



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:51 PM UTC

PDB ID : 4MXW / pdb_00004mxw
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

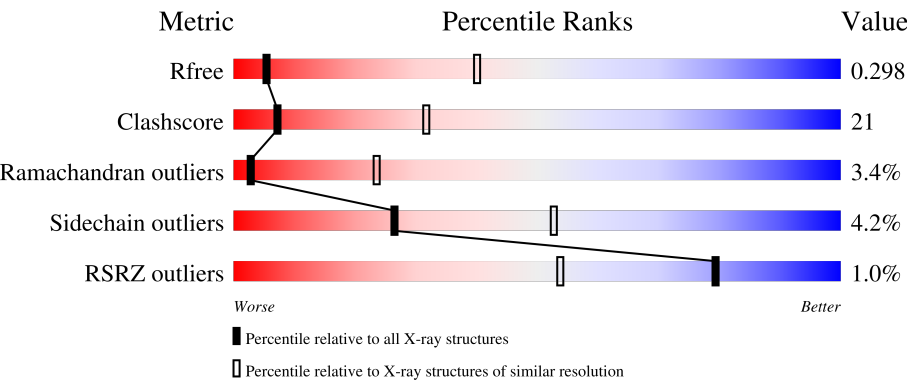
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	R	193	% 34% 34% 8% • 23%
1	S	193	2% 19% 19% • • 59%
2	A	157	49% 33% • • 15%
2	X	157	% 53% 29% • • 15%
3	B	210	% 36% 22% • 40%

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Mol	Chain	Length	Quality of chain
3	D	210	33%26%5%36%
3	Y	210	2% 36%24%.38%
3	Z	210	34%26%.36%
4	H	213	% 69%29%.
4	W	213	68%31%.
5	L	211	% 61%35%.
5	V	211	63%35%.

2 Entry composition [i](#)

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			

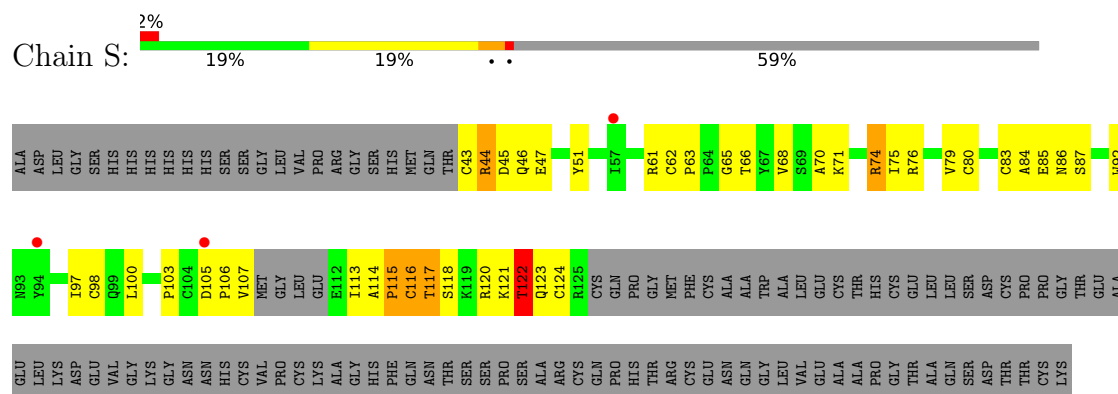
- Molecule 5 is a protein called anti-Lymphotoxin alpha antibody light chain.

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			

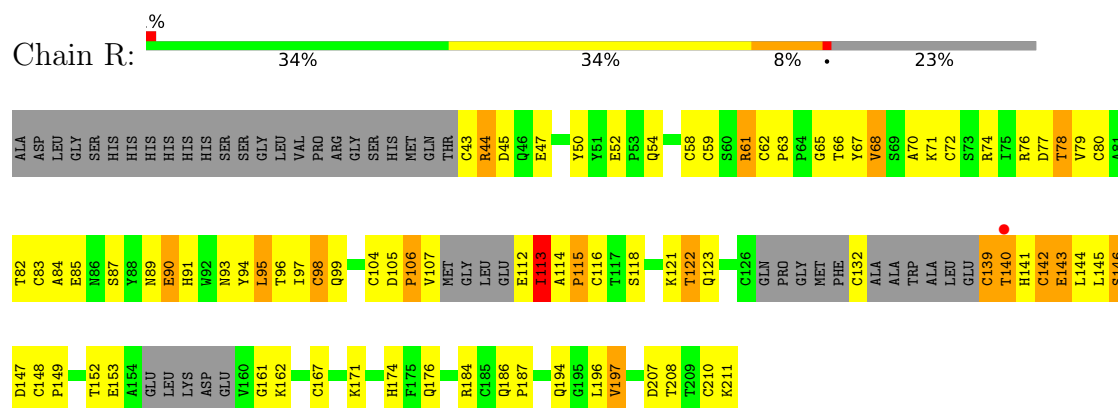
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

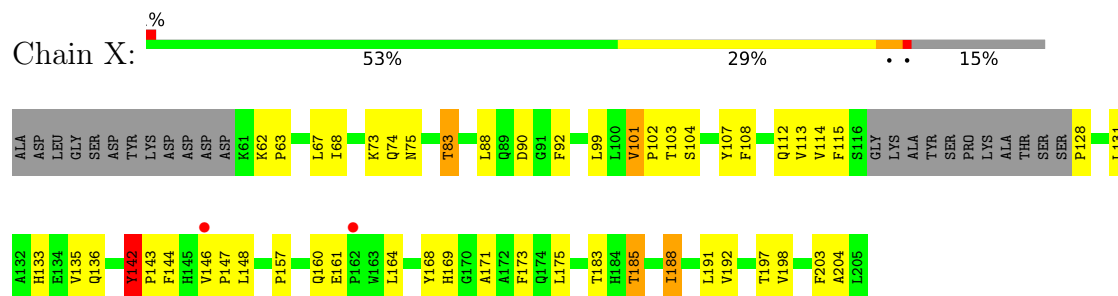
- Molecule 1: Tumor necrosis factor receptor superfamily member 3



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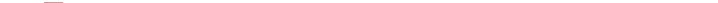


