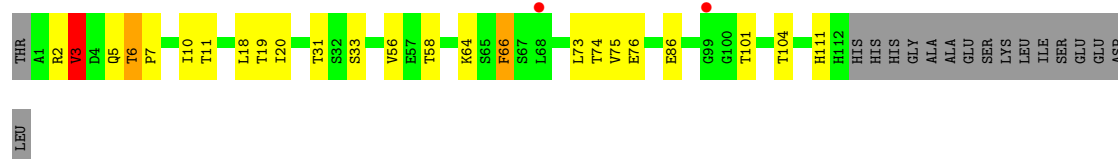
- Molecule 1: Antigen receptor

Chain c: 



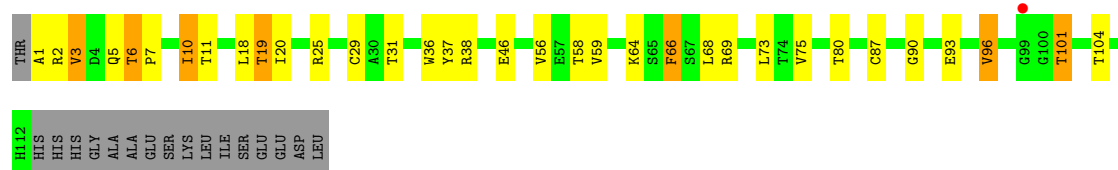
• Molecule 1: Antigen receptor

Chain d: 



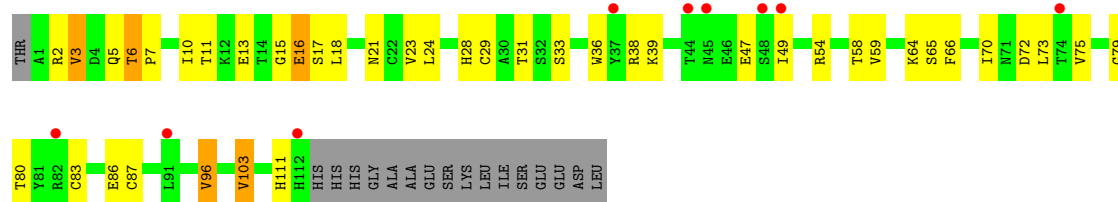
• Molecule 1: Antigen receptor

Chain h: 



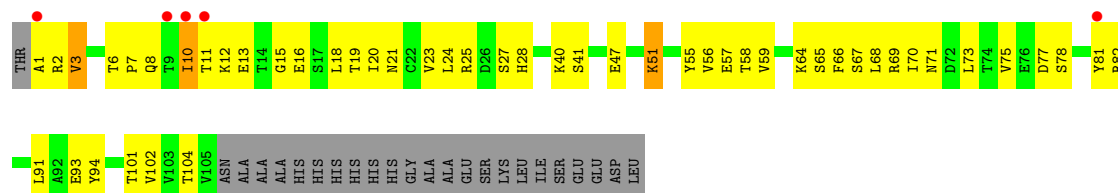
• Molecule 1: Antigen receptor

Chain i: 

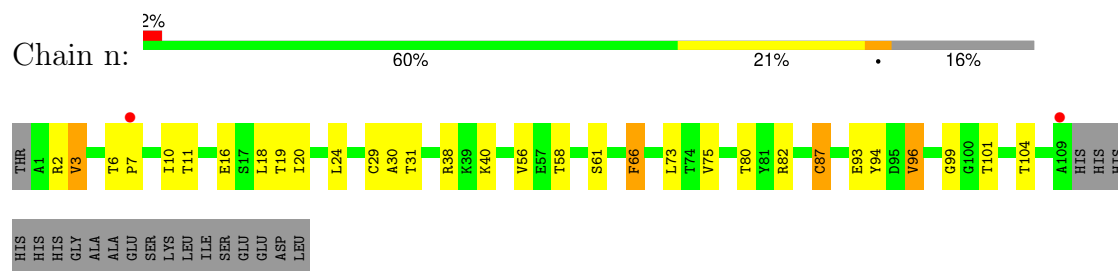


• Molecule 1: Antigen receptor

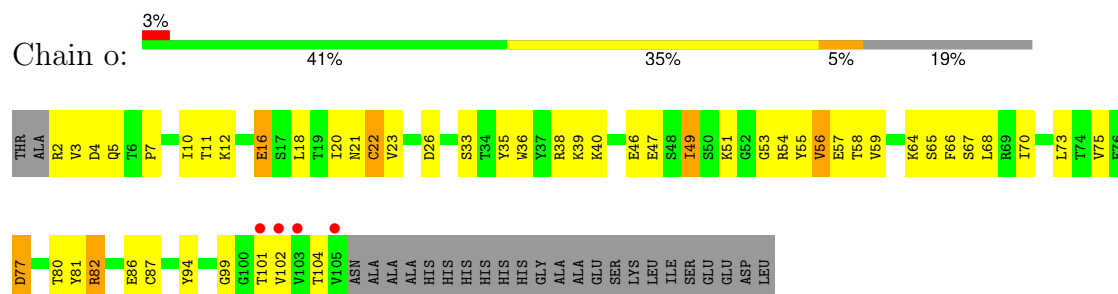
Chain j: 



