



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:20 AM UTC

PDB ID : 8I5C / pdb_00008i5c
Title : Crystal structure of a TCR in complex with HLA-A*11:01 bound to KRAS peptide (VVGAVGVGK)
Authors : Lu, D.; Chen, Y.; Jiang, M.; Tan, S.G.; Chai, Y.; Gao, G.F.
Deposited on : 2023-01-24
Resolution : 3.34 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

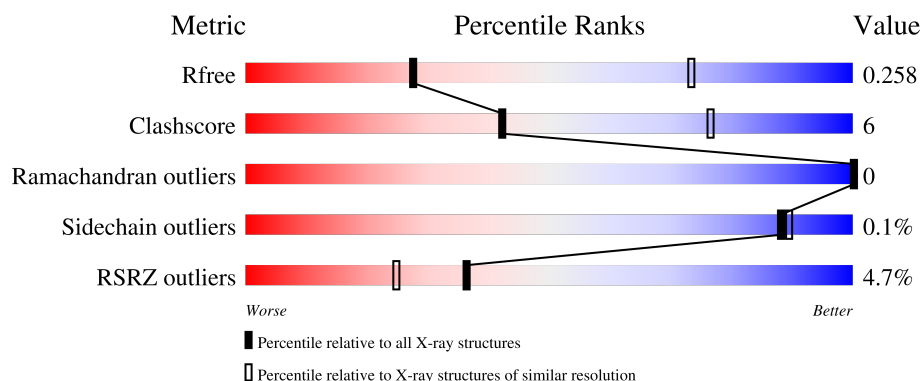
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 Å.

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



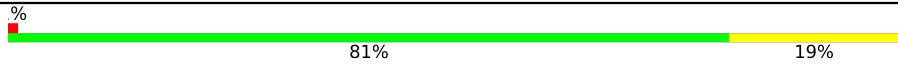
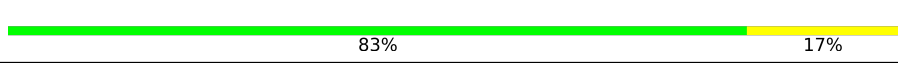
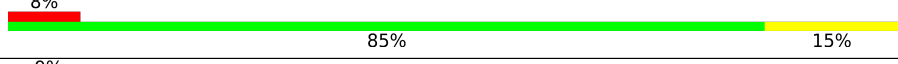
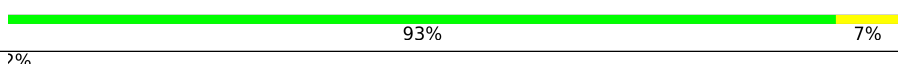
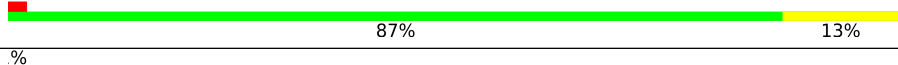
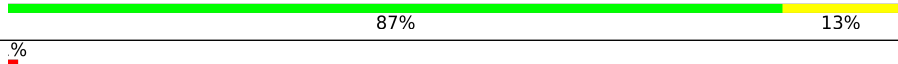
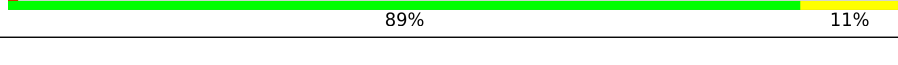
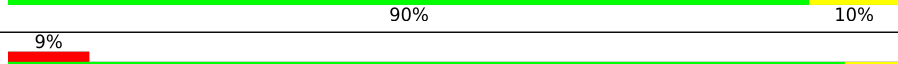
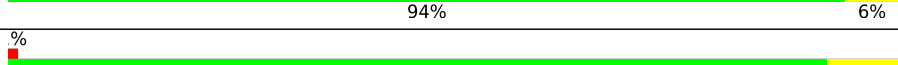
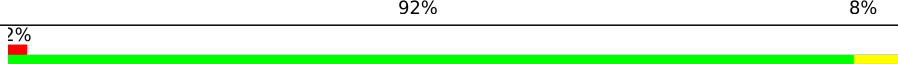
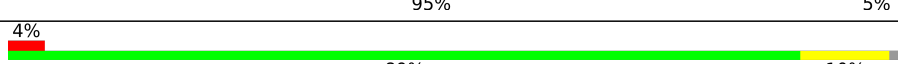
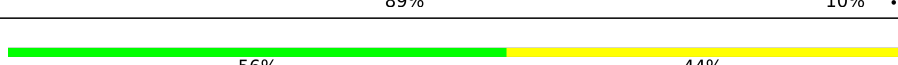
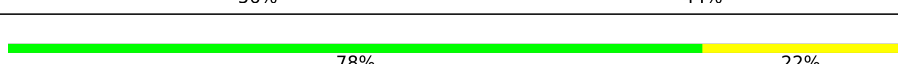
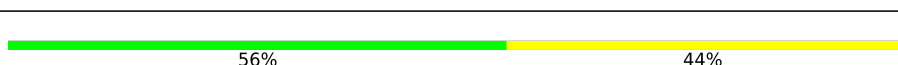
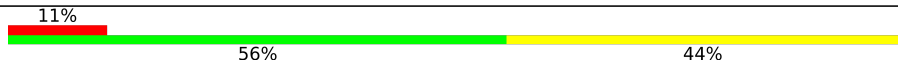
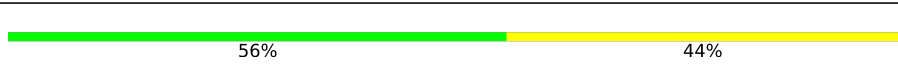
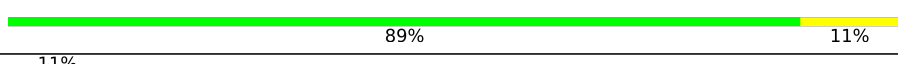
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	274	 79% 21%
1	F	274	 84% 16%
1	K	274	 82% 18%
1	P	274	 81% 19%
1	U	274	 82% 18%

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Mol	Chain	Length	Quality of chain
1	Z	274	
1	e	274	
1	j	274	
1	o	274	
1	t	274	
2	B	99	
2	G	99	
2	L	99	
2	Q	99	
2	V	99	
2	a	99	
2	f	99	
2	k	99	
2	p	99	
2	u	99	
3	C	9	
3	H	9	
3	M	9	
3	R	9	
3	W	9	
3	b	9	
3	g	9	
3	l	9	
3	q	9	
3	v	9	

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Mol	Chain	Length	Quality of chain
4	D	199	
4	I	199	
4	N	199	
4	S	199	
4	X	199	
4	c	199	
4	h	199	
4	m	199	
4	r	199	
4	w	199	
5	E	242	
5	J	242	
5	O	242	
5	T	242	
5	Y	242	
5	d	242	
5	i	242	
5	n	242	
5	s	242	
5	x	242	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 65732 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 MHC class I antigen (Fragment).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	F	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	K	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	P	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	U	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	Z	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	e	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	j	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	o	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0
1	t	274	Total 2237	C 1391	N 408	O 429	S 9	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	VAL	ALA	engineered mutation	UNP U5YJJ6
A	253	GLN	GLU	engineered mutation	UNP U5YJJ6
F	245	VAL	ALA	engineered mutation	UNP U5YJJ6
F	253	GLN	GLU	engineered mutation	UNP U5YJJ6
K	245	VAL	ALA	engineered mutation	UNP U5YJJ6
K	253	GLN	GLU	engineered mutation	UNP U5YJJ6
P	245	VAL	ALA	engineered mutation	UNP U5YJJ6
P	253	GLN	GLU	engineered mutation	UNP U5YJJ6
U	245	VAL	ALA	engineered mutation	UNP U5YJJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
U	253	GLN	GLU	engineered mutation	UNP U5YJJ6
Z	245	VAL	ALA	engineered mutation	UNP U5YJJ6
Z	253	GLN	GLU	engineered mutation	UNP U5YJJ6
e	245	VAL	ALA	engineered mutation	UNP U5YJJ6
e	253	GLN	GLU	engineered mutation	UNP U5YJJ6
j	245	VAL	ALA	engineered mutation	UNP U5YJJ6
j	253	GLN	GLU	engineered mutation	UNP U5YJJ6
o	245	VAL	ALA	engineered mutation	UNP U5YJJ6
o	253	GLN	GLU	engineered mutation	UNP U5YJJ6
t	245	VAL	ALA	engineered mutation	UNP U5YJJ6
t	253	GLN	GLU	engineered mutation	UNP U5YJJ6

