



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:07 AM GMT

PDB ID : 3E3Q
Title : Structure of the 3alpham13 high-affinity mutant of the 2C TCR in complex with Ld/QL9
Authors : Colf, L.A.; Garcia, K.C.
Deposited on : 2008-08-07
Resolution : 2.95 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

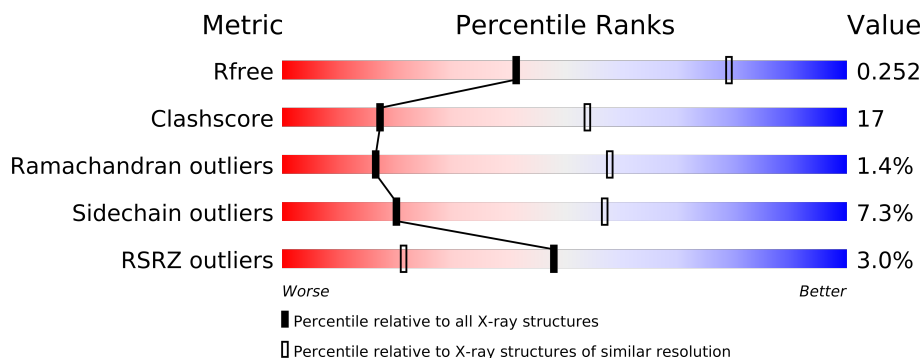
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	175	
1	B	175	
1	H	175	
1	L	175	
1	P	175	
1	U	175	
1	Y	175	
1	c	175	
2	G	9	
2	K	9	
2	O	9	
2	Q	9	
2	T	9	
2	X	9	

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Mol	Chain	Length	Quality of chain
2	b	9	
2	f	9	
3	C	109	
3	D	109	
3	I	109	
3	M	109	
3	R	109	
3	V	109	
3	Z	109	
3	d	109	
4	E	111	
4	F	111	
4	J	111	
4	N	111	
4	S	111	
4	W	111	
4	a	111	
4	e	111	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25808 atoms, of which 0 are hydrogen and 0 are deuterium.

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 H-2 class I histocompatibility antigen, L-D alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	B	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	c	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	H	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	L	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	P	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	U	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			
1	Y	175	Total	C	N	O	S	0	0	0
			1449	908	257	277	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	TYR	PHE	ENGINEERED	UNP P01897
A	12	THR	VAL	ENGINEERED	UNP P01897
A	15	ARG	PRO	ENGINEERED	UNP P01897
A	23	THR	ILE	ENGINEERED	UNP P01897
A	30	ASP	ASN	ENGINEERED	UNP P01897
A	49	VAL	ALA	ENGINEERED	UNP P01897
A	66	VAL	ILE	ENGINEERED	UNP P01897
A	97	ARG	TRP	ENGINEERED	UNP P01897
A	131	ARG	LYS	ENGINEERED	UNP P01897
B	8	TYR	PHE	ENGINEERED	UNP P01897
B	12	THR	VAL	ENGINEERED	UNP P01897
B	15	ARG	PRO	ENGINEERED	UNP P01897
B	23	THR	ILE	ENGINEERED	UNP P01897

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	ASP	ASN	ENGINEERED	UNP P01897
B	49	VAL	ALA	ENGINEERED	UNP P01897
B	66	VAL	ILE	ENGINEERED	UNP P01897
B	97	ARG	TRP	ENGINEERED	UNP P01897
B	131	ARG	LYS	ENGINEERED	UNP P01897
c	8	TYR	PHE	ENGINEERED	UNP P01897
c	12	THR	VAL	ENGINEERED	UNP P01897
c	15	ARG	PRO	ENGINEERED	UNP P01897
c	23	THR	ILE	ENGINEERED	UNP P01897
c	30	ASP	ASN	ENGINEERED	UNP P01897
c	49	VAL	ALA	ENGINEERED	UNP P01897
c	66	VAL	ILE	ENGINEERED	UNP P01897
c	97	ARG	TRP	ENGINEERED	UNP P01897
c	131	ARG	LYS	ENGINEERED	UNP P01897
H	8	TYR	PHE	ENGINEERED	UNP P01897
H	12	THR	VAL	ENGINEERED	UNP P01897
H	15	ARG	PRO	ENGINEERED	UNP P01897
H	23	THR	ILE	ENGINEERED	UNP P01897
H	30	ASP	ASN	ENGINEERED	UNP P01897
H	49	VAL	ALA	ENGINEERED	UNP P01897
H	66	VAL	ILE	ENGINEERED	UNP P01897
H	97	ARG	TRP	ENGINEERED	UNP P01897
H	131	ARG	LYS	ENGINEERED	UNP P01897
L	8	TYR	PHE	ENGINEERED	UNP P01897
L	12	THR	VAL	ENGINEERED	UNP P01897
L	15	ARG	PRO	ENGINEERED	UNP P01897
L	23	THR	ILE	ENGINEERED	UNP P01897
L	30	ASP	ASN	ENGINEERED	UNP P01897
L	49	VAL	ALA	ENGINEERED	UNP P01897
L	66	VAL	ILE	ENGINEERED	UNP P01897
L	97	ARG	TRP	ENGINEERED	UNP P01897
L	131	ARG	LYS	ENGINEERED	UNP P01897
P	8	TYR	PHE	ENGINEERED	UNP P01897
P	12	THR	VAL	ENGINEERED	UNP P01897
P	15	ARG	PRO	ENGINEERED	UNP P01897
P	23	THR	ILE	ENGINEERED	UNP P01897
P	30	ASP	ASN	ENGINEERED	UNP P01897
P	49	VAL	ALA	ENGINEERED	UNP P01897
P	66	VAL	ILE	ENGINEERED	UNP P01897
P	97	ARG	TRP	ENGINEERED	UNP P01897
P	131	ARG	LYS	ENGINEERED	UNP P01897
U	8	TYR	PHE	ENGINEERED	UNP P01897

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Chain	Residue	Modelled	Actual	Comment	Reference
U	12	THR	VAL	ENGINEERED	UNP P01897
U	15	ARG	PRO	ENGINEERED	UNP P01897
U	23	THR	ILE	ENGINEERED	UNP P01897
U	30	ASP	ASN	ENGINEERED	UNP P01897
U	49	VAL	ALA	ENGINEERED	UNP P01897
U	66	VAL	ILE	ENGINEERED	UNP P01897
U	97	ARG	TRP	ENGINEERED	UNP P01897
U	131	ARG	LYS	ENGINEERED	UNP P01897
Y	8	TYR	PHE	ENGINEERED	UNP P01897
Y	12	THR	VAL	ENGINEERED	UNP P01897
Y	15	ARG	PRO	ENGINEERED	UNP P01897
Y	23	THR	ILE	ENGINEERED	UNP P01897
Y	30	ASP	ASN	ENGINEERED	UNP P01897
Y	49	VAL	ALA	ENGINEERED	UNP P01897
Y	66	VAL	ILE	ENGINEERED	UNP P01897
Y	97	ARG	TRP	ENGINEERED	UNP P01897
Y	131	ARG	LYS	ENGINEERED	UNP P01897

- Molecule 2 is a protein called QL9 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	Q	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	G	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	f	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	K	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	O	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	T	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	X	9	Total	C	N	O	0	0	0
			76	52	10	14			
2	b	9	Total	C	N	O	0	0	0
			76	52	10	14			

- Molecule 3 is a protein called T-cell receptor alpha chain V region PHDS58.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	C	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	d	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	I	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	M	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	R	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	V	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			
3	Z	109	Total	C	N	O	S	0	0	0
			854	550	142	160	2			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	43	PRO	LEU	ENGINEERED	UNP P01738
D	82	ARG	TRP	ENGINEERED	UNP P01738
D	99	ASP	GLY	ENGINEERED	UNP P01738
D	100	PRO	PHE	ENGINEERED	UNP P01738
D	101	PRO	ALA	ENGINEERED	UNP P01738
D	102	PRO	SER	ENGINEERED	UNP P01738
D	103	LEU	ALA	ENGINEERED	UNP P01738
C	43	PRO	LEU	ENGINEERED	UNP P01738
C	82	ARG	TRP	ENGINEERED	UNP P01738
C	99	ASP	GLY	ENGINEERED	UNP P01738
C	100	PRO	PHE	ENGINEERED	UNP P01738
C	101	PRO	ALA	ENGINEERED	UNP P01738
C	102	PRO	SER	ENGINEERED	UNP P01738
C	103	LEU	ALA	ENGINEERED	UNP P01738
d	43	PRO	LEU	ENGINEERED	UNP P01738
d	82	ARG	TRP	ENGINEERED	UNP P01738
d	99	ASP	GLY	ENGINEERED	UNP P01738
d	100	PRO	PHE	ENGINEERED	UNP P01738
d	101	PRO	ALA	ENGINEERED	UNP P01738
d	102	PRO	SER	ENGINEERED	UNP P01738
d	103	LEU	ALA	ENGINEERED	UNP P01738
I	43	PRO	LEU	ENGINEERED	UNP P01738
I	82	ARG	TRP	ENGINEERED	UNP P01738
I	99	ASP	GLY	ENGINEERED	UNP P01738

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Chain	Residue	Modelled	Actual	Comment	Reference
I	100	PRO	PHE	ENGINEERED	UNP P01738
I	101	PRO	ALA	ENGINEERED	UNP P01738
I	102	PRO	SER	ENGINEERED	UNP P01738
I	103	LEU	ALA	ENGINEERED	UNP P01738
M	43	PRO	LEU	ENGINEERED	UNP P01738
M	82	ARG	TRP	ENGINEERED	UNP P01738
M	99	ASP	GLY	ENGINEERED	UNP P01738
M	100	PRO	PHE	ENGINEERED	UNP P01738
M	101	PRO	ALA	ENGINEERED	UNP P01738
M	102	PRO	SER	ENGINEERED	UNP P01738
M	103	LEU	ALA	ENGINEERED	UNP P01738
R	43	PRO	LEU	ENGINEERED	UNP P01738
R	82	ARG	TRP	ENGINEERED	UNP P01738
R	99	ASP	GLY	ENGINEERED	UNP P01738
R	100	PRO	PHE	ENGINEERED	UNP P01738
R	101	PRO	ALA	ENGINEERED	UNP P01738
R	102	PRO	SER	ENGINEERED	UNP P01738
R	103	LEU	ALA	ENGINEERED	UNP P01738
V	43	PRO	LEU	ENGINEERED	UNP P01738
V	82	ARG	TRP	ENGINEERED	UNP P01738
V	99	ASP	GLY	ENGINEERED	UNP P01738
V	100	PRO	PHE	ENGINEERED	UNP P01738
V	101	PRO	ALA	ENGINEERED	UNP P01738
V	102	PRO	SER	ENGINEERED	UNP P01738
V	103	LEU	ALA	ENGINEERED	UNP P01738
Z	43	PRO	LEU	ENGINEERED	UNP P01738
Z	82	ARG	TRP	ENGINEERED	UNP P01738
Z	99	ASP	GLY	ENGINEERED	UNP P01738
Z	100	PRO	PHE	ENGINEERED	UNP P01738
Z	101	PRO	ALA	ENGINEERED	UNP P01738
Z	102	PRO	SER	ENGINEERED	UNP P01738
Z	103	LEU	ALA	ENGINEERED	UNP P01738

- Molecule 4 is a protein called TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	111	Total	C	N	O	S	0	0	0
			847	523	147	174	3			
4	F	111	Total	C	N	O	S	0	0	0
			847	523	147	174	3			
4	e	111	Total	C	N	O	S	0	0	0
			847	523	147	174	3			

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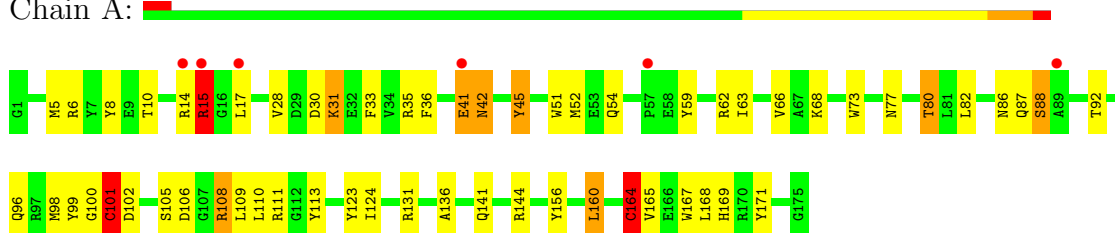
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	111	Total 847	C 523	N 147	O 174	S 3	0	0	0
4	N	111	Total 847	C 523	N 147	O 174	S 3	0	0	0
4	S	111	Total 847	C 523	N 147	O 174	S 3	0	0	0
4	W	111	Total 847	C 523	N 147	O 174	S 3	0	0	0
4	a	111	Total 847	C 523	N 147	O 174	S 3	0	0	0

3 Residue-property plots

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 ($RSRZ > 2$). 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.