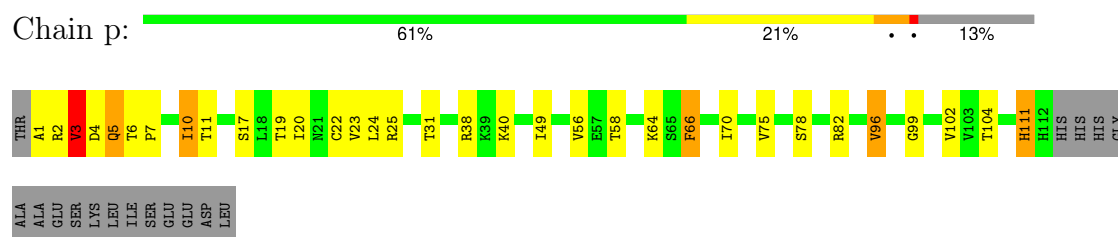
- Molecule 1: Antigen receptor



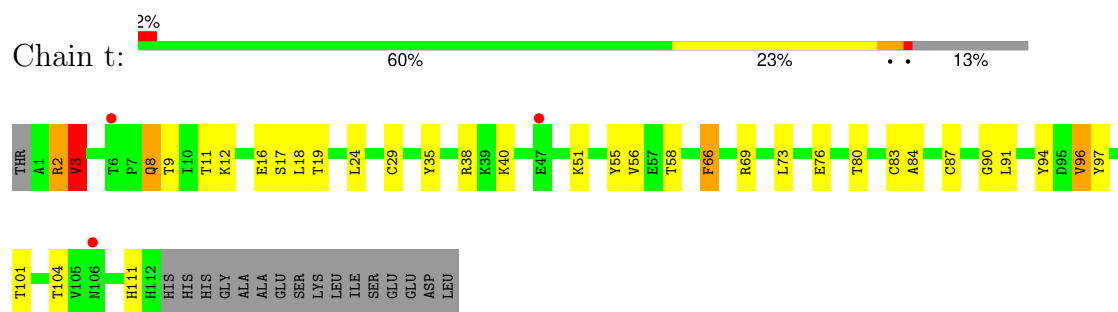
- Molecule 1: Antigen receptor



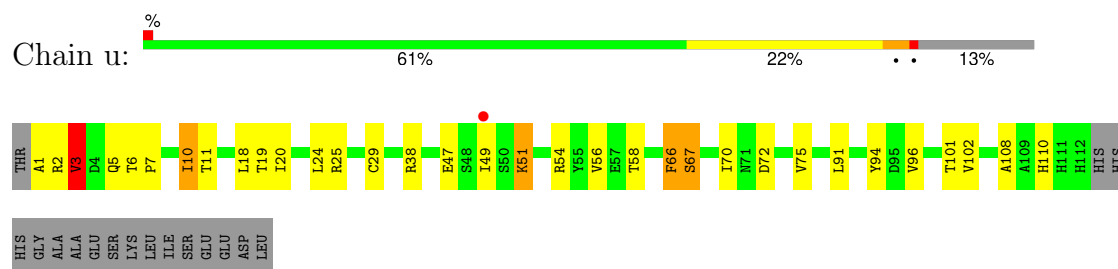
- Molecule 1: Antigen receptor



- Molecule 1: Antigen receptor

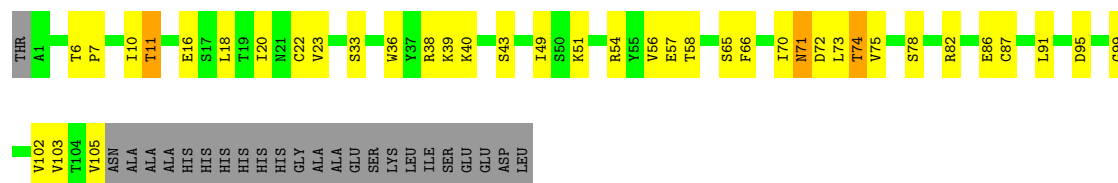


- Molecule 1: Antigen receptor



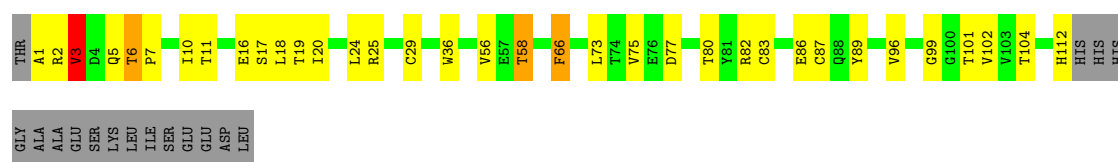
- Molecule 1: Antigen receptor

Chain v: 



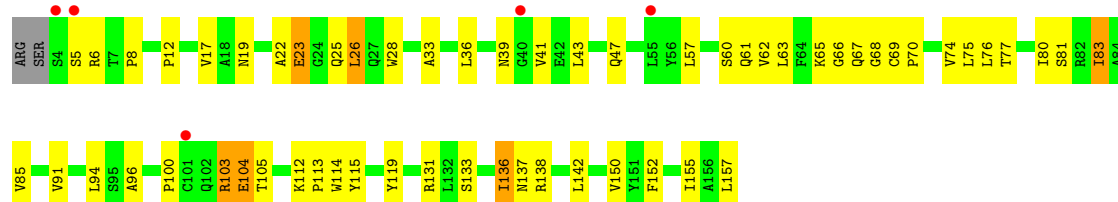
- Molecule 1: Antigen receptor

Chain z: 



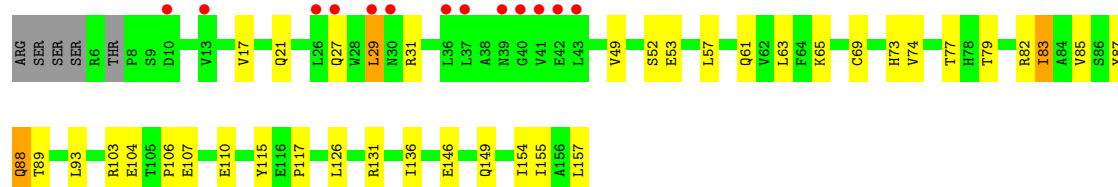
- Molecule 2: Tumor necrosis factor

Chain 2: 



- Molecule 2: Tumor necrosis factor

Chain 3: 



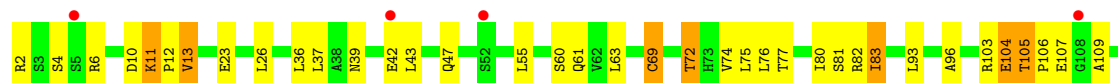
- Molecule 2: Tumor necrosis factor

Chain 4: 