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	G	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	L	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	Q	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	V	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	a	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	f	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	k	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	p	99	Total	C	N	O	S	0	0	0
			828	528	140	157	3			
2	u	98	Total	C	N	O	S	0	0	0
			820	523	139	156	2			

- Molecule 3 is a protein called peptide KRAS-G12V-9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	H	9	Total	C	N	O	0	0	0
			55	35	10	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	R	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	W	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	b	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	g	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	l	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	q	9	Total	C	N	O	0	0	0
			55	35	10	10			
3	v	9	Total	C	N	O	0	0	0
			55	35	10	10			

- Molecule 4 is a protein called TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	I	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	N	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	S	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	X	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	c	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	h	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	m	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	r	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			
4	w	198	Total	C	N	O	S	0	0	0
			1562	974	266	312	10			

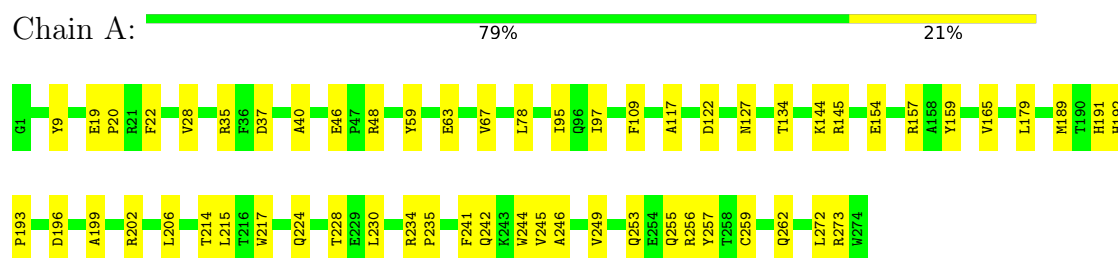
- Molecule 5 is a protein called TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	240	Total	C	N	O	S	0	0	0
			1892	1186	331	369	6			
5	J	240	Total	C	N	O	S	0	0	0
			1892	1186	331	369	6			
5	O	240	Total	C	N	O	S	0	0	0
			1892	1186	331	369	6			
5	T	240	Total	C	N	O	S	0	0	0
			1892	1186	331	369	6			
5	Y	240	Total	C	N	O	S	0	0	0
			1892	1186	331	369	6			
5	d	240	Total	C	N	O	S	0	0	0
			1892	1186	331	369	6			
5	i	240	Total	C	N	O	S	0	0	0
			1892	1186	331	369	6			
5	n	240	Total	C	N	O	S	0	0	0
			1892	1186	331	369	6			
5	s	240	Total	C	N	O	S	0	0	0
			1892	1186	331	369	6			
5	x	240	Total	C	N	O	S	0	0	0
			1892	1186	331	369	6			

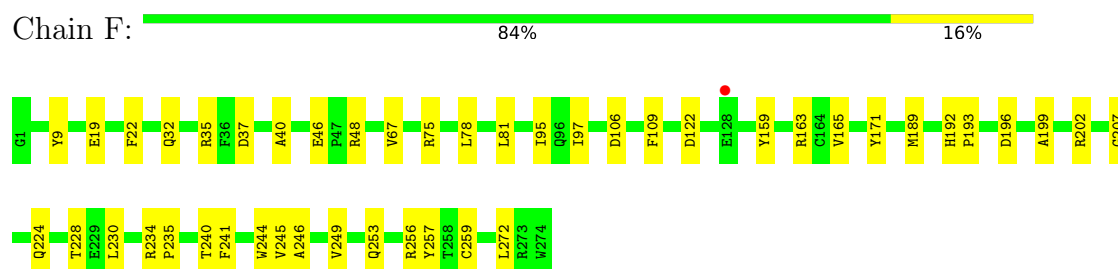
3 Residue-property plots

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.

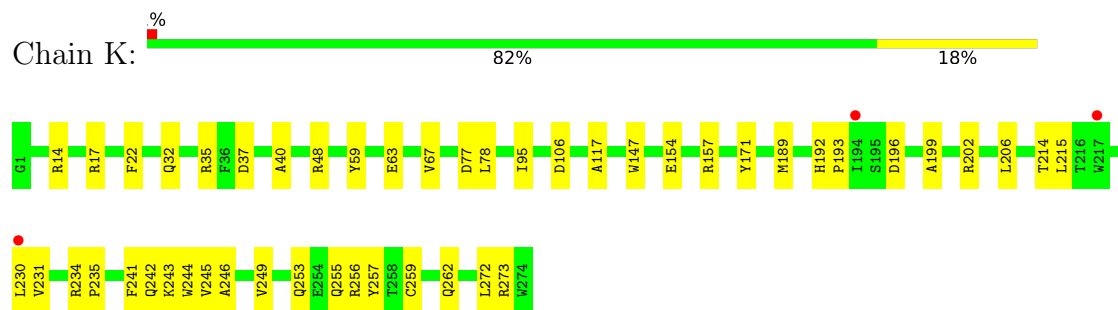
• Molecule 1: MHC class I antigen (Fragment)



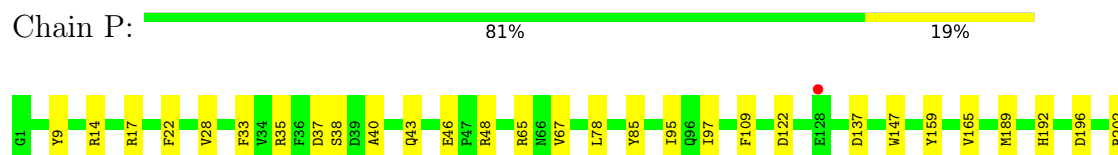
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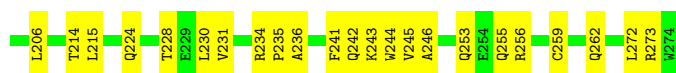


• Molecule 1: MHC class I antigen (Fragment)

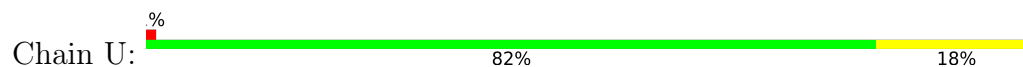


• Molecule 1: MHC class I antigen (Fragment)

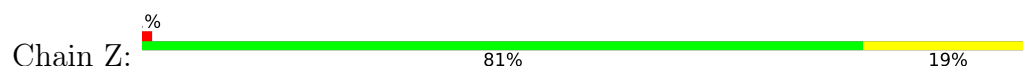




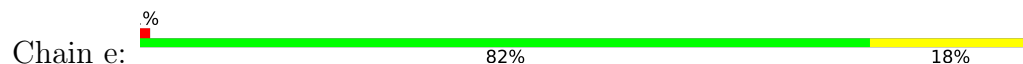
- Molecule 1: MHC class I antigen (Fragment)



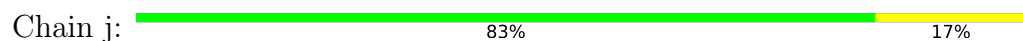
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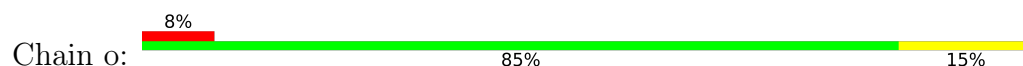
- Molecule 1: MHC class I antigen (Fragment)

