



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:51 PM GMT

PDB ID : 4MXW  
Title : Structure of heterotrimeric lymphotoxin LTa1b2 bound to lymphotoxin beta receptor LTbR and anti-LTa Fab  
Authors : Sudhamsu, J.; Yin, J.P.; Hymowitz, S.G.  
Deposited on : 2013-09-26  
Resolution : 3.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

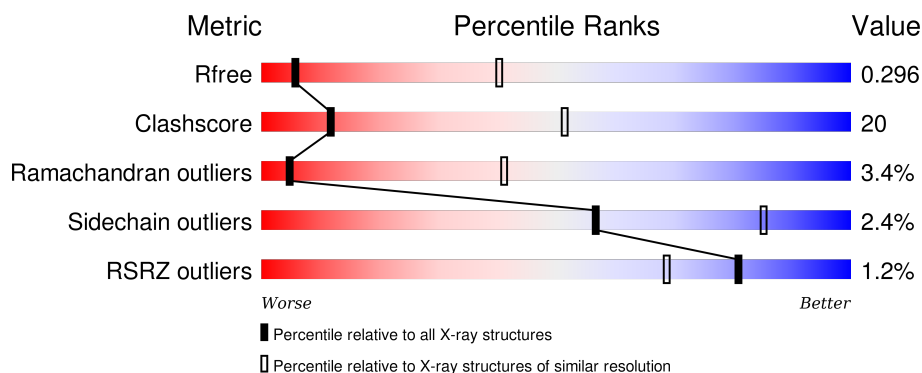
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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

Mol	Chain	Length	Quality of chain
1	R	193	<div> <div>2%</div> <div>37%</div> <div>33%</div> <div>7%</div> <div>23%</div> </div>
1	S	193	<div> <div>2%</div> <div>19%</div> <div>19%</div> <div>••</div> <div>59%</div> </div>
2	A	157	<div> <div>52%</div> <div>31%</div> <div>•</div> <div>15%</div> </div>
2	X	157	<div> <div>%</div> <div>56%</div> <div>29%</div> <div>•</div> <div>15%</div> </div>
3	B	210	<div> <div>35%</div> <div>23%</div> <div>•</div> <div>40%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	210	
3	Y	210	
3	Z	210	
4	H	213	
4	W	213	
5	L	211	
5	V	211	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14217 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 Tumor necrosis factor receptor superfamily member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	79	Total	C	N	O	S	0	0	0
			622	374	118	118	12			
1	R	149	Total	C	N	O	S	0	0	0
			1136	677	214	223	22			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	19	ALA	-	EXPRESSION TAG	UNP P36941
S	20	ASP	-	EXPRESSION TAG	UNP P36941
S	21	LEU	-	EXPRESSION TAG	UNP P36941
S	22	GLY	-	EXPRESSION TAG	UNP P36941
S	23	SER	-	EXPRESSION TAG	UNP P36941
S	24	HIS	-	EXPRESSION TAG	UNP P36941
S	25	HIS	-	EXPRESSION TAG	UNP P36941
S	26	HIS	-	EXPRESSION TAG	UNP P36941
S	27	HIS	-	EXPRESSION TAG	UNP P36941
S	28	HIS	-	EXPRESSION TAG	UNP P36941
S	29	HIS	-	EXPRESSION TAG	UNP P36941
S	30	SER	-	EXPRESSION TAG	UNP P36941
S	31	SER	-	EXPRESSION TAG	UNP P36941
S	32	GLY	-	EXPRESSION TAG	UNP P36941
S	33	LEU	-	EXPRESSION TAG	UNP P36941
S	34	VAL	-	EXPRESSION TAG	UNP P36941
S	35	PRO	-	EXPRESSION TAG	UNP P36941
S	36	ARG	-	EXPRESSION TAG	UNP P36941
S	37	GLY	-	EXPRESSION TAG	UNP P36941
S	38	SER	-	EXPRESSION TAG	UNP P36941
S	39	HIS	-	EXPRESSION TAG	UNP P36941
S	40	MET	-	EXPRESSION TAG	UNP P36941
R	19	ALA	-	EXPRESSION TAG	UNP P36941
R	20	ASP	-	EXPRESSION TAG	UNP P36941
R	21	LEU	-	EXPRESSION TAG	UNP P36941

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Chain	Residue	Modelled	Actual	Comment	Reference
R	22	GLY	-	EXPRESSION TAG	UNP P36941
R	23	SER	-	EXPRESSION TAG	UNP P36941
R	24	HIS	-	EXPRESSION TAG	UNP P36941
R	25	HIS	-	EXPRESSION TAG	UNP P36941
R	26	HIS	-	EXPRESSION TAG	UNP P36941
R	27	HIS	-	EXPRESSION TAG	UNP P36941
R	28	HIS	-	EXPRESSION TAG	UNP P36941
R	29	HIS	-	EXPRESSION TAG	UNP P36941
R	30	SER	-	EXPRESSION TAG	UNP P36941
R	31	SER	-	EXPRESSION TAG	UNP P36941
R	32	GLY	-	EXPRESSION TAG	UNP P36941
R	33	LEU	-	EXPRESSION TAG	UNP P36941
R	34	VAL	-	EXPRESSION TAG	UNP P36941
R	35	PRO	-	EXPRESSION TAG	UNP P36941
R	36	ARG	-	EXPRESSION TAG	UNP P36941
R	37	GLY	-	EXPRESSION TAG	UNP P36941
R	38	SER	-	EXPRESSION TAG	UNP P36941
R	39	HIS	-	EXPRESSION TAG	UNP P36941
R	40	MET	-	EXPRESSION TAG	UNP P36941

- Molecule 2 is a protein called Lymphotoxin-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	134	Total	C	N	O	S	0	0	0
			1055	689	173	191	2			
2	A	134	Total	C	N	O	S	0	0	0
			1055	689	173	191	2			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	49	ALA	-	EXPRESSION TAG	UNP P01374
X	50	ASP	-	EXPRESSION TAG	UNP P01374
X	51	LEU	-	EXPRESSION TAG	UNP P01374
X	52	GLY	-	EXPRESSION TAG	UNP P01374
X	53	SER	-	EXPRESSION TAG	UNP P01374
X	54	ASP	-	EXPRESSION TAG	UNP P01374
X	55	TYR	-	EXPRESSION TAG	UNP P01374
X	56	LYS	-	EXPRESSION TAG	UNP P01374
X	57	ASP	-	EXPRESSION TAG	UNP P01374
X	58	ASP	-	EXPRESSION TAG	UNP P01374
X	59	ASP	-	EXPRESSION TAG	UNP P01374

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Chain	Residue	Modelled	Actual	Comment	Reference
X	60	ASP	-	EXPRESSION TAG	UNP P01374
X	61	LYS	-	EXPRESSION TAG	UNP P01374
A	49	ALA	-	EXPRESSION TAG	UNP P01374
A	50	ASP	-	EXPRESSION TAG	UNP P01374
A	51	LEU	-	EXPRESSION TAG	UNP P01374
A	52	GLY	-	EXPRESSION TAG	UNP P01374
A	53	SER	-	EXPRESSION TAG	UNP P01374
A	54	ASP	-	EXPRESSION TAG	UNP P01374
A	55	TYR	-	EXPRESSION TAG	UNP P01374
A	56	LYS	-	EXPRESSION TAG	UNP P01374
A	57	ASP	-	EXPRESSION TAG	UNP P01374
A	58	ASP	-	EXPRESSION TAG	UNP P01374
A	59	ASP	-	EXPRESSION TAG	UNP P01374
A	60	ASP	-	EXPRESSION TAG	UNP P01374
A	61	LYS	-	EXPRESSION TAG	UNP P01374

- Molecule 3 is a protein called Lymphotoxin-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	131	Total	C	N	O	S	0	0	0
			961	617	162	179	3			
3	Z	134	Total	C	N	O	S	0	0	0
			988	637	163	185	3			
3	B	126	Total	C	N	O	S	0	0	0
			936	604	154	175	3			
3	D	135	Total	C	N	O	S	0	0	0
			1004	648	167	186	3			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	43	MET	-	EXPRESSION TAG	UNP Q06643
Y	44	LEU	-	EXPRESSION TAG	UNP Q06643
Y	45	LEU	-	EXPRESSION TAG	UNP Q06643
Y	46	VAL	-	EXPRESSION TAG	UNP Q06643
Y	47	ASN	-	EXPRESSION TAG	UNP Q06643
Y	48	GLN	-	EXPRESSION TAG	UNP Q06643
Y	49	SER	-	EXPRESSION TAG	UNP Q06643
Y	50	HIS	-	EXPRESSION TAG	UNP Q06643
Y	51	GLN	-	EXPRESSION TAG	UNP Q06643
Y	52	GLY	-	EXPRESSION TAG	UNP Q06643
Y	53	PHE	-	EXPRESSION TAG	UNP Q06643

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	54	ASN	-	EXPRESSION TAG	UNP Q06643
Y	55	LYS	-	EXPRESSION TAG	UNP Q06643
Y	56	GLU	-	EXPRESSION TAG	UNP Q06643
Y	57	HIS	-	EXPRESSION TAG	UNP Q06643
Y	58	THR	-	EXPRESSION TAG	UNP Q06643
Y	59	SER	-	EXPRESSION TAG	UNP Q06643
Y	60	LYS	-	EXPRESSION TAG	UNP Q06643
Y	61	MET	-	EXPRESSION TAG	UNP Q06643
Y	62	VAL	-	EXPRESSION TAG	UNP Q06643
Y	63	SER	-	EXPRESSION TAG	UNP Q06643
Y	64	ALA	-	EXPRESSION TAG	UNP Q06643
Y	65	ILE	-	EXPRESSION TAG	UNP Q06643
Y	66	VAL	-	EXPRESSION TAG	UNP Q06643
Y	67	LEU	-	EXPRESSION TAG	UNP Q06643
Y	68	TYR	-	EXPRESSION TAG	UNP Q06643
Y	69	VAL	-	EXPRESSION TAG	UNP Q06643
Y	70	LEU	-	EXPRESSION TAG	UNP Q06643
Y	71	LEU	-	EXPRESSION TAG	UNP Q06643
Y	72	ALA	-	EXPRESSION TAG	UNP Q06643
Y	73	ALA	-	EXPRESSION TAG	UNP Q06643
Y	74	ALA	-	EXPRESSION TAG	UNP Q06643
Y	75	ALA	-	EXPRESSION TAG	UNP Q06643
Y	76	HIS	-	EXPRESSION TAG	UNP Q06643
Y	77	SER	-	EXPRESSION TAG	UNP Q06643
Y	78	ALA	-	EXPRESSION TAG	UNP Q06643
Y	79	PHE	-	EXPRESSION TAG	UNP Q06643
Y	80	ALA	-	EXPRESSION TAG	UNP Q06643
Y	81	ALA	-	EXPRESSION TAG	UNP Q06643
Y	82	ASP	-	EXPRESSION TAG	UNP Q06643
Y	83	LEU	-	EXPRESSION TAG	UNP Q06643
Y	84	GLY	-	EXPRESSION TAG	UNP Q06643
Y	85	SER	-	EXPRESSION TAG	UNP Q06643
Y	245	HIS	-	EXPRESSION TAG	UNP Q06643
Y	246	HIS	-	EXPRESSION TAG	UNP Q06643
Y	247	HIS	-	EXPRESSION TAG	UNP Q06643
Y	248	HIS	-	EXPRESSION TAG	UNP Q06643
Y	249	HIS	-	EXPRESSION TAG	UNP Q06643
Y	250	HIS	-	EXPRESSION TAG	UNP Q06643
Y	251	HIS	-	EXPRESSION TAG	UNP Q06643
Y	252	HIS	-	EXPRESSION TAG	UNP Q06643
Z	43	MET	-	EXPRESSION TAG	UNP Q06643
Z	44	LEU	-	EXPRESSION TAG	UNP Q06643