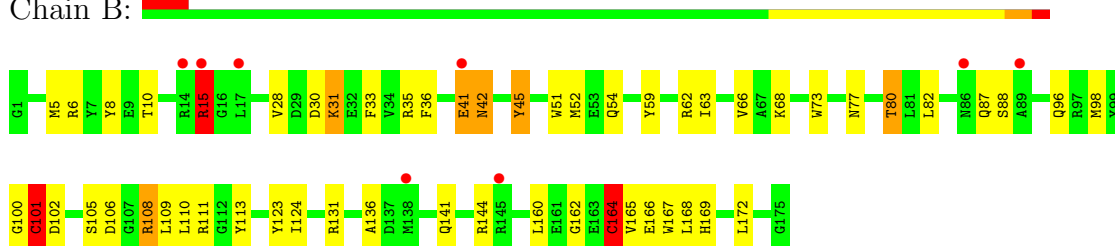
- Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

Chain A:



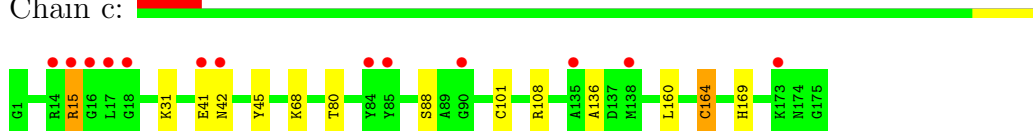
- Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

Chain B:



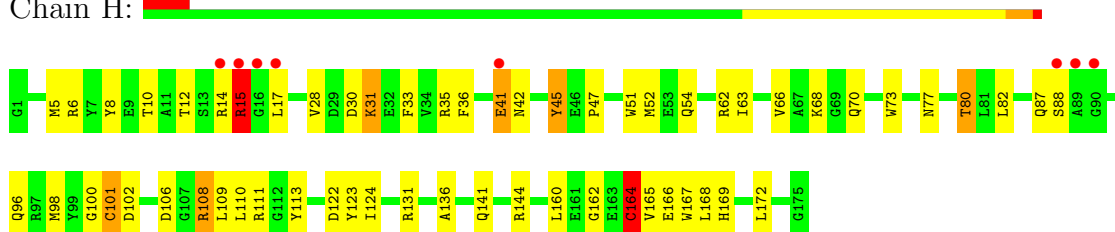
- Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

Chain c:



- Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

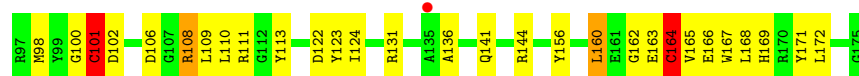
Chain H:



- Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

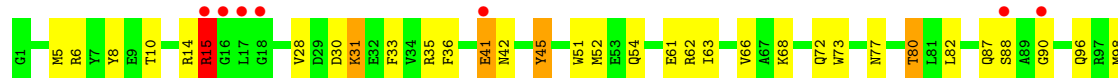
Chain L:





- Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

Chain P:



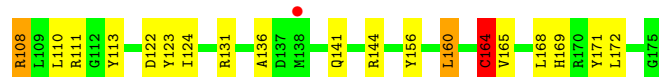
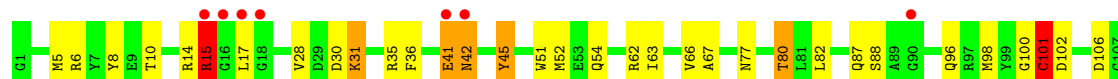
- Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

Chain U:



- Molecule 1: H-2 class I histocompatibility antigen, L-D alpha chain

Chain Y:



- Molecule 2: QL9 peptide

Chain Q:



- Molecule 2: QL9 peptide

Chain G:



- Molecule 2: QL9 peptide

Chain f: 



- Molecule 2: QL9 peptide

Chain K: 



- Molecule 2: QL9 peptide

Chain O: 



- Molecule 2: QL9 peptide

Chain T: 



- Molecule 2: QL9 peptide

Chain X: 



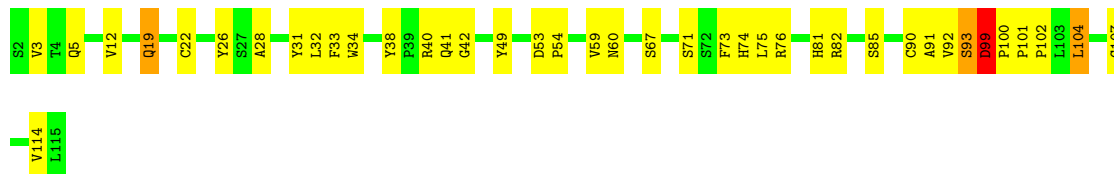
- Molecule 2: QL9 peptide

Chain b: 



- Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain D: 



- Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain C: 



- Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain d: 



- Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain I: 



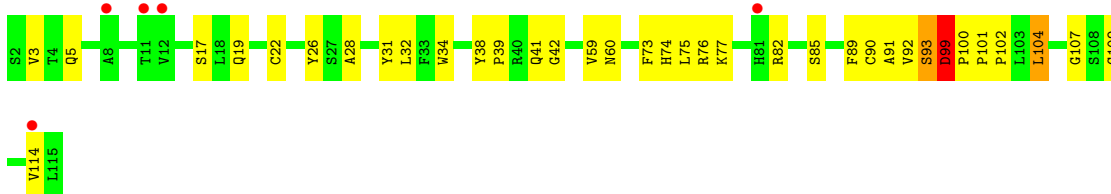
- Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain M: 



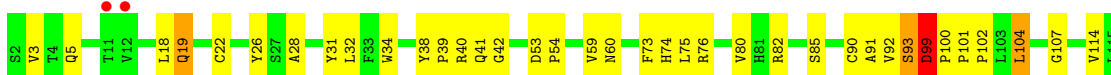
- Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain R: 



- Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain V: 



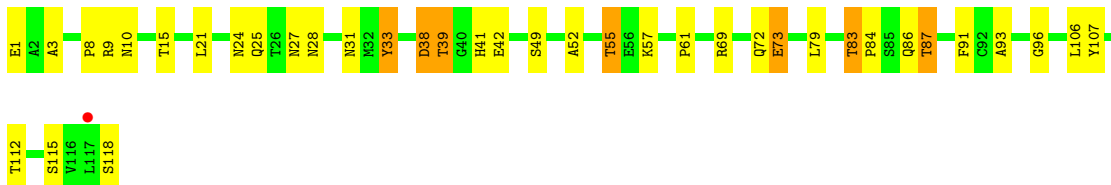
- Molecule 3: T-cell receptor alpha chain V region PHDS58

Chain Z: 

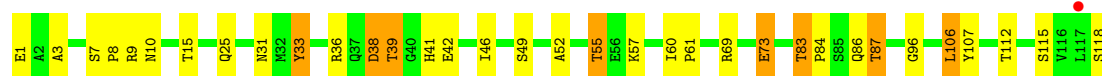


- Molecule 4: TCR beta chain

Chain E: 



- Molecule 4: TCR beta chain

Chain F: 

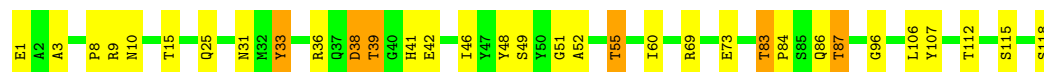
- Molecule 4: TCR beta chain

Chain e: 

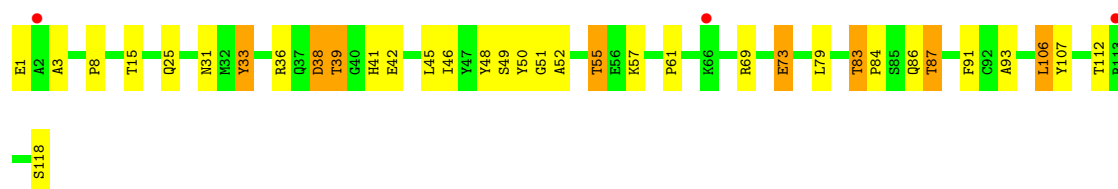
- Molecule 4: TCR beta chain

Chain J: 

- Molecule 4: TCR beta chain

Chain N: 

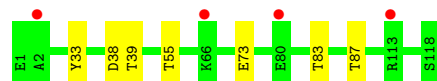
- Molecule 4: TCR beta chain

Chain S: 

- Molecule 4: TCR beta chain

Chain W: 

- Molecule 4: TCR beta chain

Chain a: 

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	158.47Å 160.46Å 357.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.52 – 2.95 41.51 – 2.93	Depositor EDS
% Data completeness (in resolution range)	97.4 (41.52-2.95) 96.7 (41.51-2.93)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.275 0.251 , 0.252	Depositor DCC
R_{free} test set	4663 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 18.4	EDS
Estimated twinning fraction	0.054 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	5 of 94226 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25808	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.77 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2603e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	A	0.48	0/1489	0.67	2/2015 (0.1%)
1	B	0.44	0/1489	0.65	2/2015 (0.1%)
1	H	0.44	0/1489	0.64	1/2015 (0.0%)
1	L	0.45	0/1489	0.65	2/2015 (0.1%)
1	P	0.43	0/1489	0.64	1/2015 (0.0%)
1	U	0.43	0/1489	0.65	1/2015 (0.0%)
1	Y	0.44	0/1489	0.65	2/2015 (0.1%)
1	c	0.42	0/1489	0.63	1/2015 (0.0%)
2	G	0.58	0/79	0.74	0/106
2	K	0.54	0/79	0.68	0/106
2	O	0.58	0/79	0.74	0/106
2	Q	0.58	0/79	0.77	0/106
2	T	0.50	0/79	0.73	0/106
2	X	0.50	0/79	0.71	0/106
2	b	0.55	0/79	0.70	0/106
2	f	0.53	0/79	0.68	0/106
3	C	0.47	0/879	0.73	1/1196 (0.1%)
3	D	0.47	0/879	0.73	1/1196 (0.1%)
3	I	0.48	0/879	0.73	1/1196 (0.1%)
3	M	0.47	0/879	0.73	0/1196
3	R	0.46	0/879	0.73	1/1196 (0.1%)
3	V	0.44	0/879	0.70	0/1196
3	Z	0.46	0/879	0.72	1/1196 (0.1%)
3	d	0.44	0/879	0.71	1/1196 (0.1%)
4	E	0.50	0/865	0.72	0/1172
4	F	0.47	0/865	0.69	0/1172
4	J	0.46	0/865	0.69	0/1172
4	N	0.45	0/865	0.69	0/1172
4	S	0.46	0/865	0.68	0/1172
4	W	0.44	0/865	0.68	0/1172
4	a	0.46	0/865	0.67	0/1172
4	e	0.43	0/865	0.66	0/1172
All	All	0.45	0/26496	0.68	18/35912 (0.1%)

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
3	D	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	164	CYS	CA-CB-SG	-7.21	101.02	114.00
1	Y	164	CYS	CA-CB-SG	-7.14	101.15	114.00
1	U	164	CYS	CA-CB-SG	-7.02	101.37	114.00
1	L	164	CYS	CA-CB-SG	-6.94	101.50	114.00
1	H	164	CYS	CA-CB-SG	-6.62	102.08	114.00
1	c	164	CYS	CA-CB-SG	-6.61	102.11	114.00
1	B	164	CYS	CA-CB-SG	-6.55	102.21	114.00
1	A	164	CYS	CA-CB-SG	-6.08	103.06	114.00
3	C	99	ASP	C-N-CD	5.84	140.68	128.40
1	A	101	CYS	CA-CB-SG	-5.64	103.84	114.00
3	I	99	ASP	C-N-CD	5.49	139.92	128.40
3	D	99	ASP	C-N-CD	5.45	139.84	128.40
1	B	101	CYS	CA-CB-SG	-5.33	104.40	114.00
3	d	99	ASP	C-N-CD	5.33	139.59	128.40
3	Z	99	ASP	C-N-CD	5.29	139.50	128.40
1	Y	101	CYS	CA-CB-SG	-5.20	104.64	114.00
1	L	101	CYS	CA-CB-SG	-5.12	104.78	114.00
3	R	99	ASP	C-N-CD	5.11	139.13	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	49	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1449	0	1337	66	3
1	B	1449	0	1337	59	0
1	H	1449	0	1337	62	0
1	L	1449	0	1337	62	0
1	P	1449	0	1337	55	0
1	U	1449	0	1337	60	0
1	Y	1449	0	1337	48	0
1	c	1449	0	1337	0	0
2	G	76	0	73	17	0
2	K	76	0	73	19	0
2	O	76	0	73	20	0
2	Q	76	0	73	19	0
2	T	76	0	73	13	0
2	X	76	0	73	17	0
2	b	76	0	73	0	0
2	f	76	0	73	0	0
3	C	854	0	832	37	0
3	D	854	0	832	51	0
3	I	854	0	832	30	0
3	M	854	0	832	23	0
3	R	854	0	832	34	0
3	V	854	0	832	37	0
3	Z	854	0	832	26	0
3	d	854	0	832	0	0
4	E	847	0	799	31	3
4	F	847	0	799	26	0
4	J	847	0	799	24	0
4	N	847	0	799	26	0
4	S	847	0	799	26	0
4	W	847	0	799	25	0
4	a	847	0	799	0	0
4	e	847	0	799	0	0
All	All	25808	0	24328	772	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (772) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:82:ARG:NH2	3:V:60:ASN:HD21	1.37	1.21