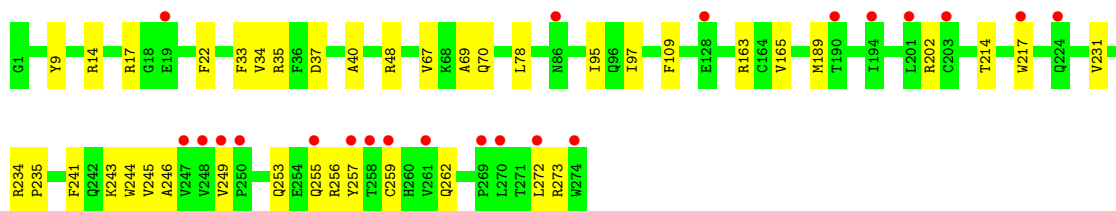


- Molecule 1: MHC class I antigen (Fragment)

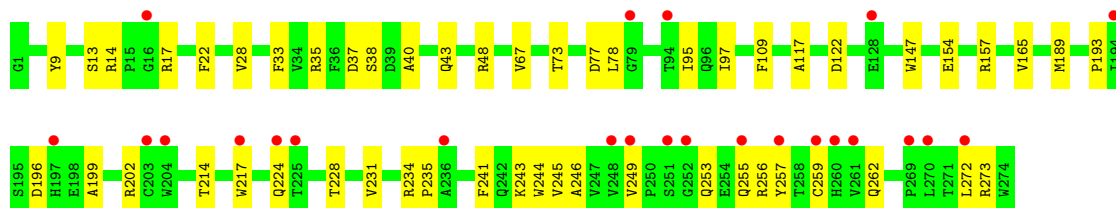
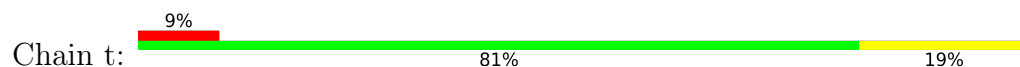


- Molecule 1: MHC class I antigen (Fragment)





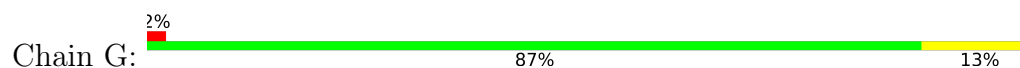
• Molecule 1: MHC class I antigen (Fragment)



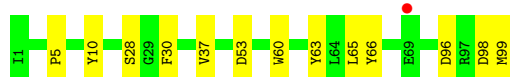
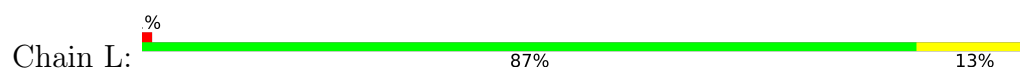
• Molecule 2: Beta-2-microglobulin



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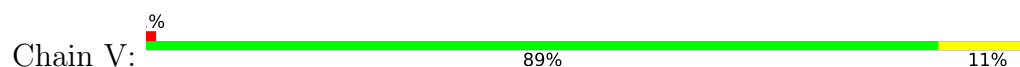
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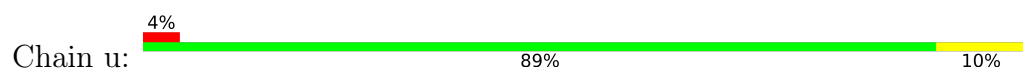
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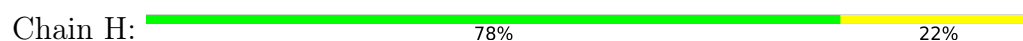
- Molecule 2: Beta-2-microglobulin



- Molecule 3: peptide KRAS-G12V-9

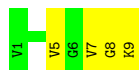


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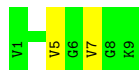
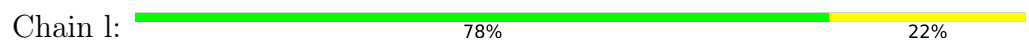
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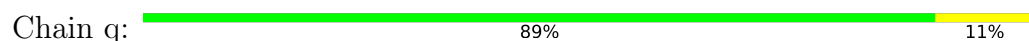
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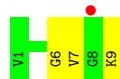


- Molecule 3: peptide KRAS-G12V-9

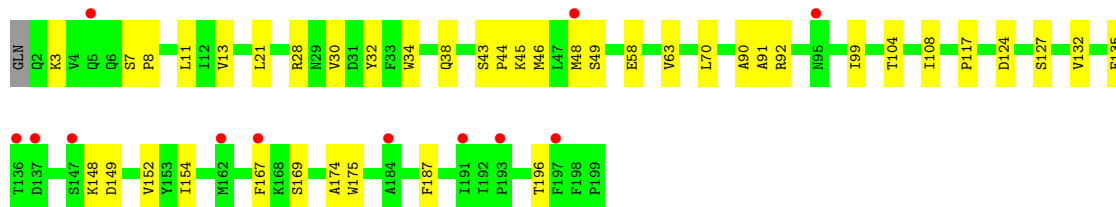
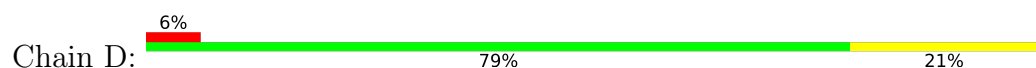




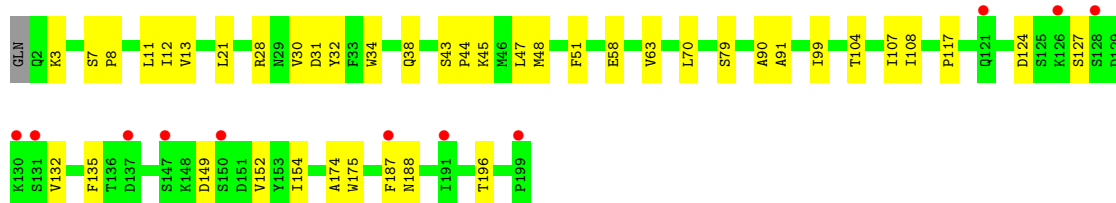
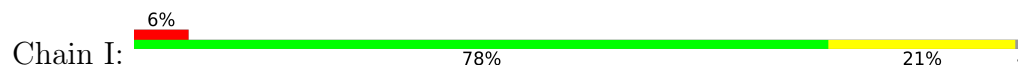
- Molecule 3: peptide KRAS-G12V-9



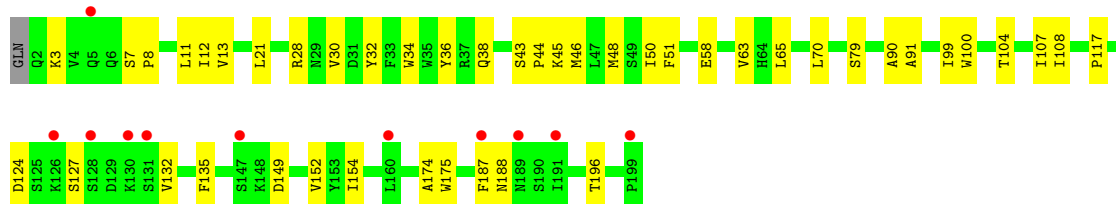
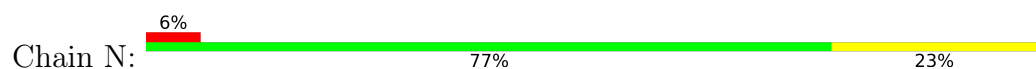
- Molecule 4: TCR alpha chain