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	45	LEU	-	EXPRESSION TAG	UNP Q06643
Z	46	VAL	-	EXPRESSION TAG	UNP Q06643
Z	47	ASN	-	EXPRESSION TAG	UNP Q06643
Z	48	GLN	-	EXPRESSION TAG	UNP Q06643
Z	49	SER	-	EXPRESSION TAG	UNP Q06643
Z	50	HIS	-	EXPRESSION TAG	UNP Q06643
Z	51	GLN	-	EXPRESSION TAG	UNP Q06643
Z	52	GLY	-	EXPRESSION TAG	UNP Q06643
Z	53	PHE	-	EXPRESSION TAG	UNP Q06643
Z	54	ASN	-	EXPRESSION TAG	UNP Q06643
Z	55	LYS	-	EXPRESSION TAG	UNP Q06643
Z	56	GLU	-	EXPRESSION TAG	UNP Q06643
Z	57	HIS	-	EXPRESSION TAG	UNP Q06643
Z	58	THR	-	EXPRESSION TAG	UNP Q06643
Z	59	SER	-	EXPRESSION TAG	UNP Q06643
Z	60	LYS	-	EXPRESSION TAG	UNP Q06643
Z	61	MET	-	EXPRESSION TAG	UNP Q06643
Z	62	VAL	-	EXPRESSION TAG	UNP Q06643
Z	63	SER	-	EXPRESSION TAG	UNP Q06643
Z	64	ALA	-	EXPRESSION TAG	UNP Q06643
Z	65	ILE	-	EXPRESSION TAG	UNP Q06643
Z	66	VAL	-	EXPRESSION TAG	UNP Q06643
Z	67	LEU	-	EXPRESSION TAG	UNP Q06643
Z	68	TYR	-	EXPRESSION TAG	UNP Q06643
Z	69	VAL	-	EXPRESSION TAG	UNP Q06643
Z	70	LEU	-	EXPRESSION TAG	UNP Q06643
Z	71	LEU	-	EXPRESSION TAG	UNP Q06643
Z	72	ALA	-	EXPRESSION TAG	UNP Q06643
Z	73	ALA	-	EXPRESSION TAG	UNP Q06643
Z	74	ALA	-	EXPRESSION TAG	UNP Q06643
Z	75	ALA	-	EXPRESSION TAG	UNP Q06643
Z	76	HIS	-	EXPRESSION TAG	UNP Q06643
Z	77	SER	-	EXPRESSION TAG	UNP Q06643
Z	78	ALA	-	EXPRESSION TAG	UNP Q06643
Z	79	PHE	-	EXPRESSION TAG	UNP Q06643
Z	80	ALA	-	EXPRESSION TAG	UNP Q06643
Z	81	ALA	-	EXPRESSION TAG	UNP Q06643
Z	82	ASP	-	EXPRESSION TAG	UNP Q06643
Z	83	LEU	-	EXPRESSION TAG	UNP Q06643
Z	84	GLY	-	EXPRESSION TAG	UNP Q06643
Z	85	SER	-	EXPRESSION TAG	UNP Q06643
Z	245	HIS	-	EXPRESSION TAG	UNP Q06643

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	246	HIS	-	EXPRESSION TAG	UNP Q06643
Z	247	HIS	-	EXPRESSION TAG	UNP Q06643
Z	248	HIS	-	EXPRESSION TAG	UNP Q06643
Z	249	HIS	-	EXPRESSION TAG	UNP Q06643
Z	250	HIS	-	EXPRESSION TAG	UNP Q06643
Z	251	HIS	-	EXPRESSION TAG	UNP Q06643
Z	252	HIS	-	EXPRESSION TAG	UNP Q06643
B	43	MET	-	EXPRESSION TAG	UNP Q06643
B	44	LEU	-	EXPRESSION TAG	UNP Q06643
B	45	LEU	-	EXPRESSION TAG	UNP Q06643
B	46	VAL	-	EXPRESSION TAG	UNP Q06643
B	47	ASN	-	EXPRESSION TAG	UNP Q06643
B	48	GLN	-	EXPRESSION TAG	UNP Q06643
B	49	SER	-	EXPRESSION TAG	UNP Q06643
B	50	HIS	-	EXPRESSION TAG	UNP Q06643
B	51	GLN	-	EXPRESSION TAG	UNP Q06643
B	52	GLY	-	EXPRESSION TAG	UNP Q06643
B	53	PHE	-	EXPRESSION TAG	UNP Q06643
B	54	ASN	-	EXPRESSION TAG	UNP Q06643
B	55	LYS	-	EXPRESSION TAG	UNP Q06643
B	56	GLU	-	EXPRESSION TAG	UNP Q06643
B	57	HIS	-	EXPRESSION TAG	UNP Q06643
B	58	THR	-	EXPRESSION TAG	UNP Q06643
B	59	SER	-	EXPRESSION TAG	UNP Q06643
B	60	LYS	-	EXPRESSION TAG	UNP Q06643
B	61	MET	-	EXPRESSION TAG	UNP Q06643
B	62	VAL	-	EXPRESSION TAG	UNP Q06643
B	63	SER	-	EXPRESSION TAG	UNP Q06643
B	64	ALA	-	EXPRESSION TAG	UNP Q06643
B	65	ILE	-	EXPRESSION TAG	UNP Q06643
B	66	VAL	-	EXPRESSION TAG	UNP Q06643
B	67	LEU	-	EXPRESSION TAG	UNP Q06643
B	68	TYR	-	EXPRESSION TAG	UNP Q06643
B	69	VAL	-	EXPRESSION TAG	UNP Q06643
B	70	LEU	-	EXPRESSION TAG	UNP Q06643
B	71	LEU	-	EXPRESSION TAG	UNP Q06643
B	72	ALA	-	EXPRESSION TAG	UNP Q06643
B	73	ALA	-	EXPRESSION TAG	UNP Q06643
B	74	ALA	-	EXPRESSION TAG	UNP Q06643
B	75	ALA	-	EXPRESSION TAG	UNP Q06643
B	76	HIS	-	EXPRESSION TAG	UNP Q06643
B	77	SER	-	EXPRESSION TAG	UNP Q06643

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Chain	Residue	Modelled	Actual	Comment	Reference
B	78	ALA	-	EXPRESSION TAG	UNP Q06643
B	79	PHE	-	EXPRESSION TAG	UNP Q06643
B	80	ALA	-	EXPRESSION TAG	UNP Q06643
B	81	ALA	-	EXPRESSION TAG	UNP Q06643
B	82	ASP	-	EXPRESSION TAG	UNP Q06643
B	83	LEU	-	EXPRESSION TAG	UNP Q06643
B	84	GLY	-	EXPRESSION TAG	UNP Q06643
B	85	SER	-	EXPRESSION TAG	UNP Q06643
B	245	HIS	-	EXPRESSION TAG	UNP Q06643
B	246	HIS	-	EXPRESSION TAG	UNP Q06643
B	247	HIS	-	EXPRESSION TAG	UNP Q06643
B	248	HIS	-	EXPRESSION TAG	UNP Q06643
B	249	HIS	-	EXPRESSION TAG	UNP Q06643
B	250	HIS	-	EXPRESSION TAG	UNP Q06643
B	251	HIS	-	EXPRESSION TAG	UNP Q06643
B	252	HIS	-	EXPRESSION TAG	UNP Q06643
D	43	MET	-	EXPRESSION TAG	UNP Q06643
D	44	LEU	-	EXPRESSION TAG	UNP Q06643
D	45	LEU	-	EXPRESSION TAG	UNP Q06643
D	46	VAL	-	EXPRESSION TAG	UNP Q06643
D	47	ASN	-	EXPRESSION TAG	UNP Q06643
D	48	GLN	-	EXPRESSION TAG	UNP Q06643
D	49	SER	-	EXPRESSION TAG	UNP Q06643
D	50	HIS	-	EXPRESSION TAG	UNP Q06643
D	51	GLN	-	EXPRESSION TAG	UNP Q06643
D	52	GLY	-	EXPRESSION TAG	UNP Q06643
D	53	PHE	-	EXPRESSION TAG	UNP Q06643
D	54	ASN	-	EXPRESSION TAG	UNP Q06643
D	55	LYS	-	EXPRESSION TAG	UNP Q06643
D	56	GLU	-	EXPRESSION TAG	UNP Q06643
D	57	HIS	-	EXPRESSION TAG	UNP Q06643
D	58	THR	-	EXPRESSION TAG	UNP Q06643
D	59	SER	-	EXPRESSION TAG	UNP Q06643
D	60	LYS	-	EXPRESSION TAG	UNP Q06643
D	61	MET	-	EXPRESSION TAG	UNP Q06643
D	62	VAL	-	EXPRESSION TAG	UNP Q06643
D	63	SER	-	EXPRESSION TAG	UNP Q06643
D	64	ALA	-	EXPRESSION TAG	UNP Q06643
D	65	ILE	-	EXPRESSION TAG	UNP Q06643
D	66	VAL	-	EXPRESSION TAG	UNP Q06643
D	67	LEU	-	EXPRESSION TAG	UNP Q06643
D	68	TYR	-	EXPRESSION TAG	UNP Q06643

