



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 12, 2023 – 07:20 AM EDT

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

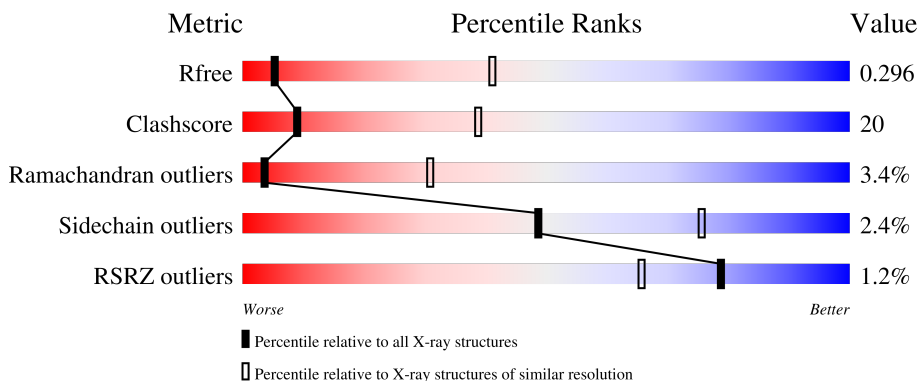
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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.



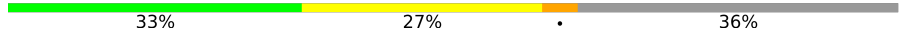
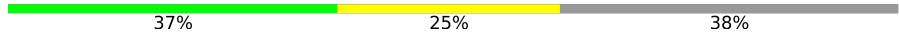
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	
1	S	193	
2	A	157	
2	X	157	
3	B	210	

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Mol	Chain	Length	Quality of chain
3	D	210	 33% 27% 36%
3	Y	210	 37% 25% 38%
3	Z	210	 36% 25% 36%
4	H	213	 72% 26% 4%
4	W	213	 71% 28%
5	L	211	 62% 36%
5	V	211	 63% 37%

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
			Total	C	N	O	S			
1	S	79	622	374	118	118	12	0	0	0
1	R	149	1136	677	214	223	22	0	0	0

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
			Total	C	N	O	S			
2	X	134	1055	689	173	191	2	0	0	0
2	A	134	1055	689	173	191	2	0	0	0

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

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			

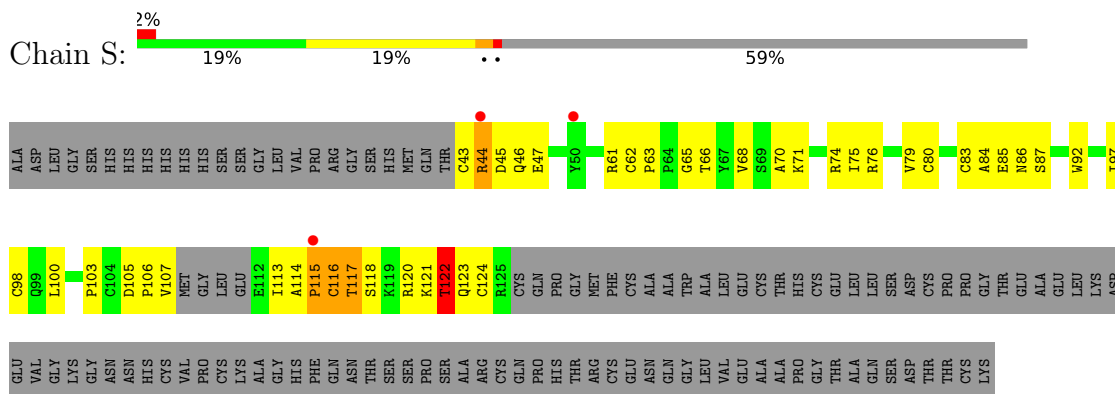
- Molecule 5 is a protein called anti-Lymphotoxin alpha antibody light chain.