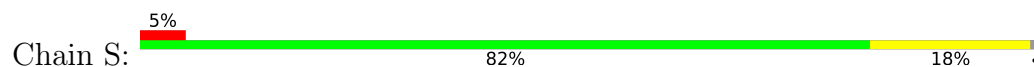
- Molecule 4: TCR alpha chain

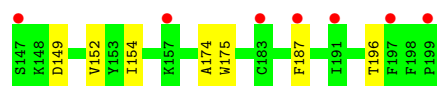


- Molecule 4: TCR alpha chain

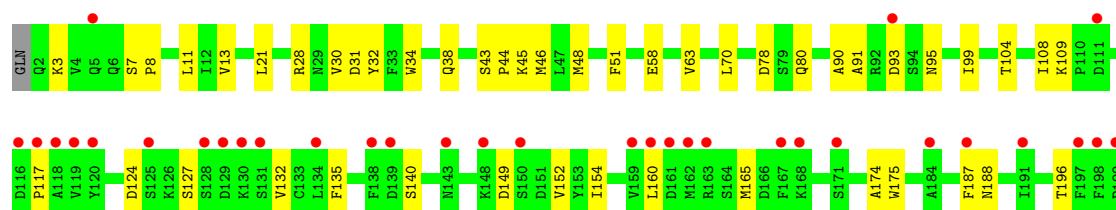
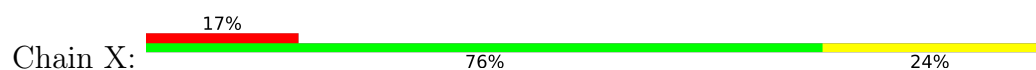


- Molecule 4: TCR alpha chain

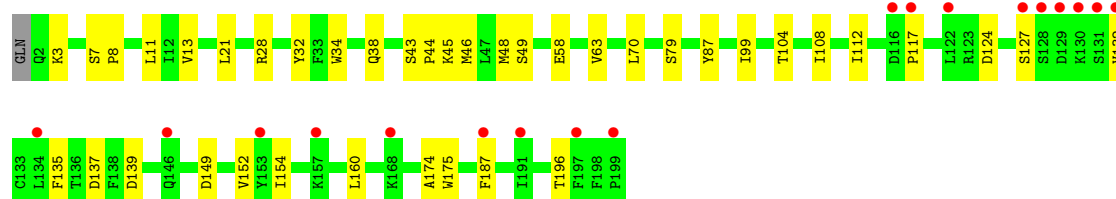
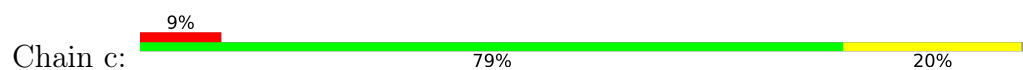




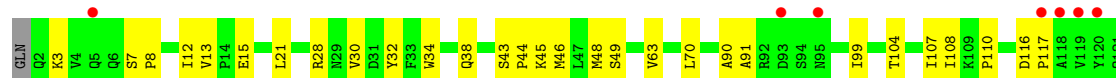
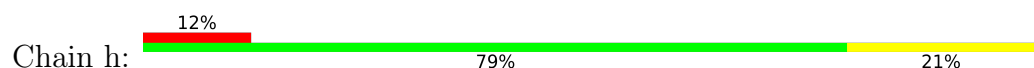
• Molecule 4: TCR alpha chain



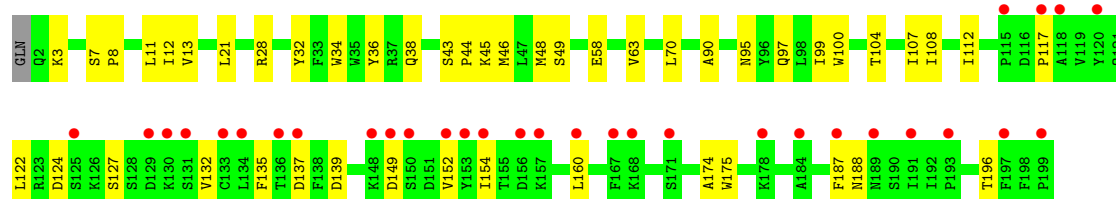
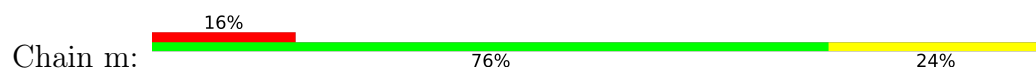
• Molecule 4: TCR alpha chain



• Molecule 4: TCR alpha chain

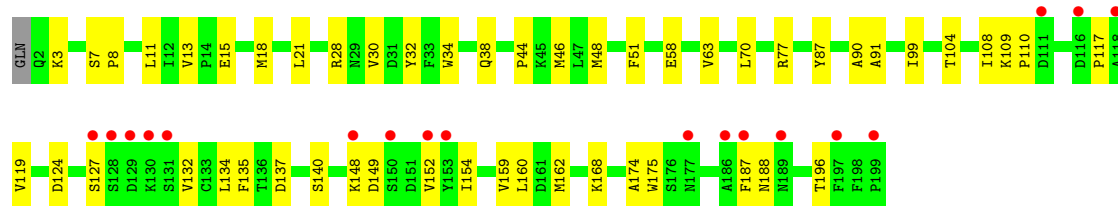


• Molecule 4: TCR alpha chain

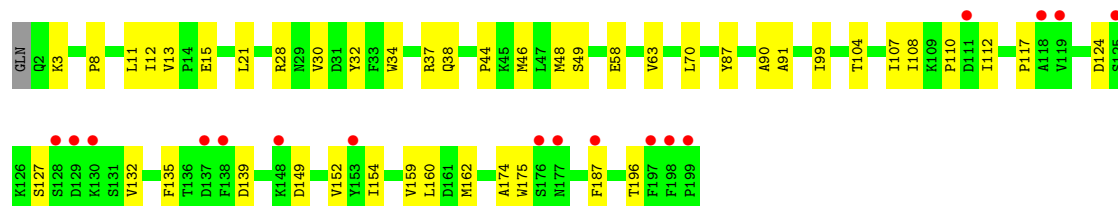
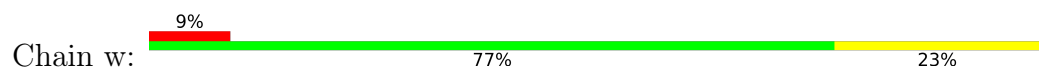


• Molecule 4: TCR alpha chain

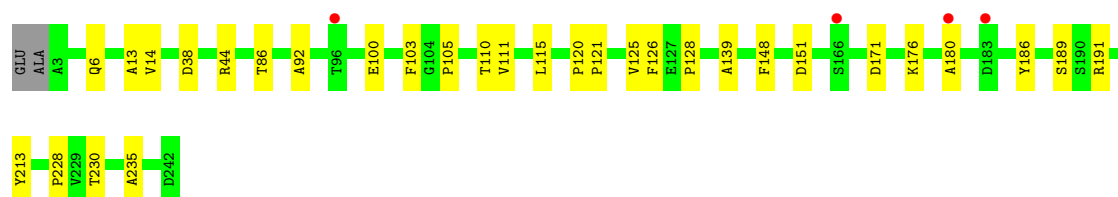
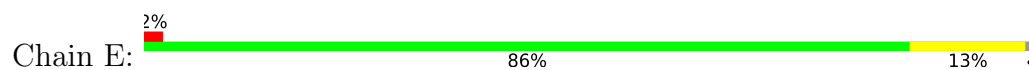