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Chain	Residue	Modelled	Actual	Comment	Reference
D	69	VAL	-	EXPRESSION TAG	UNP Q06643
D	70	LEU	-	EXPRESSION TAG	UNP Q06643
D	71	LEU	-	EXPRESSION TAG	UNP Q06643
D	72	ALA	-	EXPRESSION TAG	UNP Q06643
D	73	ALA	-	EXPRESSION TAG	UNP Q06643
D	74	ALA	-	EXPRESSION TAG	UNP Q06643
D	75	ALA	-	EXPRESSION TAG	UNP Q06643
D	76	HIS	-	EXPRESSION TAG	UNP Q06643
D	77	SER	-	EXPRESSION TAG	UNP Q06643
D	78	ALA	-	EXPRESSION TAG	UNP Q06643
D	79	PHE	-	EXPRESSION TAG	UNP Q06643
D	80	ALA	-	EXPRESSION TAG	UNP Q06643
D	81	ALA	-	EXPRESSION TAG	UNP Q06643
D	82	ASP	-	EXPRESSION TAG	UNP Q06643
D	83	LEU	-	EXPRESSION TAG	UNP Q06643
D	84	GLY	-	EXPRESSION TAG	UNP Q06643
D	85	SER	-	EXPRESSION TAG	UNP Q06643
D	245	HIS	-	EXPRESSION TAG	UNP Q06643
D	246	HIS	-	EXPRESSION TAG	UNP Q06643
D	247	HIS	-	EXPRESSION TAG	UNP Q06643
D	248	HIS	-	EXPRESSION TAG	UNP Q06643
D	249	HIS	-	EXPRESSION TAG	UNP Q06643
D	250	HIS	-	EXPRESSION TAG	UNP Q06643
D	251	HIS	-	EXPRESSION TAG	UNP Q06643
D	252	HIS	-	EXPRESSION TAG	UNP Q06643

- Molecule 4 is a protein called anti-Lymphotoxin alpha antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	W	212	Total	C	N	O	S	0	0	0
			1610	1026	268	310	6			
4	H	212	Total	C	N	O	S	0	0	0
			1604	1022	267	309	6			

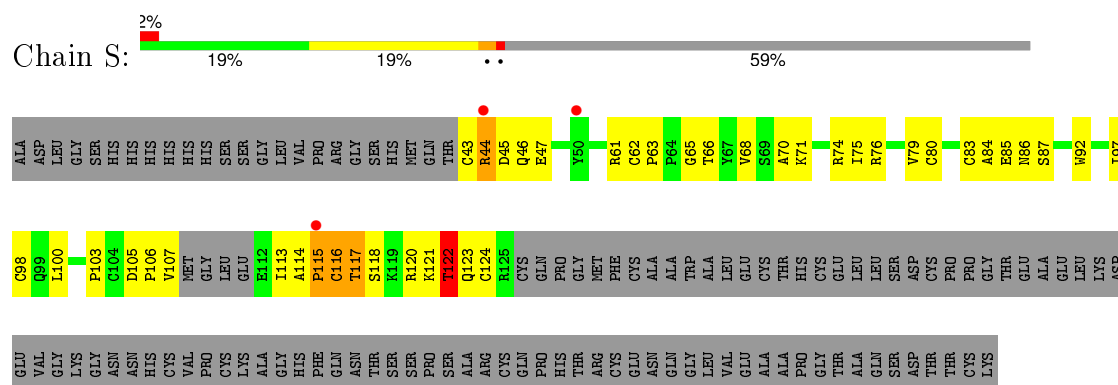
- Molecule 5 is a protein called anti-Lymphotoxin alpha antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	V	211	Total	C	N	O	S	0	0	0
			1623	1015	273	330	5			
5	L	211	Total	C	N	O	S	0	0	0
			1623	1015	273	330	5			

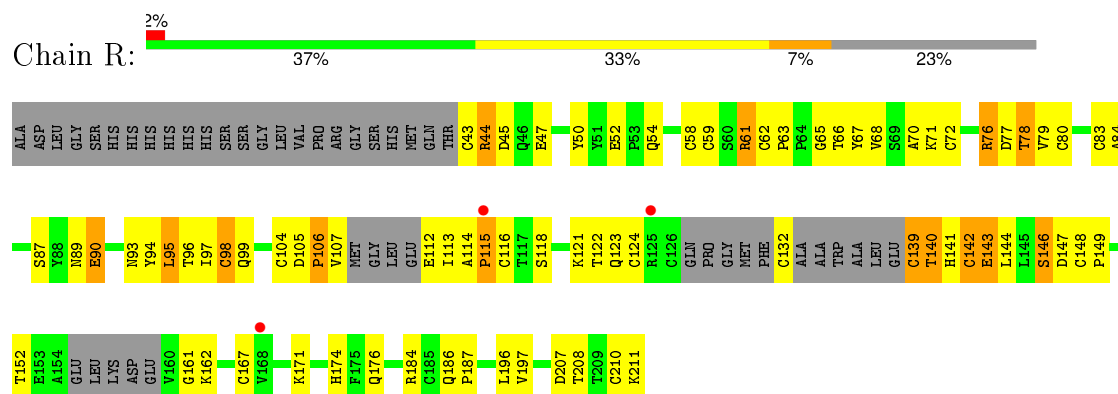
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

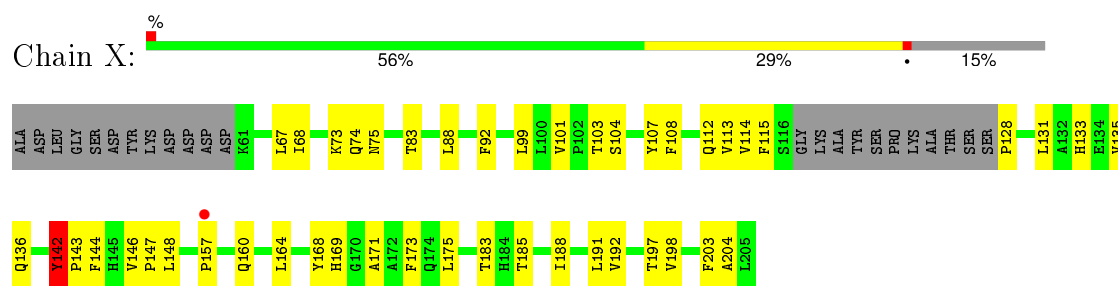
- Molecule 1: Tumor necrosis factor receptor superfamily member 3



- Molecule 1: Tumor necrosis factor receptor superfamily member 3



- Molecule 2: Lymphotoxin-alpha



- Molecule 2: Lymphotoxin-alpha





T206	K207	N210	R211	A112	P113	S114	V115	F118	P119	P120	S121	D122	E123	Q124	L125	K126	T129	V132	V133	C134	L135	Y140	P141	P142	E143	A144	K145	H148	K149	V150	D151	N152	N158	S159	Q160	Q166	Y173	S177	L181	Y186	V191	Y192	V196	T197	H198	Q199	G200	L201	V205
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.20 Å 52.43 Å 253.24 Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	49.70 – 3.60 49.70 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.70-3.60) 99.4 (49.70-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 3.57 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.231 , 0.296 0.230 , 0.296	Depositor DCC
$R_{free}$ test set	1613 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.6	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 77.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 32282 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	14217	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

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	R	0.81	5/1157 (0.4%)	0.90	2/1563 (0.1%)
1	S	0.71	0/634	0.92	1/857 (0.1%)
2	A	0.47	0/1090	0.72	1/1486 (0.1%)
2	X	0.59	3/1090 (0.3%)	0.70	1/1486 (0.1%)
3	B	0.53	0/954	0.75	0/1293
3	D	0.54	0/1027	0.75	0/1394
3	Y	0.52	0/979	0.75	0/1326
3	Z	0.52	0/1010	0.78	0/1371
4	H	0.55	0/1649	0.72	0/2253
4	W	0.56	1/1654 (0.1%)	0.69	0/2256
5	L	0.63	1/1660 (0.1%)	0.77	0/2255
5	V	0.53	0/1660	0.71	0/2255
All	All	0.58	10/14564 (0.1%)	0.76	5/19795 (0.0%)

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
1	R	0	1
1	S	0	1
3	Z	0	1
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	112	GLU	CD-OE1	10.24	1.36	1.25
1	R	112	GLU	CG-CD	9.82	1.66	1.51
1	R	112	GLU	CD-OE2	8.12	1.34	1.25
2	X	160	GLN	CB-CG	6.49	1.70	1.52
2	X	160	GLN	CG-CD	6.09	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	124	CYS	CB-SG	-5.81	1.72	1.81
1	R	112	GLU	CB-CG	5.74	1.63	1.52
2	X	160	GLN	CD-OE1	5.68	1.36	1.24
5	L	148	TRP	CB-CG	-5.23	1.40	1.50
4	W	139	CYS	CB-SG	-5.00	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	90	GLU	N-CA-C	-6.12	94.49	111.00
1	S	116	CYS	N-CA-C	-5.58	95.94	111.00
2	X	142	TYR	C-N-CD	5.43	139.81	128.40
1	R	76	ARG	NE-CZ-NH1	5.37	122.98	120.30
2	A	161	GLU	N-CA-C	-5.29	96.71	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	89	ASN	Peptide
1	S	120	ARG	Peptide
3	Z	200	LEU	Peptide

## 5.2 Too-close contacts [i](#)

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	R	1136	0	1045	64	0
1	S	622	0	574	32	1
2	A	1055	0	1017	53	0
2	X	1055	0	1017	36	1
3	B	936	0	908	61	0
3	D	1004	0	979	81	0
3	Y	961	0	929	49	0
3	Z	988	0	952	57	1
4	H	1604	0	1564	42	0
4	W	1610	0	1573	38	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	1623	0	1573	72	0
5	V	1623	0	1573	57	0
All	All	14217	0	13704	564	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 20.