- Molecule 2: Tumor necrosis factor



- Molecule 2: Tumor necrosis factor



- Molecule 2: Tumor necrosis factor

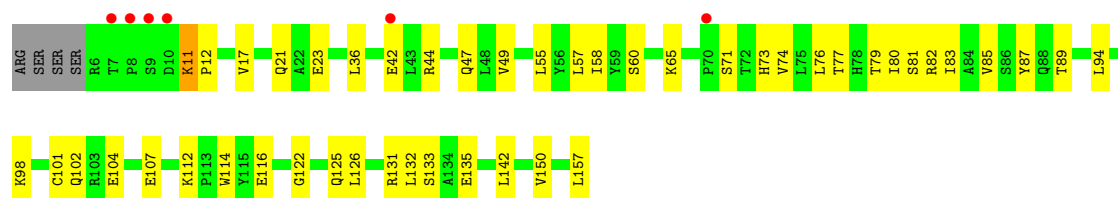


- Molecule 2: Tumor necrosis factor

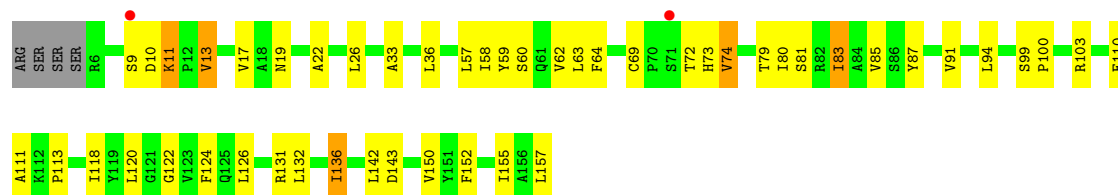


- Molecule 2: Tumor necrosis factor





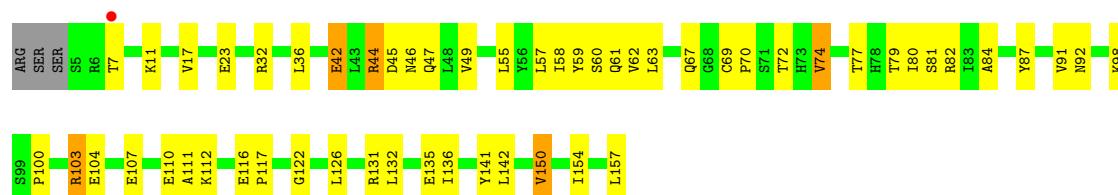
- Molecule 2: Tumor necrosis factor



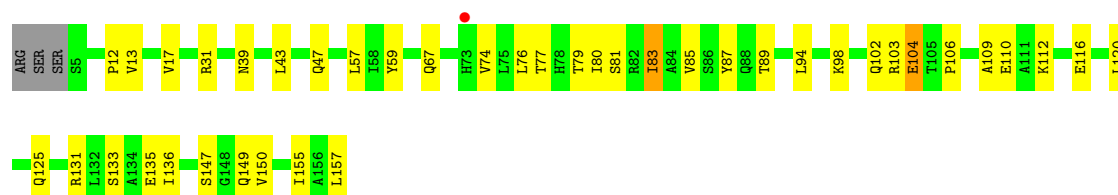
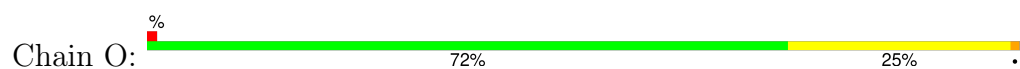
- Molecule 2: Tumor necrosis factor



- Molecule 2: Tumor necrosis factor



- Molecule 2: Tumor necrosis factor




- Molecule 2: Tumor necrosis factor

Chain S:  73% 23% ...



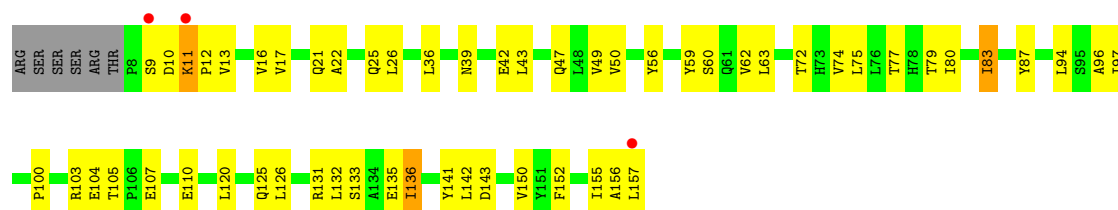
- Molecule 2: Tumor necrosis factor

Chain T:  76% 22% 3% .



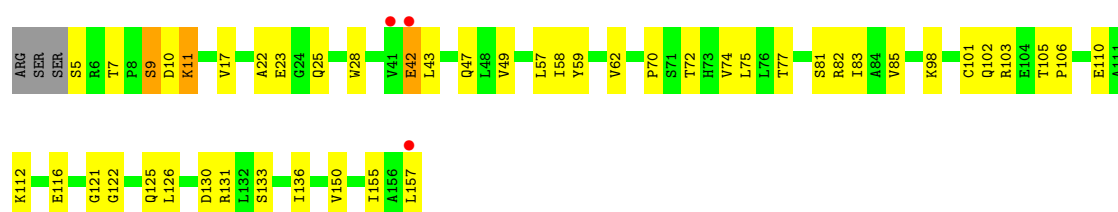
- Molecule 2: Tumor necrosis factor

Chain U:  60% 34% 2% . .



- Molecule 2: Tumor necrosis factor

Chain Y:  68% 28% 2% . .



- Molecule 2: Tumor necrosis factor

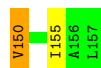
Chain Z:  74% 22% 4% . .





- Molecule 2: Tumor necrosis factor

Chain a: 78% 19% ..



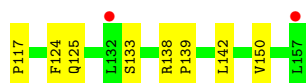
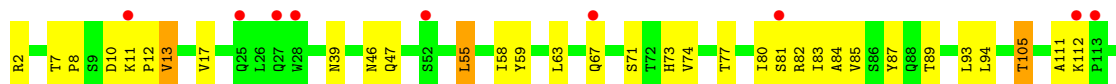
- Molecule 2: Tumor necrosis factor

Chain e: 4% 66% 29% ..



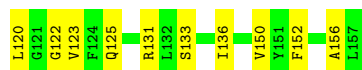
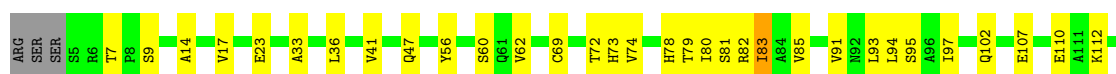
- Molecule 2: Tumor necrosis factor

Chain f: 7% 74% 24% .



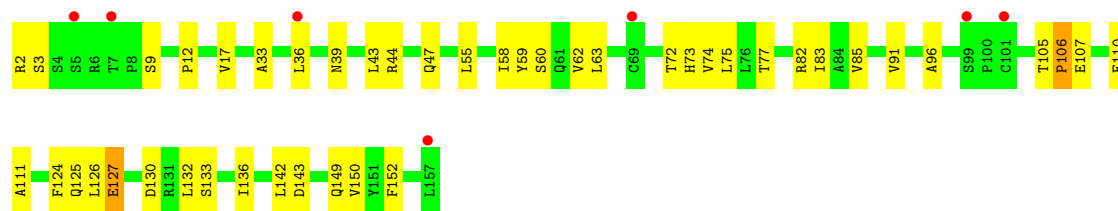
- Molecule 2: Tumor necrosis factor

Chain g: 71% 26% ..

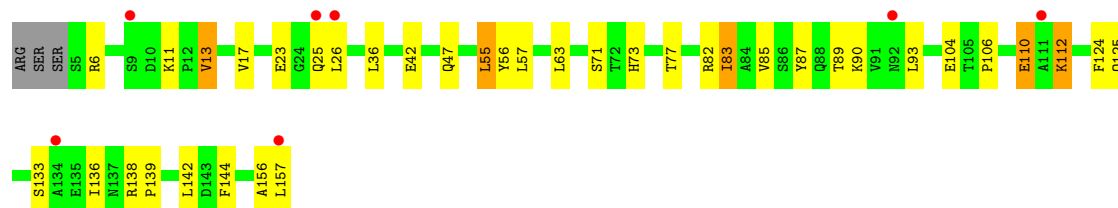


- Molecule 2: Tumor necrosis factor

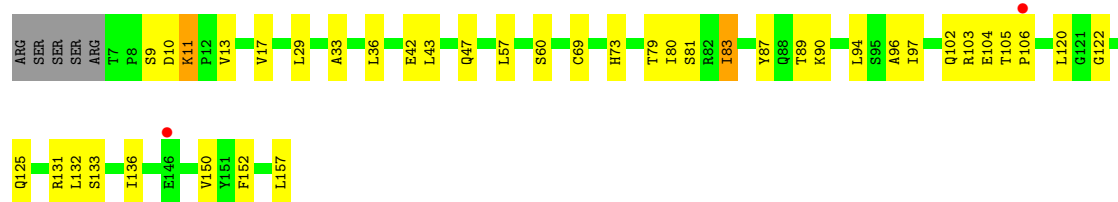
Chain k: 4% 71% 28% .