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:60:ASN:HD21	3:C:82:ARG:NH2	109.53	1.07
3:V:99:ASP:HB3	3:V:100:PRO:HD2	1.45	0.99
3:Z:99:ASP:HB3	3:Z:100:PRO:HD2	1.45	0.98
3:I:99:ASP:HB3	3:I:100:PRO:HD2	1.45	0.97
3:D:99:ASP:HB3	3:D:100:PRO:HD2	1.46	0.97
3:R:99:ASP:HB3	3:R:100:PRO:HD2	1.46	0.97
3:M:99:ASP:HB3	3:M:100:PRO:HD2	1.46	0.96
1:U:77:ASN:HD22	2:X:9:LEU:HB2	1.31	0.94
3:C:99:ASP:HB3	3:C:100:PRO:HD2	1.49	0.94
1:P:10:THR:HG22	1:P:96:GLN:HB2	1.54	0.90
3:M:99:ASP:HB3	3:M:100:PRO:CD	2.03	0.88
1:A:77:ASN:HA	1:A:80:THR:CG2	2.03	0.87
3:D:82:ARG:NH2	3:V:60:ASN:ND2	2.23	0.87
1:P:77:ASN:HA	1:P:80:THR:CG2	2.03	0.87
1:P:77:ASN:HD22	2:T:9:LEU:HB2	1.38	0.87
1:H:77:ASN:HA	1:H:80:THR:CG2	2.04	0.86
3:D:99:ASP:HB3	3:D:100:PRO:CD	2.05	0.86
1:H:10:THR:HG22	1:H:96:GLN:HB2	1.57	0.86
1:B:10:THR:HG22	1:B:96:GLN:HB2	1.57	0.86
1:L:45:TYR:CD2	1:L:63:ILE:HG22	2.11	0.85
1:L:77:ASN:HA	1:L:80:THR:CG2	2.06	0.85
3:V:99:ASP:HB3	3:V:100:PRO:CD	2.04	0.85
1:H:45:TYR:CD2	1:H:63:ILE:HG22	2.11	0.85
1:U:10:THR:HG22	1:U:96:GLN:HB2	1.58	0.85
1:Y:10:THR:HG22	1:Y:96:GLN:HB2	1.58	0.85
1:U:77:ASN:HA	1:U:80:THR:CG2	2.05	0.85
3:C:99:ASP:HB3	3:C:100:PRO:CD	2.06	0.85
1:Y:77:ASN:HA	1:Y:80:THR:CG2	2.06	0.85
1:A:10:THR:HG22	1:A:96:GLN:HB2	1.59	0.84
1:L:62:ARG:HE	2:O:1:GLN:NE2	1.75	0.84
3:D:60:ASN:HD21	3:C:82:ARG:HH21	109.53	0.84
1:B:77:ASN:HA	1:B:80:THR:CG2	2.07	0.84
3:Z:99:ASP:HB3	3:Z:100:PRO:CD	2.07	0.84
1:U:77:ASN:HD21	2:X:9:LEU:H	1.24	0.84
4:E:84:PRO:O	4:E:87:THR:HG23	1.94	0.84
3:M:22:CYS:H	3:M:74:HIS:HD2	1.24	0.84
3:R:22:CYS:H	3:R:74:HIS:CD2	1.96	0.84
3:R:99:ASP:HB3	3:R:100:PRO:CD	2.08	0.83
1:H:62:ARG:HE	2:K:1:GLN:NE2	1.77	0.83
1:B:45:TYR:CD2	1:B:63:ILE:HG22	2.14	0.82
1:L:10:THR:HG22	1:L:96:GLN:HB2	1.62	0.82
1:A:77:ASN:HD22	2:Q:9:LEU:HB2	1.44	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:TYR:CD2	1:A:63:ILE:HG22	2.15	0.82
3:I:99:ASP:HB3	3:I:100:PRO:CD	2.06	0.82
1:Y:45:TYR:CD2	1:Y:63:ILE:HG22	2.16	0.81
1:B:62:ARG:HE	2:G:1:GLN:NE2	1.79	0.80
3:M:22:CYS:H	3:M:74:HIS:CD2	1.98	0.80
3:I:22:CYS:H	3:I:74:HIS:CD2	1.99	0.80
1:B:77:ASN:HD21	2:G:9:LEU:H	1.27	0.80
1:A:77:ASN:HD21	2:Q:9:LEU:H	1.30	0.80
1:P:45:TYR:CD2	1:P:63:ILE:HG22	2.17	0.80
1:B:77:ASN:HD22	2:G:9:LEU:HB2	1.45	0.79
3:D:82:ARG:HH22	3:V:60:ASN:HD21	1.30	0.79
3:R:22:CYS:H	3:R:74:HIS:HD2	1.25	0.79
1:L:77:ASN:HD22	2:O:9:LEU:HB2	1.46	0.78
3:V:22:CYS:H	3:V:74:HIS:CD2	2.01	0.78
1:U:45:TYR:CD2	1:U:63:ILE:HG22	2.18	0.77
3:I:22:CYS:H	3:I:74:HIS:HD2	1.33	0.77
3:V:22:CYS:H	3:V:74:HIS:HD2	1.32	0.77
1:H:77:ASN:HA	1:H:80:THR:HG23	1.65	0.77
1:H:77:ASN:HD22	2:K:9:LEU:HB2	1.50	0.77
1:Y:77:ASN:HA	1:Y:80:THR:HG23	1.65	0.77
4:J:84:PRO:O	4:J:87:THR:HG23	1.85	0.77
1:P:77:ASN:HD21	2:T:9:LEU:H	1.31	0.77
3:V:85:SER:OG	3:V:114:VAL:HG12	1.83	0.77
4:W:84:PRO:O	4:W:87:THR:HG23	1.85	0.77
1:U:62:ARG:HE	2:X:1:GLN:NE2	1.83	0.76
3:D:22:CYS:H	3:D:74:HIS:CD2	2.03	0.76
1:A:77:ASN:HA	1:A:80:THR:HG23	1.68	0.76
1:L:77:ASN:HD21	2:O:9:LEU:H	1.34	0.75
1:H:52:MET:HA	1:H:52:MET:HE2	1.67	0.75
1:A:62:ARG:HE	2:Q:1:GLN:NE2	1.84	0.75
3:Z:22:CYS:H	3:Z:74:HIS:CD2	2.04	0.75
1:H:77:ASN:HD21	2:K:9:LEU:H	1.33	0.75
3:D:22:CYS:H	3:D:74:HIS:HD2	1.30	0.75
3:C:22:CYS:H	3:C:74:HIS:CD2	2.04	0.75
1:P:77:ASN:ND2	2:T:9:LEU:H	1.85	0.74
1:L:77:ASN:HA	1:L:80:THR:HG23	1.69	0.74
1:Y:8:TYR:CE1	1:Y:98:MET:HG3	2.22	0.74
4:F:84:PRO:O	4:F:87:THR:HG23	1.88	0.74
1:B:52:MET:HE2	1:B:52:MET:HA	1.69	0.74
1:U:77:ASN:HA	1:U:80:THR:HG23	1.68	0.73
1:P:77:ASN:HA	1:P:80:THR:HG23	1.69	0.73
1:U:77:ASN:ND2	2:X:9:LEU:H	1.87	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:N:84:PRO:O	4:N:87:THR:HG23	1.88	0.73
1:A:77:ASN:ND2	2:Q:9:LEU:H	1.86	0.73
1:B:77:ASN:HA	1:B:80:THR:HG23	1.70	0.72
1:P:8:TYR:CE1	1:P:98:MET:HG3	2.25	0.72
3:D:40:ARG:NH1	3:C:40:ARG:HH12	140.54	0.72
3:Z:22:CYS:H	3:Z:74:HIS:HD2	1.35	0.72
1:H:8:TYR:CE1	1:H:98:MET:HG3	2.25	0.72
1:U:8:TYR:CE1	1:U:98:MET:HG3	2.25	0.71
3:D:82:ARG:HH21	3:V:60:ASN:HD21	1.32	0.71
1:B:8:TYR:CE1	1:B:98:MET:HG3	2.26	0.71
1:L:77:ASN:ND2	2:O:9:LEU:H	1.88	0.70
1:B:77:ASN:ND2	2:G:9:LEU:H	1.89	0.70
3:Z:85:SER:OG	3:Z:114:VAL:HG12	1.91	0.70
1:Y:52:MET:HE2	1:Y:52:MET:HA	1.73	0.70
3:D:40:ARG:HH11	3:C:40:ARG:HH12	141.10	0.69
1:P:52:MET:HE2	1:P:52:MET:HA	1.72	0.69
1:U:77:ASN:HB3	2:X:9:LEU:HD22	1.73	0.69
1:H:82:LEU:HD23	1:H:87:GLN:HE21	1.59	0.68
1:B:167:TRP:CE2	2:G:1:GLN:HG2	2.29	0.68
3:D:76:ARG:NH1	1:L:106:ASP:OD2	94.09	0.68
1:U:52:MET:HA	1:U:52:MET:HE2	1.76	0.68
3:D:85:SER:OG	3:D:114:VAL:HG12	1.95	0.67
1:L:62:ARG:O	1:L:66:VAL:HG23	1.95	0.67
1:U:77:ASN:ND2	2:X:9:LEU:HB2	2.07	0.67
1:A:8:TYR:CE1	1:A:98:MET:HG3	2.29	0.67
1:B:167:TRP:NE1	2:G:1:GLN:HG2	2.10	0.67
3:C:22:CYS:H	3:C:74:HIS:HD2	1.43	0.67
1:H:77:ASN:ND2	2:K:9:LEU:H	1.93	0.66
1:A:106:ASP:OD2	3:R:76:ARG:NH1	2.25	0.66
4:E:38:ASP:N	4:E:38:ASP:OD2	2.38	0.66
3:V:38:TYR:O	3:V:41:GLN:HB2	1.96	0.66
3:R:38:TYR:O	3:R:41:GLN:HB2	1.96	0.66
1:L:8:TYR:CE1	1:L:98:MET:HG3	2.29	0.66
3:M:82:ARG:HA	3:M:114:VAL:HG11	1.78	0.65
1:A:52:MET:HE2	1:A:52:MET:HA	1.76	0.65
2:G:8:ASP:OD2	4:F:96:GLY:HA2	1.96	0.65
1:Y:5:MET:HB2	1:Y:168:LEU:HD13	1.79	0.65
1:A:82:LEU:HD23	1:A:87:GLN:HE21	1.61	0.65
1:P:131:ARG:HG3	1:P:131:ARG:HH11	1.62	0.65
3:M:85:SER:OG	3:M:114:VAL:HG12	1.97	0.64
3:D:38:TYR:O	3:D:41:GLN:HB2	2.07	0.64
3:D:82:ARG:HA	3:D:114:VAL:HG11	1.88	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:62:ARG:O	1:H:66:VAL:HG23	1.98	0.64
4:E:84:PRO:O	4:E:87:THR:CG2	2.61	0.64
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.78	0.64
1:Y:82:LEU:HD23	1:Y:87:GLN:HE21	1.61	0.64
1:U:82:LEU:HD23	1:U:87:GLN:HE21	1.62	0.63
3:R:85:SER:OG	3:R:114:VAL:HG12	1.98	0.63
4:N:38:ASP:OD2	4:N:38:ASP:N	2.30	0.63
4:E:39:THR:OG1	4:E:41:HIS:HB2	2.08	0.63
3:M:82:ARG:HA	3:M:114:VAL:CG1	2.29	0.63
3:D:40:ARG:HH11	3:C:40:ARG:NH1	141.88	0.63
1:H:5:MET:HB2	1:H:168:LEU:HD13	1.79	0.63
3:Z:38:TYR:O	3:Z:41:GLN:HB2	1.97	0.63
1:L:123:TYR:HD1	1:L:124:ILE:HG22	1.64	0.63
1:A:105:SER:OG	3:R:17:SER:N	2.26	0.63
1:P:77:ASN:HB3	2:T:9:LEU:HD22	1.80	0.62
1:A:167:TRP:NE1	2:Q:1:GLN:HG2	2.15	0.62
4:S:38:ASP:O	4:S:39:THR:HG23	2.00	0.62
4:E:55:THR:HG22	4:E:55:THR:O	1.98	0.62
1:A:167:TRP:CE2	2:Q:1:GLN:HG2	2.34	0.62
3:D:82:ARG:HA	3:D:114:VAL:CG1	2.33	0.62
3:I:85:SER:OG	3:I:114:VAL:HG12	2.00	0.62
1:L:52:MET:HE2	1:L:52:MET:HA	1.80	0.62
1:B:62:ARG:O	1:B:66:VAL:HG23	2.00	0.61
1:P:123:TYR:HD1	1:P:124:ILE:HG22	1.64	0.61
1:Y:123:TYR:HD1	1:Y:124:ILE:HG22	1.64	0.61
3:R:5:GLN:HE21	3:R:107:GLY:HA3	1.65	0.61
1:B:5:MET:HB2	1:B:168:LEU:HD13	1.82	0.61
4:W:1:GLU:HB2	4:W:107:TYR:HB3	1.83	0.61
4:W:38:ASP:N	4:W:38:ASP:OD2	2.31	0.61
3:C:85:SER:OG	3:C:114:VAL:HG12	2.00	0.61
3:R:82:ARG:HA	3:R:114:VAL:CG1	2.31	0.61
1:B:82:LEU:HD23	1:B:87:GLN:HE21	1.66	0.60
4:S:84:PRO:O	4:S:87:THR:CG2	2.49	0.60
1:P:10:THR:HG22	1:P:96:GLN:CB	2.31	0.60
4:W:38:ASP:O	4:W:39:THR:HG23	2.02	0.60
2:K:8:ASP:OD2	4:J:96:GLY:HA2	2.01	0.60
3:Z:82:ARG:HA	3:Z:114:VAL:CG1	2.31	0.60
4:J:38:ASP:N	4:J:38:ASP:OD2	2.32	0.60
1:H:167:TRP:NE1	2:K:1:GLN:HG2	2.16	0.60
4:W:84:PRO:O	4:W:87:THR:CG2	2.49	0.60
1:L:5:MET:HB2	1:L:168:LEU:HD13	1.83	0.60
4:S:39:THR:OG1	4:S:41:HIS:HB2	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:82:LEU:HD23	1:P:87:GLN:HE21	1.67	0.60
4:S:38:ASP:N	4:S:38:ASP:OD2	2.35	0.60
1:P:5:MET:HB2	1:P:168:LEU:HD13	1.84	0.60
1:L:82:LEU:HD23	1:L:87:GLN:HE21	1.66	0.60
3:C:99:ASP:O	3:C:101:PRO:HD3	2.02	0.59
1:B:51:TRP:O	1:B:54:GLN:HG2	2.02	0.59
4:S:84:PRO:O	4:S:87:THR:HG23	2.02	0.59
1:B:123:TYR:HD1	1:B:124:ILE:HG22	1.68	0.59
3:I:82:ARG:HA	3:I:114:VAL:CG1	2.32	0.59
1:U:123:TYR:HD1	1:U:124:ILE:HG22	1.67	0.59
3:C:82:ARG:HA	3:C:114:VAL:CG1	2.33	0.59
3:V:82:ARG:HA	3:V:114:VAL:HG11	1.84	0.59
1:A:62:ARG:O	1:A:66:VAL:HG23	2.01	0.59
1:A:108:ARG:HB3	3:R:76:ARG:CZ	2.33	0.59
4:N:1:GLU:HB2	4:N:107:TYR:HB3	1.84	0.59
3:Z:5:GLN:HE21	3:Z:107:GLY:HA3	1.68	0.59
3:D:99:ASP:O	3:D:101:PRO:HD3	2.03	0.59
1:U:5:MET:HB2	1:U:168:LEU:HD13	1.84	0.59
3:D:60:ASN:ND2	3:C:82:ARG:NH2	109.21	0.58
4:E:87:THR:HB	4:E:115:SER:HA	1.84	0.58
1:B:10:THR:HG22	1:B:96:GLN:CB	2.32	0.58
4:W:39:THR:OG1	4:W:41:HIS:HB2	2.03	0.58
3:R:82:ARG:HA	3:R:114:VAL:HG11	1.84	0.58
3:I:82:ARG:HA	3:I:114:VAL:HG11	1.85	0.58
3:I:26:TYR:CE2	3:I:28:ALA:HB3	2.39	0.58
1:H:123:TYR:HD1	1:H:124:ILE:HG22	1.66	0.58
1:P:167:TRP:NE1	2:T:1:GLN:HG2	2.19	0.58
1:H:109:LEU:O	3:V:76:ARG:NH2	2.36	0.58
1:B:131:ARG:HG3	1:B:131:ARG:HH11	1.68	0.58
4:J:1:GLU:HB2	4:J:107:TYR:HB3	1.86	0.58
1:L:62:ARG:NE	2:O:1:GLN:NE2	2.50	0.58
3:D:40:ARG:NH1	3:C:40:ARG:NH1	141.33	0.58
3:Z:82:ARG:HA	3:Z:114:VAL:HG11	1.85	0.58
1:Y:30:ASP:H	1:Y:31:LYS:HD2	1.69	0.58
1:A:51:TRP:O	1:A:54:GLN:HG2	2.03	0.57
1:P:62:ARG:HE	2:T:1:GLN:NE2	2.01	0.57
1:U:131:ARG:HG3	1:U:131:ARG:HH11	1.69	0.57
4:N:55:THR:HG22	4:N:55:THR:O	2.04	0.57
3:C:31:TYR:HB2	3:C:93:SER:HB2	1.87	0.57
1:H:131:ARG:HG3	1:H:131:ARG:HH11	1.68	0.57
3:D:26:TYR:CE2	3:D:28:ALA:HB3	2.40	0.57
4:E:1:GLU:HB2	4:E:107:TYR:HB3	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:82:ARG:HA	3:C:114:VAL:HG11	1.88	0.56
3:C:26:TYR:CE2	3:C:28:ALA:HB3	2.41	0.56
1:H:141:GLN:NE2	1:H:144:ARG:NH1	2.54	0.56
1:Y:131:ARG:HG3	1:Y:131:ARG:HH11	1.71	0.56
3:D:42:GLY:HA2	4:E:91:PHE:CE2	2.86	0.56
1:H:45:TYR:CG	1:H:63:ILE:HG22	2.41	0.56
3:Z:26:TYR:CE2	3:Z:28:ALA:HB3	2.41	0.56
3:V:26:TYR:CE2	3:V:28:ALA:HB3	2.41	0.56
4:N:87:THR:HB	4:N:115:SER:HA	1.87	0.56
3:V:82:ARG:HA	3:V:114:VAL:CG1	2.35	0.56
3:M:31:TYR:HB2	3:M:93:SER:HB2	1.86	0.56
1:U:62:ARG:O	1:U:66:VAL:HG23	2.06	0.56
1:B:106:ASP:OD2	3:Z:76:ARG:NH1	2.33	0.56
4:W:55:THR:O	4:W:55:THR:HG22	2.05	0.55
2:Q:1:GLN:N	2:Q:1:GLN:OE1	2.39	0.55
4:F:38:ASP:O	4:F:39:THR:HG23	2.05	0.55
3:R:26:TYR:CE2	3:R:28:ALA:HB3	2.41	0.55
1:L:45:TYR:CG	1:L:63:ILE:HG22	2.41	0.55
1:H:164:CYS:SG	1:H:165:VAL:N	2.78	0.55
1:Y:141:GLN:NE2	1:Y:144:ARG:NH1	2.54	0.55
1:H:62:ARG:NE	2:K:1:GLN:NE2	2.52	0.55
3:R:42:GLY:HA2	4:S:91:PHE:CE2	2.41	0.55
1:Y:111:ARG:HG2	1:Y:113:TYR:CZ	2.41	0.55
4:F:55:THR:HG22	4:F:55:THR:O	2.05	0.55
1:U:141:GLN:NE2	1:U:144:ARG:NH1	2.54	0.55
3:D:3:VAL:HG13	3:D:92:VAL:HG12	1.99	0.55
1:U:6:ARG:NH2	1:U:102:ASP:OD1	2.39	0.55
3:D:31:TYR:HB2	3:D:93:SER:HB2	1.87	0.55
4:W:15:THR:OG1	4:W:118:SER:HA	2.07	0.55
1:P:51:TRP:O	1:P:54:GLN:HG2	2.07	0.55
1:H:10:THR:HG22	1:H:96:GLN:CB	2.33	0.55
4:J:39:THR:OG1	4:J:41:HIS:HB2	2.07	0.55
2:X:5:PHE:CG	3:V:102:PRO:HD3	2.42	0.55
4:F:52:ALA:HA	4:F:69:ARG:HG3	1.89	0.55
3:C:76:ARG:NH1	1:Y:106:ASP:OD2	2.38	0.55
1:H:167:TRP:CE2	2:K:1:GLN:HG2	2.41	0.54
1:H:51:TRP:O	1:H:54:GLN:HG2	2.06	0.54
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.71	0.54
1:B:45:TYR:CG	1:B:63:ILE:HG22	2.43	0.54
1:A:45:TYR:CG	1:A:63:ILE:HG22	2.42	0.54
1:Y:62:ARG:O	1:Y:66:VAL:HG23	2.07	0.54
1:Y:51:TRP:O	1:Y:54:GLN:HG2	2.06	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:31:TYR:HB2	3:I:93:SER:HB2	1.88	0.54