All (564) 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)
3:Z:159:LEU:HG	3:Z:207:PHE:CE2	1.81	1.14
5:V:197:THR:HG22	5:V:204:PRO:HB3	1.30	1.14
3:B:241:VAL:HG11	3:D:243:VAL:CG1	1.80	1.11
3:Z:159:LEU:HG	3:Z:207:PHE:HE2	0.98	1.10
2:A:205:LEU:CD1	3:D:241:VAL:HG11	1.84	1.07
5:L:120:PRO:HD3	5:L:132:VAL:HG22	1.13	1.07
3:B:241:VAL:HG11	3:D:243:VAL:HG11	1.08	1.06
2:A:205:LEU:HD13	3:D:241:VAL:CG1	1.86	1.06
1:R:44:ARG:HG3	1:R:45:ASP:H	1.24	1.03
1:R:196:LEU:HD11	1:R:210:CYS:HB3	1.40	1.01
3:Y:163:LEU:HD12	3:Y:218:ARG:O	1.61	1.00
3:B:156:SER:HA	3:B:184:THR:HG22	1.43	1.00
3:Y:156:SER:HA	3:Y:184:THR:HG22	1.44	1.00
1:S:121:LYS:HG2	1:S:122:THR:H	1.26	0.98
5:V:54:ARG:HH11	5:V:60:SER:HA	1.25	0.98
3:B:158:THR:HG22	3:B:182:ALA:HB1	1.46	0.97
5:V:197:THR:CG2	5:V:204:PRO:HB3	1.96	0.95
2:A:67:LEU:HD11	2:A:99:LEU:HD13	1.46	0.94
3:Z:230:ASP:OD2	3:Z:235:LYS:NZ	2.00	0.94
5:L:54:ARG:HH11	5:L:60:SER:HA	1.35	0.91
5:V:197:THR:HG22	5:V:204:PRO:CB	2.01	0.90
5:L:115:VAL:C	5:L:207:LYS:HZ1	1.74	0.90
3:B:87:LEU:O	3:B:87:LEU:HD12	1.72	0.90
4:W:194:ILE:HD11	4:W:207:ASP:HB3	1.53	0.90
1:R:54:GLN:OE1	1:R:71:LYS:NZ	2.05	0.89
1:S:121:LYS:HG2	1:S:122:THR:N	1.88	0.88
4:H:6:GLU:OE2	4:H:96:CYS:N	2.06	0.88
3:Y:163:LEU:HD13	3:Y:163:LEU:O	1.75	0.87
3:B:158:THR:HG22	3:B:182:ALA:CB	2.04	0.87
3:B:241:VAL:HG23	3:D:210:LEU:HD11	1.54	0.87
3:B:241:VAL:HG12	3:B:242:MET:O	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:156:SER:HA	3:Z:184:THR:HG22	1.57	0.85
5:V:120:PRO:HD3	5:V:132:VAL:HG22	1.59	0.85
5:V:149:LYS:NZ	5:V:195:GLU:OE1	2.10	0.85
3:D:170:TYR:CD1	1:R:95:LEU:HG	2.11	0.84
3:B:159:LEU:HD22	3:B:205:VAL:HG12	1.60	0.83
5:L:120:PRO:CD	5:L:132:VAL:HG22	2.04	0.82
2:X:73:LYS:O	2:X:75:ASN:N	2.12	0.82
3:Z:164:TYR:CE1	3:Z:175:PRO:HG3	2.14	0.82
3:Y:163:LEU:C	3:Y:163:LEU:HD13	1.99	0.81
5:L:83:PHE:CD1	5:L:104:VAL:HG12	2.13	0.81
3:D:156:SER:HA	3:D:184:THR:HG22	1.61	0.81
1:R:146:SER:O	1:R:147:ASP:OD1	1.97	0.81
3:Y:241:VAL:HG23	3:Z:210:LEU:HD11	1.60	0.81
2:A:153:LYS:HZ2	3:D:203:THR:HG22	1.46	0.81
5:V:54:ARG:NH1	5:V:60:SER:HA	1.96	0.80
4:H:67:ARG:NH1	4:H:90:ASP:OD2	2.13	0.80
3:D:144:ARG:HA	3:D:200:LEU:H	1.47	0.80
5:L:201:LEU:CD2	5:L:205:VAL:HB	2.11	0.80
2:A:73:LYS:O	2:A:75:ASN:N	2.13	0.80
3:D:170:TYR:CE1	1:R:95:LEU:HG	2.17	0.80
4:W:67:ARG:NH1	4:W:90:ASP:OD2	2.15	0.79
3:Y:233:ARG:HD2	3:Z:177:LEU:HD23	1.64	0.79
1:R:196:LEU:CD1	1:R:210:CYS:HB3	2.13	0.79
2:A:205:LEU:HD13	3:D:241:VAL:HG11	0.90	0.79
5:L:158:ASN:HD22	5:L:181:LEU:HD21	1.48	0.78
5:L:50:SER:HB3	5:L:53:HIS:HD2	1.47	0.78
3:D:158:THR:HG22	3:D:182:ALA:CB	2.14	0.78
3:D:158:THR:HG22	3:D:182:ALA:HB1	1.66	0.78
4:W:124:PRO:HB3	4:W:144:TYR:HB3	1.65	0.78
2:A:153:LYS:NZ	3:D:203:THR:HG22	1.98	0.78
3:Z:137:CYS:SG	3:Z:159:LEU:HD11	2.23	0.77
5:L:54:ARG:NH1	5:L:60:SER:HA	1.99	0.77
5:L:2:ILE:HG12	5:L:27:GLN:HE21	1.51	0.76
3:B:163:LEU:HD23	3:B:178:LEU:HD11	1.69	0.75
3:D:233:ARG:O	3:D:235:LYS:N	2.19	0.75
4:W:6:GLU:OE2	4:W:96:CYS:N	2.19	0.75
3:Y:241:VAL:HG12	3:Y:242:MET:O	1.87	0.74
3:B:233:ARG:HH22	1:R:99:GLN:HE21	1.34	0.74
1:R:132:CYS:SG	1:R:143:GLU:N	2.58	0.74
3:D:157:VAL:HG22	3:D:183:GLU:O	1.89	0.73
1:R:63:PRO:O	1:R:66:THR:OG1	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:76:ARG:HG2	1:R:77:ASP:N	2.05	0.72
3:B:241:VAL:CG2	3:D:210:LEU:HD11	2.19	0.72
3:Y:159:LEU:HG	3:Y:207:PHE:HE2	1.54	0.72
3:B:154:GLY:HA2	3:B:186:THR:HG22	1.72	0.72
2:A:161:GLU:HG3	3:B:186:THR:HG21	1.71	0.71
1:S:114:ALA:HB1	1:S:115:PRO:HA	1.71	0.71
3:B:241:VAL:CG1	3:D:243:VAL:HG11	2.04	0.70
3:D:170:TYR:HE1	1:R:95:LEU:CD1	2.04	0.70
1:R:171:LYS:HB2	1:R:174:HIS:HD2	1.52	0.70
5:L:83:PHE:CE1	5:L:104:VAL:HG12	2.26	0.70
4:W:194:ILE:CD1	4:W:207:ASP:HB3	2.21	0.70
5:V:38:GLN:O	5:V:39:LYS:HB2	1.91	0.69
3:D:87:LEU:HD22	3:D:88:PRO:HD2	1.73	0.69
3:D:154:GLY:HA2	3:D:186:THR:HA	1.74	0.69
5:L:145:LYS:HB3	5:L:197:THR:HB	1.73	0.69
3:B:158:THR:O	3:B:159:LEU:HD12	1.92	0.69
5:V:150:VAL:HB	5:V:155:GLN:HE21	1.58	0.69
4:H:124:PRO:HB3	4:H:144:TYR:HB3	1.75	0.69
3:D:126:ALA:HB2	3:D:218:ARG:HG2	1.75	0.69
5:V:2:ILE:HG12	5:V:27:GLN:HE21	1.59	0.68
1:R:196:LEU:HD11	1:R:210:CYS:CB	2.20	0.68
4:W:194:ILE:HD11	4:W:207:ASP:CB	2.23	0.68
4:W:192:THR:HG23	4:W:209:LYS:HE3	1.73	0.68
2:A:154:MET:HG2	3:D:202:TYR:HD2	1.59	0.68
1:R:65:GLY:HA2	1:R:118:SER:O	1.94	0.67
5:L:106:ILE:H	5:L:166:GLN:HE22	1.40	0.67
4:W:131:PRO:HG2	4:W:212:PRO:HG3	1.76	0.67
3:Y:106:THR:HB	3:Y:113:LEU:HD11	1.76	0.67
3:B:159:LEU:C	3:B:160:ARG:HG3	2.15	0.67
3:B:106:THR:HB	3:B:113:LEU:HD11	1.76	0.67
2:X:133:HIS:ND1	2:X:185:THR:HG22	2.09	0.67
3:D:170:TYR:N	1:R:94:TYR:CE2	2.63	0.66
1:R:196:LEU:HD12	1:R:197:VAL:N	2.09	0.66
2:X:148:LEU:HB3	2:X:173:PHE:CZ	2.31	0.66
1:R:50:TYR:O	1:R:58:CYS:HB2	1.96	0.66
2:X:164:LEU:N	3:Y:184:THR:OG1	2.29	0.66
3:B:160:ARG:HG2	3:B:180:GLU:HG3	1.77	0.66
2:X:115:PHE:CD2	2:X:131:LEU:HD22	2.31	0.66
3:D:170:TYR:CE1	1:R:95:LEU:CD1	2.80	0.65
5:L:115:VAL:HB	5:L:207:LYS:HZ2	1.62	0.65
3:Z:93:ILE:HG13	3:Z:111:ALA:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:6:GLU:OE2	4:W:95:TYR:HA	1.96	0.65
3:Y:159:LEU:HG	3:Y:207:PHE:CE2	2.32	0.64
2:X:112:GLN:HB2	2:X:168:TYR:HD2	1.63	0.64
2:A:146:VAL:HG13	3:D:233:ARG:NH2	2.12	0.64
5:L:198:HIS:HD2	5:L:199:GLN:H	1.46	0.64
5:V:37:GLN:HB3	5:V:47:LEU:HD11	1.80	0.64
3:Y:154:GLY:HA2	3:Y:186:THR:HA	1.80	0.64
3:B:158:THR:C	3:B:159:LEU:HD12	2.18	0.64
2:A:153:LYS:HE2	2:A:165:HIS:CE1	2.33	0.64
1:R:44:ARG:HG3	1:R:45:ASP:N	2.05	0.64
2:A:146:VAL:HG13	3:D:233:ARG:CZ	2.28	0.63
3:Z:145:ALA:CB	3:Z:187:PRO:HG3	2.28	0.63
5:V:11:LEU:HD11	5:V:104:VAL:HG22	1.81	0.63
3:B:159:LEU:C	3:B:160:ARG:CG	2.67	0.63
3:D:230:ASP:OD2	3:D:235:LYS:NZ	2.31	0.63
3:D:170:TYR:CG	3:D:171:GLY:N	2.64	0.63
3:D:170:TYR:CE1	1:R:95:LEU:CG	2.82	0.63
3:Z:159:LEU:HD12	3:Z:160:ARG:H	1.63	0.63
1:R:114:ALA:HB1	1:R:115:PRO:HA	1.81	0.63
3:Z:163:LEU:HD23	3:Z:178:LEU:HD11	1.80	0.63
2:A:191:LEU:HD22	2:A:198:VAL:HG21	1.81	0.62
2:A:133:HIS:ND1	2:A:185:THR:HG22	2.14	0.62
3:Y:140:GLY:H	3:Y:236:THR:HG22	1.64	0.62
3:B:233:ARG:O	3:B:235:LYS:N	2.29	0.62
3:Z:127:LEU:HD13	3:Z:133:TYR:CE1	2.35	0.62
4:W:167:ALA:HB2	4:W:177:LEU:HD23	1.81	0.62
4:H:120:SER:OG	4:H:121:THR:N	2.33	0.62
1:R:84:ALA:O	1:R:87:SER:OG	2.09	0.61
4:H:126:VAL:HG22	4:H:141:VAL:HG22	1.82	0.61
3:D:170:TYR:O	1:R:61:ARG:NH2	2.33	0.61
3:Y:106:THR:HB	3:Y:113:LEU:CD1	2.29	0.61
3:B:113:LEU:HB3	3:B:117:THR:OG1	2.01	0.61
3:Z:126:ALA:HB2	3:Z:218:ARG:HG2	1.81	0.60
4:H:105:PHE:HD2	5:L:36:TYR:HH	1.49	0.60
1:R:207:ASP:OD1	1:R:208:THR:N	2.34	0.60
5:V:170:ASP:OD1	5:V:172:THR:OG1	2.15	0.60
1:R:149:PRO:O	1:R:152:THR:OG1	2.19	0.60
3:D:106:THR:HB	3:D:113:LEU:HD11	1.83	0.60
3:B:159:LEU:HD22	3:B:205:VAL:CG1	2.29	0.60
3:Y:241:VAL:CG2	3:Z:210:LEU:HD11	2.32	0.60
5:L:4:MET:HE2	5:L:25:ALA:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:4:MET:HE3	5:V:90:GLU:HB3	1.84	0.59
3:Z:159:LEU:CG	3:Z:207:PHE:HE2	1.93	0.59
5:V:201:LEU:HD13	5:V:205:VAL:HB	1.84	0.59
3:B:120:SER:OG	3:B:123:GLU:HB2	2.02	0.59
1:S:61:ARG:HH12	3:Z:171:GLY:HA2	1.68	0.59
2:X:164:LEU:H	3:Y:184:THR:HG1	1.51	0.59
3:D:139:VAL:HB	3:D:159:LEU:HD11	1.85	0.59
1:R:96:THR:O	1:R:97:ILE:HG13	2.02	0.59
2:X:114:VAL:CG2	2:X:197:THR:HB	2.33	0.58
2:A:135:VAL:HG22	2:A:183:THR:HG22	1.84	0.58
2:X:148:LEU:HB3	2:X:173:PHE:CE1	2.38	0.58
2:A:142:TYR:HB2	2:A:143:PRO:HD3	1.84	0.58
1:R:67:TYR:HD2	1:R:98:CYS:SG	2.26	0.58
5:V:7:SER:OG	5:V:8:PRO:HD3	2.03	0.58
2:A:203:PHE:CD1	3:B:210:LEU:HD21	2.38	0.58
3:Y:163:LEU:CD1	3:Y:163:LEU:C	2.69	0.58
3:D:170:TYR:N	1:R:94:TYR:CZ	2.71	0.58
3:B:233:ARG:HH12	1:R:99:GLN:NE2	2.02	0.58
2:A:114:VAL:HG21	2:A:197:THR:HB	1.85	0.58
2:A:91:GLY:O	2:A:102:PRO:HB3	2.03	0.58
3:D:106:THR:HB	3:D:113:LEU:CD1	2.33	0.58
3:B:107:THR:O	1:R:97:ILE:HG21	2.03	0.58
5:L:198:HIS:CD2	5:L:199:GLN:H	2.21	0.58
4:W:12:VAL:HG11	4:W:86:LEU:HD12	1.86	0.58
3:D:157:VAL:CG2	3:D:183:GLU:O	2.52	0.57
3:Z:159:LEU:HD12	3:Z:160:ARG:N	2.18	0.57
5:L:7:SER:OG	5:L:8:PRO:HD3	2.03	0.57
5:L:85:THR:HG22	5:L:103:LYS:HG2	1.85	0.57
2:A:116:SER:HB3	2:A:192:VAL:HG21	1.86	0.57
2:A:114:VAL:CG2	2:A:197:THR:HB	2.34	0.57
1:R:43:CYS:SG	1:R:44:ARG:N	2.74	0.57
5:L:38:GLN:O	5:L:84:ALA:HB1	2.05	0.57
1:S:107:VAL:CG2	3:Y:142:ARG:NH1	2.68	0.57
5:L:83:PHE:HD1	5:L:104:VAL:HG12	1.65	0.57