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			

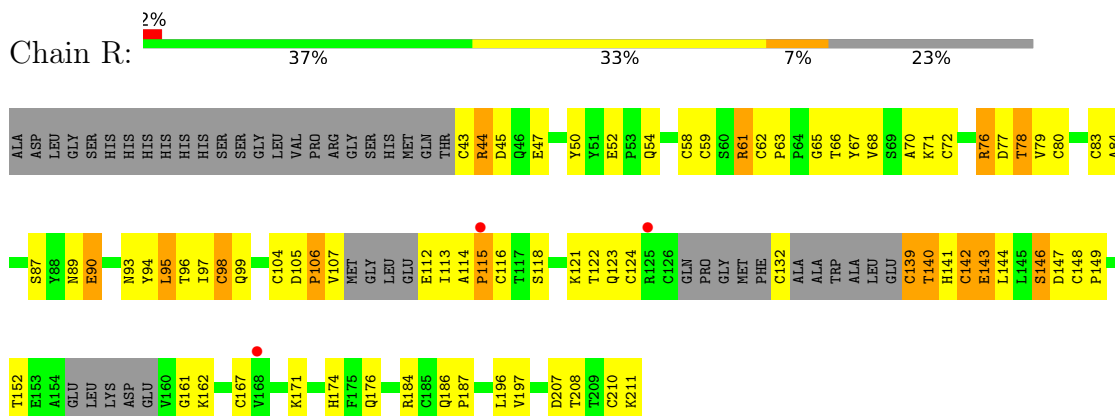
3 Residue-property plots [i](#)

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.

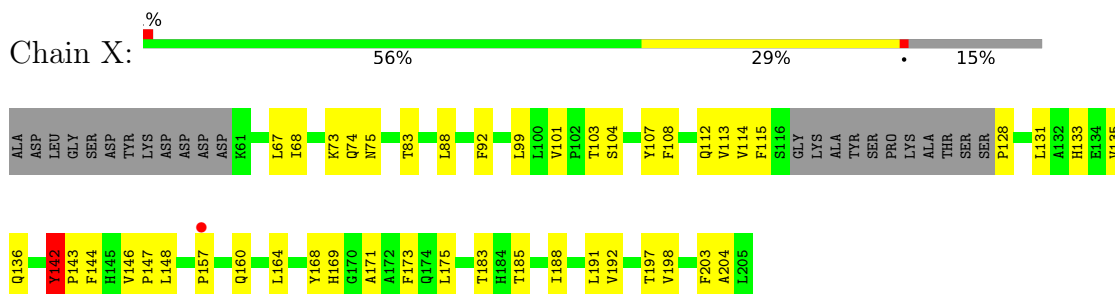
- Molecule 1: Tumor necrosis factor receptor superfamily member 3



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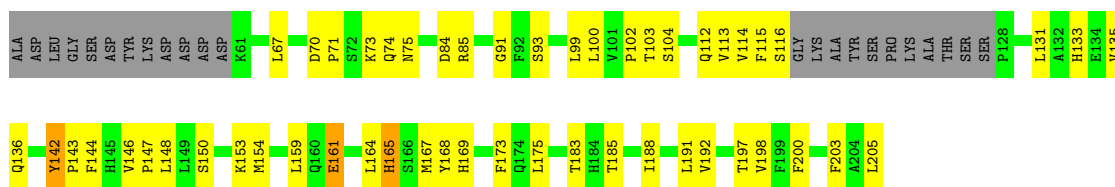


- Molecule 2: Lymphotoxin-alpha

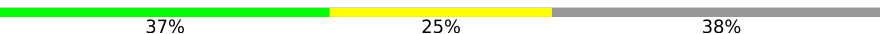


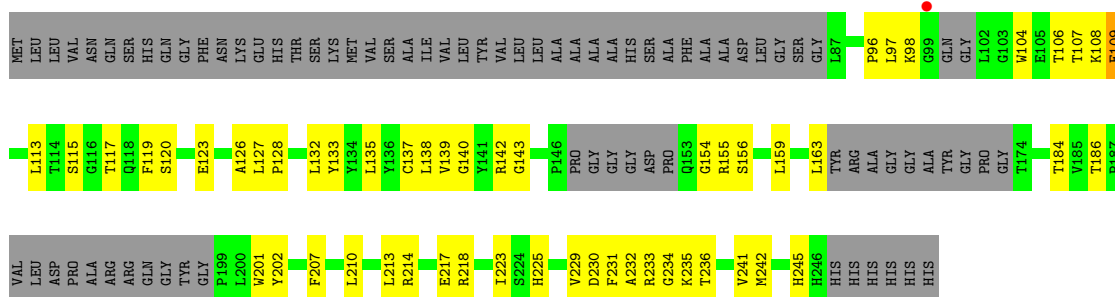
- Molecule 2: Lymphotoxin-alpha

Chain A: 