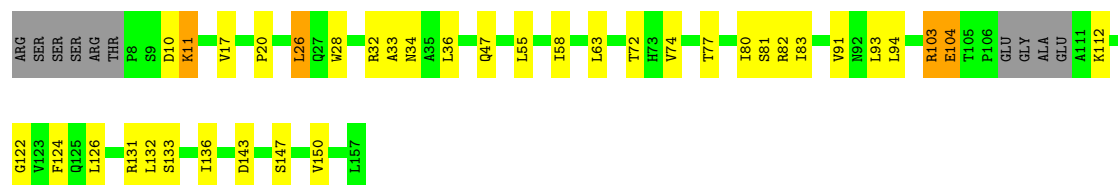
• Molecule 2: Tumor necrosis factor



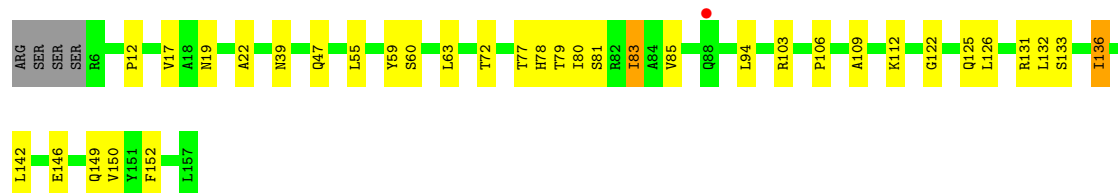
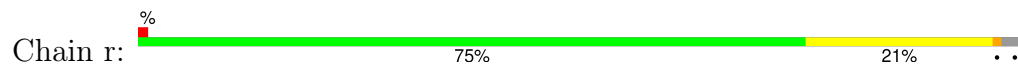
• Molecule 2: Tumor necrosis factor