3:Z:106:THR:HB	3:Z:113:LEU:CD1	2.34	0.57
1:S:65:GLY:HA2	1:S:118:SER:O	2.05	0.57
5:L:118:PHE:O	5:L:132:VAL:HG13	2.05	0.56
2:A:146:VAL:CG1	3:D:233:ARG:NH2	2.67	0.56
3:D:158:THR:HG22	3:D:182:ALA:HB2	1.87	0.56
1:R:152:THR:HB	1:R:167:CYS:HB3	1.88	0.56
5:L:39:LYS:HB3	5:L:40:PRO:HD2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:183:GLU:HG2	3:Z:185:VAL:HG23	1.87	0.56
1:R:171:LYS:HB2	1:R:174:HIS:CD2	2.38	0.56
2:A:148:LEU:HB3	2:A:173:PHE:CZ	2.40	0.56
1:S:116:CYS:O	1:S:117:THR:HG23	2.05	0.56
1:R:87:SER:HB2	1:R:98:CYS:HB2	1.87	0.56
5:V:17:ASP:OD1	5:V:18:ARG:N	2.38	0.56
3:Z:137:CYS:HB3	3:Z:207:PHE:CZ	2.40	0.56
5:L:196:VAL:HB	5:L:205:VAL:HG12	1.86	0.56
1:S:107:VAL:HG21	3:Y:142:ARG:NH1	2.21	0.56
3:B:97:LEU:O	3:B:98:LYS:HB3	2.04	0.56
3:Y:233:ARG:O	3:Y:235:LYS:N	2.37	0.56
3:D:127:LEU:HD13	3:D:133:TYR:CE1	2.41	0.56
5:V:80:PRO:HA	5:V:106:ILE:HD12	1.88	0.56
1:S:83:CYS:HB3	1:S:87:SER:HB3	1.89	0.55
3:B:230:ASP:OD2	3:B:235:LYS:NZ	2.36	0.55
5:L:6:GLN:NE2	5:L:102:THR:OG1	2.39	0.55
3:B:154:GLY:CA	3:B:186:THR:HG22	2.34	0.55
4:W:167:ALA:HA	4:W:177:LEU:HB3	1.87	0.55
5:V:4:MET:CE	5:V:90:GLU:HB3	2.37	0.55
3:Y:135:LEU:HD11	3:Y:213:LEU:HD11	1.88	0.55
1:R:76:ARG:CG	1:R:77:ASP:N	2.70	0.55
5:L:34:ALA:HA	5:L:48:ILE:O	2.07	0.55
4:W:73:ASP:OD1	4:W:75:SER:OG	2.19	0.55
1:R:196:LEU:HD13	1:R:211:LYS:OXT	2.07	0.55
3:B:139:VAL:HA	3:B:236:THR:HG22	1.89	0.55
3:B:140:GLY:H	3:B:236:THR:HG22	1.72	0.55
3:Z:137:CYS:HB3	3:Z:207:PHE:CE1	2.42	0.55
3:D:233:ARG:CG	3:D:234:GLY:H	2.19	0.55
4:W:93:VAL:HA	4:W:113:LEU:HD23	1.88	0.55
3:B:110:GLN:NE2	3:D:176:GLU:OE2	2.40	0.55
5:V:50:SER:HB2	5:V:53:HIS:HD2	1.72	0.55
2:A:112:GLN:HB2	2:A:168:TYR:HD2	1.71	0.54
5:V:106:ILE:O	5:V:166:GLN:NE2	2.38	0.54
1:R:105:ASP:O	1:R:107:VAL:N	2.40	0.54
5:L:201:LEU:HD23	5:L:205:VAL:HB	1.88	0.54
2:X:114:VAL:HG21	2:X:197:THR:HB	1.88	0.54
5:V:113:PRO:HD3	5:V:198:HIS:HD1	1.72	0.54
5:V:150:VAL:HB	5:V:155:GLN:NE2	2.20	0.54
4:H:192:THR:HG23	4:H:209:LYS:HE3	1.89	0.54
5:L:39:LYS:HB3	5:L:40:PRO:CD	2.37	0.54
5:L:115:VAL:C	5:L:207:LYS:NZ	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:140:GLY:H	3:Z:236:THR:HG22	1.72	0.54
3:D:132:LEU:HD21	3:D:210:LEU:HD22	1.90	0.54
3:Z:164:TYR:HE1	3:Z:175:PRO:HG3	1.67	0.54
1:R:107:VAL:HG12	1:R:139:CYS:N	2.23	0.54
3:Z:160:ARG:HG2	3:Z:177:LEU:HD11	1.88	0.53
3:Z:160:ARG:HG2	3:Z:177:LEU:CD1	2.38	0.53
4:H:184:PRO:HG2	4:H:187:SER:OG	2.08	0.53
4:W:151:VAL:HG11	4:W:179:SER:CB	2.38	0.53
4:H:91:THR:OG1	4:H:115:THR:HA	2.08	0.53
4:H:183:VAL:HG11	4:H:193:TYR:CE1	2.43	0.53
3:Z:139:VAL:HA	3:Z:236:THR:HG22	1.90	0.53
3:Z:92:LEU:HD23	3:Z:106:THR:HG22	1.91	0.53
3:Z:158:THR:HG22	3:Z:182:ALA:CB	2.39	0.53
1:R:76:ARG:HG2	1:R:77:ASP:H	1.73	0.53
3:Y:97:LEU:O	3:Y:98:LYS:HG2	2.09	0.53
3:B:106:THR:HB	3:B:113:LEU:CD1	2.38	0.53
4:H:167:ALA:HB2	4:H:177:LEU:HD23	1.91	0.53
2:X:142:TYR:HB2	2:X:143:PRO:HD3	1.91	0.53
3:D:172:PRO:HA	1:R:61:ARG:HH12	1.74	0.53
5:L:35:TRP:CZ3	5:L:88:CYS:HB3	2.44	0.53
1:S:44:ARG:HG2	1:S:45:ASP:H	1.74	0.52
3:Z:120:SER:OG	3:Z:123:GLU:HB2	2.10	0.52
2:A:115:PHE:CD2	2:A:131:LEU:HD22	2.44	0.52
4:W:51:ASN:HD22	4:W:58:THR:HG22	1.73	0.52
4:W:50:TYR:CE2	4:W:102:LEU:HD21	2.45	0.52
2:X:68:ILE:HD11	2:X:83:THR:HG21	1.92	0.52
3:B:159:LEU:O	3:B:160:ARG:CG	2.57	0.52
4:H:149:VAL:HG23	4:H:199:HIS:HB2	1.91	0.52
3:D:159:LEU:HB3	3:D:207:PHE:HE2	1.74	0.52
3:Z:183:GLU:HG2	3:Z:185:VAL:CG2	2.40	0.52
3:Z:102:LEU:HD22	3:Z:223:ILE:HD12	1.92	0.52
2:A:112:GLN:O	2:A:198:VAL:HA	2.10	0.52
3:Z:106:THR:HB	3:Z:113:LEU:HD11	1.92	0.52
5:L:150:VAL:HG22	5:L:192:TYR:CD1	2.45	0.52
4:H:194:ILE:HD12	4:H:207:ASP:HB3	1.90	0.52
1:S:97:ILE:HG21	3:Y:107:THR:O	2.10	0.52
4:H:39:GLN:HB3	4:H:45:LEU:HD23	1.91	0.52
3:B:241:VAL:CG2	3:D:210:LEU:CD1	2.87	0.52
1:R:196:LEU:CD1	1:R:197:VAL:N	2.73	0.52
5:L:37:GLN:HB3	5:L:47:LEU:HD11	1.90	0.51
2:X:88:LEU:HD13	2:X:92:PHE:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:214:ARG:O	3:B:217:GLU:HB2	2.09	0.51
5:L:37:GLN:HB3	5:L:86:TYR:CE2	2.46	0.51
2:X:88:LEU:HD22	2:X:92:PHE:HB3	1.92	0.51
3:B:140:GLY:N	3:B:235:LYS:O	2.44	0.51
5:V:80:PRO:HA	5:V:106:ILE:CD1	2.40	0.51
4:H:180:VAL:HG11	5:L:135:LEU:HD22	1.91	0.51
3:Y:155:ARG:O	3:Y:184:THR:HA	2.11	0.51
4:H:129:LEU:HD13	5:L:133:VAL:HG11	1.93	0.51
3:D:93:ILE:CG2	3:D:94:GLY:N	2.74	0.51
3:D:92:LEU:HD23	3:D:106:THR:HG22	1.93	0.50
1:S:61:ARG:HH22	3:Z:171:GLY:N	2.09	0.50
4:W:138:GLY:O	4:W:210:VAL:HG21	2.11	0.50
3:Z:132:LEU:O	3:Z:243:VAL:HG22	2.11	0.50
4:H:169:LEU:HD23	4:H:175:TYR:CE1	2.45	0.50
3:Y:132:LEU:HD11	3:Y:210:LEU:HB3	1.94	0.50
3:B:87:LEU:O	3:B:87:LEU:CD1	2.54	0.50
4:W:103:PRO:HB2	5:V:91:SER:HB2	1.94	0.50
4:H:127:PHE:HB3	5:L:121:SER:OG	2.11	0.50
2:A:133:HIS:HB3	2:A:167:MET:HE3	1.93	0.50
5:V:118:PHE:HB2	5:V:133:VAL:HG12	1.94	0.50
4:W:129:LEU:HD13	5:V:133:VAL:HG11	1.94	0.50
4:H:135:ALA:HB3	4:H:183:VAL:O	2.11	0.50
4:W:136:ALA:HB2	4:W:182:THR:HG22	1.92	0.50
4:W:93:VAL:HG22	4:W:113:LEU:HD21	1.94	0.50
3:B:202:TYR:N	3:D:184:THR:OG1	2.45	0.50
2:A:154:MET:HG2	3:D:202:TYR:CD2	2.43	0.50
1:S:105:ASP:O	1:S:107:VAL:N	2.44	0.50
2:X:135:VAL:HG22	2:X:183:THR:HG22	1.93	0.50
4:H:99:PRO:HB2	4:H:101:MET:O	2.12	0.49
3:Z:145:ALA:HB2	3:Z:187:PRO:HG3	1.94	0.49
3:Y:104:TRP:HB2	3:Y:119:PHE:CZ	2.46	0.49
2:A:93:SER:OG	2:A:100:LEU:HB2	2.12	0.49
3:D:185:VAL:HG13	3:D:187:PRO:HD2	1.94	0.49
2:A:116:SER:HB3	2:A:192:VAL:CG2	2.42	0.49
5:L:143:GLU:N	5:L:143:GLU:OE1	2.28	0.49
4:H:18:LEU:HD12	4:H:19:ARG:H	1.78	0.49
3:Y:241:VAL:CG2	3:Z:210:LEU:CD1	2.91	0.49
3:D:117:THR:HG22	3:D:128:PRO:HD3	1.94	0.49
4:H:167:ALA:HA	4:H:177:LEU:HB3	1.94	0.49
5:L:123:GLU:O	5:L:126:LYS:HB2	2.13	0.49
1:S:103:PRO:HD2	3:Y:96:PRO:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:158:THR:HG22	3:B:182:ALA:HB2	1.90	0.49
4:H:183:VAL:HB	4:H:184:PRO:HD2	1.94	0.49
1:R:70:ALA:HB3	1:R:79:VAL:HB	1.94	0.49
3:Y:127:LEU:HD13	3:Y:133:TYR:CE1	2.48	0.49
5:L:85:THR:HA	5:L:102:THR:O	2.13	0.49
5:L:85:THR:HG22	5:L:103:LYS:CG	2.43	0.49
2:X:103:THR:OG1	4:W:101:MET:SD	2.71	0.49
5:L:198:HIS:CD2	5:L:199:GLN:N	2.81	0.48
5:V:34:ALA:HA	5:V:48:ILE:O	2.13	0.48
1:S:123:GLN:HG3	1:S:123:GLN:O	2.13	0.48
4:W:13:GLN:HA	4:W:117:SER:O	2.13	0.48
5:V:190:LYS:HG2	5:V:210:ASN:HB2	1.95	0.48
2:A:113:VAL:HG13	2:A:133:HIS:CD2	2.48	0.48
2:A:185:THR:OG1	2:A:188:ILE:HD13	2.13	0.48
2:A:191:LEU:HD22	2:A:198:VAL:CG2	2.43	0.48
3:D:96:PRO:HB3	3:D:231:PHE:CE2	2.47	0.48
5:L:148:TRP:HZ2	5:L:177:SER:O	1.96	0.48
4:H:129:LEU:HB3	5:L:118:PHE:CD1	2.48	0.48
2:A:85:ARG:HH22	3:B:163:LEU:HD21	1.78	0.48
5:V:2:ILE:CG1	5:V:27:GLN:HE21	2.24	0.48
3:D:93:ILE:HG22	3:D:94:GLY:N	2.27	0.48
3:B:154:GLY:HA2	3:B:186:THR:HA	1.96	0.48
3:Z:158:THR:HG22	3:Z:182:ALA:HB1	1.96	0.48
5:V:106:ILE:N	5:V:166:GLN:HE22	2.11	0.48
1:S:68:VAL:HG11	1:S:71:LYS:HD3	1.95	0.48
3:D:170:TYR:CE1	1:R:95:LEU:HD11	2.48	0.48
1:S:85:GLU:O	1:S:86:ASN:HB2	2.12	0.48
3:B:241:VAL:CG1	3:D:243:VAL:CG1	2.72	0.47
1:S:61:ARG:HH12	3:Z:172:PRO:HD2	1.79	0.47
4:W:18:LEU:HD12	4:W:19:ARG:H	1.78	0.47
3:D:89:ALA:HB1	3:D:241:VAL:HG22	1.96	0.47
1:S:61:ARG:HG2	1:S:92:TRP:HB3	1.96	0.47
3:Z:233:ARG:O	3:Z:235:LYS:N	2.39	0.47
3:Y:223:ILE:HG22	3:Y:225:HIS:H	1.79	0.47
3:B:93:ILE:HG13	3:B:111:ALA:HB2	1.97	0.47
3:Z:160:ARG:HG3	3:Z:180:GLU:HG3	1.96	0.47
5:L:115:VAL:O	5:L:207:LYS:NZ	2.36	0.47
5:L:83:PHE:CD1	5:L:104:VAL:O	2.68	0.47
2:A:85:ARG:NH2	3:B:163:LEU:HD21	2.29	0.47
2:A:168:TYR:HH	3:B:134:TYR:HH	1.62	0.47
1:S:70:ALA:HB3	1:S:79:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:123:GLU:OE1	3:D:218:ARG:NE	2.48	0.47
5:V:36:TYR:CE1	5:V:46:LEU:HD13	2.50	0.47
4:W:165:PHE:CZ	5:V:176:SER:HB3	2.50	0.47
3:Z:113:LEU:HB3	3:Z:117:THR:OG1	2.15	0.47
3:D:143:GLY:O	3:D:201:TRP:N	2.36	0.47
3:B:159:LEU:O	3:B:160:ARG:HG2	2.15	0.47
3:D:170:TYR:N	1:R:94:TYR:HH	2.13	0.47
1:R:68:VAL:HG13	1:R:78:THR:CG2	2.45	0.47
1:R:140:THR:OG1	1:R:141:HIS:N	2.48	0.47
3:Y:120:SER:OG	3:Y:123:GLU:HB2	2.14	0.47
3:B:98:LYS:NZ	3:B:226:PRO:HB2	2.30	0.46
3:Y:241:VAL:HG21	3:Z:210:LEU:HD21	1.96	0.46
1:R:76:ARG:CG	1:R:77:ASP:H	2.29	0.46
1:R:104:CYS:O	1:R:106:PRO:HD3	2.14	0.46
5:L:150:VAL:HG22	5:L:192:TYR:HD1	1.79	0.46
3:Y:143:GLY:O	3:Y:201:TRP:N	2.47	0.46
1:R:50:TYR:CZ	1:R:52:GLU:HB2	2.50	0.46
5:L:2:ILE:CG1	5:L:27:GLN:HE21	2.25	0.46