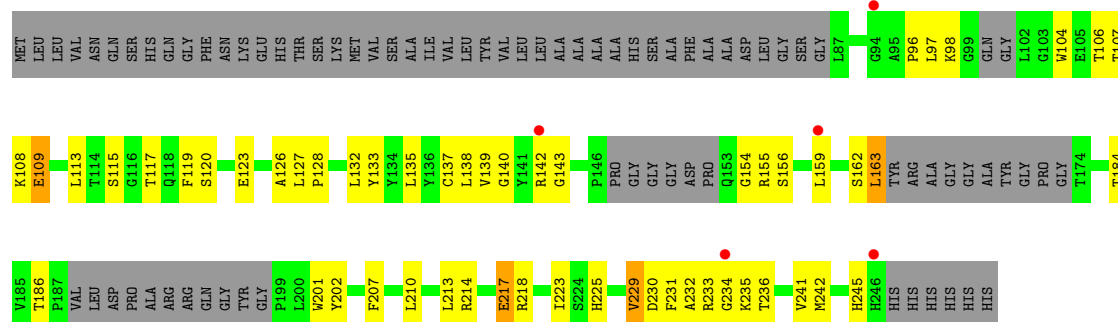
- Molecule 2: Lymphotoxin-alpha



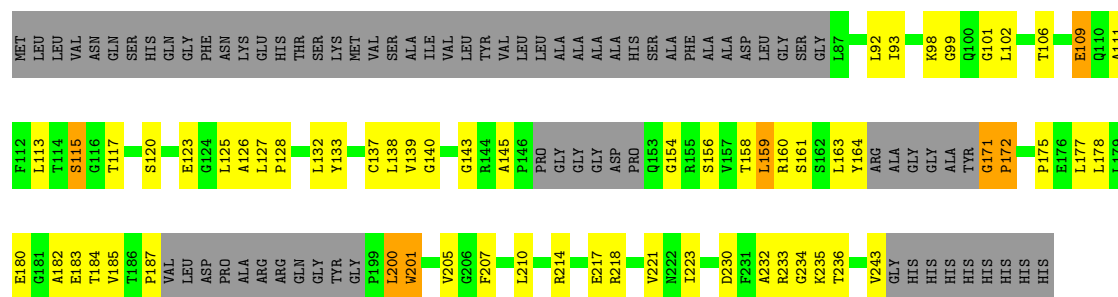
- Molecule 2: Lymphotoxin-alpha

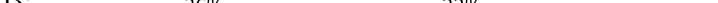
P128	L131	A132	H133	E134	V135	Q136	T142	P143	F144	H145	V146	P147	L148	L149	S150	K153	M154	V155	L159	Q160	E161	L164	H165	S166	M167	V168	H169	F173	Q174	L175	T183	H184	T185	I188	L191	V192	T197	V198	F199	F200	F203	A204	L205								
ALA	ASP	LEU	GLY	SER	ASP	TYR	LYS	ASP	ASP	ASP	R61	K62	P63	L67	D70	P71	S72	K73	Q74	N75	D84	R85	A86	F87	D90	G91	F92	S93	L99	L100	V101	P102	T103	S104	V109	Q112	V113	V114	F115	S116	GLY	LYS	ALA	TVR	SER	PRO	LYS	ALA	THR	SER	SEP