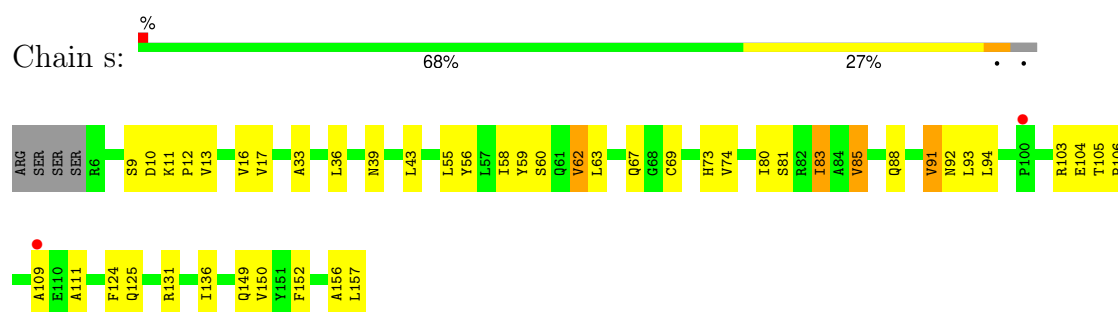
• Molecule 2: Tumor necrosis factor



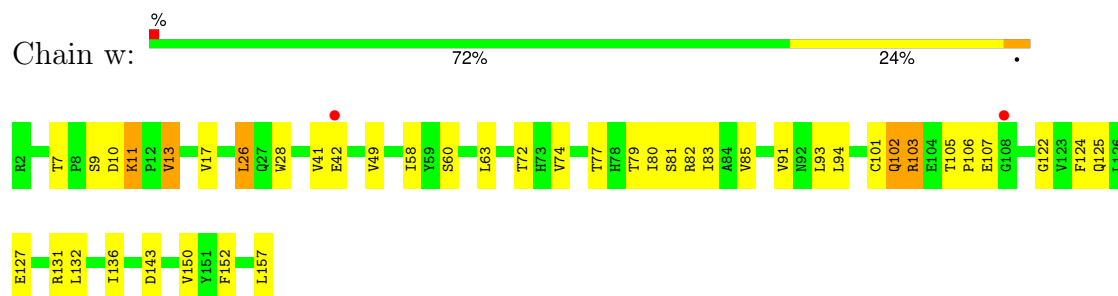
• Molecule 2: Tumor necrosis factor



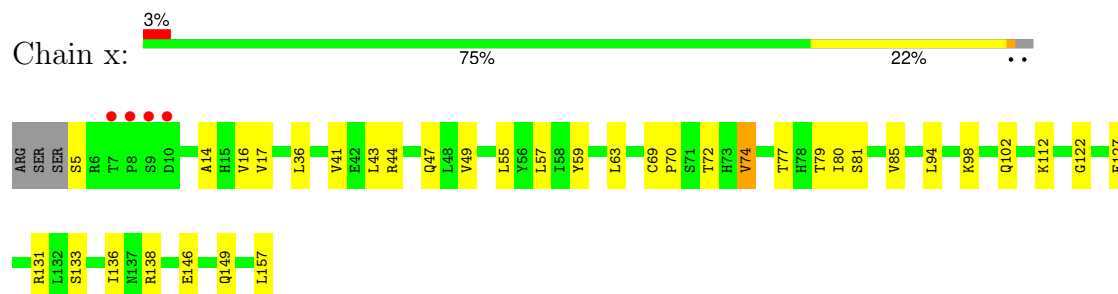
• Molecule 2: Tumor necrosis factor



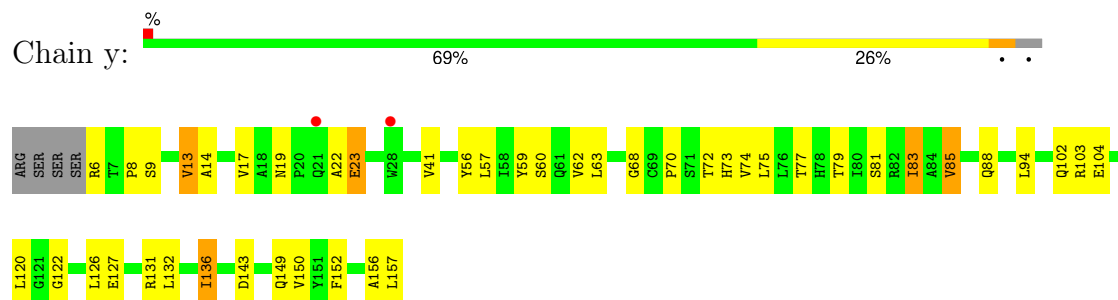
- Molecule 2: Tumor necrosis factor



- Molecule 2: Tumor necrosis factor



- Molecule 2: Tumor necrosis factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.32Å 218.13Å 236.49Å 90.00° 96.28° 90.00°	Depositor
Resolution (Å)	109.06 – 3.31 109.06 – 3.31	Depositor EDS
% Data completeness (in resolution range)	92.8 (109.06-3.31) 92.7 (109.06-3.31)	Depositor EDS
R_{merge}	0.58	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.235 , 0.294 0.235 , 0.293	Depositor DCC
R_{free} test set	7793 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 81.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	60848	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, 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	0.16	0/826	0.45	0/1118
1	1	0.17	0/808	0.48	0/1093
1	5	0.16	0/831	0.46	0/1125
1	6	0.17	0/826	0.51	0/1118
1	7	0.17	0/826	0.58	0/1118
1	D	0.18	0/821	0.48	0/1111
1	E	0.20	0/831	0.53	0/1125
1	F	0.19	0/821	0.62	0/1111
1	J	0.16	0/831	0.43	0/1125
1	K	0.15	0/821	0.43	0/1111
1	L	0.17	0/869	0.53	0/1177
1	P	0.16	0/826	0.46	0/1118
1	Q	0.17	0/869	0.45	0/1177
1	R	0.14	0/826	0.41	0/1118
1	V	0.16	0/832	0.43	0/1125
1	W	0.15	0/821	0.42	0/1111
1	X	0.16	0/826	0.44	0/1118
1	b	0.15	0/869	0.43	0/1177
1	c	0.15	0/869	0.47	0/1177
1	d	0.17	0/869	0.42	0/1177
1	h	0.15	0/869	0.46	0/1177
1	i	0.20	0/869	0.49	0/1177
1	j	0.16	0/813	0.52	0/1100
1	n	0.16	0/836	0.43	0/1132
1	o	0.17	0/808	0.58	0/1093
1	p	0.14	0/869	0.39	0/1177
1	t	0.17	0/869	0.45	0/1177
1	u	0.14	0/869	0.43	0/1177
1	v	0.14	0/813	0.48	0/1100
1	z	0.17	0/869	0.46	0/1177
2	2	0.16	0/1229	0.51	0/1672
2	3	0.13	0/1209	0.46	0/1642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	4	0.14	0/1235	0.44	0/1680
2	A	0.17	0/1246	0.49	0/1694
2	B	0.13	0/1223	0.43	0/1664
2	C	0.15	0/1223	0.49	0/1664
2	G	0.14	0/1223	0.44	0/1664
2	H	0.13	0/1215	0.41	0/1653
2	I	0.12	0/1217	0.44	0/1656
2	M	0.15	0/1223	0.44	0/1664
2	N	0.14	0/1223	0.40	0/1664
2	O	0.13	0/1223	0.45	0/1664
2	S	0.13	0/1229	0.47	0/1672
2	T	0.15	0/1246	0.43	0/1694
2	U	0.13	0/1199	0.44	0/1631
2	Y	0.13	0/1223	0.45	0/1664
2	Z	0.13	0/1217	0.42	0/1656
2	a	0.13	0/1229	0.42	0/1672
2	e	0.13	0/1223	0.47	0/1664
2	f	0.14	0/1246	0.41	0/1694
2	g	0.12	0/1223	0.45	0/1664
2	k	0.11	0/1246	0.43	0/1694
2	l	0.12	0/1223	0.39	0/1664
2	m	0.12	0/1206	0.43	0/1642
2	q	0.11	0/1171	0.46	0/1592
2	r	0.12	0/1217	0.41	0/1656
2	s	0.13	0/1217	0.45	0/1656
2	w	0.13	0/1246	0.48	0/1694
2	x	0.14	0/1223	0.41	0/1664
2	y	0.13	0/1217	0.43	0/1656
All	All	0.15	0/61892	0.46	0/84027

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	105	THR	Peptide

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	815	0	775	21	0
1	1	797	0	756	21	0
1	5	820	0	780	21	0
1	6	815	0	775	30	0
1	7	815	0	775	29	0
1	D	810	0	770	25	0
1	E	820	0	780	28	0
1	F	810	0	772	28	0
1	J	820	0	780	21	0
1	K	810	0	770	23	0
1	L	855	0	806	27	0
1	P	815	0	775	25	0
1	Q	855	0	806	19	0
1	R	815	0	775	34	0
1	V	821	0	782	18	0
1	W	810	0	770	19	0
1	X	815	0	775	18	0
1	b	855	0	806	18	0
1	c	855	0	806	29	0
1	d	855	0	806	12	0
1	h	855	0	806	21	0
1	i	855	0	806	24	0
1	j	802	0	764	28	0
1	n	825	0	785	17	0
1	o	797	0	756	33	0
1	p	855	0	806	22	0
1	t	855	0	806	22	0
1	u	855	0	806	23	0
1	v	802	0	764	21	0
1	z	855	0	806	23	0
2	2	1202	0	1195	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3	1183	0	1178	20	0
2	4	1208	0	1200	19	0
2	A	1219	0	1213	39	0
2	B	1196	0	1190	31	0
2	C	1196	0	1190	27	0
2	G	1196	0	1190	21	0
2	H	1188	0	1180	25	0
2	I	1190	0	1185	26	0
2	M	1196	0	1190	27	0
2	N	1196	0	1190	32	0
2	O	1196	0	1190	18	0
2	S	1202	0	1195	19	0
2	T	1219	0	1213	19	0
2	U	1172	0	1166	32	0
2	Y	1196	0	1190	25	0
2	Z	1190	0	1185	22	0
2	a	1202	0	1195	21	0
2	e	1196	0	1190	33	0
2	f	1219	0	1213	22	0
2	g	1196	0	1190	25	0
2	k	1219	0	1213	27	0
2	l	1196	0	1190	23	0
2	m	1179	0	1172	20	0
2	q	1145	0	1145	23	0
2	r	1190	0	1185	20	0
2	s	1190	0	1185	29	0
2	w	1219	0	1213	23	0
2	x	1196	0	1190	24	0
2	y	1190	0	1185	24	0
3	0	6	0	8	0	0
3	1	6	0	8	0	0
3	5	6	0	8	0	0
3	D	6	0	8	0	0
3	J	6	0	8	1	0
3	P	6	0	8	0	0
3	V	6	0	8	0	0
3	W	6	0	8	2	0
3	a	6	0	8	1	0
3	b	18	0	24	1	0
3	h	6	0	8	1	0
3	n	6	0	8	0	0
3	t	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	z	6	0	8	1	0
4	P	5	0	0	0	0
4	h	5	0	0	0	0
4	t	5	0	0	0	0
5	S	1	0	0	0	0
6	D	2	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	P	1	0	0	0	0
6	U	1	0	0	0	0
6	V	2	0	0	0	0
6	X	1	0	0	0	0
All	All	60848	0	59387	1285	0

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 11.