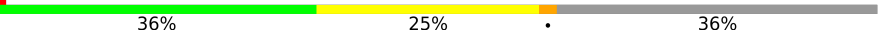


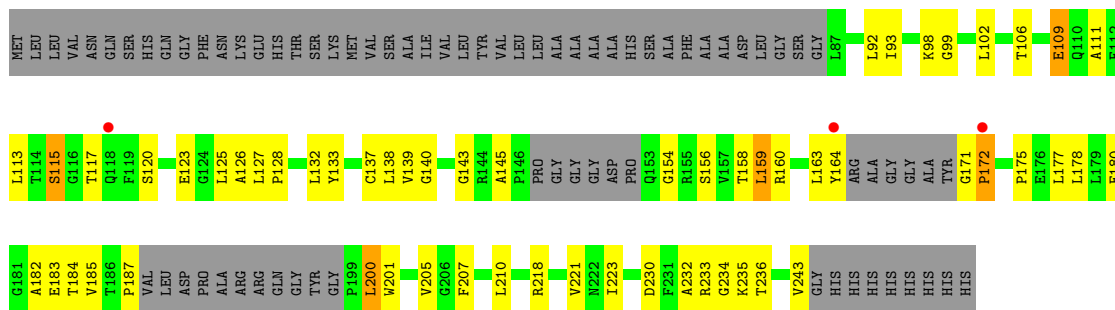
- Molecule 3: Lymphotoxin-beta

Chain Y: 

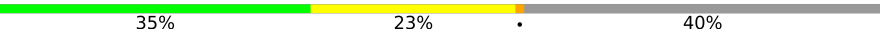


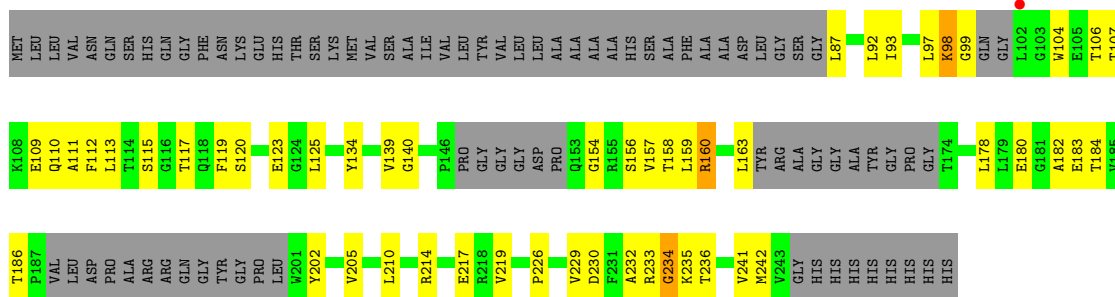
- Molecule 3: Lymphotoxin-beta

Chain Z: 

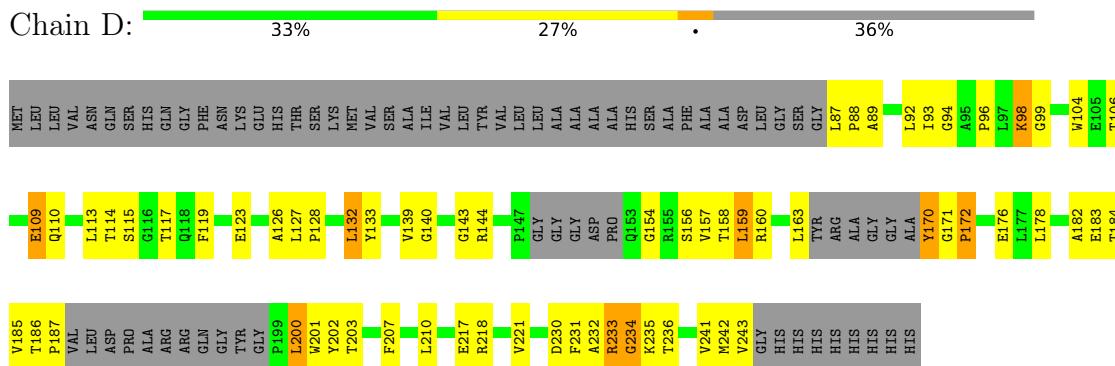


- Molecule 3: Lymphotoxin-beta

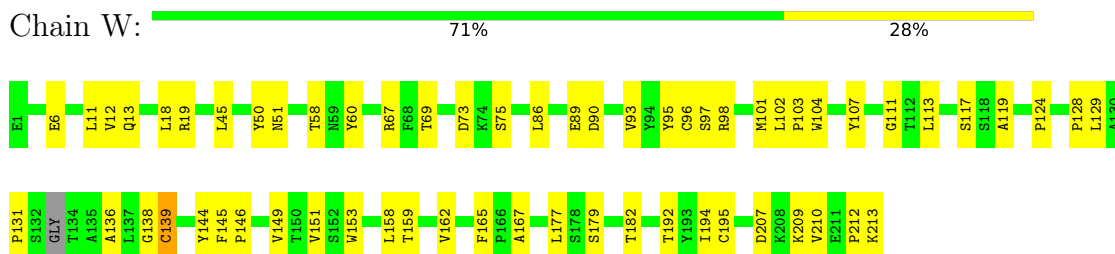
Chain B: 