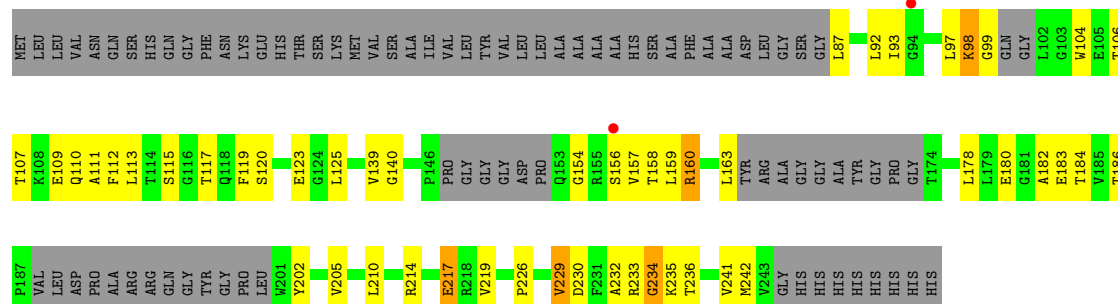
Chain Y:  2% 36% 24% 38%



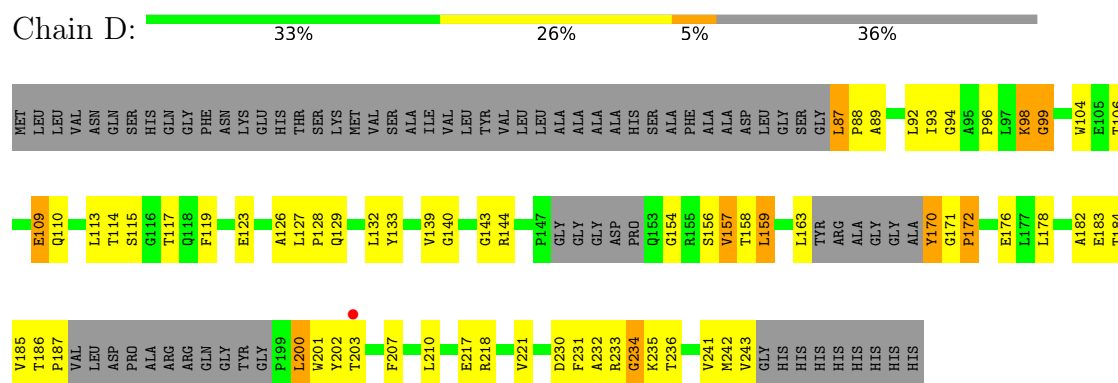
Chain Z: 34% 26% . 39%



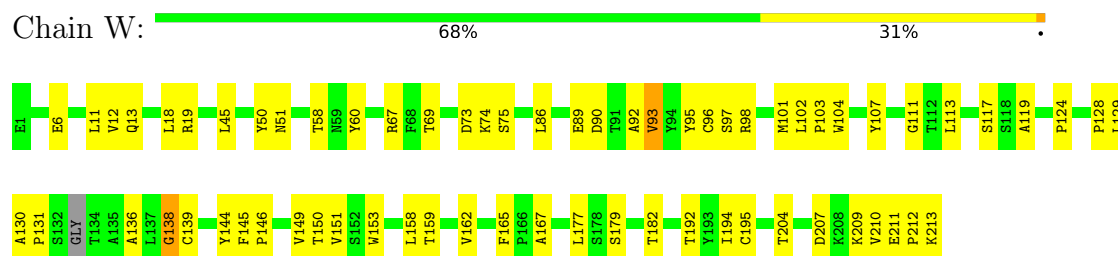
Chain B:  %



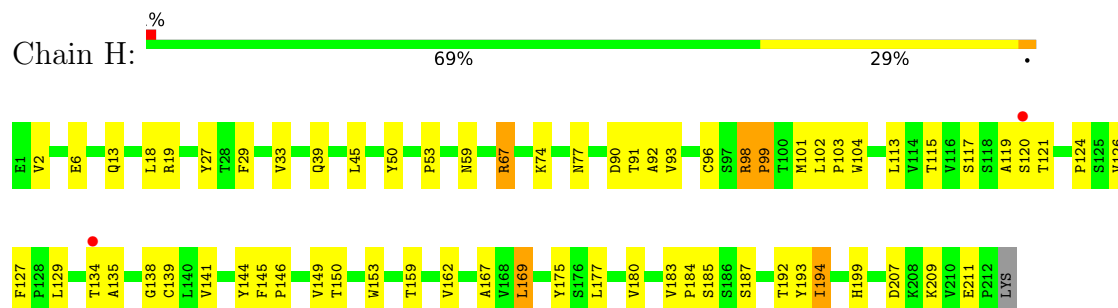
- Molecule 3: Lymphotoxin-beta



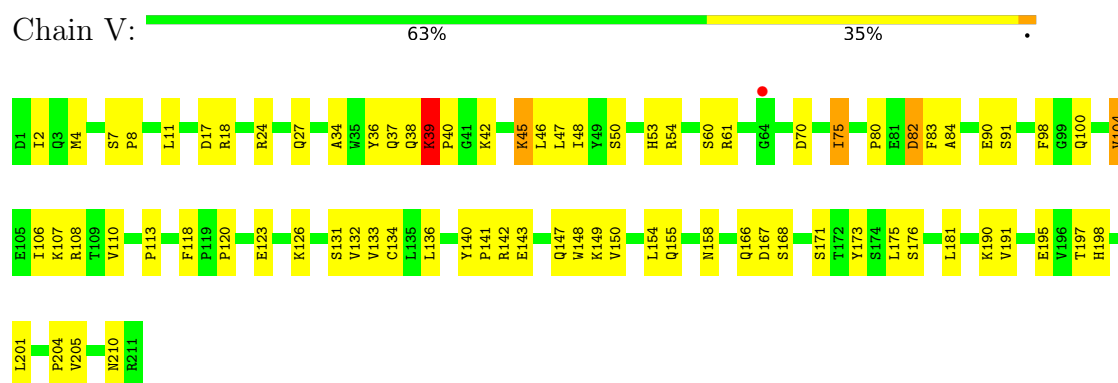
- Molecule 4: anti-Lymphotoxin alpha antibody heavy chain



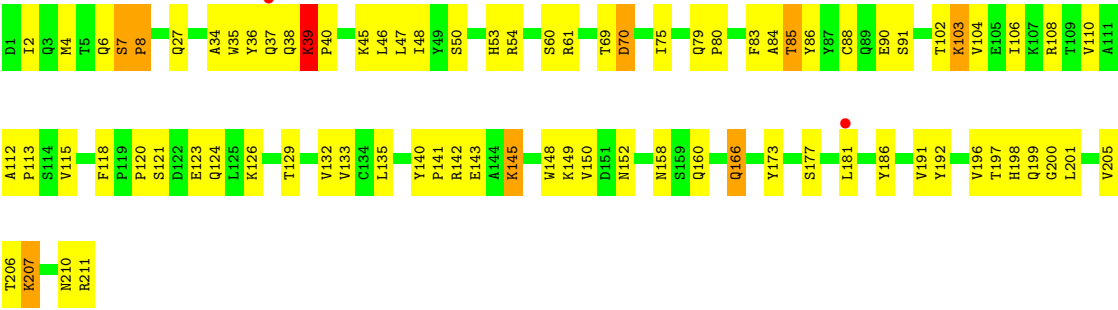
- Molecule 4: anti-Lymphotoxin alpha antibody heavy chain



- Molecule 5: anti-Lymphotoxin alpha antibody light chain



- Molecule 5: anti-Lymphotoxin alpha antibody light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.20Å 52.43Å 253.24Å 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) 99.3 (49.70-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.231 , 0.296 0.233 , 0.298	Depositor DCC
R_{free} test set	1615 reflections (4.14%)	wwPDB-VP
Wilson B-factor (Å ²)	93.6	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 101.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14217	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

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	0.83	3/1157 (0.3%)	1.22	7/1563 (0.4%)
1	S	0.88	1/634 (0.2%)	1.21	2/857 (0.2%)
2	A	0.64	1/1090 (0.1%)	1.11	7/1486 (0.5%)
2	X	0.71	3/1090 (0.3%)	1.10	8/1486 (0.5%)
3	B	0.68	0/954	0.99	0/1293
3	D	0.68	1/1027 (0.1%)	1.03	2/1394 (0.1%)
3	Y	0.66	0/979	1.03	2/1326 (0.2%)
3	Z	0.67	0/1010	1.12	4/1371 (0.3%)
4	H	0.68	0/1649	1.05	4/2253 (0.2%)
4	W	0.72	0/1654	1.00	6/2256 (0.3%)
5	L	0.75	0/1660	1.10	5/2255 (0.2%)
5	V	0.67	0/1660	1.03	4/2255 (0.2%)
All	All	0.71	9/14564 (0.1%)	1.08	51/19795 (0.3%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	160	GLN	CD-OE1	6.79	1.36	1.23
1	R	113	ILE	CA-CB	6.15	1.62	1.54
1	R	112	GLU	CD-OE1	6.09	1.36	1.25
3	D	157	VAL	CA-CB	5.91	1.61	1.53
2	X	160	GLN	CB-CG	5.88	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	112	GLU	CG-CD	5.85	1.66	1.52
2	X	160	GLN	CG-CD	5.21	1.65	1.52
1	S	51	TYR	C-O	-5.14	1.17	1.24
2	A	188	ILE	CA-CB	-5.06	1.51	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	142	TYR	CA-C-N	-10.19	109.14	120.45
2	X	142	TYR	C-N-CA	-10.19	109.14	120.45
2	A	161	GLU	N-CA-C	-9.84	96.71	110.29
3	Z	171	GLY	CA-C-N	9.24	131.39	119.84
3	Z	171	GLY	C-N-CA	9.24	131.39	119.84
5	L	39	LYS	CA-C-N	-9.04	108.54	119.84
5	L	39	LYS	C-N-CA	-9.04	108.54	119.84
2	A	142	TYR	CA-C-N	-9.02	110.44	120.45
2	A	142	TYR	C-N-CA	-9.02	110.44	120.45
1	S	116	CYS	N-CA-C	-8.67	95.94	108.60
2	A	188	ILE	CB-CA-C	-8.30	105.81	113.70
2	X	188	ILE	CB-CA-C	-8.27	105.85	113.70
1	R	90	GLU	N-CA-C	-7.66	94.49	110.80
3	Z	201	TRP	N-CA-C	7.50	120.67	110.55
4	H	92	ALA	N-CA-C	7.22	118.06	107.88
1	R	85	GLU	N-CA-C	7.05	120.21	110.35
4	H	2	VAL	N-CA-C	6.86	117.94	108.89
5	L	85	THR	N-CA-C	-6.58	98.18	108.90
4	W	138	GLY	N-CA-C	6.36	120.42	111.19
2	X	101	VAL	CA-C-N	6.12	125.52	118.85
2	X	101	VAL	C-N-CA	6.12	125.52	118.85
4	W	211	GLU	CA-C-N	5.96	127.29	119.84
4	W	211	GLU	C-N-CA	5.96	127.29	119.84
5	V	39	LYS	CA-C-N	-5.90	112.46	119.84
5	V	39	LYS	C-N-CA	-5.90	112.46	119.84
3	D	87	LEU	CA-C-N	5.82	126.01	119.90
3	D	87	LEU	C-N-CA	5.82	126.01	119.90
4	W	92	ALA	N-CA-C	5.81	116.07	107.88
2	A	70	ASP	CA-C-N	5.79	125.89	119.87
2	A	70	ASP	C-N-CA	5.79	125.89	119.87
1	R	112	GLU	CA-C-N	5.77	132.35	121.97
1	R	112	GLU	C-N-CA	5.77	132.35	121.97
2	X	161	GLU	N-CA-C	5.68	119.14	110.50
1	R	74	ARG	N-CA-C	-5.68	105.66	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	7	SER	CA-C-N	-5.61	112.83	119.84
5	L	7	SER	C-N-CA	-5.61	112.83	119.84
1	S	74	ARG	N-CA-C	-5.57	105.17	112.41
4	H	119	ALA	N-CA-C	5.57	119.62	113.21
5	V	82	ASP	N-CA-C	-5.51	104.76	112.25
4	H	138	GLY	N-CA-C	5.47	119.13	111.19
5	V	104	VAL	N-CA-C	5.33	115.54	107.75
2	A	87	PHE	N-CA-C	5.21	116.20	108.60
1	R	194	GLN	N-CA-C	-5.18	105.81	111.82
2	X	62	LYS	CA-C-N	5.14	125.05	119.85
2	X	62	LYS	C-N-CA	5.14	125.05	119.85
1	R	197	VAL	N-CA-C	5.08	116.03	108.46
4	W	130	ALA	CA-C-N	5.08	124.98	119.85
4	W	130	ALA	C-N-CA	5.08	124.98	119.85
3	Z	101	GLY	N-CA-C	5.07	118.87	112.79
3	Y	162	SER	CA-C-N	5.01	130.72	121.70
3	Y	162	SER	C-N-CA	5.01	130.72	121.70