The worst 5 of 1285 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)
2:w:103:ARG:HD2	2:w:105:THR:H	1.28	0.95
1:7:7:PRO:HG2	1:7:20:ILE:HA	1.46	0.94
2:B:57:LEU:HB2	2:B:157:LEU:HD11	1.51	0.90
2:A:112:LYS:HG3	2:C:103:ARG:HG3	1.56	0.86
1:F:7:PRO:HG2	1:F:20:ILE:HA	1.59	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	105/129 (81%)	92 (88%)	13 (12%)	0	100	100
1	1	102/129 (79%)	86 (84%)	16 (16%)	0	100	100
1	5	106/129 (82%)	92 (87%)	14 (13%)	0	100	100
1	6	105/129 (81%)	93 (89%)	12 (11%)	0	100	100
1	7	105/129 (81%)	86 (82%)	19 (18%)	0	100	100
1	D	104/129 (81%)	90 (86%)	13 (12%)	1 (1%)	13	42
1	E	106/129 (82%)	87 (82%)	17 (16%)	2 (2%)	6	30
1	F	104/129 (81%)	77 (74%)	26 (25%)	1 (1%)	13	42
1	J	106/129 (82%)	93 (88%)	12 (11%)	1 (1%)	14	44
1	K	104/129 (81%)	87 (84%)	16 (15%)	1 (1%)	13	42
1	L	110/129 (85%)	88 (80%)	21 (19%)	1 (1%)	14	44
1	P	105/129 (81%)	88 (84%)	16 (15%)	1 (1%)	13	42
1	Q	110/129 (85%)	88 (80%)	20 (18%)	2 (2%)	7	31
1	R	105/129 (81%)	89 (85%)	15 (14%)	1 (1%)	13	42
1	V	105/129 (81%)	90 (86%)	14 (13%)	1 (1%)	13	42
1	W	104/129 (81%)	91 (88%)	13 (12%)	0	100	100
1	X	105/129 (81%)	86 (82%)	18 (17%)	1 (1%)	13	42
1	b	110/129 (85%)	92 (84%)	17 (16%)	1 (1%)	14	44
1	c	110/129 (85%)	91 (83%)	18 (16%)	1 (1%)	14	44
1	d	110/129 (85%)	91 (83%)	18 (16%)	1 (1%)	14	44
1	h	110/129 (85%)	93 (84%)	17 (16%)	0	100	100
1	i	110/129 (85%)	93 (84%)	16 (14%)	1 (1%)	14	44
1	j	103/129 (80%)	88 (85%)	14 (14%)	1 (1%)	13	42
1	n	107/129 (83%)	93 (87%)	13 (12%)	1 (1%)	14	44
1	o	102/129 (79%)	78 (76%)	23 (22%)	1 (1%)	13	42
1	p	110/129 (85%)	93 (84%)	16 (14%)	1 (1%)	14	44
1	t	110/129 (85%)	93 (84%)	15 (14%)	2 (2%)	7	31
1	u	110/129 (85%)	91 (83%)	18 (16%)	1 (1%)	14	44
1	v	103/129 (80%)	90 (87%)	13 (13%)	0	100	100
1	z	110/129 (85%)	90 (82%)	19 (17%)	1 (1%)	14	44
2	2	152/156 (97%)	126 (83%)	24 (16%)	2 (1%)	10	37
2	3	148/156 (95%)	129 (87%)	18 (12%)	1 (1%)	19	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	4	153/156 (98%)	135 (88%)	17 (11%)	1 (1%)	19	50
2	A	154/156 (99%)	133 (86%)	18 (12%)	3 (2%)	6	30
2	B	151/156 (97%)	128 (85%)	22 (15%)	1 (1%)	19	50
2	C	151/156 (97%)	128 (85%)	21 (14%)	2 (1%)	10	37
2	G	151/156 (97%)	127 (84%)	21 (14%)	3 (2%)	6	29
2	H	150/156 (96%)	130 (87%)	20 (13%)	0	100	100
2	I	150/156 (96%)	128 (85%)	20 (13%)	2 (1%)	10	37
2	M	151/156 (97%)	125 (83%)	25 (17%)	1 (1%)	19	50
2	N	151/156 (97%)	135 (89%)	16 (11%)	0	100	100
2	O	151/156 (97%)	131 (87%)	19 (13%)	1 (1%)	19	50
2	S	152/156 (97%)	124 (82%)	24 (16%)	4 (3%)	4	24
2	T	154/156 (99%)	132 (86%)	21 (14%)	1 (1%)	22	53
2	U	148/156 (95%)	127 (86%)	20 (14%)	1 (1%)	19	50
2	Y	151/156 (97%)	130 (86%)	18 (12%)	3 (2%)	6	29
2	Z	150/156 (96%)	128 (85%)	22 (15%)	0	100	100
2	a	152/156 (97%)	133 (88%)	18 (12%)	1 (1%)	19	50
2	e	151/156 (97%)	126 (83%)	23 (15%)	2 (1%)	10	37
2	f	154/156 (99%)	130 (84%)	23 (15%)	1 (1%)	22	53
2	g	151/156 (97%)	126 (83%)	25 (17%)	0	100	100
2	k	154/156 (99%)	129 (84%)	23 (15%)	2 (1%)	10	37
2	l	151/156 (97%)	133 (88%)	18 (12%)	0	100	100
2	m	149/156 (96%)	130 (87%)	18 (12%)	1 (1%)	19	50
2	q	142/156 (91%)	124 (87%)	15 (11%)	3 (2%)	5	28
2	r	150/156 (96%)	132 (88%)	18 (12%)	0	100	100
2	s	150/156 (96%)	123 (82%)	27 (18%)	0	100	100
2	w	154/156 (99%)	132 (86%)	20 (13%)	2 (1%)	10	37
2	x	151/156 (97%)	130 (86%)	21 (14%)	0	100	100
2	y	150/156 (96%)	131 (87%)	19 (13%)	0	100	100
All	All	7723/8550 (90%)	6554 (85%)	1106 (14%)	63 (1%)	16	47

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	33	ALA
2	C	72	THR
1	E	49	ILE
2	G	9	SER
2	S	104	GLU