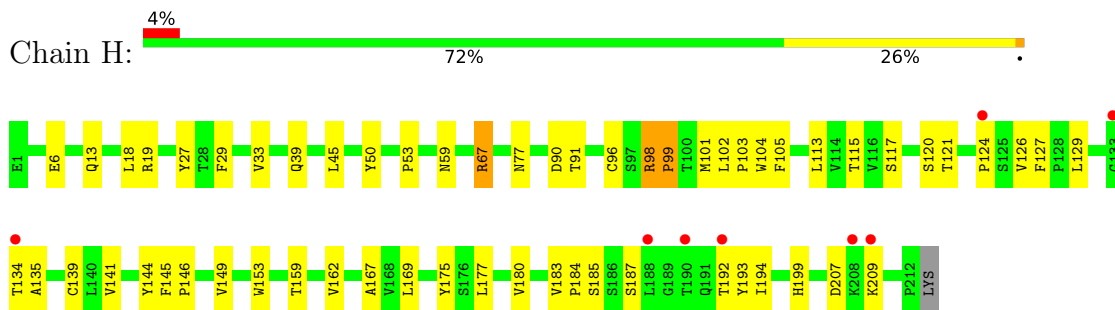
- Molecule 3: Lymphotoxin-beta



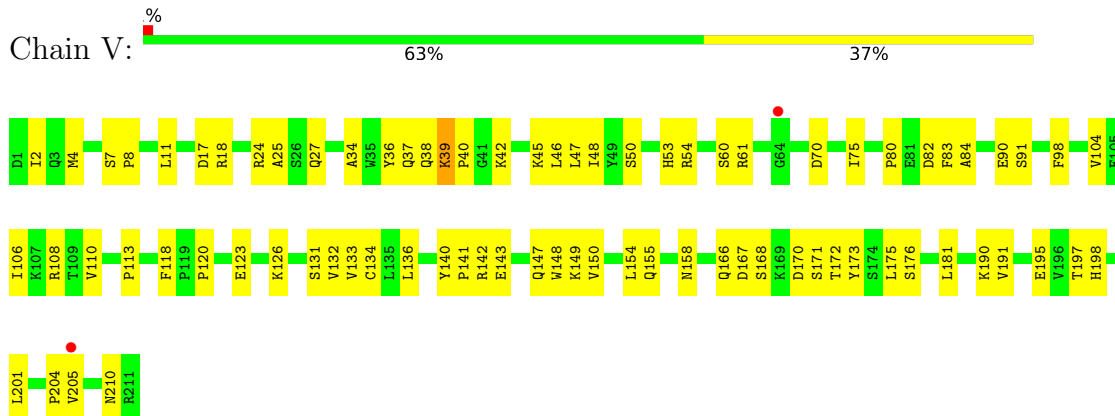
- Molecule 4: anti-Lymphotoxin alpha antibody heavy chain



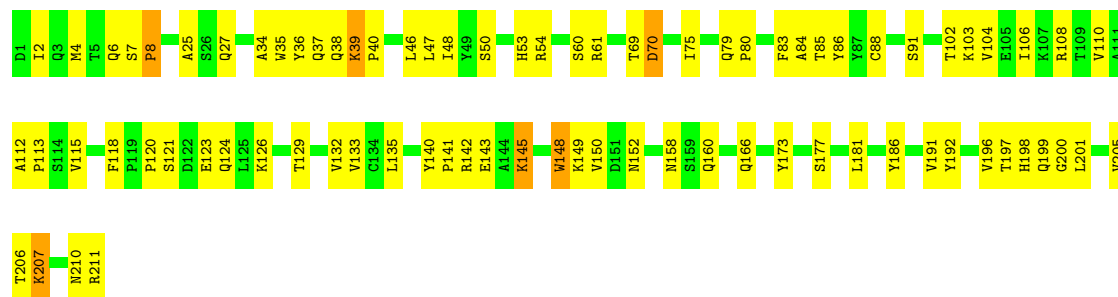
- Molecule 4: anti-Lymphotoxin alpha antibody heavy chain



- 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) 99.4 (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)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.231 , 0.296 0.231 , 0.296	Depositor DCC
R_{free} test set	1615 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	93.6	Xtrriage
Anisotropy	0.098	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 77.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	14217	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtrriage'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 i

5.1 Standard geometry i

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

The worst 5 of 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

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
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.