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

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	67	0
1	S	622	0	574	33	1
2	A	1055	0	1017	55	0
2	X	1055	0	1017	39	1
3	B	936	0	908	59	0
3	D	1004	0	979	83	0
3	Y	961	0	929	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Z	988	0	952	58	1
4	H	1604	0	1564	44	0
4	W	1610	0	1573	41	1
5	L	1623	0	1573	73	0
5	V	1623	0	1573	58	0
All	All	14217	0	13704	577	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 21.

All (577) 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
5:L:115:VAL:C	5:L:207:LYS:HZ1	1.74	0.95
3:Z:230:ASP:OD2	3:Z:235:LYS:NZ	2.00	0.94
2:A:67:LEU:HD11	2:A:99:LEU:HD13	1.46	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
3:B:87:LEU:HD12	3:B:87:LEU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Y:163:LEU:HD13	3:Y:163:LEU:C	1.99	0.86
3:B:241:VAL:HG12	3:B:242:MET:O	1.76	0.86
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:V:4:MET:HE3	5:V:90:GLU:HB3	1.60	0.83
2:X:73:LYS:O	2:X:75:ASN:N	2.12	0.82
5:L:120:PRO:CD	5:L:132:VAL:HG22	2.04	0.82
3:Z:164:TYR:CE1	3:Z:175:PRO:HG3	2.14	0.82
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
5:L:83:PHE:CD1	5:L:104:VAL:HG12	2.13	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
4:H:67:ARG:NH1	4:H:90:ASP:OD2	2.13	0.80
5:V:54:ARG:NH1	5:V:60:SER:HA	1.96	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:50:SER:HB3	5:L:53:HIS:HD2	1.47	0.78
5:L:158:ASN:HD22	5:L:181:LEU:HD21	1.48	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
2:A:102:PRO:HB2	4:H:101:MET:HE3	1.65	0.77
5:L:2:ILE:HG12	5:L:27:GLN:HE21	1.51	0.76
2:X:102:PRO:HB2	4:W:101:MET:HE3	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:B:241:VAL:CG2	3:D:210:LEU:HD11	2.19	0.72
1:R:76:ARG:HG2	1:R:77:ASP:N	2.05	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
3:B:159:LEU:C	3:B:160:ARG:HG3	2.15	0.71
1:S:114:ALA:HB1	1:S:115:PRO:HA	1.71	0.71
2:A:161:GLU:HG3	3:B:186:THR:HG21	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
4:H:124:PRO:HB3	4:H:144:TYR:HB3	1.75	0.69
5:V:150:VAL:HB	5:V:155:GLN:HE21	1.58	0.69
3:D:126:ALA:HB2	3:D:218:ARG:HG2	1.75	0.69
3:B:158:THR:C	3:B:159:LEU:HD12	2.18	0.68
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
3:Y:106:THR:HB	3:Y:113:LEU:HD11	1.76	0.67
4:W:131:PRO:HG2	4:W:212:PRO:HG3	1.76	0.67
2:X:133:HIS:ND1	2:X:185:THR:HG22	2.09	0.67
3:B:106:THR:HB	3:B:113:LEU:HD11	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:50:TYR:O	1:R:58:CYS:HB2	1.96	0.66
2:X:115:PHE:CD2	2:X:131:LEU:HD22	2.31	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
3:B:159:LEU:C	3:B:160:ARG:CG	2.67	0.65
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
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:V:37:GLN:HB3	5:V:47:LEU:HD11	1.80	0.64
5:L:198:HIS:HD2	5:L:199:GLN:H	1.46	0.64
3:Y:154:GLY:HA2	3:Y:186:THR:HA	1.80	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
3:Z:145:ALA:CB	3:Z:187:PRO:HG3	2.28	0.63
2:A:146:VAL:HG13	3:D:233:ARG:CZ	2.28	0.63
5:V:11:LEU:HD11	5:V:104:VAL:HG22	1.81	0.63
3:D:230:ASP:OD2	3:D:235:LYS:NZ	2.31	0.63
3:D:170:TYR:CE1	1:R:95:LEU:CG	2.82	0.63
3:D:170:TYR:CG	3:D:171:GLY:N	2.64	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
1:R:84:ALA:O	1:R:87:SER:OG	2.09	0.61
3:Y:163:LEU:C	3:Y:163:LEU:CD1	2.69	0.61
4:H:126:VAL:HG22	4:H:141:VAL:HG22	1.82	0.61
3:Y:106:THR:HB	3:Y:113:LEU:CD1	2.29	0.61
3:D:170:TYR:O	1:R:61:ARG:NH2	2.33	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
1:R:207:ASP:OD1	1:R:208:THR:N	2.34	0.60
3:D:106:THR:HB	3:D:113:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:149:PRO:O	1:R:152:THR:OG1	2.19	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
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
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:D:170:TYR:N	1:R:94:TYR:CZ	2.71	0.58
2:A:114:VAL:HG21	2:A:197:THR:HB	1.85	0.58
3:B:233:ARG:HH12	1:R:99:GLN:NE2	2.02	0.58
5:L:115:VAL:C	5:L:207:LYS:NZ	2.56	0.58
2:A:91:GLY:O	2:A:102:PRO:HB3	2.03	0.58
3:B:107:THR:O	1:R:97:ILE:HG21	2.03	0.58
3:D:106:THR:HB	3:D:113:LEU:CD1	2.33	0.58
4:W:12:VAL:HG11	4:W:86:LEU:HD12	1.86	0.58
5:L:198:HIS:CD2	5:L:199:GLN:H	2.21	0.58
3:D:157:VAL:CG2	3:D:183:GLU:O	2.52	0.57
2:X:164:LEU:H	3:Y:184:THR:HG1	1.51	0.57
3:Z:159:LEU:HD12	3:Z:160:ARG:N	2.18	0.57
2:A:116:SER:HB3	2:A:192:VAL:HG21	1.86	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: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
1:S:107:VAL:CG2	3:Y:142:ARG:NH1	2.68	0.57
5:L:38:GLN:O	5:L:84:ALA:HB1	2.05	0.57
1:S:65:GLY:HA2	1:S:118:SER:O	2.05	0.57
3:Z:106:THR:HB	3:Z:113:LEU:CD1	2.34	0.57
5:L:83:PHE:HD1	5:L:104:VAL:HG12	1.65	0.57
4:H:120:SER:OG	4:H:121:THR:N	2.33	0.56
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