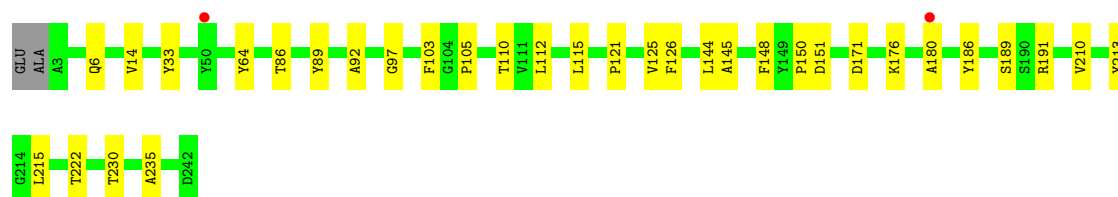
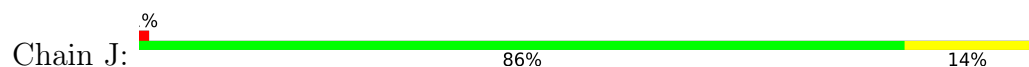
• Molecule 4: TCR alpha chain



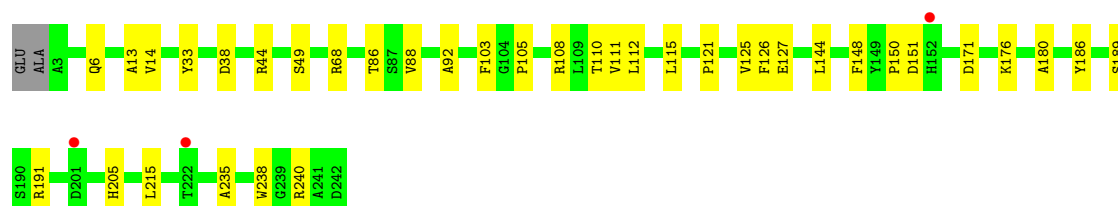
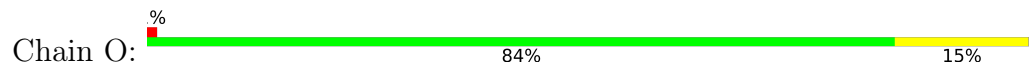
• Molecule 5: TCR beta chain



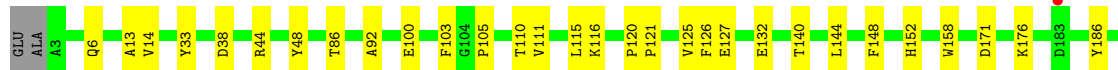
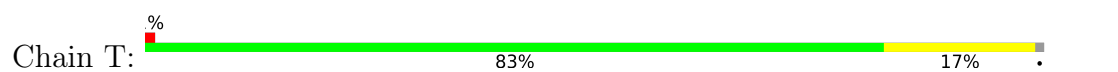
• Molecule 5: TCR beta chain



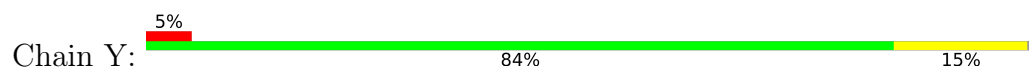
• Molecule 5: TCR beta chain



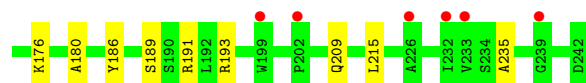
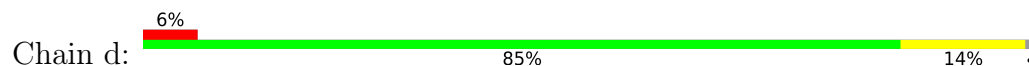
• Molecule 5: TCR beta chain



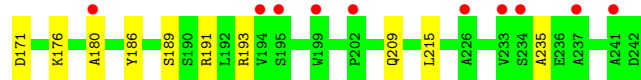
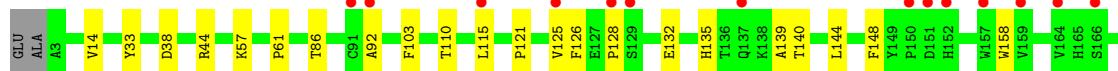
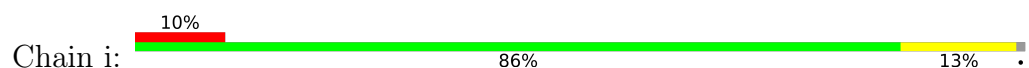
- Molecule 5: TCR beta chain