The worst 5 of 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

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	8
1	S	75/193 (39%)	56 (75%)	13 (17%)	6 (8%)	1	11
2	A	130/157 (83%)	114 (88%)	13 (10%)	3 (2%)	6	38
2	X	130/157 (83%)	113 (87%)	14 (11%)	3 (2%)	6	38
3	B	116/210 (55%)	98 (84%)	13 (11%)	5 (4%)	2	24
3	D	127/210 (60%)	105 (83%)	14 (11%)	8 (6%)	1	17
3	Y	121/210 (58%)	104 (86%)	12 (10%)	5 (4%)	3	26
3	Z	126/210 (60%)	111 (88%)	6 (5%)	9 (7%)	1	14
4	H	210/213 (99%)	185 (88%)	23 (11%)	2 (1%)	15	55
4	W	208/213 (98%)	185 (89%)	22 (11%)	1 (0%)	29	68
5	L	209/211 (99%)	188 (90%)	18 (9%)	3 (1%)	11	48
5	V	209/211 (99%)	184 (88%)	22 (10%)	3 (1%)	11	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1801/2388 (75%)	1549 (86%)	190 (10%)	62 (3%)	3	31

5 of 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

5.3.2 Protein sidechains [i](#)

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%)	18	53
1	S	71/167 (42%)	69 (97%)	2 (3%)	43	72
2	A	116/135 (86%)	114 (98%)	2 (2%)	60	82
2	X	116/135 (86%)	115 (99%)	1 (1%)	78	90
3	B	94/159 (59%)	93 (99%)	1 (1%)	73	88
3	D	101/159 (64%)	94 (93%)	7 (7%)	15	49
3	Y	95/159 (60%)	95 (100%)	0	100	100
3	Z	98/159 (62%)	97 (99%)	1 (1%)	76	88
4	H	178/179 (99%)	175 (98%)	3 (2%)	60	82
4	W	179/179 (100%)	176 (98%)	3 (2%)	60	82
5	L	185/185 (100%)	179 (97%)	6 (3%)	39	70
5	V	185/185 (100%)	182 (98%)	3 (2%)	62	83
All	All	1550/1968 (79%)	1513 (98%)	37 (2%)	49	75

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	V	83	PHE
5	L	207	LYS
5	V	108	ARG
5	L	108	ARG
3	D	221	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
5	V	89	GLN
5	V	210	ASN
5	V	155	GLN
5	L	27	GLN
4	W	39	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	149/193 (77%)	0.13	3 (2%) 65 49	52, 138, 190, 219	0
1	S	79/193 (40%)	0.51	3 (3%) 40 26	78, 146, 211, 263	0
2	A	134/157 (85%)	-0.28	0 100 100	56, 102, 178, 222	0
2	X	134/157 (85%)	-0.13	1 (0%) 87 78	58, 104, 169, 238	0
3	B	126/210 (60%)	-0.18	1 (0%) 86 75	69, 111, 172, 220	0
3	D	135/210 (64%)	-0.27	0 100 100	67, 115, 178, 233	0
3	Y	131/210 (62%)	-0.09	1 (0%) 86 75	63, 118, 201, 271	0
3	Z	134/210 (63%)	-0.09	3 (2%) 62 45	64, 121, 185, 304	0
4	H	212/213 (99%)	0.02	8 (3%) 40 26	38, 90, 168, 267	0
4	W	212/213 (99%)	-0.34	0 100 100	49, 85, 128, 169	0
5	L	211/211 (100%)	-0.30	0 100 100	43, 89, 126, 170	0
5	V	211/211 (100%)	-0.04	2 (0%) 84 73	46, 101, 157, 212	0
All	All	1868/2388 (78%)	-0.12	22 (1%) 79 66	38, 104, 178, 304	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	172	PRO	3.9
1	S	44	ARG	3.8
3	Y	99	GLY	3.8
1	S	115	PRO	3.7
3	B	102	LEU	3.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.