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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
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
2:A:148:LEU:HB3	2:A:173:PHE:CZ	2.40	0.56
1:R:171:LYS:HB2	1:R:174:HIS:CD2	2.38	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
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
5:L:196:VAL:HB	5:L:205:VAL:HG12	1.86	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:Y:135:LEU:HD11	3:Y:213:LEU:HD11	1.88	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
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
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
1:R:196:LEU:HD13	1:R:211:LYS:OXT	2.07	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
3:B:110:GLN:NE2	3:D:176:GLU:OE2	2.40	0.55
4:W:93:VAL:HA	4:W:113:LEU:HD23	1.88	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
1:R:105:ASP:O	1:R:107:VAL:N	2.40	0.54
5:V:106:ILE:O	5:V:166:GLN:NE2	2.38	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:L:201:LEU:HD23	5:L:205:VAL:HB	1.88	0.54
4:H:192:THR:HG23	4:H:209:LYS:HE3	1.89	0.54
5:V:150:VAL:HB	5:V:155:GLN:NE2	2.20	0.54
5:L:39:LYS:HB3	5:L:40:PRO:CD	2.37	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:Z:164:TYR:HE1	3:Z:175:PRO:HG3	1.67	0.54
3:D:132:LEU:HD21	3:D:210:LEU:HD22	1.90	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: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:184:PRO:HG2	4:H:187:SER:OG	2.08	0.53
4:H:183:VAL:HG11	4:H:193:TYR:CE1	2.43	0.53
3:Z:92:LEU:HD23	3:Z:106:THR:HG22	1.91	0.53
3:Z:139:VAL:HA	3:Z:236:THR:HG22	1.90	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
2:X:142:TYR:HB2	2:X:143:PRO:HD3	1.91	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
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:50:TYR:CE2	4:W:102:LEU:HD21	2.45	0.52
4:W:51:ASN:HD22	4:W:58:THR:HG22	1.73	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
3:Z:102:LEU:HD22	3:Z:223:ILE:HD12	1.92	0.52
3:Z:183:GLU:HG2	3:Z:185:VAL:CG2	2.40	0.52
3:D:159:LEU:HB3	3:D:207:PHE:HE2	1.74	0.52
4:H:149:VAL:HG23	4:H:199:HIS:HB2	1.91	0.52
3:Z:106:THR:HB	3:Z:113:LEU:HD11	1.92	0.52
2:A:112:GLN:O	2:A:198:VAL:HA	2.10	0.52
4:H:194:ILE:HD12	4:H:207:ASP:HB3	1.90	0.52
5:L:150:VAL:HG22	5:L:192:TYR:CD1	2.45	0.52
1:S:97:ILE:HG21	3:Y:107:THR:O	2.10	0.52
4:W:73:ASP:OD1	4:W:75:SER:OG	2.19	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
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)
5:L:37:GLN:HB3	5:L:47:LEU:HD11	1.90	0.51
3:B:214:ARG:O	3:B:217:GLU:HB2	2.09	0.51
2:X:88:LEU:HD22	2:X:92:PHE:HB3	1.92	0.51
5:L:37:GLN:HB3	5:L:86:TYR:CE2	2.46	0.51
3:B:140:GLY:N	3:B:235:LYS:O	2.44	0.51
4:H:180:VAL:HG11	5:L:135:LEU:HD22	1.91	0.51
5:V:80:PRO:HA	5:V:106:ILE:CD1	2.40	0.51
3:Y:155:ARG:O	3:Y:184:THR:HA	2.11	0.51
5:V:4:MET:CE	5:V:90:GLU:HB3	2.37	0.51
3:D:93:ILE:CG2	3:D:94:GLY:N	2.74	0.51
4:H:129:LEU:HD13	5:L:133:VAL:HG11	1.93	0.51
1:S:61:ARG:HH22	3:Z:171:GLY:N	2.09	0.50
3:D:92:LEU:HD23	3:D:106:THR:HG22	1.93	0.50
4:W:138:GLY:O	4:W:210:VAL:HG21	2.11	0.50
3:Y:132:LEU:HD11	3:Y:210:LEU:HB3	1.94	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: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
4:W:129:LEU:HD13	5:V:133:VAL:HG11	1.94	0.50
4:W:136:ALA:HB2	4:W:182:THR:HG22	1.92	0.50
4:H:135:ALA:HB3	4:H:183:VAL:O	2.11	0.50
5:V:118:PHE:HB2	5:V:133:VAL:HG12	1.94	0.50
4:W:93:VAL:HG22	4:W:113:LEU:HD21	1.94	0.50
1:S:105:ASP:O	1:S:107:VAL:N	2.44	0.50
2:A:154:MET:HG2	3:D:202:TYR:CD2	2.43	0.50
3:B:202:TYR:N	3:D:184:THR:OG1	2.45	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:Y:104:TRP:HB2	3:Y:119:PHE:CZ	2.46	0.49
3:Z:145:ALA:HB2	3:Z:187:PRO:HG3	1.94	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
1:R:196:LEU:HD12	1:R:196:LEU:C	2.38	0.49
2:A:116:SER:HB3	2:A:192:VAL:CG2	2.42	0.49
5:L:143:GLU:OE1	5:L:143:GLU:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Y:127:LEU:HD13	3:Y:133:TYR:CE1	2.48	0.49
3:B:158:THR:HG22	3:B:182:ALA:HB2	1.90	0.49
1:R:70:ALA:HB3	1:R:79:VAL:HB	1.94	0.49
4:H:183:VAL:HB	4:H:184:PRO:HD2	1.94	0.49
5:L:85:THR:HA	5:L:102:THR:O	2.13	0.49
2:X:103:THR:OG1	4:W:101:MET:SD	2.71	0.49
5:L:85:THR:HG22	5:L:103:LYS:CG	2.43	0.49
5:L:200:GLY:C	5:L:201:LEU:HD12	2.38	0.49
1:S:123:GLN:O	1:S:123:GLN:HG3	2.13	0.48
5:V:34:ALA:HA	5:V:48:ILE:O	2.13	0.48
5:L:198:HIS:CD2	5:L:199:GLN:N	2.81	0.48
2:A:115:PHE:HE2	2:A:167:MET:HE2	1.76	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
1:R:96:THR:C	1:R:97:ILE:HG13	2.39	0.48
5:L:148:TRP:HZ2	5:L:177:SER:O	1.96	0.48
2:A:85:ARG:HH22	3:B:163:LEU:HD21	1.78	0.48
3:D:93:ILE:HG22	3:D:94:GLY:N	2.27	0.48
4:H:129:LEU:HB3	5:L:118:PHE:CD1	2.48	0.48
5:V:2:ILE:CG1	5:V:27:GLN:HE21	2.24	0.48
3:Z:158:THR:HG22	3:Z:182:ALA:HB1	1.96	0.48
3:B:154:GLY:HA2	3:B:186:THR:HA	1.96	0.48
1:S:68:VAL:HG11	1:S:71:LYS:HD3	1.95	0.48
5:V:106:ILE:N	5:V:166:GLN:HE22	2.11	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
1:S:61:ARG:HH12	3:Z:172:PRO:HD2	1.79	0.47
3:B:241:VAL:CG1	3:D:243:VAL:CG1	2.72	0.47
4:W:18:LEU:HD12	4:W:19:ARG:H	1.78	0.47
1:S:61:ARG:HG2	1:S:92:TRP:HB3	1.96	0.47
3:D:89:ALA:HB1	3:D:241:VAL:HG22	1.96	0.47
2:X:90:ASP:O	4:W:101:MET:HE2	2.14	0.47
3:Y:223:ILE:HG22	3:Y:225:HIS:H	1.79	0.47
3:Z:233:ARG:O	3:Z:235:LYS:N	2.39	0.47
5:L:4:MET:HE3	5:L:90:GLU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:93:ILE:HG13	3:B:111:ALA:HB2	1.97	0.47
1:S:70:ALA:HB3	1:S:79:VAL:HB	1.96	0.47
3:Z:160:ARG:HG3	3:Z:180:GLU:HG3	1.96	0.47
2:A:85:ARG:NH2	3:B:163:LEU:HD21	2.29	0.47
5:L:83:PHE:CD1	5:L:104:VAL:O	2.68	0.47
5:L:115:VAL:O	5:L:207:LYS:NZ	2.36	0.47
3:D:123:GLU:OE1	3:D:218:ARG:NE	2.48	0.47
4:W:165:PHE:CZ	5:V:176:SER:HB3	2.50	0.47
5:V:36:TYR:CE1	5:V:46:LEU:HD13	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:Y:120:SER:OG	3:Y:123:GLU:HB2	2.14	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: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
3:D:171:GLY:O	3:D:172:PRO:C	2.58	0.46
1:S:63:PRO:O	1:S:66:THR:OG1	2.32	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
3:Y:143:GLY:O	3:Y:201:TRP:N	2.47	0.46
5:L:150:VAL:HG22	5:L:192:TYR:HD1	1.79	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
2:A:104:SER:HA	2:A:175:LEU:O	2.16	0.46
3:D:241:VAL:HG12	3:D:242:MET:O	2.16	0.46
4:W:45:LEU:HD12	5:V:98:PHE:CE2	2.51	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
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:S:75:ILE:HG13	1:S:76:ARG:HG2	1.96	0.46
1:R:121:LYS:O	1:R:123:GLN:N	2.49	0.46
5:V:40:PRO:C	5:V:42:LYS:H	2.23	0.46
3:Z:140:GLY:O	3:Z:230:ASP:N	2.43	0.45
1:R:142:CYS:O	1:R:144:LEU:N	2.46	0.45
5:L:206:THR:O	5:L:207:LYS:HG2	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Y:108:LYS:O	3:Y:109:GLU:C	2.58	0.45
3:B:104:TRP:HB2	3:B:119:PHE:CZ	2.52	0.45
5:L:83:PHE:CZ	5:L:106:ILE:HG13	2.51	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