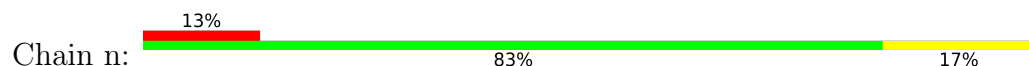
- Molecule 5: TCR beta chain

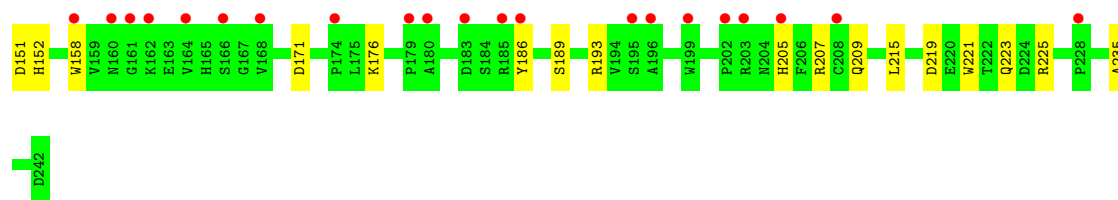


- Molecule 5: TCR beta chain

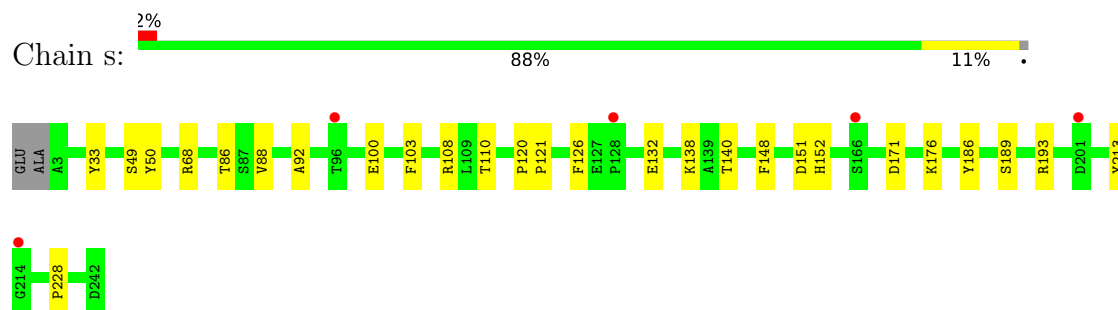


- Molecule 5: TCR beta chain

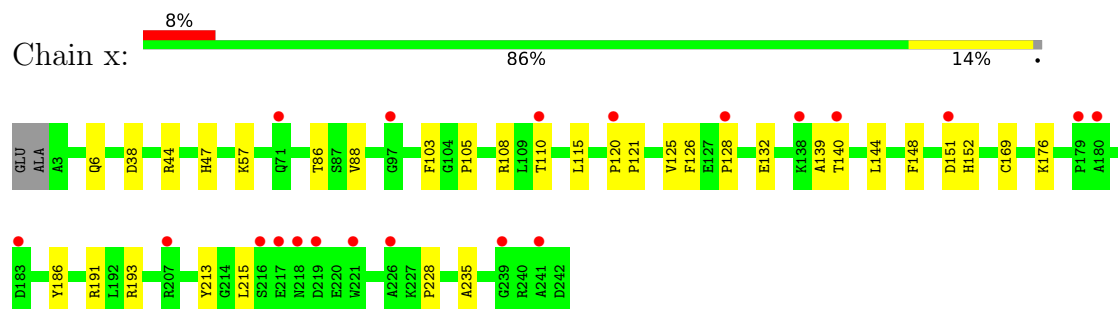




- Molecule 5: TCR beta chain



- Molecule 5: TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	156.86Å 156.89Å 191.97Å 77.37° 78.13° 82.27°	Depositor
Resolution (Å)	49.82 – 3.34 49.82 – 3.34	Depositor EDS
% Data completeness (in resolution range)	92.3 (49.82-3.34) 92.4 (49.82-3.34)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.224 , 0.258 0.224 , 0.258	Depositor DCC
R_{free} test set	11643 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	65732	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.07	0/2298	0.23	0/3120
1	F	0.07	0/2298	0.23	0/3120
1	K	0.07	0/2298	0.23	0/3120
1	P	0.07	0/2298	0.23	0/3120
1	U	0.07	0/2298	0.22	0/3120
1	Z	0.07	0/2298	0.22	0/3120
1	e	0.07	0/2298	0.23	0/3120
1	j	0.08	0/2298	0.22	0/3120
1	o	0.08	0/2298	0.24	0/3120
1	t	0.07	0/2298	0.22	0/3120
2	B	0.09	0/851	0.27	0/1152
2	G	0.09	0/851	0.27	0/1152
2	L	0.09	0/851	0.27	0/1152
2	Q	0.09	0/851	0.28	0/1152
2	V	0.09	0/851	0.27	0/1152
2	a	0.12	0/851	0.27	0/1152
2	f	0.09	0/851	0.26	0/1152
2	k	0.11	0/851	0.25	0/1152
2	p	0.10	0/851	0.24	0/1152
2	u	0.08	0/843	0.24	0/1142
3	C	0.11	0/54	0.28	0/70
3	H	0.13	0/54	0.26	0/70
3	M	0.11	0/54	0.33	0/70
3	R	0.12	0/54	0.36	0/70
3	W	0.13	0/54	0.40	0/70
3	b	0.08	0/54	0.24	0/70
3	g	0.07	0/54	0.26	0/70
3	l	0.09	0/54	0.29	0/70
3	q	0.07	0/54	0.20	0/70
3	v	0.11	0/54	0.28	0/70
4	D	0.08	0/1598	0.22	0/2163
4	I	0.08	0/1598	0.24	0/2163
4	N	0.08	0/1598	0.24	0/2163
4	S	0.07	0/1598	0.22	0/2163

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	X	0.08	0/1598	0.24	0/2163
4	c	0.07	0/1598	0.22	0/2163
4	h	0.07	0/1598	0.21	0/2163
4	m	0.07	0/1598	0.21	0/2163
4	r	0.08	0/1598	0.24	0/2163
4	w	0.08	0/1598	0.24	0/2163
5	E	0.07	0/1944	0.24	0/2650
5	J	0.07	0/1944	0.24	0/2650
5	O	0.08	0/1944	0.24	0/2650
5	T	0.08	0/1944	0.24	0/2650
5	Y	0.10	0/1944	0.25	0/2650
5	d	0.07	0/1944	0.23	0/2650
5	i	0.07	0/1944	0.23	0/2650
5	n	0.08	0/1944	0.25	0/2650
5	s	0.07	0/1944	0.24	0/2650
5	x	0.08	0/1944	0.26	0/2650
All	All	0.08	0/67442	0.24	0/91540