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	92/109 (84%)	74 (80%)	18 (20%)	1	5
1	1	91/109 (84%)	75 (82%)	16 (18%)	1	7
1	5	92/109 (84%)	78 (85%)	14 (15%)	2	11
1	6	92/109 (84%)	73 (79%)	19 (21%)	1	4
1	7	92/109 (84%)	73 (79%)	19 (21%)	1	4
1	D	92/109 (84%)	79 (86%)	13 (14%)	3	13
1	E	92/109 (84%)	73 (79%)	19 (21%)	1	4
1	F	92/109 (84%)	74 (80%)	18 (20%)	1	5
1	J	92/109 (84%)	78 (85%)	14 (15%)	2	11
1	K	92/109 (84%)	79 (86%)	13 (14%)	3	13
1	L	95/109 (87%)	72 (76%)	23 (24%)	0	2
1	P	92/109 (84%)	72 (78%)	20 (22%)	1	3
1	Q	95/109 (87%)	73 (77%)	22 (23%)	0	3
1	R	92/109 (84%)	78 (85%)	14 (15%)	2	11
1	V	93/109 (85%)	81 (87%)	12 (13%)	3	15
1	W	92/109 (84%)	73 (79%)	19 (21%)	1	4
1	X	92/109 (84%)	73 (79%)	19 (21%)	1	4
1	b	95/109 (87%)	82 (86%)	13 (14%)	3	14
1	c	95/109 (87%)	84 (88%)	11 (12%)	4	18
1	d	95/109 (87%)	84 (88%)	11 (12%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	h	95/109 (87%)	81 (85%)	14 (15%)	2	12
1	i	95/109 (87%)	85 (90%)	10 (10%)	5	22
1	j	91/109 (84%)	78 (86%)	13 (14%)	2	13
1	n	92/109 (84%)	78 (85%)	14 (15%)	2	11
1	o	91/109 (84%)	75 (82%)	16 (18%)	1	7
1	p	95/109 (87%)	81 (85%)	14 (15%)	2	12
1	t	95/109 (87%)	83 (87%)	12 (13%)	3	16
1	u	95/109 (87%)	82 (86%)	13 (14%)	3	14
1	v	91/109 (84%)	80 (88%)	11 (12%)	4	17
1	z	95/109 (87%)	82 (86%)	13 (14%)	3	14
2	2	130/132 (98%)	114 (88%)	16 (12%)	4	16
2	3	127/132 (96%)	114 (90%)	13 (10%)	6	23
2	4	131/132 (99%)	111 (85%)	20 (15%)	2	11
2	A	132/132 (100%)	117 (89%)	15 (11%)	4	19
2	B	129/132 (98%)	118 (92%)	11 (8%)	8	31
2	C	129/132 (98%)	113 (88%)	16 (12%)	4	16
2	G	129/132 (98%)	117 (91%)	12 (9%)	7	27
2	H	127/132 (96%)	110 (87%)	17 (13%)	3	14
2	I	128/132 (97%)	116 (91%)	12 (9%)	7	26
2	M	129/132 (98%)	116 (90%)	13 (10%)	6	23
2	N	129/132 (98%)	107 (83%)	22 (17%)	1	8
2	O	129/132 (98%)	114 (88%)	15 (12%)	4	18
2	S	130/132 (98%)	116 (89%)	14 (11%)	5	21
2	T	132/132 (100%)	119 (90%)	13 (10%)	6	25
2	U	126/132 (96%)	112 (89%)	14 (11%)	5	20
2	Y	129/132 (98%)	114 (88%)	15 (12%)	4	18
2	Z	128/132 (97%)	119 (93%)	9 (7%)	12	38
2	a	130/132 (98%)	121 (93%)	9 (7%)	13	39
2	e	129/132 (98%)	116 (90%)	13 (10%)	6	23
2	f	132/132 (100%)	119 (90%)	13 (10%)	6	25
2	g	129/132 (98%)	118 (92%)	11 (8%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	k	132/132 (100%)	120 (91%)	12 (9%)	7	28
2	l	129/132 (98%)	116 (90%)	13 (10%)	6	23
2	m	127/132 (96%)	115 (91%)	12 (9%)	7	26
2	q	124/132 (94%)	113 (91%)	11 (9%)	8	29
2	r	128/132 (97%)	120 (94%)	8 (6%)	15	41
2	s	128/132 (97%)	119 (93%)	9 (7%)	12	38
2	w	132/132 (100%)	114 (86%)	18 (14%)	3	14
2	x	129/132 (98%)	121 (94%)	8 (6%)	15	42
2	y	128/132 (97%)	115 (90%)	13 (10%)	6	23
All	All	6661/7230 (92%)	5807 (87%)	854 (13%)	3	15

5 of 854 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	U	155	ILE
1	d	6	THR
1	v	87	CYS
1	V	106	ASN
2	U	150	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
2	f	39	ASN
2	m	92	ASN
2	f	47	GLN
2	l	46	ASN
2	q	47	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