2:X:171:ALA:HB3	2:X:173:PHE:CE2	2.52	0.45
3:Y:137:CYS:SG	3:Y:159:LEU:HD11	2.56	0.45
2:A:90:ASP:O	4:H:101:MET:HE2	2.16	0.45
2:A:148:LEU:HB3	2:A:173:PHE:CE1	2.52	0.45
5:V:147:GLN:NE2	5:V:154:LEU:HD11	2.31	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:HD2	5:V:42:LYS:HA	1.69	0.45
1:S:115:PRO:HB2	1:S:116:CYS:H	1.42	0.45
4:W:101:MET:HG2	4:W:104:TRP:CZ3	2.52	0.45
5:L:36:TYR:CE1	5:L:46:LEU:HD13	2.52	0.45
2:X:67:LEU:HD11	2:X:99:LEU:HD13	1.99	0.45
2:X:107:TYR:CE1	2:X:204:ALA:HB2	2.52	0.45
2:X:203:PHE:CD1	3:Y:210:LEU:HD21	2.52	0.45
3:Y:202:TYR:N	3:Z:184:THR:OG1	2.48	0.45
3:D:98:LYS:HB3	3:D:98:LYS:HE3	1.68	0.45
1:R:121:LYS:O	1:R:122:THR:C	2.59	0.45
4:H:135:ALA:HB2	4:H:185:SER:HA	1.99	0.45
5:L:113:PRO:HD3	5:L:198:HIS:ND1	2.31	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
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
2:A:84:ASP:OD1	2:A:85:ARG:N	2.51	0.44
5:V:61:ARG:HE	5:V:82:ASP:CG	2.25	0.44
5:L:112:ALA:HB1	5:L:201:LEU:CD1	2.47	0.44
3:Y:229:VAL:CG2	3:Y:236:THR:HG21	2.48	0.44
1:S:100:LEU:HB2	3:Y:108:LYS:HG3	1.99	0.44
3:Y:113:LEU:HB3	3:Y:117:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:214:ARG:H	3:Z:217:GLU:CD	2.26	0.44
3:D:88:PRO:HA	3:D:114:THR:OG1	2.16	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
1:R:196:LEU:CD1	1:R:197:VAL:H	2.31	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
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
5:L:4:MET:HE3	5:L:90:GLU:HG2	2.00	0.43
5:L:186:TYR:O	5:L:192:TYR:OH	2.33	0.43
1:S:87:SER:HB3	1:S:98:CYS:HB2	2.01	0.43
3:Z:127:LEU:HA	3:Z:128:PRO:HD3	1.69	0.43
2:A:136:GLN:HA	2:A:147:PRO:HA	1.99	0.43
2:X:113:VAL:HG13	2:X:133:HIS:CD2	2.52	0.43
3:D:98:LYS:O	3:D:99:GLY:C	2.61	0.43
5:L:201:LEU:HD12	5:L:201:LEU:N	2.32	0.43
1:R:186:GLN:HB3	1:R:187:PRO:HD2	2.00	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:S:62:CYS:O	1:S:92:TRP:HA	2.18	0.43
4:H:29:PHE:HB2	4:H:77:ASN:ND2	2.33	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
2:A:188:ILE:H	2:A:188:ILE:HG12	1.60	0.43
3:B:202:TYR:HB2	3:D:184:THR:HG23	1.99	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
2:X:136:GLN:HA	2:X:147:PRO:HA	2.01	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:B:233:ARG:HB3	3:B:234:GLY:H	1.56	0.43
3:D:170:TYR:CD2	3:D:171:GLY:N	2.86	0.43
4:H:50:TYR:CZ	4:H:59:ASN:HB3	2.54	0.43
3:Z:138:LEU:HD23	3:Z:235:LYS:O	2.19	0.43
2:A:103:THR:OG1	4:H:101:MET:SD	2.77	0.43
3:B:98:LYS:HG3	3:B:99:GLY:N	2.34	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
1:S:100:LEU:HD13	3:Y:108:LYS:HG3	2.01	0.42
3:D:140:GLY:H	3:D:236:THR:HG22	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:141:HIS:O	1:R:142:CYS:HB2	2.18	0.42
4:W:159:THR:O	4:W:162:VAL:HG12	2.19	0.42
5:L:158:ASN:ND2	5:L:181:LEU:HD21	2.26	0.42
2:X:112:GLN:HB2	2:X:168:TYR:CD2	2.48	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
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
2:X:185:THR:OG1	2:X:188:ILE:HD13	2.20	0.42
3:Y:139:VAL:HA	3:Y:236:THR:HG22	2.01	0.42
3:D:104:TRP:HB2	3:D:119:PHE:CZ	2.54	0.42
5:V:158:ASN:HD22	5:V:181:LEU:HD21	1.85	0.42
5:L:2:ILE:HG12	5:L:27:GLN:NE2	2.27	0.42
1:S:63:PRO:HD2	1:S:80:CYS:SG	2.59	0.42
2:A:203:PHE:HE2	2:A:205:LEU:HD21	1.84	0.42
5:V:100:GLN:H	5:V:100:GLN:CD	2.26	0.42
5:V:166:GLN:HE21	5:V:171:SER:HB3	1.85	0.42
5:L:191:VAL:HA	5:L:210:ASN:HB3	2.01	0.42
2:X:108:PHE:HA	2:X:171:ALA:O	2.20	0.42
5:L:83:PHE:HD1	5:L:104:VAL:O	2.02	0.42
4:W:128:PRO:CB	4:W:210:VAL:HG22	2.50	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
3:Z:159:LEU:HD23	3:Z:205:VAL:HG12	2.00	0.42
3:B:92:LEU:HD11	3:B:125:LEU:HD13	2.02	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
5:L:206:THR:C	5:L:207:LYS:HG2	2.44	0.42
3:Y:154:GLY:HA2	3:Y:186:THR:HG22	2.02	0.42
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
3:B:241:VAL:HG21	3:D:210:LEU:HD21	2.02	0.41
3:D:202:TYR:O	3:D:203:THR:CG2	2.68	0.41
1:R:143:GLU:C	1:R:145:LEU:H	2.27	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
5:L:186:TYR:HE1	5:L:192:TYR:CE2	2.39	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
2:A:70:ASP:HA	2:A:71:PRO:HD2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:66:THR:HB	1:R:80:CYS:HB3	2.02	0.41
5:V:24:ARG:HG3	5:V:70:ASP:OD1	2.21	0.41
5:L:124:GLN:HG2	5:L:129:THR:O	2.21	0.41
2:X:104:SER:HA	2:X:175:LEU:O	2.20	0.41
3:Z:115:SER:O	3:Z:128:PRO:HG2	2.20	0.41
4:W:129:LEU:HB3	5:V:118:PHE:CD1	2.55	0.41
5:V:197:THR:HG22	5:V:204:PRO:CG	2.49	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
3:D:170:TYR:HA	1:R:94:TYR:CE2	2.55	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
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
2:X:128:PRO:HA	2:X:157:PRO:HD3	2.02	0.41
2:A:175:LEU:HA	2:A:175:LEU:HD23	1.77	0.41
3:Y:230:ASP:OD1	3:Y:231:PHE:N	2.54	0.41
2:A:63:PRO:HG3	4:H:101:MET:HE1	2.03	0.41
2:A:164:LEU:HA	2:A:164:LEU:HD12	1.84	0.41
4:H:102:LEU:HB3	4:H:103:PRO:HD3	2.01	0.41
4:H:144:TYR:CD2	4:H:199:HIS:CD2	3.09	0.41
5:V:61:ARG:O	5:V:75:ILE:HA	2.20	0.41
5:L:141:PRO:HB2	5:L:143:GLU:OE1	2.21	0.41
1:S:46:GLN:O	1:S:47:GLU:HG2	2.21	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
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
1:R:153:GLU:CD	1:R:184:ARG:HA	2.46	0.41
2:X:63:PRO:HG3	4:W:101:MET:HE1	2.01	0.40
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
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
2:A:146:VAL:CG1	3:D:233:ARG:HH21	2.34	0.40
3:B:157:VAL:HB	3:B:183:GLU:O	2.21	0.40
3:D:129:GLN:O	3:D:133:TYR:OH	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:145:PHE:HA	4:H:146:PRO:HA	1.84	0.40
4:H:159:THR:O	4:H:162:VAL:HG12	2.22	0.40
5:V:54:ARG:HE	5:V:54:ARG:HB2	1.29	0.40
5:V:123:GLU:O	5:V:126:LYS:HB2	2.22	0.40
5:L:140:TYR:CD2	5:L:141:PRO:HA	2.56	0.40
5:L:142:ARG:HB2	5:L:173:TYR:CD1	2.55	0.40
2:X:101:VAL:HG21	2:X:175:LEU:HD13	2.02	0.40
3:Z:160:ARG:O	3:Z:221:VAL:HA	2.22	0.40
5:V:167:ASP:OD1	5:V:168:SER:N	2.54	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:B:163:LEU:HB3	3:B:219:VAL:HG22	2.04	0.40
1:R:95:LEU:C	1:R:97:ILE:N	2.79	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
5:V:80:PRO:C	5:V:82:ASP:H	2.29	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%)	0 5
1	S	75/193 (39%)	56 (75%)	13 (17%)	6 (8%)	1 8
2	A	130/157 (83%)	114 (88%)	13 (10%)	3 (2%)	5 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	X	130/157 (83%)	113 (87%)	14 (11%)	3 (2%)	5	30
3	B	116/210 (55%)	98 (84%)	13 (11%)	5 (4%)	2	18
3	D	127/210 (60%)	105 (83%)	14 (11%)	8 (6%)	1	12
3	Y	121/210 (58%)	104 (86%)	12 (10%)	5 (4%)	2	19
3	Z	126/210 (60%)	111 (88%)	6 (5%)	9 (7%)	1	10
4	H	210/213 (99%)	185 (88%)	23 (11%)	2 (1%)	12	45
4	W	208/213 (98%)	185 (89%)	22 (11%)	1 (0%)	24	57
5	L	209/211 (99%)	188 (90%)	18 (9%)	3 (1%)	9	38
5	V	209/211 (99%)	184 (88%)	22 (10%)	3 (1%)	9	38
All	All	1801/2388 (75%)	1549 (86%)	190 (10%)	62 (3%)	3	23