1:L:141:GLN:NE2	1:L:144:ARG:NH1	2.56	0.54
4:S:3:ALA:O	4:S:25:GLN:HA	2.07	0.54
1:P:100:GLY:C	1:P:101:CYS:SG	2.86	0.54
1:P:164:CYS:SG	1:P:165:VAL:N	2.77	0.54
4:N:83:THR:HG23	4:N:86:GLN:HG3	1.88	0.54
4:F:1:GLU:HB2	4:F:107:TYR:HB3	1.88	0.54
4:J:33:TYR:CZ	4:J:106:LEU:HD11	2.43	0.53
1:Y:10:THR:HG22	1:Y:96:GLN:CB	2.35	0.53
1:U:167:TRP:NE1	2:X:1:GLN:HG2	2.23	0.53
2:T:5:PHE:CG	3:R:102:PRO:HD3	2.44	0.53
4:F:38:ASP:OD2	4:F:38:ASP:N	2.39	0.53
3:M:26:TYR:CE2	3:M:28:ALA:HB3	2.44	0.53
1:Y:100:GLY:C	1:Y:101:CYS:SG	2.85	0.53
4:W:33:TYR:N	4:W:33:TYR:CD1	2.76	0.53
1:U:10:THR:HG22	1:U:96:GLN:CB	2.32	0.53
1:A:10:THR:HG22	1:A:96:GLN:CB	2.34	0.53
1:Y:45:TYR:CG	1:Y:63:ILE:HG22	2.43	0.53
4:N:38:ASP:O	4:N:39:THR:HG23	2.07	0.53
4:N:39:THR:OG1	4:N:41:HIS:HB2	2.08	0.53
4:F:33:TYR:N	4:F:33:TYR:CD1	2.77	0.53
4:S:1:GLU:HB2	4:S:107:TYR:HB3	1.91	0.53
1:U:110:LEU:O	1:U:110:LEU:HD23	2.09	0.53
4:J:1:GLU:HG2	4:J:107:TYR:CD1	2.44	0.53
1:B:109:LEU:O	3:Z:76:ARG:NH2	2.42	0.53
1:H:162:GLY:O	1:H:166:GLU:HG3	2.09	0.53
3:C:3:VAL:HG13	3:C:92:VAL:HG12	1.91	0.53
1:U:52:MET:CE	1:U:52:MET:HA	2.39	0.53
1:Y:164:CYS:SG	1:Y:165:VAL:N	2.79	0.53
4:E:33:TYR:CZ	4:E:106:LEU:HD11	2.43	0.53
1:L:131:ARG:HH11	1:L:131:ARG:HG3	1.72	0.53
4:J:83:THR:HG23	4:J:86:GLN:HG3	1.90	0.53
2:G:2:LEU:HD13	2:G:2:LEU:N	2.24	0.53
3:D:5:GLN:HE21	3:D:107:GLY:HA3	1.77	0.53
1:Y:110:LEU:O	1:Y:110:LEU:HD23	2.09	0.53
4:F:33:TYR:CZ	4:F:106:LEU:HD11	2.44	0.52
4:J:87:THR:HB	4:J:115:SER:HA	1.90	0.52
4:F:1:GLU:HG2	4:F:107:TYR:CD1	2.45	0.52
4:N:3:ALA:O	4:N:25:GLN:HA	2.10	0.52
1:L:164:CYS:SG	1:L:165:VAL:N	2.77	0.52
3:D:40:ARG:HH12	3:V:40:ARG:HH11	1.57	0.52
1:H:35:ARG:NH2	1:P:35:ARG:NH2	2.57	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:P:167:TRP:CE2	2:T:1:GLN:HG2	2.44	0.52
1:U:167:TRP:CE2	2:X:1:GLN:HG2	2.44	0.52
2:Q:5:PHE:CG	3:D:102:PRO:HD3	2.44	0.52
1:H:122:ASP:OD1	1:P:31:LYS:HE2	2.09	0.52
4:J:84:PRO:O	4:J:87:THR:CG2	2.57	0.52
1:L:41:GLU:H	1:L:41:GLU:CD	2.13	0.52
1:L:35:ARG:NH2	1:Y:35:ARG:NH2	2.57	0.52
2:Q:8:ASP:OD2	4:E:96:GLY:HA2	2.10	0.52
4:F:87:THR:HB	4:F:115:SER:HA	1.92	0.52
1:A:109:LEU:O	3:R:76:ARG:NH2	2.42	0.52
4:J:38:ASP:O	4:J:39:THR:HG23	2.10	0.52
3:M:5:GLN:NE2	3:M:90:CYS:H	2.08	0.52
3:D:32:LEU:HD13	3:D:73:PHE:HB2	1.90	0.52
1:L:62:ARG:HE	2:O:1:GLN:HE22	1.56	0.52
1:B:105:SER:OG	3:Z:17:SER:N	2.31	0.52
1:U:15:ARG:HD2	1:U:15:ARG:N	2.25	0.52
1:U:100:GLY:C	1:U:101:CYS:SG	2.88	0.52
4:F:9:ARG:HG3	4:F:10:ASN:ND2	2.25	0.52
1:U:41:GLU:H	1:U:41:GLU:CD	2.12	0.52
1:A:123:TYR:HD1	1:A:124:ILE:HG22	1.75	0.51
1:U:51:TRP:O	1:U:54:GLN:HG2	2.10	0.51
1:P:45:TYR:CG	1:P:63:ILE:HG22	2.45	0.51
1:L:62:ARG:NE	2:O:1:GLN:HE22	2.08	0.51
1:A:41:GLU:CD	1:A:41:GLU:H	2.14	0.51
1:B:141:GLN:NE2	1:B:144:ARG:NH1	2.58	0.51
1:L:31:LYS:HE2	1:Y:122:ASP:OD1	2.11	0.51
4:N:84:PRO:O	4:N:87:THR:CG2	2.59	0.51
1:P:30:ASP:H	1:P:31:LYS:HD2	1.76	0.51
1:L:6:ARG:NH2	1:L:102:ASP:OD1	2.43	0.51
4:J:55:THR:HG22	4:J:55:THR:O	2.09	0.51
4:E:38:ASP:O	4:E:39:THR:HG23	2.11	0.51
4:N:52:ALA:HA	4:N:69:ARG:HG3	1.91	0.51
3:R:31:TYR:HB2	3:R:93:SER:HB2	1.93	0.51
2:O:1:GLN:OE1	2:O:1:GLN:CA	2.59	0.51
1:U:62:ARG:NE	2:X:1:GLN:NE2	2.57	0.51
4:J:52:ALA:HA	4:J:69:ARG:HG3	1.93	0.51
4:N:15:THR:OG1	4:N:118:SER:HA	2.10	0.51
1:U:30:ASP:H	1:U:31:LYS:HD2	1.75	0.51
1:B:15:ARG:HD2	1:B:15:ARG:N	2.26	0.51
3:I:99:ASP:O	3:I:100:PRO:C	2.48	0.51
1:U:45:TYR:CG	1:U:63:ILE:HG22	2.44	0.51
3:R:32:LEU:HD13	3:R:73:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:S:52:ALA:HA	4:S:69:ARG:HG3	1.93	0.51
4:N:33:TYR:CZ	4:N:106:LEU:HD11	2.45	0.51
3:I:3:VAL:HG13	3:I:92:VAL:HG12	1.92	0.51
3:M:99:ASP:O	3:M:101:PRO:HD3	2.10	0.51
2:O:1:GLN:OE1	2:O:1:GLN:N	2.43	0.51
1:B:77:ASN:ND2	2:G:9:LEU:HB2	2.20	0.51
4:E:79:LEU:N	4:E:79:LEU:HD12	2.35	0.51
1:B:15:ARG:HD2	1:B:15:ARG:H	1.76	0.51
1:U:72:GLN:HG3	4:W:50:TYR:CD2	2.46	0.51
4:E:15:THR:OG1	4:E:118:SER:HA	2.19	0.51
3:Z:59:VAL:HG12	3:Z:60:ASN:N	2.25	0.51
3:M:3:VAL:HG13	3:M:92:VAL:HG12	1.93	0.51
4:E:1:GLU:HG2	4:E:107:TYR:CD1	2.46	0.50
1:B:6:ARG:NH2	1:B:102:ASP:OD1	2.44	0.50
1:A:141:GLN:NE2	1:A:144:ARG:NH1	2.59	0.50
1:U:77:ASN:HA	1:U:80:THR:HG22	1.93	0.50
1:L:51:TRP:O	1:L:54:GLN:HG2	2.12	0.50
2:X:2:LEU:N	2:X:2:LEU:HD13	2.26	0.50
3:I:99:ASP:O	3:I:101:PRO:HD3	2.11	0.50
3:D:99:ASP:CB	3:D:100:PRO:CD	2.87	0.50
1:A:77:ASN:ND2	2:Q:9:LEU:HB2	2.21	0.50
4:N:1:GLU:HG2	4:N:107:TYR:CD1	2.45	0.50
1:L:122:ASP:OD1	1:Y:31:LYS:HE2	2.12	0.50
1:H:6:ARG:NH2	1:H:102:ASP:OD1	2.44	0.50
3:M:38:TYR:O	3:M:41:GLN:HB2	2.12	0.50
3:I:32:LEU:HD13	3:I:73:PHE:HB2	1.92	0.50
1:Y:30:ASP:N	1:Y:31:LYS:HD2	2.27	0.50
1:P:31:LYS:HD2	1:P:31:LYS:N	2.27	0.50
3:R:3:VAL:HG13	3:R:92:VAL:HG12	1.94	0.50
1:L:15:ARG:N	1:L:15:ARG:HD2	2.27	0.50
1:U:111:ARG:HG2	1:U:113:TYR:CZ	2.47	0.50
1:L:10:THR:HG22	1:L:96:GLN:CB	2.37	0.50
2:Q:1:GLN:CA	2:Q:1:GLN:OE1	2.59	0.50
1:A:41:GLU:CD	1:A:42:ASN:H	2.15	0.50
1:P:141:GLN:NE2	1:P:144:ARG:NH1	2.60	0.50
4:F:73:GLU:CD	4:F:73:GLU:H	2.15	0.50
1:Y:82:LEU:HD23	1:Y:87:GLN:NE2	2.27	0.50
4:S:83:THR:HG23	4:S:86:GLN:HG3	1.94	0.50
3:V:99:ASP:O	3:V:101:PRO:HD3	2.11	0.49
1:L:77:ASN:HA	1:L:80:THR:HG22	1.93	0.49
4:F:84:PRO:O	4:F:87:THR:CG2	2.57	0.49
4:J:33:TYR:N	4:J:33:TYR:CD1	2.80	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.45	0.49
3:V:42:GLY:HA2	4:W:91:PHE:CE2	2.46	0.49
4:F:15:THR:OG1	4:F:118:SER:HA	2.12	0.49
3:V:99:ASP:O	3:V:100:PRO:C	2.46	0.49
1:P:77:ASN:HA	1:P:80:THR:HG22	1.89	0.49
1:H:82:LEU:HD23	1:H:87:GLN:NE2	2.24	0.49
1:P:72:GLN:HG3	4:S:50:TYR:CD2	2.47	0.49
1:A:31:LYS:N	1:A:31:LYS:HD2	2.27	0.49
1:H:106:ASP:OD2	3:V:76:ARG:NH1	2.41	0.49
4:W:33:TYR:CZ	4:W:106:LEU:HD11	2.47	0.49
4:S:51:GLY:O	4:S:69:ARG:HG2	2.12	0.49
4:E:57:LYS:HB3	4:E:61:PRO:HG3	1.98	0.49
1:H:111:ARG:HG2	1:H:113:TYR:CZ	2.47	0.49
4:S:55:THR:HG22	4:S:55:THR:O	2.12	0.49
1:B:52:MET:CE	1:B:52:MET:HA	2.41	0.49
3:Z:91:ALA:HB1	3:Z:104:LEU:HD22	1.94	0.49
3:C:38:TYR:O	3:C:41:GLN:HB2	2.11	0.49
4:N:9:ARG:HG3	4:N:10:ASN:ND2	2.27	0.49
1:Y:41:GLU:CD	1:Y:41:GLU:H	2.15	0.49
1:H:28:VAL:HG23	1:H:33:PHE:CE1	2.48	0.49
4:J:3:ALA:O	4:J:25:GLN:HA	2.12	0.49
3:V:31:TYR:HB2	3:V:93:SER:HB2	1.94	0.49
1:H:77:ASN:HB3	2:K:9:LEU:HD22	1.94	0.49
2:T:1:GLN:HA	2:T:1:GLN:OE1	2.12	0.49
1:B:31:LYS:HD2	1:B:31:LYS:N	2.27	0.49
1:A:100:GLY:C	1:A:101:CYS:SG	2.88	0.49
4:E:33:TYR:CD1	4:E:33:TYR:N	2.79	0.49
4:F:3:ALA:O	4:F:25:GLN:HA	2.12	0.49
2:G:5:PHE:CG	3:C:102:PRO:HD3	2.47	0.49
3:C:12:VAL:O	3:C:114:VAL:HA	2.13	0.49
1:L:41:GLU:CD	1:L:42:ASN:H	2.16	0.49
1:L:30:ASP:H	1:L:31:LYS:HD2	1.78	0.49
1:A:164:CYS:SG	1:A:165:VAL:N	2.85	0.49
4:E:3:ALA:O	4:E:25:GLN:HA	2.13	0.49
1:H:41:GLU:H	1:H:41:GLU:CD	2.16	0.49
4:N:60:ILE:HG13	4:N:60:ILE:O	2.13	0.49
1:A:28:VAL:HG23	1:A:33:PHE:CD1	2.48	0.49
4:E:52:ALA:HA	4:E:69:ARG:HG3	1.94	0.49
1:L:167:TRP:NE1	2:O:1:GLN:HG2	2.28	0.49
1:A:15:ARG:HD2	1:A:15:ARG:N	2.28	0.49
1:B:100:GLY:C	1:B:101:CYS:SG	2.86	0.49
3:Z:3:VAL:HG13	3:Z:92:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:Z:99:ASP:CB	3:Z:100:PRO:CD	2.87	0.48
1:B:30:ASP:H	1:B:31:LYS:HD2	1.78	0.48
3:V:91:ALA:HB1	3:V:104:LEU:HD22	1.95	0.48
3:M:99:ASP:O	3:M:100:PRO:C	2.46	0.48
4:S:8:PRO:O	4:S:112:THR:HG23	2.13	0.48
1:A:111:ARG:HG2	1:A:113:TYR:CZ	2.48	0.48
1:Y:15:ARG:N	1:Y:15:ARG:HD2	2.28	0.48
1:P:41:GLU:CD	1:P:41:GLU:H	2.16	0.48
3:I:99:ASP:CB	3:I:100:PRO:CD	2.87	0.48
1:H:73:TRP:HZ2	2:K:9:LEU:HD13	1.77	0.48
2:K:1:GLN:OE1	2:K:1:GLN:CA	2.61	0.48
1:A:52:MET:HA	1:A:52:MET:CE	2.43	0.48
3:I:91:ALA:HB1	3:I:104:LEU:HD22	1.95	0.48
2:K:5:PHE:CG	3:I:102:PRO:HD3	2.48	0.48
4:F:60:ILE:HG13	4:F:60:ILE:O	2.13	0.48
2:T:2:LEU:N	2:T:2:LEU:HD13	2.28	0.48
1:B:77:ASN:HA	1:B:80:THR:HG22	1.93	0.48
1:L:111:ARG:HG2	1:L:113:TYR:CZ	2.48	0.48
3:R:99:ASP:O	3:R:101:PRO:HD3	2.13	0.48
1:U:82:LEU:HD23	1:U:87:GLN:NE2	2.28	0.48
1:B:28:VAL:HG23	1:B:33:PHE:CD1	2.48	0.48
3:I:38:TYR:O	3:I:41:GLN:HB2	2.13	0.48
1:B:111:ARG:HG2	1:B:113:TYR:CZ	2.48	0.48
3:V:5:GLN:NE2	3:V:90:CYS:H	2.10	0.48
3:V:5:GLN:HE21	3:V:107:GLY:HA3	1.78	0.48
4:W:60:ILE:O	4:W:60:ILE:HG13	2.13	0.48
3:D:91:ALA:HB1	3:D:104:LEU:HD22	1.95	0.48
1:B:28:VAL:HG23	1:B:33:PHE:CE1	2.49	0.48
1:H:30:ASP:H	1:H:31:LYS:HD2	1.79	0.48
3:R:34:TRP:CE2	3:R:75:LEU:HB2	2.49	0.48
1:P:15:ARG:HD2	1:P:15:ARG:N	2.27	0.48
1:B:108:ARG:HB3	3:Z:76:ARG:CZ	2.44	0.48
1:L:100:GLY:C	1:L:101:CYS:SG	2.89	0.48
3:Z:32:LEU:HD13	3:Z:73:PHE:HB2	1.96	0.48
2:O:5:PHE:CG	3:M:102:PRO:HD3	2.49	0.48
4:W:8:PRO:O	4:W:112:THR:HG23	2.14	0.48
1:U:164:CYS:SG	1:U:165:VAL:N	2.80	0.48
1:A:62:ARG:NE	2:Q:1:GLN:NE2	2.59	0.48
4:N:33:TYR:N	4:N:33:TYR:CD1	2.81	0.48
4:S:33:TYR:CZ	4:S:106:LEU:HD11	2.49	0.48
1:Y:6:ARG:NH2	1:Y:102:ASP:OD1	2.47	0.48
1:L:77:ASN:HB3	2:O:9:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:J:73:GLU:CD	4:J:73:GLU:H	2.16	0.47
1:Y:168:LEU:O	1:Y:172:LEU:HG	2.14	0.47
1:H:108:ARG:HG2	1:H:108:ARG:HH11	1.80	0.47
1:H:110:LEU:O	1:H:110:LEU:HD23	2.14	0.47
2:K:1:GLN:N	2:K:1:GLN:OE1	2.46	0.47
1:P:52:MET:CE	1:P:52:MET:HA	2.41	0.47
3:C:99:ASP:CB	3:C:100:PRO:CD	2.88	0.47
1:B:167:TRP:CZ2	2:G:1:GLN:HG2	2.50	0.47
1:H:31:LYS:HD2	1:H:31:LYS:N	2.30	0.47
1:A:14:ARG:CB	1:A:17:LEU:HD12	2.44	0.47
3:R:59:VAL:HG12	3:R:60:ASN:N	2.30	0.47
3:Z:99:ASP:O	3:Z:101:PRO:HD3	2.14	0.47
1:A:108:ARG:HB3	3:R:76:ARG:NH1	2.30	0.47
1:L:41:GLU:N	1:L:41:GLU:CD	2.68	0.47
1:H:28:VAL:HG23	1:H:33:PHE:CD1	2.50	0.47
4:S:33:TYR:CD1	4:S:33:TYR:N	2.82	0.47
4:S:15:THR:OG1	4:S:118:SER:HA	2.14	0.47
1:H:100:GLY:C	1:H:101:CYS:SG	2.90	0.47
3:I:5:GLN:HE21	3:I:107:GLY:HA3	1.80	0.47
1:A:41:GLU:N	1:A:41:GLU:CD	2.68	0.47
1:A:15:ARG:HD2	1:A:15:ARG:H	1.78	0.47
2:T:1:GLN:CA	2:T:1:GLN:OE1	2.62	0.47
4:W:3:ALA:O	4:W:25:GLN:HA	2.14	0.47
2:Q:2:LEU:HD13	2:Q:2:LEU:N	2.28	0.47
1:A:77:ASN:HB3	2:Q:9:LEU:HD22	1.96	0.47
1:A:82:LEU:HD23	1:A:87:GLN:NE2	2.28	0.47
4:W:1:GLU:HG2	4:W:107:TYR:CD1	2.49	0.47
4:W:41:HIS:HB3	4:W:42:GLU:H	1.53	0.47
1:L:82:LEU:HD23	1:L:87:GLN:NE2	2.30	0.47
1:A:14:ARG:HB2	1:A:17:LEU:HD12	1.97	0.47
4:W:83:THR:HG23	4:W:86:GLN:HG3	1.97	0.47
4:E:24:ASN:HA	4:E:73:GLU:O	2.24	0.47
1:U:156:TYR:O	1:U:160:LEU:HD22	2.15	0.47
4:N:73:GLU:CD	4:N:73:GLU:H	2.18	0.47
1:P:62:ARG:O	1:P:66:VAL:HG23	2.15	0.46
1:U:28:VAL:HG23	1:U:33:PHE:CE1	2.50	0.46
4:J:15:THR:OG1	4:J:118:SER:HA	2.14	0.46
1:H:62:ARG:NE	2:K:1:GLN:HE22	2.13	0.46
3:D:76:ARG:NH2	1:L:109:LEU:O	89.61	0.46
1:L:48:GLN:HE22	1:Y:14:ARG:HH22	1.64	0.46
1:B:41:GLU:CD	1:B:41:GLU:H	2.19	0.46
1:Y:31:LYS:HD2	1:Y:31:LYS:N	2.29	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:41:GLU:CD	1:U:41:GLU:N	2.69	0.46
4:E:73:GLU:CD	4:E:73:GLU:H	2.27	0.46
3:V:34:TRP:CE2	3:V:75:LEU:HB2	2.51	0.46
4:N:31:ASN:HA	4:N:49:SER:O	2.14	0.46
1:P:6:ARG:NH2	1:P:102:ASP:OD1	2.49	0.46
3:R:93:SER:C	3:R:99:ASP:O	2.53	0.46
1:Y:52:MET:CE	1:Y:52:MET:HA	2.43	0.46
4:E:55:THR:CG2	4:E:55:THR:O	2.64	0.46
2:X:5:PHE:CD1	3:V:102:PRO:HD3	2.51	0.46
1:L:31:LYS:N	1:L:31:LYS:HD2	2.30	0.46