3:D:241:VAL:HG12	3:D:242:MET:O	2.16	0.46
4:W:95:TYR:CE1	4:W:111:GLY:HA3	2.51	0.46
4:H:103:PRO:HB2	5:L:91:SER:HB2	1.97	0.46
4:W:45:LEU:HD12	5:V:98:PHE:CE2	2.51	0.46
2:A:104:SER:HA	2:A:175:LEU:O	2.16	0.46
2:A:159:LEU:HB3	2:A:161:GLU:OE2	2.16	0.46
5:V:113:PRO:HD3	5:V:198:HIS:ND1	2.30	0.46
1:R:121:LYS:O	1:R:123:GLN:N	2.49	0.46
1:S:75:ILE:HG13	1:S:76:ARG:HG2	1.96	0.46
3:Z:140:GLY:O	3:Z:230:ASP:N	2.43	0.45
5:L:206:THR:O	5:L:207:LYS:HG2	2.17	0.45
1:R:142:CYS:O	1:R:144:LEU:N	2.46	0.45
3:D:127:LEU:HA	3:D:128:PRO:HD3	1.68	0.45
4:H:101:MET:HG2	4:H:104:TRP:CZ3	2.52	0.45
1:S:66:THR:HB	1:S:80:CYS:HB3	1.98	0.45
3:Z:143:GLY:N	3:Z:201:TRP:O	2.49	0.45
5:L:83:PHE:CZ	5:L:106:ILE:HG13	2.51	0.45
3:B:104:TRP:HB2	3:B:119:PHE:CZ	2.52	0.45
1:S:43:CYS:SG	1:S:44:ARG:N	2.85	0.45
4:W:153:TRP:CZ3	4:W:195:CYS:HB3	2.52	0.45
3:Y:137:CYS:SG	3:Y:159:LEU:HD11	2.56	0.45
2:X:171:ALA:HB3	2:X:173:PHE:CE2	2.52	0.45
2:A:148:LEU:HB3	2:A:173:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:V:147:GLN:NE2	5:V:154:LEU:HD11	2.31	0.45
1:R:44:ARG:CG	1:R:45:ASP:N	2.74	0.45
3:Z:145:ALA:HB3	3:Z:187:PRO:HG3	1.99	0.45
2:A:135:VAL:HG22	2:A:183:THR:CG2	2.46	0.45
1:R:62:CYS:HB2	1:R:93:ASN:O	2.17	0.45
1:R:83:CYS:HB3	1:R:87:SER:OG	2.16	0.45
5:V:42:LYS:HA	5:V:42:LYS:HD2	1.69	0.45
1:R:196:LEU:C	1:R:196:LEU:HD12	2.38	0.45
1:S:115:PRO:HB2	1:S:116:CYS:H	1.42	0.45
5:L:36:TYR:CE1	5:L:46:LEU:HD13	2.52	0.45
4:W:101:MET:HG2	4:W:104:TRP:CZ3	2.52	0.45
3:Y:202:TYR:N	3:Z:184:THR:OG1	2.48	0.45
5:L:113:PRO:HD3	5:L:198:HIS:ND1	2.31	0.45
4:H:135:ALA:HB2	4:H:185:SER:HA	1.99	0.45
2:X:203:PHE:CD1	3:Y:210:LEU:HD21	2.52	0.45
2:X:107:TYR:CE1	2:X:204:ALA:HB2	2.52	0.45
2:X:67:LEU:HD11	2:X:99:LEU:HD13	1.99	0.45
3:D:98:LYS:HB3	3:D:98:LYS:HE3	1.68	0.45
1:S:83:CYS:HB3	1:S:87:SER:CB	2.48	0.44
3:Y:241:VAL:HG21	3:Z:210:LEU:CD2	2.47	0.44
5:V:4:MET:HE2	5:V:25:ALA:HA	1.98	0.44
1:R:68:VAL:HG13	1:R:78:THR:HG23	1.98	0.44
5:V:136:LEU:HB2	5:V:175:LEU:HB3	1.98	0.44
3:D:163:LEU:HD23	3:D:178:LEU:HD11	1.99	0.44
2:A:150:SER:OG	3:D:235:LYS:HG2	2.17	0.44
2:X:197:THR:OG1	2:X:198:VAL:N	2.51	0.44
5:L:112:ALA:HB1	5:L:201:LEU:CD1	2.47	0.44
2:A:84:ASP:OD1	2:A:85:ARG:N	2.51	0.44
3:Y:229:VAL:CG2	3:Y:236:THR:HG21	2.48	0.44
5:L:200:GLY:C	5:L:201:LEU:HD12	2.38	0.44
3:D:88:PRO:HA	3:D:114:THR:OG1	2.16	0.44
3:Y:113:LEU:HB3	3:Y:117:THR:OG1	2.18	0.44
1:S:100:LEU:HB2	3:Y:108:LYS:HG3	1.99	0.44
1:R:196:LEU:CD1	1:R:197:VAL:H	2.31	0.44
2:A:153:LYS:HZ1	3:D:203:THR:HG22	1.82	0.44
3:D:127:LEU:HD13	3:D:133:TYR:CD1	2.53	0.44
4:H:113:LEU:HD21	4:H:115:THR:HG23	2.00	0.44
5:V:140:TYR:CG	5:V:141:PRO:HA	2.53	0.44
4:W:145:PHE:CE2	4:W:146:PRO:HB3	2.53	0.44
4:H:13:GLN:HA	4:H:117:SER:O	2.18	0.44
5:L:186:TYR:O	5:L:192:TYR:OH	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:127:LEU:HA	3:Z:128:PRO:HD3	1.69	0.43
1:R:96:THR:C	1:R:97:ILE:HG13	2.39	0.43
1:S:87:SER:HB3	1:S:98:CYS:HB2	2.01	0.43
2:A:136:GLN:HA	2:A:147:PRO:HA	1.99	0.43
5:L:201:LEU:HD12	5:L:201:LEU:N	2.32	0.43
2:X:113:VAL:HG13	2:X:133:HIS:CD2	2.52	0.43
4:W:149:VAL:HG12	4:W:177:LEU:HD21	2.00	0.43
4:H:153:TRP:CD1	4:H:162:VAL:HG21	2.54	0.43
1:R:186:GLN:HB3	1:R:187:PRO:HD2	2.00	0.43
1:S:62:CYS:O	1:S:92:TRP:HA	2.18	0.43
4:H:33:VAL:CG1	4:H:50:TYR:HB2	2.49	0.43
5:V:61:ARG:NE	5:V:82:ASP:OD2	2.36	0.43
4:H:29:PHE:HB2	4:H:77:ASN:ND2	2.33	0.43
3:B:202:TYR:HB2	3:D:184:THR:HG23	1.99	0.43
2:A:188:ILE:H	2:A:188:ILE:HG12	1.60	0.43
3:D:117:THR:HG22	3:D:128:PRO:CD	2.48	0.43
5:V:191:VAL:HA	5:V:210:ASN:HB3	2.00	0.43
3:Y:126:ALA:HB2	3:Y:218:ARG:HG2	2.01	0.43
2:A:67:LEU:HD12	2:A:200:PHE:CD2	2.54	0.43
3:D:170:TYR:CD2	3:D:171:GLY:N	2.86	0.43
3:B:233:ARG:HB3	3:B:234:GLY:H	1.56	0.43
4:H:50:TYR:CZ	4:H:59:ASN:HB3	2.54	0.43
2:X:136:GLN:HA	2:X:147:PRO:HA	2.01	0.43
3:Z:138:LEU:HD23	3:Z:235:LYS:O	2.19	0.43
3:B:98:LYS:HG3	3:B:99:GLY:N	2.34	0.43
2:A:103:THR:OG1	4:H:101:MET:SD	2.77	0.43
1:R:176:GLN:NE2	1:R:184:ARG:O	2.51	0.43
5:V:142:ARG:HB2	5:V:173:TYR:CD1	2.53	0.43
5:L:158:ASN:ND2	5:L:181:LEU:HD21	2.26	0.42
3:D:140:GLY:H	3:D:236:THR:HG22	1.83	0.42
3:B:98:LYS:HZ2	3:B:226:PRO:HB2	1.84	0.42
1:R:141:HIS:O	1:R:142:CYS:HB2	2.18	0.42
1:S:100:LEU:HD13	3:Y:108:LYS:HG3	2.01	0.42
4:W:159:THR:O	4:W:162:VAL:HG12	2.19	0.42
3:Z:140:GLY:H	3:Z:236:THR:CG2	2.33	0.42
5:V:118:PHE:O	5:V:132:VAL:HG13	2.18	0.42
2:X:112:GLN:HB2	2:X:168:TYR:CD2	2.48	0.42
3:D:233:ARG:HG2	3:D:234:GLY:H	1.84	0.42
4:W:97:SER:HB2	4:W:107:TYR:O	2.20	0.42
5:L:2:ILE:HG12	5:L:27:GLN:NE2	2.27	0.42
2:X:185:THR:OG1	2:X:188:ILE:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:139:VAL:HA	3:Y:236:THR:HG22	2.01	0.42
5:V:158:ASN:HD22	5:V:181:LEU:HD21	1.85	0.42
3:D:104:TRP:HB2	3:D:119:PHE:CZ	2.54	0.42
2:A:203:PHE:HE2	2:A:205:LEU:HD21	1.84	0.42
5:V:166:GLN:HE21	5:V:171:SER:HB3	1.85	0.42
1:S:63:PRO:HD2	1:S:80:CYS:SG	2.59	0.42
5:L:191:VAL:HA	5:L:210:ASN:HB3	2.01	0.42
5:L:83:PHE:HD1	5:L:104:VAL:O	2.02	0.42
2:X:108:PHE:HA	2:X:171:ALA:O	2.20	0.42
5:L:113:PRO:HD2	5:L:201:LEU:CD1	2.49	0.42
5:L:186:TYR:CE1	5:L:192:TYR:CE2	3.07	0.42
4:W:128:PRO:CB	4:W:210:VAL:HG22	2.50	0.42
3:Z:159:LEU:HD23	3:Z:205:VAL:HG12	2.00	0.42
3:D:140:GLY:O	3:D:230:ASP:N	2.50	0.42
4:H:98:ARG:NE	4:H:99:PRO:O	2.40	0.42
5:L:69:THR:HG23	5:L:70:ASP:OD1	2.19	0.42
3:B:92:LEU:HD11	3:B:125:LEU:HD13	2.02	0.42
3:Y:154:GLY:HA2	3:Y:186:THR:HG22	2.02	0.42
3:B:241:VAL:HG21	3:D:210:LEU:HD21	2.02	0.41
3:D:171:GLY:O	3:D:172:PRO:C	2.58	0.41
3:D:202:TYR:O	3:D:203:THR:CG2	2.68	0.41
2:X:191:LEU:HD22	2:X:198:VAL:HG21	2.02	0.41
3:Y:214:ARG:O	3:Y:217:GLU:HB2	2.19	0.41
5:L:186:TYR:HE1	5:L:192:TYR:CE2	2.39	0.41
5:L:61:ARG:O	5:L:75:ILE:HA	2.19	0.41
5:L:79:GLN:HB3	5:L:80:PRO:HD2	2.02	0.41
1:R:66:THR:HB	1:R:80:CYS:HB3	2.02	0.41
1:S:84:ALA:N	1:S:87:SER:HB2	2.35	0.41
2:X:143:PRO:HG2	2:X:146:VAL:HG22	2.02	0.41
5:L:124:GLN:HG2	5:L:129:THR:O	2.21	0.41
5:V:24:ARG:HG3	5:V:70:ASP:OD1	2.21	0.41
2:A:70:ASP:HA	2:A:71:PRO:HD2	1.94	0.41
5:V:197:THR:HG22	5:V:204:PRO:CG	2.49	0.41
4:W:129:LEU:HB3	5:V:118:PHE:CD1	2.55	0.41
3:Z:115:SER:O	3:Z:128:PRO:HG2	2.20	0.41
2:X:104:SER:HA	2:X:175:LEU:O	2.20	0.41
3:D:170:TYR:HA	1:R:94:TYR:CE2	2.55	0.41
2:X:112:GLN:O	2:X:198:VAL:HA	2.19	0.41
3:Y:127:LEU:HA	3:Y:128:PRO:HD3	1.81	0.41
4:W:60:TYR:OH	4:W:69:THR:HA	2.21	0.41
5:L:149:LYS:HB3	5:L:152:ASN:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:229:VAL:CG2	3:B:236:THR:HG21	2.50	0.41
4:H:27:TYR:CE1	4:H:98:ARG:HD3	2.56	0.41
5:V:36:TYR:HA	5:V:45:LYS:O	2.20	0.41
5:V:40:PRO:C	5:V:42:LYS:H	2.23	0.41
3:Y:108:LYS:O	3:Y:109:GLU:C	2.58	0.41
2:A:175:LEU:HA	2:A:175:LEU:HD23	1.77	0.41
2:X:128:PRO:HA	2:X:157:PRO:HD3	2.02	0.41
4:H:144:TYR:CD2	4:H:199:HIS:CD2	3.09	0.41
5:L:141:PRO:HB2	5:L:143:GLU:OE1	2.21	0.41
4:H:102:LEU:HB3	4:H:103:PRO:HD3	2.01	0.41
5:V:61:ARG:O	5:V:75:ILE:HA	2.20	0.41
2:A:164:LEU:HD12	2:A:164:LEU:HA	1.84	0.41
3:Y:230:ASP:OD1	3:Y:231:PHE:N	2.54	0.41
2:X:115:PHE:CE2	2:X:131:LEU:HD22	2.55	0.41
2:X:115:PHE:CG	2:X:131:LEU:HD22	2.55	0.41
3:Z:117:THR:HG22	3:Z:128:PRO:CD	2.51	0.41
2:A:100:LEU:HD22	4:H:50:TYR:OH	2.20	0.41
4:H:29:PHE:CE1	4:H:53:PRO:HB3	2.56	0.41
1:S:46:GLN:O	1:S:47:GLU:HG2	2.21	0.41
5:V:143:GLU:OE1	5:V:143:GLU:N	2.31	0.41
2:X:133:HIS:ND1	2:X:185:THR:CG2	2.82	0.41
3:B:112:PHE:CZ	3:D:132:LEU:HD11	2.57	0.40
5:V:134:CYS:HB2	5:V:148:TRP:CZ2	2.55	0.40
5:V:54:ARG:HE	5:V:54:ARG:HB2	1.29	0.40
2:A:146:VAL:CG1	3:D:233:ARG:HH21	2.34	0.40
3:Y:138:LEU:O	3:Y:236:THR:HA	2.20	0.40
3:Z:92:LEU:HD11	3:Z:125:LEU:HD13	2.03	0.40
5:L:140:TYR:CD2	5:L:141:PRO:HA	2.56	0.40
4:H:159:THR:O	4:H:162:VAL:HG12	2.22	0.40
5:V:123:GLU:O	5:V:126:LYS:HB2	2.22	0.40
3:B:157:VAL:HB	3:B:183:GLU:O	2.21	0.40
5:L:142:ARG:HB2	5:L:173:TYR:CD1	2.55	0.40
4:H:145:PHE:HA	4:H:146:PRO:HA	1.84	0.40
3:Z:160:ARG:O	3:Z:221:VAL:HA	2.22	0.40
2:X:101:VAL:HG21	2:X:175:LEU:HD13	2.02	0.40
5:V:167:ASP:OD1	5:V:168:SER:N	2.54	0.40
3:B:163:LEU:HB3	3:B:219:VAL:HG22	2.04	0.40
2:X:192:VAL:O	2:X:197:THR:OG1	2.36	0.40
3:Z:127:LEU:HD13	3:Z:133:TYR:CD1	2.56	0.40
3:D:109:GLU:HB2	3:D:110:GLN:H	1.67	0.40
4:W:11:LEU:HD21	4:W:119:ALA:O	2.20	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:S:74:ARG:NH1	3:Z:109:GLU:O[4_554]	2.04	0.16
2:X:75:ASN:ND2	4:W:89:GLU:OE1[2_554]	2.15	0.05