All (62) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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%)	120 (91%)	12 (9%)	9	33
1	S	71/167 (42%)	69 (97%)	2 (3%)	38	60
2	A	116/135 (86%)	112 (97%)	4 (3%)	32	57
2	X	116/135 (86%)	113 (97%)	3 (3%)	40	62
3	B	94/159 (59%)	91 (97%)	3 (3%)	34	58
3	D	101/159 (64%)	97 (96%)	4 (4%)	28	54
3	Y	95/159 (60%)	92 (97%)	3 (3%)	34	58
3	Z	98/159 (62%)	96 (98%)	2 (2%)	48	66
4	H	178/179 (99%)	169 (95%)	9 (5%)	21	49
4	W	179/179 (100%)	172 (96%)	7 (4%)	28	54
5	L	185/185 (100%)	176 (95%)	9 (5%)	22	49
5	V	185/185 (100%)	178 (96%)	7 (4%)	29	55
All	All	1550/1968 (79%)	1485 (96%)	65 (4%)	26	53

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	122	THR
1	S	124	CYS
2	X	83	THR
2	X	169	HIS
2	X	185	THR
3	Y	163	LEU
3	Y	217	GLU
3	Y	229	VAL
3	Z	159	LEU
3	Z	161	SER
2	A	109	VAL
2	A	155	VAL
2	A	165	HIS
2	A	169	HIS
3	B	160	ARG
3	B	217	GLU
3	B	229	VAL
3	D	159	LEU