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2237	0	2091	38	0
1	F	2237	0	2091	31	0
1	K	2237	0	2091	33	0
1	P	2237	0	2091	36	0
1	U	2237	0	2091	32	0
1	Z	2237	0	2091	32	0
1	e	2237	0	2091	31	0
1	j	2237	0	2091	28	0
1	o	2237	0	2091	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	t	2237	0	2091	34	0
2	B	828	0	794	8	0
2	G	828	0	794	11	0
2	L	828	0	794	11	0
2	Q	828	0	794	11	0
2	V	828	0	794	9	0
2	a	828	0	794	9	0
2	f	828	0	794	5	0
2	k	828	0	794	7	0
2	p	828	0	794	4	0
2	u	820	0	785	8	0
3	C	55	0	65	3	0
3	H	55	0	65	3	0
3	M	55	0	65	3	0
3	R	55	0	65	3	0
3	W	55	0	65	5	0
3	b	55	0	65	2	0
3	g	55	0	65	5	0
3	l	55	0	65	1	0
3	q	55	0	65	1	0
3	v	55	0	65	5	0
4	D	1562	0	1484	30	0
4	I	1562	0	1484	29	0
4	N	1562	0	1484	31	0
4	S	1562	0	1484	23	0
4	X	1562	0	1484	32	0
4	c	1562	0	1484	29	0
4	h	1562	0	1484	26	0
4	m	1562	0	1484	31	0
4	r	1562	0	1484	37	0
4	w	1562	0	1484	27	0
5	E	1892	0	1779	20	0
5	J	1892	0	1779	23	0
5	O	1892	0	1779	23	0
5	T	1892	0	1779	25	0
5	Y	1892	0	1779	23	0
5	d	1892	0	1779	24	0
5	i	1892	0	1779	20	0
5	n	1892	0	1779	24	0
5	s	1892	0	1779	20	0
5	x	1892	0	1779	20	0
All	All	65732	0	62121	810	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (810) 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)
1:t:255:GLN:O	1:t:273:ARG:NH1	2.21	0.73
1:o:255:GLN:O	1:o:273:ARG:NH1	2.23	0.72
1:P:14:ARG:HB3	1:P:17:ARG:HB2	1.73	0.70
5:n:221:TRP:HH2	5:n:225:ARG:HB2	1.56	0.70
1:A:35:ARG:HD3	1:A:48:ARG:HE	1.57	0.69
1:F:35:ARG:HD3	1:F:48:ARG:HE	1.58	0.68
4:w:110:PRO:HG3	4:w:159:VAL:HG11	1.75	0.68
1:o:35:ARG:HD3	1:o:48:ARG:HE	1.59	0.68
1:F:19:GLU:OE1	1:F:75:ARG:NH1	2.27	0.68
1:K:35:ARG:HD3	1:K:48:ARG:HE	1.59	0.67
4:N:34:TRP:HB2	4:N:90:ALA:HB3	1.76	0.67
1:o:78:LEU:HD22	1:o:95:ILE:HD12	1.77	0.67
1:U:35:ARG:HD3	1:U:48:ARG:HE	1.60	0.67
1:A:214:THR:HB	1:A:262:GLN:HB2	1.76	0.66
4:S:3:LYS:HD2	4:S:99:ILE:HD13	1.75	0.66
1:P:78:LEU:HD22	1:P:95:ILE:HD12	1.77	0.66
1:U:192:HIS:NE2	2:V:98:ASP:OD2	2.28	0.66
1:P:192:HIS:NE2	2:Q:98:ASP:OD2	2.28	0.66
1:A:192:HIS:NE2	2:B:98:ASP:OD2	2.29	0.66
4:h:7:SER:HB2	4:m:13:VAL:HG23	1.78	0.66
4:N:117:PRO:HB2	4:N:196:THR:HG22	1.78	0.66
3:H:5:VAL:HG13	5:J:97:GLY:HA3	1.78	0.65
4:I:32:TYR:CD1	4:I:51:PHE:HB3	2.31	0.65
5:x:38:ASP:OD2	5:x:44:ARG:NH2	2.29	0.65
1:F:192:HIS:NE2	2:G:98:ASP:OD2	2.29	0.65
1:j:35:ARG:HD3	1:j:48:ARG:HE	1.62	0.65
1:A:78:LEU:HD22	1:A:95:ILE:HD12	1.78	0.64
4:I:149:ASP:HB3	4:I:152:VAL:HG12	1.79	0.64
4:I:34:TRP:HB2	4:I:90:ALA:HB3	1.79	0.64
4:I:117:PRO:HB2	4:I:196:THR:HG22	1.79	0.63
4:S:117:PRO:HB2	4:S:196:THR:HG22	1.80	0.63
4:N:32:TYR:CD1	4:N:51:PHE:HB3	2.33	0.63
5:E:180:ALA:HB2	4:r:188:ASN:HB3	1.80	0.63
4:N:149:ASP:HB3	4:N:152:VAL:HG12	1.81	0.63
1:P:35:ARG:HD3	1:P:48:ARG:HE	1.63	0.63
4:X:7:SER:HB2	4:c:13:VAL:HG23	1.80	0.63
1:Z:214:THR:HB	1:Z:262:GLN:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:35:ARG:HD3	1:e:48:ARG:HE	1.63	0.62
1:F:78:LEU:HD22	1:F:95:ILE:HD12	1.81	0.62
4:D:117:PRO:HB2	4:D:196:THR:HG22	1.80	0.62
4:r:34:TRP:HB2	4:r:90:ALA:HB3	1.80	0.62
1:K:59:TYR:HH	1:K:171:TYR:HH	1.48	0.62
1:K:192:HIS:NE2	2:L:98:ASP:OD2	2.33	0.61
4:r:3:LYS:HD2	4:r:99:ILE:HG12	1.81	0.61
1:t:235:PRO:HG2	2:u:65:LEU:HD22	1.82	0.61
4:h:13:VAL:HG23	4:m:7:SER:HB2	1.83	0.61
1:t:35:ARG:HD3	1:t:48:ARG:HE	1.66	0.61
4:w:34:TRP:HB2	4:w:90:ALA:HB3	1.82	0.61
4:S:149:ASP:HB3	4:S:152:VAL:HG12	1.83	0.61
1:Z:78:LEU:HD22	1:Z:95:ILE:HD12	1.83	0.61
1:j:78:LEU:HD22	1:j:95:ILE:HD12	1.83	0.60
4:r:32:TYR:CD1	4:r:51:PHE:HB3	2.36	0.60
1:j:214:THR:HB	1:j:262:GLN:HB2	1.82	0.60
1:K:78:LEU:HD22	1:K:95:ILE:HD12	1.82	0.60
4:c:3:LYS:HD2	4:c:99:ILE:HG12	1.83	0.60
1:F:235:PRO:HG2	2:G:65:LEU:HD22	1.84	0.59
4:X:32:TYR:CD1	4:X:51:PHE:HB3	2.37	0.59
4:w:149:ASP:HB3	4:w:152:VAL:HG12	1.84	0.59
4:h:34:TRP:HB2	4:h:90:ALA:HB3	1.84	0.59
1:e:78:LEU:HD22	1:e:95:ILE:HD12	1.84	0.59
4:D:149:ASP:HB3	4:D:152:VAL:HG12	1.85	0.59
4:I:7:SER:HB2	4:N:13:VAL:HG23	1.85	0.59
4:w:117:PRO:HB2	4:w:196:THR:HG22	1.84	0.59
4:D:7:SER:HB2	4:r:13:VAL:HG23	1.84	0.59
4:X:3:LYS:HB3	4:X:99:ILE:HG21	1.84	0.59
5:J:6:GLN:HG3	5:J:105:PRO:HD2	1.85	0.58
1:e:192:HIS:NE2	2:f:98:ASP:OD2	2.34	0.58
4:h:3:LYS:HB3	4:h:99:ILE:HG21	1.84	0.58
1:t:14:ARG:HB3	1:t:17:ARG:HB2	1.85	0.58
1:K:14:ARG:HB3	1:K:17:ARG:HG3	1.85	0.58
4:m:43:SER:OG	4:m:45:LYS:NZ	2.34	0.58
1:Z:35:ARG:HD3	1:Z:48:ARG:HE	1.66	0.58
4:w:38:GLN:HB2	4:w:44:PRO:HB3	1.86	0.58
1:A:193:PRO:HA	1:A:199:ALA:HA	1.85	0.58
1:F:253:GLN:HB3	1:F:256:ARG:HD3	1.85	0.58
4:I:13:VAL:HG23	4:N:7:SER:HB2	1.85	0.58
1:K:255:GLN:O	1:K:273:ARG:NH1	2.37	0.58
5:Y:86:THR:HG23	5:Y:110:THR:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:253:GLN:HB3	1:e:256:ARG:HD3	1.85	0.58
4:S:32:TYR:HE1	4:S:49:SER:HB2	1.68	0.58
1:Z:14:ARG:HB3	1:Z:17:ARG:HB2	1.85	0.58
4:N:3:LYS:HB3	4:N:99:ILE:HG21	1.85	0.58
1:j:9:TYR:HB2	1:j:97:ILE:HB	1.85	0.58
1:U:14:ARG:HB3	1:U:17:ARG:HB2	1.86	0.57
1:o:9:TYR:HB2	1:o:97:ILE:HB	1.86	0.57
5:x:121:PRO:HB3	5:x:148:PHE:HB3	1.86	0.57
1:U:78:LEU:HD22	1:U:95:ILE:HD12	1.86	0.57
4:m:3:LYS:HD2	4:m:99:ILE:HG12	1.86	0.57
1:F:9:TYR:HB2	1:F:97:ILE:HB	1.86	0.57
5:J:86:THR:HG23	5:J:110:THR:HA	1.86	0.57
4:w:21:LEU:HD22	4:w:104:THR:HG21	1.86	0.57
5:O:86:THR:HG23	5:O:110:THR:HA	1.86	0.57
1:U:255:GLN:O	1:U:273:ARG:NH1	2.38	0.57
1:j:14:ARG:HB3	1:j:17:ARG:HB2	1.86	0.57
4:I:30:VAL:HG11	4:I:91:ALA:HB1	1.86	0.57