1:P:111:ARG:HG2	1:P:113:TYR:CZ	2.51	0.46
4:E:83:THR:HG23	4:E:86:GLN:HG3	1.96	0.46
3:R:99:ASP:CB	3:R:100:PRO:CD	2.87	0.46
1:H:66:VAL:O	1:H:70:GLN:HG2	2.15	0.46
2:G:1:GLN:CA	2:G:1:GLN:OE1	2.64	0.46
1:U:31:LYS:N	1:U:31:LYS:HD2	2.30	0.46
4:F:57:LYS:HB3	4:F:61:PRO:HG3	1.98	0.46
1:A:73:TRP:HZ2	2:Q:9:LEU:HD13	1.80	0.46
1:B:77:ASN:HB3	2:G:9:LEU:HD22	1.97	0.46
4:F:39:THR:OG1	4:F:41:HIS:HB2	2.16	0.46
1:B:110:LEU:HD23	1:B:110:LEU:O	2.16	0.46
3:V:59:VAL:HG12	3:V:60:ASN:N	2.30	0.46
3:M:99:ASP:CB	3:M:100:PRO:CD	2.85	0.46
4:E:41:HIS:HB3	4:E:42:GLU:H	1.49	0.46
1:U:162:GLY:O	1:U:166:GLU:HG3	2.15	0.46
1:H:15:ARG:N	1:H:15:ARG:HD2	2.30	0.46
2:X:1:GLN:CA	2:X:1:GLN:OE1	2.63	0.46
1:H:12:THR:HG21	1:H:14:ARG:HE	1.81	0.46
4:J:60:ILE:HG13	4:J:60:ILE:O	2.14	0.46
3:M:91:ALA:HB1	3:M:104:LEU:HD22	1.98	0.46
1:Y:41:GLU:CD	1:Y:41:GLU:N	2.68	0.45
1:A:35:ARG:HG2	1:A:36:PHE:N	2.32	0.45
4:E:8:PRO:O	4:E:112:THR:HG23	2.22	0.45
1:U:77:ASN:HD22	2:X:9:LEU:CB	2.16	0.45
3:V:3:VAL:HG13	3:V:92:VAL:HG12	1.98	0.45
1:P:77:ASN:ND2	2:T:9:LEU:HB2	2.17	0.45
1:H:41:GLU:CD	1:H:42:ASN:H	2.19	0.45
1:P:41:GLU:CD	1:P:41:GLU:N	2.69	0.45
3:D:40:ARG:NH1	3:V:40:ARG:HH11	2.15	0.45
1:P:131:ARG:HG3	1:P:131:ARG:NH1	2.29	0.45
1:Y:31:LYS:CD	1:Y:31:LYS:N	2.80	0.45
4:N:51:GLY:O	4:N:69:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Y:41:GLU:CD	1:Y:42:ASN:H	2.19	0.45
2:O:8:ASP:OD2	4:N:96:GLY:HA2	2.16	0.45
3:V:93:SER:C	3:V:99:ASP:O	2.54	0.45
3:R:91:ALA:HB1	3:R:104:LEU:HD22	1.98	0.45
3:Z:99:ASP:O	3:Z:100:PRO:C	2.53	0.45
1:B:62:ARG:NE	2:G:1:GLN:NE2	2.55	0.45
1:L:108:ARG:HG2	1:L:108:ARG:HH11	1.80	0.45
4:N:41:HIS:HB3	4:N:42:GLU:H	1.49	0.45
3:C:59:VAL:HG12	3:C:60:ASN:N	2.31	0.45
3:D:59:VAL:HG12	3:D:60:ASN:N	2.37	0.45
2:X:1:GLN:N	2:X:1:GLN:OE1	2.46	0.45
3:C:5:GLN:NE2	3:C:90:CYS:H	2.15	0.45
3:V:19:GLN:HE21	3:V:19:GLN:HB3	1.66	0.45
1:B:108:ARG:HH11	1:B:108:ARG:HG2	1.82	0.45
2:K:2:LEU:HD13	2:K:2:LEU:N	2.32	0.44
1:B:62:ARG:NE	2:G:1:GLN:HE22	2.15	0.44
3:C:72:SER:HB2	3:C:74:HIS:CD2	2.52	0.44
4:S:41:HIS:HB3	4:S:42:GLU:H	1.55	0.44
1:U:108:ARG:HH11	1:U:108:ARG:HG2	1.82	0.44
1:L:52:MET:HE3	1:L:171:TYR:CD1	2.52	0.44
1:B:82:LEU:HD23	1:B:87:GLN:NE2	2.32	0.44
1:A:110:LEU:HD23	1:A:110:LEU:O	2.16	0.44
3:C:99:ASP:O	3:C:101:PRO:CD	2.65	0.44
1:H:47:PRO:O	1:P:14:ARG:NH2	2.50	0.44
1:B:59:TYR:O	1:B:63:ILE:HG12	2.17	0.44
1:H:41:GLU:N	1:H:41:GLU:CD	2.70	0.44
1:P:108:ARG:HH11	1:P:108:ARG:HG2	1.83	0.44
1:Y:108:ARG:HG2	1:Y:108:ARG:HH11	1.81	0.44
1:U:73:TRP:HZ2	2:X:9:LEU:HD13	1.82	0.44
1:A:30:ASP:H	1:A:31:LYS:HD2	1.83	0.44
3:I:34:TRP:CE2	3:I:75:LEU:HB2	2.53	0.44
4:F:31:ASN:HA	4:F:49:SER:O	2.17	0.44
3:R:99:ASP:O	3:R:100:PRO:C	2.53	0.44
1:Y:52:MET:HE3	1:Y:171:TYR:CD1	2.53	0.44
1:A:106:ASP:CG	3:R:76:ARG:NH1	2.71	0.44
1:H:168:LEU:O	1:H:172:LEU:HG	2.17	0.44
1:L:35:ARG:HG2	1:L:36:PHE:N	2.33	0.44
1:B:31:LYS:CD	1:B:31:LYS:N	2.80	0.44
1:B:41:GLU:CD	1:B:42:ASN:H	2.20	0.44
4:J:31:ASN:HA	4:J:49:SER:O	2.16	0.44
3:D:99:ASP:O	3:D:100:PRO:C	2.53	0.44
1:Y:35:ARG:HG2	1:Y:36:PHE:N	2.33	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Y:156:TYR:O	1:Y:160:LEU:HD22	2.18	0.44
3:Z:19:GLN:HB3	3:Z:19:GLN:HE21	1.67	0.44
4:J:9:ARG:HG3	4:J:10:ASN:ND2	2.33	0.44
3:V:99:ASP:CB	3:V:100:PRO:CD	2.86	0.43
3:D:76:ARG:NH1	1:P:106:ASP:OD2	2.51	0.43
4:S:73:GLU:H	4:S:73:GLU:CD	2.20	0.43
3:Z:93:SER:C	3:Z:99:ASP:O	2.56	0.43
1:L:66:VAL:O	1:L:70:GLN:HG2	2.19	0.43
1:L:123:TYR:CD1	1:L:124:ILE:HG22	2.50	0.43
1:H:35:ARG:HG2	1:H:36:PHE:N	2.33	0.43
1:P:30:ASP:N	1:P:31:LYS:HD2	2.33	0.43
3:D:93:SER:C	3:D:99:ASP:O	2.57	0.43
2:O:1:GLN:OE1	2:O:1:GLN:HA	2.18	0.43
1:L:168:LEU:O	1:L:172:LEU:HG	2.18	0.43
1:Y:14:ARG:O	1:Y:17:LEU:HB2	2.18	0.43
3:V:32:LEU:HD13	3:V:73:PHE:HB2	2.00	0.43
3:M:32:LEU:HD13	3:M:73:PHE:HB2	1.99	0.43
4:W:24:ASN:HA	4:W:73:GLU:O	2.17	0.43
3:Z:34:TRP:CE2	3:Z:75:LEU:HB2	2.53	0.43
4:S:57:LYS:HB3	4:S:61:PRO:HG3	2.00	0.43
3:M:103:LEU:HD21	4:N:48:TYR:CZ	2.53	0.43
1:L:156:TYR:O	1:L:160:LEU:HD22	2.19	0.43
3:I:59:VAL:HG12	3:I:60:ASN:N	2.33	0.43
1:A:77:ASN:HA	1:A:80:THR:HG22	1.91	0.43
1:P:15:ARG:HA	1:P:90:GLY:O	2.19	0.43
4:W:52:ALA:HA	4:W:69:ARG:HG3	2.01	0.43
1:A:106:ASP:OD1	3:R:76:ARG:NH1	2.51	0.43
1:H:35:ARG:NH2	1:P:35:ARG:HH21	2.17	0.43
1:P:35:ARG:HG2	1:P:36:PHE:N	2.32	0.43
3:M:34:TRP:CE2	3:M:75:LEU:HB2	2.53	0.43
1:B:41:GLU:CD	1:B:41:GLU:N	2.71	0.43
3:D:99:ASP:O	3:D:101:PRO:CD	2.65	0.43
1:A:52:MET:HE3	1:A:171:TYR:CD1	2.54	0.43
1:U:15:ARG:HA	1:U:90:GLY:O	2.19	0.43
1:H:108:ARG:NH1	1:H:108:ARG:HG2	2.33	0.43
1:P:110:LEU:O	1:P:110:LEU:HD23	2.18	0.43
3:D:81:HIS:O	3:D:114:VAL:HG11	2.19	0.43
1:L:59:TYR:O	1:L:63:ILE:HG12	2.19	0.43
3:I:81:HIS:O	3:I:114:VAL:HG11	2.18	0.43
1:P:31:LYS:CD	1:P:31:LYS:N	2.81	0.43
1:A:31:LYS:N	1:A:31:LYS:CD	2.82	0.43
1:B:30:ASP:N	1:B:31:LYS:HD2	2.33	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:9:ARG:HG3	4:E:10:ASN:ND2	2.33	0.43
1:B:35:ARG:HG2	1:B:36:PHE:N	2.34	0.43
4:W:31:ASN:HA	4:W:49:SER:O	2.18	0.43
1:A:108:ARG:NH2	3:R:76:ARG:HD3	2.34	0.42
1:H:14:ARG:HB2	1:H:17:LEU:HD12	2.01	0.42
1:U:97:ARG:HG3	1:U:116:PHE:CZ	2.54	0.42
1:B:164:CYS:SG	1:B:165:VAL:N	2.84	0.42
1:H:77:ASN:ND2	2:K:9:LEU:HB2	2.25	0.42
3:V:32:LEU:HD23	3:V:92:VAL:HG23	2.01	0.42
1:L:73:TRP:CZ2	2:O:9:LEU:HD13	2.54	0.42
1:Y:28:VAL:O	1:Y:31:LYS:HD3	2.20	0.42
1:U:30:ASP:N	1:U:31:LYS:HD2	2.34	0.42
2:G:1:GLN:N	2:G:1:GLN:OE1	2.50	0.42
3:D:40:ARG:HH12	3:V:40:ARG:NH1	2.17	0.42
3:R:76:ARG:HG2	3:R:77:LYS:N	2.35	0.42
3:D:5:GLN:NE2	3:D:90:CYS:H	2.24	0.42
1:L:110:LEU:HD23	1:L:110:LEU:O	2.19	0.42
4:E:31:ASN:HA	4:E:49:SER:O	2.23	0.42
4:J:57:LYS:HB3	4:J:61:PRO:HG3	2.02	0.42
1:P:73:TRP:HZ2	2:T:9:LEU:HD13	1.85	0.42
1:H:36:PHE:C	1:H:36:PHE:CD1	2.93	0.42
1:A:156:TYR:O	1:A:160:LEU:HD22	2.20	0.42
1:U:66:VAL:O	1:U:70:GLN:HG2	2.19	0.42
4:F:7:SER:HA	4:F:8:PRO:HA	1.89	0.42
1:L:31:LYS:N	1:L:31:LYS:CD	2.82	0.42
4:F:83:THR:HG23	4:F:86:GLN:HG3	2.00	0.42
3:I:93:SER:C	3:I:99:ASP:O	2.58	0.42
1:U:73:TRP:CZ2	2:X:9:LEU:HD13	2.55	0.42
3:C:99:ASP:O	3:C:100:PRO:C	2.54	0.42
1:L:73:TRP:HZ2	2:O:9:LEU:HD13	1.84	0.42
1:H:63:ILE:HG23	2:K:2:LEU:HD21	2.00	0.42
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.54	0.42
1:A:51:TRP:CZ3	1:A:52:MET:HG2	2.54	0.42
1:U:168:LEU:O	1:U:172:LEU:HG	2.20	0.42
4:S:93:ALA:HA	4:S:107:TYR:O	2.19	0.42
1:H:31:LYS:CD	1:H:31:LYS:N	2.83	0.42
1:U:28:VAL:HG23	1:U:33:PHE:CD1	2.55	0.42
4:N:8:PRO:O	4:N:112:THR:HG23	2.20	0.42
1:L:162:GLY:O	1:L:166:GLU:HG3	2.20	0.42
3:D:60:ASN:HD21	3:C:82:ARG:HH22	108.82	0.42
1:L:30:ASP:N	1:L:31:LYS:HD2	2.34	0.42
1:A:30:ASP:N	1:A:31:LYS:HD2	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:5:GLN:NE2	3:I:90:CYS:H	2.17	0.42
1:L:108:ARG:NH1	1:L:108:ARG:HG2	2.35	0.42
1:P:28:VAL:HG23	1:P:33:PHE:CD1	2.55	0.42
1:A:73:TRP:CZ2	2:Q:9:LEU:HD13	2.54	0.42
3:I:72:SER:HB2	3:I:74:HIS:CD2	2.55	0.42
3:I:72:SER:HB2	3:I:74:HIS:NE2	2.34	0.42
1:Y:111:ARG:HG2	1:Y:113:TYR:OH	2.19	0.42
3:V:53:ASP:OD1	3:V:54:PRO:HD2	2.20	0.42
3:M:93:SER:C	3:M:99:ASP:O	2.58	0.42
1:H:73:TRP:CZ2	2:K:9:LEU:HD13	2.53	0.42
2:Q:1:GLN:HA	2:Q:1:GLN:OE1	2.19	0.42
4:W:21:LEU:HD22	4:W:112:THR:HG21	2.01	0.42
4:E:21:LEU:HD22	4:E:112:THR:HG21	2.10	0.42
1:Y:108:ARG:HG2	1:Y:108:ARG:NH1	2.35	0.42
3:D:67:SER:O	3:D:71:SER:N	2.59	0.42
4:J:8:PRO:O	4:J:112:THR:HG23	2.20	0.42
1:U:35:ARG:HG2	1:U:36:PHE:N	2.35	0.42
3:I:12:VAL:O	3:I:114:VAL:HA	2.20	0.41
3:C:104:LEU:HD12	4:F:106:LEU:HD22	2.02	0.41
3:R:104:LEU:HD12	4:S:106:LEU:HB2	2.02	0.41
4:E:27:ASN:O	4:E:28:ASN:HB3	2.20	0.41
1:H:51:TRP:CZ3	1:H:52:MET:HG2	2.55	0.41
3:D:34:TRP:CE2	3:D:75:LEU:HB2	2.55	0.41
3:D:19:GLN:HB3	3:D:19:GLN:HE21	1.61	0.41
3:D:40:ARG:HD3	3:C:40:ARG:HH11	144.69	0.41
1:Y:110:LEU:HD23	1:Y:110:LEU:C	2.40	0.41
3:Z:92:VAL:HG13	3:Z:92:VAL:O	2.20	0.41
3:C:34:TRP:CE2	3:C:75:LEU:HB2	2.55	0.41
1:A:92:THR:O	1:A:92:THR:HG23	2.20	0.41
1:L:77:ASN:ND2	2:O:9:LEU:HB2	2.25	0.41
4:W:73:GLU:CD	4:W:73:GLU:H	2.23	0.41
1:L:28:VAL:HG23	1:L:33:PHE:CE1	2.56	0.41
3:I:45:LEU:HD22	4:J:105:THR:CG2	2.50	0.41
2:O:2:LEU:HD13	2:O:2:LEU:N	2.35	0.41
3:C:19:GLN:HB3	3:C:19:GLN:HE21	1.64	0.41
1:L:73:TRP:CE2	2:O:6:PRO:HG2	2.55	0.41
3:I:104:LEU:HD12	4:J:106:LEU:HD22	2.03	0.41
1:U:110:LEU:HD23	1:U:110:LEU:C	2.41	0.41
4:F:8:PRO:O	4:F:112:THR:HG23	2.20	0.41
1:P:41:GLU:CD	1:P:42:ASN:H	2.23	0.41
1:L:78:LEU:HA	1:L:78:LEU:HD23	1.94	0.41
1:U:45:TYR:CE2	1:U:67:ALA:HB2	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:72:SER:HB2	3:C:74:HIS:NE2	2.35	0.41
1:U:97:ARG:HG3	1:U:116:PHE:CE1	2.56	0.41
4:F:36:ARG:HB3	4:F:46:ILE:HD11	2.03	0.41
3:M:19:GLN:HB3	3:M:19:GLN:HE21	1.68	0.41
3:D:12:VAL:O	3:D:114:VAL:HA	2.21	0.41
1:Y:45:TYR:CE2	1:Y:67:ALA:HB2	2.55	0.41
1:B:162:GLY:O	1:B:166:GLU:HG3	2.21	0.41
4:S:36:ARG:HB3	4:S:46:ILE:HD11	2.03	0.41
4:S:45:LEU:HD21	4:S:48:TYR:CD1	2.55	0.41
3:I:76:ARG:NH1	1:U:106:ASP:OD2	2.51	0.41
3:D:60:ASN:ND2	3:C:82:ARG:HH21	109.21	0.41
1:B:168:LEU:O	1:B:172:LEU:HG	2.21	0.41
4:E:93:ALA:HA	4:E:107:TYR:O	2.25	0.41
4:F:41:HIS:HB3	4:F:42:GLU:H	1.51	0.41
1:B:15:ARG:CD	1:B:15:ARG:H	2.33	0.41
1:U:72:GLN:HG3	4:W:50:TYR:CE2	2.56	0.41
1:H:30:ASP:N	1:H:31:LYS:HD2	2.36	0.41
1:A:36:PHE:CD1	1:A:36:PHE:C	2.94	0.41
4:N:36:ARG:HB3	4:N:46:ILE:HD11	2.03	0.41
1:U:22:TYR:CB	1:U:71:GLU:HG3	2.50	0.41
3:V:18:LEU:HB2	3:V:80:VAL:HG11	2.03	0.41
1:L:163:GLU:OE2	2:O:1:GLN:HB3	2.21	0.41
3:C:32:LEU:HD13	3:C:73:PHE:HB2	2.03	0.40
2:K:1:GLN:HA	2:K:1:GLN:OE1	2.20	0.40
1:B:51:TRP:CZ3	1:B:52:MET:HG2	2.56	0.40
3:R:5:GLN:NE2	3:R:90:CYS:H	2.19	0.40
1:P:168:LEU:O	1:P:172:LEU:HG	2.20	0.40
1:U:123:TYR:CZ	1:U:140:ALA:HA	2.56	0.40
1:Y:36:PHE:C	1:Y:36:PHE:CD1	2.94	0.40
4:E:79:LEU:N	4:E:79:LEU:CD1	2.94	0.40
1:A:99:TYR:OH	2:Q:2:LEU:HB3	2.20	0.40
4:S:31:ASN:HA	4:S:49:SER:O	2.21	0.40
1:B:73:TRP:HZ2	2:G:9:LEU:HD13	1.86	0.40
1:U:41:GLU:CD	1:U:42:ASN:H	2.24	0.40
4:N:33:TYR:CE1	4:N:106:LEU:HD11	2.56	0.40
1:B:36:PHE:C	1:B:36:PHE:CD1	2.94	0.40
3:D:53:ASP:OD1	3:D:54:PRO:HD2	2.21	0.40
3:I:99:ASP:O	3:I:101:PRO:CD	2.69	0.40
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.85	0.40
1:Y:141:GLN:NE2	1:Y:144:ARG:CZ	2.84	0.40
3:C:91:ALA:HB1	3:C:104:LEU:HD22	2.02	0.40
1:P:36:PHE:CD1	1:P:36:PHE:C	2.93	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:31:LYS:HE2	1:P:122:ASP:OD1	2.22	0.40
1:H:12:THR:CG2	1:H:14:ARG:HE	2.35	0.40
4:W:57:LYS:HB3	4:W:61:PRO:HG3	2.03	0.40
3:M:20:LEU:HD22	3:M:110:THR:HG21	2.02	0.40
3:Z:5:GLN:HA	3:Z:6:PRO:HD2	1.91	0.40
1:A:131:ARG:NH1	1:A:131:ARG:HG3	2.36	0.40
3:D:104:LEU:HD12	4:E:106:LEU:HD22	2.08	0.40
3:R:89:PHE:CE1	3:R:109:GLY:HA3	2.56	0.40
3:D:33:PHE:N	3:D:33:PHE:CD1	2.89	0.40
4:S:79:LEU:HD12	4:S:79:LEU:N	2.37	0.40
1:A:59:TYR:O	1:A:63:ILE:HG12	2.21	0.40
1:P:63:ILE:HA	1:P:63:ILE:HD13	1.90	0.40
1:A:167:TRP:CZ2	2:Q:1:GLN:HG2	2.56	0.40
1:P:82:LEU:HD23	1:P:87:GLN:NE2	2.32	0.40
1:B:108:ARG:HG2	1:B:108:ARG:NH1	2.36	0.40