## 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	R	140/193 (72%)	106 (76%)	20 (14%)	14 (10%)	1	11
1	S	75/193 (39%)	56 (75%)	13 (17%)	6 (8%)	1	16
2	A	130/157 (83%)	114 (88%)	13 (10%)	3 (2%)	8	50
2	X	130/157 (83%)	113 (87%)	14 (11%)	3 (2%)	8	50
3	B	116/210 (55%)	98 (84%)	13 (11%)	5 (4%)	3	33
3	D	127/210 (60%)	105 (83%)	14 (11%)	8 (6%)	2	23
3	Y	121/210 (58%)	104 (86%)	12 (10%)	5 (4%)	3	34
3	Z	126/210 (60%)	111 (88%)	6 (5%)	9 (7%)	1	19
4	H	210/213 (99%)	185 (88%)	23 (11%)	2 (1%)	19	66
4	W	208/213 (98%)	185 (89%)	22 (11%)	1 (0%)	34	77
5	L	209/211 (99%)	188 (90%)	18 (9%)	3 (1%)	14	59
5	V	209/211 (99%)	184 (88%)	22 (10%)	3 (1%)	14	59
All	All	1801/2388 (75%)	1549 (86%)	190 (10%)	62 (3%)	5	41

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	113	ILE
1	S	115	PRO
1	S	122	THR