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	$\# Z > 2$
3	GOL	5	201	-	5,5,5	0.37	0	5,5,5	0.50	0
3	GOL	b	201	-	5,5,5	0.35	0	5,5,5	0.46	0
3	GOL	t	203	-	5,5,5	0.35	0	5,5,5	0.42	0
3	GOL	a	201	-	5,5,5	0.35	0	5,5,5	0.42	0
3	GOL	h	202	-	5,5,5	0.35	0	5,5,5	0.43	0
3	GOL	t	202	-	5,5,5	0.33	0	5,5,5	0.42	0
3	GOL	z	201	-	5,5,5	0.34	0	5,5,5	0.36	0
4	SO4	h	201	-	4,4,4	0.64	0	6,6,6	0.09	0
4	SO4	t	201	-	4,4,4	0.66	0	6,6,6	0.09	0
3	GOL	D	201	-	5,5,5	0.34	0	5,5,5	0.40	0
3	GOL	J	201	-	5,5,5	0.35	0	5,5,5	0.42	0
3	GOL	P	202	-	5,5,5	0.34	0	5,5,5	0.40	0
3	GOL	W	201	-	5,5,5	0.34	0	5,5,5	0.40	0
3	GOL	0	201	-	5,5,5	0.35	0	5,5,5	0.39	0
4	SO4	P	201	-	4,4,4	0.67	0	6,6,6	0.07	0
3	GOL	V	201	-	5,5,5	0.35	0	5,5,5	0.42	0
3	GOL	b	202	-	5,5,5	0.33	0	5,5,5	0.41	0
3	GOL	1	201	-	5,5,5	0.34	0	5,5,5	0.36	0
3	GOL	b	203	-	5,5,5	0.34	0	5,5,5	0.42	0
3	GOL	n	201	-	5,5,5	0.34	0	5,5,5	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	t	202	-	-	2/4/4/4	-
3	GOL	P	202	-	-	2/4/4/4	-
3	GOL	5	201	-	-	0/4/4/4	-
3	GOL	1	201	-	-	2/4/4/4	-
3	GOL	b	203	-	-	4/4/4/4	-
3	GOL	W	201	-	-	1/4/4/4	-
3	GOL	z	201	-	-	0/4/4/4	-
3	GOL	b	201	-	-	0/4/4/4	-
3	GOL	0	201	-	-	0/4/4/4	-
3	GOL	n	201	-	-	0/4/4/4	-
3	GOL	V	201	-	-	0/4/4/4	-
3	GOL	D	201	-	-	0/4/4/4	-
3	GOL	t	203	-	-	2/4/4/4	-
3	GOL	J	201	-	-	4/4/4/4	-
3	GOL	b	202	-	-	0/4/4/4	-
3	GOL	a	201	-	-	0/4/4/4	-
3	GOL	h	202	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	201	GOL	O1-C1-C2-C3
3	J	201	GOL	C1-C2-C3-O3
3	P	202	GOL	O1-C1-C2-O2
3	P	202	GOL	O1-C1-C2-C3
3	b	203	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	b	201	GOL	1	0
3	a	201	GOL	1	0
3	h	202	GOL	1	0
3	t	202	GOL	1	0
3	z	201	GOL	1	0
3	J	201	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	W	201	GOL	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	107/129 (82%)	0.13	1 (0%) 81 70	71, 120, 172, 228	0
1	1	104/129 (80%)	0.12	2 (1%) 66 51	51, 129, 181, 218	0
1	5	108/129 (83%)	-0.16	0 100 100	42, 66, 98, 143	0
1	6	107/129 (82%)	0.02	0 100 100	95, 131, 165, 188	0
1	7	107/129 (82%)	0.37	3 (2%) 55 40	94, 169, 221, 233	0
1	D	106/129 (82%)	0.10	2 (1%) 66 51	43, 70, 111, 152	0
1	E	108/129 (83%)	0.03	1 (0%) 81 70	81, 131, 194, 213	0
1	F	106/129 (82%)	-0.01	1 (0%) 81 70	82, 156, 218, 248	0
1	J	108/129 (83%)	-0.14	0 100 100	44, 65, 91, 132	0
1	K	106/129 (82%)	-0.02	0 100 100	69, 110, 162, 211	0
1	L	112/129 (86%)	0.35	5 (4%) 39 29	71, 140, 195, 255	0
1	P	107/129 (82%)	-0.13	0 100 100	45, 68, 95, 111	0
1	Q	112/129 (86%)	0.26	2 (1%) 67 53	87, 133, 182, 199	0
1	R	107/129 (82%)	0.18	1 (0%) 81 70	56, 132, 192, 225	0
1	V	106/129 (82%)	-0.05	3 (2%) 55 40	39, 64, 96, 124	1 (0%)
1	W	106/129 (82%)	0.07	0 100 100	72, 110, 154, 203	0
1	X	107/129 (82%)	0.19	0 100 100	71, 107, 154, 172	0
1	b	112/129 (86%)	0.04	1 (0%) 81 70	49, 77, 152, 294	0
1	c	112/129 (86%)	0.02	0 100 100	56, 102, 196, 239	0
1	d	112/129 (86%)	0.24	2 (1%) 67 53	65, 126, 187, 246	0
1	h	112/129 (86%)	-0.09	1 (0%) 81 70	38, 72, 151, 247	0
1	i	112/129 (86%)	0.66	9 (8%) 20 17	89, 153, 210, 227	0
1	j	105/129 (81%)	0.52	5 (4%) 36 28	127, 168, 202, 245	0
1	n	109/129 (84%)	-0.01	2 (1%) 67 53	50, 72, 117, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	o	104/129 (80%)	0.40	4 (3%) 44 33	112, 196, 248, 268	0
1	p	112/129 (86%)	0.15	0 100 100	86, 130, 170, 196	0
1	t	112/129 (86%)	0.17	3 (2%) 56 41	42, 74, 242, 307	0
1	u	112/129 (86%)	0.24	1 (0%) 81 70	67, 129, 196, 236	0
1	v	105/129 (81%)	0.33	0 100 100	76, 161, 221, 244	0
1	z	112/129 (86%)	-0.15	0 100 100	40, 63, 116, 209	0
2	2	154/156 (98%)	-0.00	5 (3%) 50 36	43, 86, 208, 353	0
2	3	151/156 (96%)	0.39	13 (8%) 18 16	64, 110, 228, 296	0
2	4	155/156 (99%)	-0.10	3 (1%) 66 51	44, 85, 210, 233	0
2	A	156/156 (100%)	-0.06	4 (2%) 57 42	36, 77, 189, 239	0
2	B	153/156 (98%)	0.01	2 (1%) 74 62	54, 90, 202, 259	0
2	C	153/156 (98%)	0.03	3 (1%) 64 49	45, 82, 184, 233	0
2	G	153/156 (98%)	-0.15	2 (1%) 74 62	37, 65, 165, 206	0
2	H	152/156 (97%)	0.24	6 (3%) 44 32	40, 71, 196, 260	0
2	I	152/156 (97%)	-0.10	2 (1%) 74 62	33, 66, 166, 231	0
2	M	153/156 (98%)	-0.11	2 (1%) 74 62	37, 75, 273, 309	0
2	N	153/156 (98%)	-0.00	1 (0%) 84 75	54, 96, 199, 231	0
2	O	153/156 (98%)	-0.01	1 (0%) 84 75	47, 83, 233, 283	0
2	S	154/156 (98%)	0.00	0 100 100	33, 66, 170, 200	0
2	T	156/156 (100%)	0.12	5 (3%) 50 36	32, 69, 177, 265	0
2	U	150/156 (96%)	-0.25	3 (2%) 64 49	33, 61, 142, 215	0
2	Y	153/156 (98%)	-0.08	3 (1%) 64 49	36, 60, 134, 195	0
2	Z	152/156 (97%)	0.01	6 (3%) 44 32	23, 66, 162, 212	0
2	a	154/156 (98%)	-0.23	0 100 100	35, 62, 145, 181	0
2	e	153/156 (98%)	0.20	6 (3%) 44 32	47, 94, 178, 221	0
2	f	156/156 (100%)	0.54	11 (7%) 23 19	87, 128, 202, 245	0
2	g	153/156 (98%)	0.05	0 100 100	56, 110, 186, 210	0
2	k	156/156 (100%)	0.37	7 (4%) 39 29	55, 92, 203, 305	0
2	l	153/156 (98%)	0.45	7 (4%) 38 29	81, 122, 211, 278	0
2	m	151/156 (96%)	0.20	2 (1%) 74 62	60, 101, 191, 244	0
2	q	146/156 (93%)	-0.32	0 100 100	37, 75, 164, 264	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	r	152/156 (97%)	-0.10	1 (0%) 84 75	51, 87, 183, 230	0
2	s	152/156 (97%)	-0.04	2 (1%) 74 62	42, 77, 209, 263	0
2	w	156/156 (100%)	-0.08	2 (1%) 74 62	40, 70, 176, 244	0
2	x	153/156 (98%)	0.07	4 (2%) 57 42	40, 75, 175, 208	0
2	y	152/156 (97%)	-0.16	2 (1%) 74 62	34, 67, 161, 217	0
All	All	7845/8550 (91%)	0.07	154 (1%) 64 49	23, 93, 196, 353	1 (0%)

The worst 5 of 154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	42	GLU	5.2
2	3	42	GLU	5.1
2	3	41	VAL	4.7
1	j	1	ALA	4.4
2	3	43	LEU	4.1

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
3	GOL	1	201	6/6	0.68	0.13	58,66,78,79	0
3	GOL	0	201	6/6	0.72	0.14	60,62,78,81	0
3	GOL	t	203	6/6	0.76	0.12	59,89,97,113	0
3	GOL	b	203	6/6	0.77	0.12	56,71,77,88	0
3	GOL	a	201	6/6	0.77	0.15	58,71,79,81	0
3	GOL	z	201	6/6	0.77	0.12	53,61,82,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	P	202	6/6	0.78	0.10	61,66,83,91	0
3	GOL	5	201	6/6	0.82	0.14	52,63,65,78	0
3	GOL	n	201	6/6	0.86	0.09	60,70,89,103	0
3	GOL	t	202	6/6	0.87	0.09	66,69,85,88	0
3	GOL	W	201	6/6	0.88	0.08	61,74,90,96	0
3	GOL	h	202	6/6	0.88	0.09	54,61,72,75	0
3	GOL	D	201	6/6	0.88	0.08	52,62,81,81	0
3	GOL	b	202	6/6	0.89	0.07	47,69,81,88	0
4	SO4	h	201	5/5	0.89	0.10	56,91,117,136	0
3	GOL	J	201	6/6	0.91	0.10	31,36,52,72	0
3	GOL	b	201	6/6	0.91	0.10	33,58,66,81	0
3	GOL	V	201	6/6	0.92	0.11	48,61,62,78	0
4	SO4	t	201	5/5	0.92	0.16	68,70,90,139	0
4	SO4	P	201	5/5	0.94	0.09	64,71,96,103	0
5	CL	S	201	1/1	0.96	0.04	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.