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Mol	Chain	Res	Type
3	D	170	TYR
3	D	217	GLU
3	D	221	VAL
1	R	59	CYS
1	R	61	ARG
1	R	68	VAL
1	R	72	CYS
1	R	82	THR
1	R	91	HIS
1	R	95	LEU
1	R	98	CYS
1	R	113	ILE
1	R	139	CYS
1	R	146	SER
1	R	148	CYS
4	W	74	LYS
4	W	93	VAL
4	W	98	ARG
4	W	139	CYS
4	W	150	THR
4	W	204	THR
4	W	213	LYS
4	H	67	ARG
4	H	74	LYS
4	H	93	VAL
4	H	98	ARG
4	H	139	CYS
4	H	150	THR
4	H	169	LEU
4	H	194	ILE
4	H	211	GLU
5	V	39	LYS
5	V	45	LYS
5	V	75	ILE
5	V	83	PHE
5	V	107	LYS
5	V	108	ARG
5	V	131	SER
5	L	45	LYS
5	L	70	ASP
5	L	103	LYS
5	L	108	ARG

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Mol	Chain	Res	Type
5	L	145	LYS
5	L	160	GLN
5	L	166	GLN
5	L	207	LYS
5	L	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
2	X	66	HIS
2	X	145	HIS
2	X	160	GLN
2	X	165	HIS
1	R	99	GLN
1	R	165	ASN
1	R	174	HIS
1	R	176	GLN
4	W	39	GLN
4	W	51	ASN
4	W	84	ASN
4	H	51	ASN
4	H	77	ASN
4	H	84	ASN
4	H	198	ASN
5	V	27	GLN
5	V	37	GLN
5	V	38	GLN
5	V	53	HIS
5	V	147	GLN
5	V	155	GLN
5	L	27	GLN
5	L	37	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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, 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	R	149/193 (77%)	-0.02	1 (0%) 84 61	52, 138, 190, 219	0
1	S	79/193 (40%)	0.36	3 (3%) 44 25	78, 146, 211, 263	0
2	A	134/157 (85%)	-0.09	0 100 100	56, 102, 178, 222	0
2	X	134/157 (85%)	-0.04	2 (1%) 72 44	58, 104, 169, 238	0
3	B	126/210 (60%)	0.09	2 (1%) 70 43	69, 111, 172, 220	0
3	D	135/210 (64%)	0.19	1 (0%) 84 61	67, 115, 178, 233	0
3	Y	131/210 (62%)	0.23	5 (3%) 44 25	63, 118, 201, 271	0
3	Z	134/210 (63%)	0.22	0 100 100	64, 121, 185, 304	0
4	H	212/213 (99%)	-0.15	2 (0%) 81 56	38, 90, 168, 267	0
4	W	212/213 (99%)	-0.27	0 100 100	49, 85, 128, 169	0
5	L	211/211 (100%)	-0.21	2 (0%) 81 56	43, 89, 126, 170	0
5	V	211/211 (100%)	-0.05	1 (0%) 87 66	46, 101, 157, 212	0
All	All	1868/2388 (78%)	-0.02	19 (1%) 79 54	38, 104, 178, 304	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	246	HIS	3.1
3	B	156	SER	2.9
5	L	37	GLN	2.5
4	H	134	THR	2.5
3	Y	234	GLY	2.5
2	X	162	PRO	2.5
4	H	120	SER	2.4
3	B	94	GLY	2.3
3	D	203	THR	2.3
1	S	94	TYR	2.3
1	S	105	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
5	V	64	GLY	2.2
3	Y	142	ARG	2.1
5	L	181	LEU	2.1
3	Y	159	LEU	2.1
2	X	146	VAL	2.0
1	S	57	ILE	2.0
1	R	140	THR	2.0
3	Y	94	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.