All (3) 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	Distance(Å)	Clash(Å)
1:A:88:SER:OG	4:E:73:GLU:OE2[6_545]	1.93	0.27
1:A:88:SER:OG	4:E:73:GLU:OE1[6_545]	2.12	0.08
1:A:86:ASN:O	4:E:28:ASN:OD1[6_545]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	173/175 (99%)	158 (91%)	12 (7%)	3 (2%)	14 52
1	B	173/175 (99%)	155 (90%)	15 (9%)	3 (2%)	14 52
1	H	173/175 (99%)	155 (90%)	15 (9%)	3 (2%)	14 52
1	L	173/175 (99%)	157 (91%)	13 (8%)	3 (2%)	14 52
1	P	173/175 (99%)	156 (90%)	14 (8%)	3 (2%)	14 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	173/175 (99%)	158 (91%)	12 (7%)	3 (2%)	14	52
1	Y	173/175 (99%)	157 (91%)	13 (8%)	3 (2%)	14	52
1	c	173/175 (99%)	156 (90%)	14 (8%)	3 (2%)	14	52
2	G	7/9 (78%)	7 (100%)	0	0	100	100
2	K	7/9 (78%)	7 (100%)	0	0	100	100
2	O	7/9 (78%)	7 (100%)	0	0	100	100
2	Q	7/9 (78%)	7 (100%)	0	0	100	100
2	T	7/9 (78%)	7 (100%)	0	0	100	100
2	X	7/9 (78%)	7 (100%)	0	0	100	100
2	b	7/9 (78%)	7 (100%)	0	0	100	100
2	f	7/9 (78%)	7 (100%)	0	0	100	100
3	C	107/109 (98%)	98 (92%)	7 (6%)	2 (2%)	12	49
3	D	107/109 (98%)	101 (94%)	5 (5%)	1 (1%)	25	71
3	I	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	25	71
3	M	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	25	71
3	R	107/109 (98%)	100 (94%)	5 (5%)	2 (2%)	12	49
3	V	107/109 (98%)	100 (94%)	5 (5%)	2 (2%)	12	49
3	Z	107/109 (98%)	101 (94%)	4 (4%)	2 (2%)	12	49
3	d	107/109 (98%)	100 (94%)	5 (5%)	2 (2%)	12	49
4	E	109/111 (98%)	105 (96%)	3 (3%)	1 (1%)	25	71
4	F	109/111 (98%)	105 (96%)	3 (3%)	1 (1%)	25	71
4	J	109/111 (98%)	106 (97%)	2 (2%)	1 (1%)	25	71
4	N	109/111 (98%)	105 (96%)	3 (3%)	1 (1%)	25	71
4	S	109/111 (98%)	106 (97%)	2 (2%)	1 (1%)	25	71
4	W	109/111 (98%)	106 (97%)	2 (2%)	1 (1%)	25	71
4	a	109/111 (98%)	106 (97%)	2 (2%)	1 (1%)	25	71
4	e	109/111 (98%)	106 (97%)	2 (2%)	1 (1%)	25	71
All	All	3168/3232 (98%)	2953 (93%)	170 (5%)	45 (1%)	16	58