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Mol	Chain	Res	Type
2	X	74	GLN
2	X	142	TYR
3	Y	245	HIS
3	Z	172	PRO
2	A	74	GLN
2	A	142	TYR
3	D	172	PRO
3	D	234	GLY
1	R	47	GLU
1	R	113	ILE
1	R	115	PRO
1	R	116	CYS
1	R	140	THR
1	R	142	CYS
4	H	134	THR
5	V	39	LYS
5	L	39	LYS
1	S	117	THR
3	Y	234	GLY
3	Z	234	GLY
3	B	98	LYS
3	B	232	ALA
3	B	234	GLY
3	D	99	GLY
3	D	232	ALA
1	R	78	THR
1	R	106	PRO
1	R	122	THR
5	L	110	VAL
3	Y	232	ALA
3	Z	98	LYS
3	Z	115	SER
3	Z	154	GLY
3	Z	200	LEU
3	B	115	SER
3	D	115	SER
3	D	200	LEU
1	R	44	ARG
1	R	90	GLU
1	S	106	PRO
3	Y	109	GLU
3	Z	99	GLY

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Mol	Chain	Res	Type
3	Z	109	GLU
3	B	109	GLU
3	D	98	LYS
3	D	109	GLU
1	R	143	GLU
1	R	162	LYS
4	W	158	LEU
1	S	44	ARG
2	X	144	PHE
3	Y	115	SER
3	Z	232	ALA
2	A	144	PHE
1	R	161	GLY
5	V	84	ALA
5	V	110	VAL
4	H	99	PRO
5	L	8	PRO

### 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	R	132/167 (79%)	124 (94%)	8 (6%)	23	65
1	S	71/167 (42%)	69 (97%)	2 (3%)	51	82
2	A	116/135 (86%)	114 (98%)	2 (2%)	68	89
2	X	116/135 (86%)	115 (99%)	1 (1%)	84	94
3	B	94/159 (59%)	93 (99%)	1 (1%)	80	92
3	D	101/159 (64%)	94 (93%)	7 (7%)	19	60
3	Y	95/159 (60%)	95 (100%)	0	100	100
3	Z	98/159 (62%)	97 (99%)	1 (1%)	82	93
4	H	178/179 (99%)	175 (98%)	3 (2%)	68	89
4	W	179/179 (100%)	176 (98%)	3 (2%)	68	89
5	L	185/185 (100%)	179 (97%)	6 (3%)	46	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	V	185/185 (100%)	182 (98%)	3 (2%)	70	90
All	All	1550/1968 (79%)	1513 (98%)	37 (2%)	57	85

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	122	THR
1	S	124	CYS
2	X	169	HIS
3	Z	159	LEU
2	A	165	HIS
2	A	169	HIS
3	B	160	ARG
3	D	132	LEU
3	D	159	LEU
3	D	160	ARG
3	D	170	TYR
3	D	217	GLU
3	D	221	VAL
3	D	233	ARG
1	R	59	CYS
1	R	61	ARG
1	R	72	CYS
1	R	95	LEU
1	R	98	CYS
1	R	139	CYS
1	R	146	SER
1	R	148	CYS
4	W	98	ARG
4	W	139	CYS
4	W	213	LYS
4	H	67	ARG
4	H	98	ARG
4	H	139	CYS
5	V	83	PHE
5	V	108	ARG
5	V	131	SER
5	L	70	ASP
5	L	108	ARG
5	L	145	LYS
5	L	160	GLN
5	L	207	LYS

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Mol	Chain	Res	Type
5	L	211	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	X	66	HIS
2	X	145	HIS
2	X	165	HIS
1	R	99	GLN
1	R	165	ASN
1	R	174	HIS
4	W	39	GLN
4	W	51	ASN
4	W	84	ASN
4	H	82	GLN
4	H	84	ASN
5	V	27	GLN
5	V	38	GLN
5	V	53	HIS
5	V	89	GLN
5	V	147	GLN
5	V	155	GLN
5	V	210	ASN
5	L	27	GLN
5	L	53	HIS
5	L	89	GLN
5	L	160	GLN
5	L	166	GLN
5	L	198	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	R	149/193 (77%)	0.16	3 (2%) 68 54	52, 138, 190, 219	0
1	S	79/193 (40%)	0.54	3 (3%) 44 32	78, 146, 211, 263	0
2	A	134/157 (85%)	-0.25	0 100 100	56, 102, 178, 222	0
2	X	134/157 (85%)	-0.10	1 (0%) 89 81	58, 104, 169, 238	0
3	B	126/210 (60%)	-0.15	1 (0%) 87 78	69, 111, 173, 220	0
3	D	135/210 (64%)	-0.25	0 100 100	67, 115, 178, 233	0
3	Y	131/210 (62%)	-0.07	1 (0%) 87 78	63, 118, 201, 271	0
3	Z	134/210 (63%)	-0.07	3 (2%) 65 50	64, 121, 185, 304	0
4	H	212/213 (99%)	0.04	8 (3%) 44 32	38, 90, 168, 267	0
4	W	212/213 (99%)	-0.31	0 100 100	49, 85, 128, 169	0
5	L	211/211 (100%)	-0.27	0 100 100	43, 89, 126, 170	0
5	V	211/211 (100%)	-0.02	2 (0%) 85 75	46, 101, 157, 212	0
All	All	1868/2388 (78%)	-0.09	22 (1%) 81 69	38, 104, 178, 304	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	172	PRO	3.9
3	Y	99	GLY	3.7
1	S	115	PRO	3.7
1	S	44	ARG	3.7
3	B	102	LEU	3.1
4	H	188	LEU	2.8
1	S	50	TYR	2.8
4	H	192	THR	2.7
5	V	64	GLY	2.6
2	X	157	PRO	2.6
3	Z	118	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
3	Z	164	TYR	2.5
4	H	190	THR	2.5
4	H	133	GLY	2.4
4	H	134	THR	2.4
4	H	208	LYS	2.4
1	R	115	PRO	2.3
1	R	168	VAL	2.3
1	R	125	ARG	2.3
4	H	124	PRO	2.2
5	V	205	VAL	2.2
4	H	209	LYS	2.2

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.