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	99	ASP

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Mol	Chain	Res	Type
3	C	99	ASP
3	d	99	ASP
3	I	99	ASP
3	M	99	ASP
3	R	99	ASP
3	V	99	ASP
3	Z	99	ASP
1	A	136	ALA
1	B	88	SER
1	B	136	ALA
1	c	88	SER
1	c	136	ALA
1	H	136	ALA
1	L	15	ARG
1	L	88	SER
1	L	136	ALA
1	P	15	ARG
1	P	88	SER
1	P	136	ALA
1	U	88	SER
1	U	136	ALA
1	Y	15	ARG
1	Y	88	SER
1	Y	136	ALA
1	c	15	ARG
1	H	15	ARG
1	H	88	SER
4	S	39	THR
1	U	15	ARG
4	a	39	THR
1	A	15	ARG
1	A	88	SER
1	B	15	ARG
4	F	39	THR
4	e	39	THR
4	J	39	THR
4	N	39	THR
4	W	39	THR
4	E	39	THR
3	d	39	PRO
3	R	39	PRO
3	Z	39	PRO

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Mol	Chain	Res	Type
3	V	39	PRO
3	C	39	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	A	144/144 (100%)	132 (92%)	12 (8%)	16	50
1	B	144/144 (100%)	132 (92%)	12 (8%)	16	50
1	H	144/144 (100%)	133 (92%)	11 (8%)	19	55
1	L	144/144 (100%)	133 (92%)	11 (8%)	19	55
1	P	144/144 (100%)	132 (92%)	12 (8%)	16	50
1	U	144/144 (100%)	132 (92%)	12 (8%)	16	50
1	Y	144/144 (100%)	133 (92%)	11 (8%)	19	55
1	c	144/144 (100%)	132 (92%)	12 (8%)	16	50
2	G	9/9 (100%)	6 (67%)	3 (33%)	0	1
2	K	9/9 (100%)	6 (67%)	3 (33%)	0	1
2	O	9/9 (100%)	7 (78%)	2 (22%)	1	6
2	Q	9/9 (100%)	6 (67%)	3 (33%)	0	1
2	T	9/9 (100%)	6 (67%)	3 (33%)	0	1
2	X	9/9 (100%)	6 (67%)	3 (33%)	0	1
2	b	9/9 (100%)	6 (67%)	3 (33%)	0	1
2	f	9/9 (100%)	6 (67%)	3 (33%)	0	1
3	C	95/95 (100%)	91 (96%)	4 (4%)	40	82
3	D	95/95 (100%)	91 (96%)	4 (4%)	40	82
3	I	95/95 (100%)	91 (96%)	4 (4%)	40	82
3	M	95/95 (100%)	91 (96%)	4 (4%)	40	82
3	R	95/95 (100%)	92 (97%)	3 (3%)	51	87
3	V	95/95 (100%)	91 (96%)	4 (4%)	40	82
3	Z	95/95 (100%)	91 (96%)	4 (4%)	40	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	d	95/95 (100%)	91 (96%)	4 (4%)	40	82
4	E	91/91 (100%)	84 (92%)	7 (8%)	18	54
4	F	91/91 (100%)	84 (92%)	7 (8%)	18	54
4	J	91/91 (100%)	85 (93%)	6 (7%)	24	63
4	N	91/91 (100%)	86 (94%)	5 (6%)	30	71
4	S	91/91 (100%)	84 (92%)	7 (8%)	18	54
4	W	91/91 (100%)	84 (92%)	7 (8%)	18	54
4	a	91/91 (100%)	85 (93%)	6 (7%)	24	63
4	e	91/91 (100%)	85 (93%)	6 (7%)	24	63
All	All	2712/2712 (100%)	2514 (93%)	198 (7%)	20	57

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	31	LYS
1	A	41	GLU
1	A	42	ASN
1	A	45	TYR
1	A	68	LYS
1	A	80	THR
1	A	101	CYS
1	A	108	ARG
1	A	160	LEU
1	A	164	CYS
1	A	169	HIS
2	Q	1	GLN
2	Q	2	LEU
2	Q	9	LEU
3	D	19	GLN
3	D	93	SER
3	D	99	ASP
3	D	104	LEU
4	E	33	TYR
4	E	38	ASP
4	E	55	THR
4	E	72	GLN
4	E	73	GLU
4	E	83	THR

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Mol	Chain	Res	Type
4	E	87	THR
1	B	15	ARG
1	B	31	LYS
1	B	41	GLU
1	B	42	ASN
1	B	45	TYR
1	B	68	LYS
1	B	80	THR
1	B	101	CYS
1	B	108	ARG
1	B	160	LEU
1	B	164	CYS
1	B	169	HIS
2	G	1	GLN
2	G	2	LEU
2	G	9	LEU
3	C	19	GLN
3	C	93	SER
3	C	99	ASP
3	C	104	LEU
4	F	33	TYR
4	F	38	ASP
4	F	55	THR
4	F	73	GLU
4	F	83	THR
4	F	87	THR
4	F	106	LEU
1	c	15	ARG
1	c	31	LYS
1	c	41	GLU
1	c	42	ASN
1	c	45	TYR
1	c	68	LYS
1	c	80	THR
1	c	101	CYS
1	c	108	ARG
1	c	160	LEU
1	c	164	CYS
1	c	169	HIS
2	f	1	GLN
2	f	2	LEU
2	f	9	LEU

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Mol	Chain	Res	Type
3	d	19	GLN
3	d	93	SER
3	d	99	ASP
3	d	104	LEU
4	e	33	TYR
4	e	38	ASP
4	e	55	THR
4	e	73	GLU
4	e	83	THR
4	e	87	THR
1	H	15	ARG
1	H	31	LYS
1	H	41	GLU
1	H	45	TYR
1	H	68	LYS
1	H	80	THR
1	H	101	CYS
1	H	108	ARG
1	H	160	LEU
1	H	164	CYS
1	H	169	HIS
2	K	1	GLN
2	K	2	LEU
2	K	9	LEU
3	I	19	GLN
3	I	93	SER
3	I	99	ASP
3	I	104	LEU
4	J	33	TYR
4	J	38	ASP
4	J	55	THR
4	J	73	GLU
4	J	83	THR
4	J	87	THR
1	L	15	ARG
1	L	31	LYS
1	L	41	GLU
1	L	45	TYR
1	L	68	LYS
1	L	80	THR
1	L	101	CYS
1	L	108	ARG

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Mol	Chain	Res	Type
1	L	160	LEU
1	L	164	CYS
1	L	169	HIS
2	O	1	GLN
2	O	2	LEU
3	M	19	GLN
3	M	93	SER
3	M	99	ASP
3	M	104	LEU
4	N	33	TYR
4	N	38	ASP
4	N	55	THR
4	N	83	THR
4	N	87	THR
1	P	15	ARG
1	P	31	LYS
1	P	41	GLU
1	P	45	TYR
1	P	61	GLU
1	P	68	LYS
1	P	80	THR
1	P	101	CYS
1	P	108	ARG
1	P	160	LEU
1	P	164	CYS
1	P	169	HIS
2	T	1	GLN
2	T	2	LEU
2	T	9	LEU
3	R	19	GLN
3	R	93	SER
3	R	104	LEU
4	S	33	TYR
4	S	38	ASP
4	S	55	THR
4	S	73	GLU
4	S	83	THR
4	S	87	THR
4	S	106	LEU
1	U	15	ARG
1	U	31	LYS
1	U	41	GLU

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Mol	Chain	Res	Type
1	U	42	ASN
1	U	45	TYR
1	U	68	LYS
1	U	80	THR
1	U	101	CYS
1	U	108	ARG
1	U	160	LEU
1	U	164	CYS
1	U	169	HIS
2	X	1	GLN
2	X	2	LEU
2	X	9	LEU
3	V	19	GLN
3	V	93	SER
3	V	99	ASP
3	V	104	LEU
4	W	33	TYR
4	W	38	ASP
4	W	55	THR
4	W	73	GLU
4	W	83	THR
4	W	87	THR
4	W	106	LEU
1	Y	15	ARG
1	Y	31	LYS
1	Y	41	GLU
1	Y	42	ASN
1	Y	45	TYR
1	Y	80	THR
1	Y	101	CYS
1	Y	108	ARG
1	Y	160	LEU
1	Y	164	CYS
1	Y	169	HIS
2	b	1	GLN
2	b	2	LEU
2	b	9	LEU
3	Z	19	GLN
3	Z	93	SER
3	Z	99	ASP
3	Z	104	LEU
4	a	33	TYR

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Mol	Chain	Res	Type
4	a	38	ASP
4	a	55	THR
4	a	73	GLU
4	a	83	THR
4	a	87	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	54	GLN
1	A	70	GLN
1	A	77	ASN
1	A	87	GLN
1	A	127	ASN
3	D	5	GLN
3	D	19	GLN
3	D	41	GLN
3	D	74	HIS
4	E	10	ASN
4	E	30	ASN
4	E	72	GLN
1	B	42	ASN
1	B	54	GLN
1	B	70	GLN
1	B	77	ASN
1	B	87	GLN
1	B	127	ASN
3	C	5	GLN
3	C	19	GLN
3	C	41	GLN
3	C	74	HIS
4	F	10	ASN
4	F	30	ASN
4	F	72	GLN
1	c	42	ASN
1	c	54	GLN
1	c	70	GLN
1	c	77	ASN
1	c	87	GLN
1	c	127	ASN
3	d	5	GLN

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Mol	Chain	Res	Type
3	d	19	GLN
3	d	41	GLN
3	d	60	ASN
3	d	74	HIS
4	e	10	ASN
4	e	30	ASN
4	e	72	GLN
1	H	42	ASN
1	H	54	GLN
1	H	70	GLN
1	H	77	ASN
1	H	87	GLN
1	H	127	ASN
3	I	5	GLN
3	I	19	GLN
3	I	41	GLN
3	I	74	HIS
4	J	10	ASN
4	J	30	ASN
4	J	72	GLN
1	L	42	ASN
1	L	48	GLN
1	L	70	GLN
1	L	77	ASN
1	L	87	GLN
1	L	127	ASN
3	M	5	GLN
3	M	19	GLN
3	M	41	GLN
3	M	74	HIS
4	N	10	ASN
4	N	30	ASN
4	N	72	GLN
1	P	42	ASN
1	P	70	GLN
1	P	77	ASN
1	P	87	GLN
1	P	127	ASN
3	R	5	GLN
3	R	19	GLN
3	R	41	GLN
3	R	74	HIS

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Mol	Chain	Res	Type
4	S	30	ASN
4	S	72	GLN
1	U	42	ASN
1	U	70	GLN
1	U	77	ASN
1	U	87	GLN
1	U	127	ASN
3	V	5	GLN
3	V	19	GLN
3	V	41	GLN
3	V	60	ASN
3	V	74	HIS
4	W	30	ASN
4	W	72	GLN
1	Y	42	ASN
1	Y	48	GLN
1	Y	70	GLN
1	Y	77	ASN
1	Y	87	GLN
1	Y	127	ASN
3	Z	5	GLN
3	Z	19	GLN
3	Z	41	GLN
3	Z	74	HIS
4	a	10	ASN
4	a	30	ASN
4	a	72	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	175/175 (100%)	0.05	6 (3%)	43	19	24, 40, 68, 92	0
1	B	175/175 (100%)	0.21	8 (4%)	31	15	33, 49, 74, 92	0
1	H	175/175 (100%)	0.26	8 (4%)	31	15	31, 50, 76, 97	0
1	L	175/175 (100%)	0.15	7 (4%)	36	17	32, 46, 69, 89	0
1	P	175/175 (100%)	0.25	9 (5%)	27	13	30, 49, 70, 92	0
1	U	175/175 (100%)	0.27	8 (4%)	31	15	28, 49, 74, 93	0
1	Y	175/175 (100%)	0.19	8 (4%)	31	15	30, 46, 69, 89	0
1	c	175/175 (100%)	0.31	13 (7%)	14	8	38, 53, 76, 94	0
2	G	9/9 (100%)	0.04	0	100	100	37, 42, 44, 51	0
2	K	9/9 (100%)	-0.09	0	100	100	39, 41, 48, 54	0
2	O	9/9 (100%)	0.06	0	100	100	36, 38, 46, 48	0
2	Q	9/9 (100%)	0.03	0	100	100	35, 37, 42, 49	0
2	T	9/9 (100%)	0.42	0	100	100	35, 43, 46, 55	0
2	X	9/9 (100%)	0.09	0	100	100	39, 43, 47, 52	0
2	b	9/9 (100%)	-0.02	0	100	100	32, 36, 43, 45	0
2	f	9/9 (100%)	0.36	0	100	100	45, 47, 53, 56	0
3	C	109/109 (100%)	-0.02	0	100	100	30, 44, 59, 69	0
3	D	109/109 (100%)	-0.01	0	100	100	25, 39, 56, 65	0
3	I	109/109 (100%)	-0.01	0	100	100	32, 44, 58, 68	0
3	M	109/109 (100%)	0.05	3 (2%)	50	22	32, 46, 62, 75	0
3	R	109/109 (100%)	0.08	5 (4%)	31	15	31, 44, 58, 71	0
3	V	109/109 (100%)	0.11	2 (1%)	65	29	34, 46, 60, 74	0
3	Z	109/109 (100%)	-0.02	0	100	100	32, 41, 55, 66	0
3	d	109/109 (100%)	0.24	4 (3%)	39	18	35, 49, 61, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
4	E	111/111 (100%)	-0.11	1 (0%) 81 39	26, 38, 58, 74	0
4	F	111/111 (100%)	0.04	1 (0%) 81 39	29, 45, 63, 77	0
4	J	111/111 (100%)	-0.04	3 (2%) 52 23	32, 45, 65, 80	0
4	N	111/111 (100%)	-0.14	0 100 100	30, 42, 58, 80	0
4	S	111/111 (100%)	0.12	3 (2%) 52 23	33, 45, 62, 75	0
4	W	111/111 (100%)	0.26	3 (2%) 52 23	32, 48, 63, 78	0
4	a	111/111 (100%)	0.10	4 (3%) 41 19	31, 44, 59, 72	0
4	e	111/111 (100%)	0.03	1 (0%) 81 39	35, 49, 64, 79	0
All	All	3232/3232 (100%)	0.12	97 (3%) 48 21	24, 46, 68, 97	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	16	GLY	6.5
1	H	89	ALA	5.6
1	c	16	GLY	4.7
1	U	17	LEU	4.6
1	Y	17	LEU	4.3
1	U	16	GLY	4.3
1	A	17	LEU	4.2
1	c	15	ARG	4.0
1	H	15	ARG	3.9
1	P	17	LEU	3.8
1	Y	15	ARG	3.8
1	U	15	ARG	3.7
1	H	16	GLY	3.7
1	H	17	LEU	3.6
3	d	12	VAL	3.5
1	L	15	ARG	3.5
3	V	11	THR	3.4
1	B	15	ARG	3.4
1	A	15	ARG	3.2
1	c	17	LEU	3.2
1	P	16	GLY	3.2
1	U	107	GLY	3.1
1	Y	18	GLY	3.1
1	H	41	GLU	3.1
1	B	138	MET	3.1
1	H	14	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	90	GLY	3.0
1	c	41	GLU	3.0
3	R	11	THR	3.0
1	P	15	ARG	3.0
1	L	88	SER	2.9
1	B	14	ARG	2.9
3	V	12	VAL	2.9
1	A	89	ALA	2.9
1	B	89	ALA	2.8
3	M	10	VAL	2.8
1	c	138	MET	2.8
1	c	14	ARG	2.7
1	B	41	GLU	2.7
1	L	16	GLY	2.7
1	B	17	LEU	2.7
1	Y	42	ASN	2.7
1	A	41	GLU	2.7
1	c	18	GLY	2.7
4	a	113	ARG	2.6
1	P	41	GLU	2.6
1	Y	90	GLY	2.6
1	Y	41	GLU	2.6
4	S	113	ARG	2.6
1	L	135	ALA	2.6
4	a	66	LYS	2.5
1	B	86	ASN	2.5
1	U	1	GLY	2.4
1	H	90	GLY	2.4
1	U	41	GLU	2.4
1	P	107	GLY	2.4
4	W	61	PRO	2.4
4	e	80	GLU	2.4
1	A	14	ARG	2.4
4	E	117	LEU	2.3
1	P	18	GLY	2.3
3	M	81	HIS	2.3
3	d	18	LEU	2.3
1	c	84	TYR	2.3
3	R	12	VAL	2.3
1	U	14	ARG	2.3
1	c	135	ALA	2.2
3	d	112	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	U	42	ASN	2.2
1	c	90	GLY	2.2
1	Y	138	MET	2.2
1	P	173	LYS	2.2
1	P	90	GLY	2.2
4	J	1	GLU	2.2
3	d	10	VAL	2.2
1	L	41	GLU	2.2
1	c	173	LYS	2.2
1	A	57	PRO	2.2
4	W	80	GLU	2.1
1	H	88	SER	2.1
3	R	114	VAL	2.1
3	R	81	HIS	2.1
1	P	88	SER	2.1
4	a	2	ALA	2.1
1	c	85	TYR	2.1
1	c	42	ASN	2.1
4	W	71	SER	2.1
1	B	145	ARG	2.1
3	M	15	GLY	2.1
3	R	8	ALA	2.1
4	S	2	ALA	2.1
4	J	2	ALA	2.0
4	a	80	GLU	2.0
4	S	66	LYS	2.0
1	L	89	ALA	2.0
4	J	117	LEU	2.0
4	F	117	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.