4:m:21:LEU:HD22	4:m:104:THR:HG21	1.87	0.57
1:o:14:ARG:HB3	1:o:17:ARG:HB2	1.86	0.57
1:o:214:THR:HB	1:o:262:GLN:HB2	1.87	0.57
4:X:13:VAL:HG23	4:c:7:SER:HB2	1.85	0.57
1:K:214:THR:HB	1:K:262:GLN:HB2	1.87	0.57
1:K:235:PRO:HG2	2:L:65:LEU:HD22	1.87	0.57
1:t:78:LEU:HD22	1:t:95:ILE:HD12	1.85	0.57
4:I:3:LYS:HD2	4:I:99:ILE:HG12	1.87	0.56
4:X:117:PRO:HB2	4:X:196:THR:HG22	1.87	0.56
4:h:117:PRO:HB2	4:h:196:THR:HG22	1.87	0.56
2:V:37:VAL:HB	2:V:66:TYR:CE2	2.41	0.56
4:c:149:ASP:HB3	4:c:152:VAL:HG12	1.88	0.56
1:e:235:PRO:HG2	2:f:65:LEU:HD22	1.87	0.56
4:m:137:ASP:OD1	5:n:193:ARG:NH1	2.35	0.56
4:S:34:TRP:HB2	4:S:90:ALA:HB3	1.88	0.56
4:X:13:VAL:HG13	4:X:108:ILE:HG12	1.87	0.56
4:m:32:TYR:HE1	4:m:49:SER:HB2	1.70	0.56
4:w:162:MET:HE2	5:x:193:ARG:HB3	1.86	0.56
5:T:152:HIS:HB3	5:T:213:TYR:HB2	1.88	0.56
4:X:78:ASP:O	4:X:80:GLN:NE2	2.39	0.56
4:h:149:ASP:HB3	4:h:152:VAL:HG12	1.88	0.56
4:I:43:SER:OG	4:I:45:LYS:NZ	2.34	0.56
1:Z:189:MET:HE3	1:Z:272:LEU:HB3	1.88	0.56
5:i:121:PRO:HB3	5:i:148:PHE:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:3:LYS:HB3	4:r:99:ILE:HG21	1.87	0.56
1:F:163:ARG:NH1	4:I:31:ASP:OD2	2.38	0.55
1:U:163:ARG:NH1	4:X:31:ASP:OD2	2.38	0.55
5:Y:121:PRO:HB3	5:Y:148:PHE:HB3	1.88	0.55
4:c:117:PRO:HB2	4:c:196:THR:HG22	1.87	0.55
5:d:121:PRO:HB3	5:d:148:PHE:HB3	1.87	0.55
1:o:235:PRO:HG2	2:p:65:LEU:HD22	1.88	0.55
4:X:149:ASP:HB3	4:X:152:VAL:HG12	1.87	0.55
4:r:21:LEU:HD22	4:r:104:THR:HG21	1.88	0.55
1:e:189:MET:HE3	1:e:272:LEU:HB3	1.88	0.55
1:A:255:GLN:O	1:A:273:ARG:NH1	2.40	0.55
1:K:235:PRO:O	2:L:10:TYR:OH	2.21	0.55
1:P:235:PRO:HG2	2:Q:65:LEU:HD22	1.88	0.55
4:w:44:PRO:HG2	5:x:103:PHE:CD2	2.42	0.55
5:x:108:ARG:HE	5:x:152:HIS:HB3	1.72	0.55
4:I:3:LYS:HB3	4:I:99:ILE:HG21	1.88	0.55
4:I:38:GLN:HB2	4:I:44:PRO:HB3	1.88	0.55
1:K:253:GLN:HB3	1:K:256:ARG:HD3	1.87	0.55
4:c:32:TYR:HE1	4:c:49:SER:HB2	1.70	0.55
5:E:121:PRO:HB3	5:E:148:PHE:HB3	1.88	0.55
1:e:231:VAL:O	1:e:243:LYS:NZ	2.35	0.55
4:h:32:TYR:HE1	4:h:49:SER:HB2	1.72	0.55
5:i:86:THR:HG23	5:i:110:THR:HA	1.89	0.55
1:j:255:GLN:O	1:j:273:ARG:NH1	2.40	0.55
4:D:13:VAL:HG23	4:r:7:SER:HB2	1.89	0.55
4:D:34:TRP:HB2	4:D:90:ALA:HB3	1.89	0.55
3:R:5:VAL:HG12	3:R:7:VAL:HG23	1.89	0.55
1:Z:37:ASP:HB3	1:Z:40:ALA:HB2	1.89	0.54
4:m:149:ASP:HB3	4:m:152:VAL:HG12	1.89	0.54
4:r:117:PRO:HB2	4:r:196:THR:HG22	1.90	0.54
2:L:37:VAL:HB	2:L:66:TYR:CE2	2.43	0.54
1:P:147:TRP:NE1	3:R:8:GLY:O	2.35	0.54
5:n:6:GLN:HG3	5:n:105:PRO:HD2	1.89	0.54
5:s:171:ASP:OD2	5:s:189:SER:OG	2.23	0.54
1:F:224:GLN:O	1:F:228:THR:OG1	2.21	0.54
5:E:171:ASP:OD2	5:E:189:SER:OG	2.21	0.54
4:N:3:LYS:HD2	4:N:99:ILE:HG12	1.89	0.54
1:U:9:TYR:HB2	1:U:97:ILE:HB	1.90	0.54
5:Y:132:GLU:OE2	5:Y:140:THR:OG1	2.25	0.54
1:Z:253:GLN:HB3	1:Z:256:ARG:HD3	1.89	0.54
1:o:231:VAL:O	1:o:243:LYS:NZ	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLN:HB3	1:A:256:ARG:HD3	1.89	0.54
4:h:21:LEU:HD22	4:h:104:THR:HG21	1.90	0.54
4:h:38:GLN:HB2	4:h:44:PRO:HB3	1.89	0.54
4:m:44:PRO:HG2	5:n:103:PHE:CD2	2.42	0.54
1:A:37:ASP:HB3	1:A:40:ALA:HB2	1.90	0.54
1:t:224:GLN:O	1:t:228:THR:OG1	2.22	0.54
1:F:19:GLU:HB3	1:F:75:ARG:HH12	1.73	0.53
4:c:38:GLN:HB2	4:c:44:PRO:HB3	1.89	0.53
1:j:235:PRO:HG2	2:k:65:LEU:HD22	1.90	0.53
5:s:108:ARG:HE	5:s:152:HIS:HB3	1.72	0.53
4:m:3:LYS:HB3	4:m:99:ILE:HG21	1.90	0.53
5:E:13:ALA:HB3	5:E:111:VAL:HG22	1.89	0.53
4:r:149:ASP:HB3	4:r:152:VAL:HG12	1.90	0.53
5:s:86:THR:HG23	5:s:110:THR:HA	1.89	0.53
4:X:44:PRO:HG2	5:Y:103:PHE:CD2	2.43	0.53
4:c:3:LYS:HB3	4:c:99:ILE:HG21	1.90	0.53
4:c:13:VAL:HG13	4:c:108:ILE:HG12	1.91	0.53
4:D:30:VAL:HG11	4:D:91:ALA:HB1	1.91	0.53
5:J:189:SER:OG	5:J:191:ARG:NH1	2.41	0.53
4:c:137:ASP:OD1	5:d:193:ARG:NH1	2.40	0.53
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.91	0.53
1:P:9:TYR:HB2	1:P:97:ILE:HB	1.91	0.53
1:U:147:TRP:NE1	3:W:8:GLY:O	2.29	0.53
5:T:6:GLN:HG3	5:T:105:PRO:HD2	1.91	0.53
4:X:21:LEU:HD22	4:X:104:THR:HG21	1.91	0.53
4:X:34:TRP:HB2	4:X:90:ALA:HB3	1.90	0.53
3:b:5:VAL:HG12	3:b:7:VAL:HG13	1.90	0.53
1:e:235:PRO:HA	1:e:241:PHE:HD1	1.72	0.53
1:t:38:SER:O	1:t:43:GLN:NE2	2.36	0.53
2:B:37:VAL:HB	2:B:66:TYR:CE2	2.44	0.53
4:N:124:ASP:HA	5:O:126:PHE:HD1	1.74	0.53
5:d:86:THR:HG23	5:d:110:THR:HA	1.91	0.53
4:r:44:PRO:HG2	5:s:103:PHE:CD2	2.43	0.53
4:r:48:MET:HG3	4:r:63:VAL:HG21	1.90	0.53
5:s:121:PRO:HB3	5:s:148:PHE:HB3	1.90	0.53
4:N:44:PRO:HG2	5:O:103:PHE:CD2	2.44	0.52
5:T:171:ASP:OD2	5:T:189:SER:OG	2.26	0.52
1:U:235:PRO:HG2	2:V:65:LEU:HD22	1.90	0.52
2:p:37:VAL:HB	2:p:66:TYR:CE2	2.44	0.52
1:A:144:LYS:NZ	2:a:44:GLU:OE2	2.32	0.52
4:D:3:LYS:HD2	4:D:99:ILE:HG12	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:MET:HG3	4:D:63:VAL:HG21	1.90	0.52
4:N:13:VAL:HG13	4:N:108:ILE:HG12	1.92	0.52
4:S:124:ASP:HA	5:T:126:PHE:HD1	1.74	0.52
2:k:37:VAL:HB	2:k:66:TYR:CE2	2.44	0.52
1:K:230:LEU:HD12	1:K:245:VAL:HG22	1.90	0.52
5:T:86:THR:HG23	5:T:110:THR:HA	1.91	0.52
5:i:171:ASP:OD2	5:i:189:SER:OG	2.24	0.52
1:o:37:ASP:HB3	1:o:40:ALA:HB2	1.90	0.52
1:F:37:ASP:HB3	1:F:40:ALA:HB2	1.91	0.52
1:K:202:ARG:NH1	2:L:98:ASP:O	2.42	0.52
1:Z:235:PRO:HA	1:Z:241:PHE:HD1	1.74	0.52
4:r:30:VAL:HG11	4:r:91:ALA:HB1	1.92	0.52
5:E:86:THR:HG23	5:E:110:THR:HA	1.91	0.52
3:M:5:VAL:HG12	3:M:7:VAL:HG13	1.92	0.52
2:Q:37:VAL:HB	2:Q:66:TYR:CE2	2.44	0.52
5:Y:171:ASP:OD2	5:Y:189:SER:OG	2.26	0.52
4:c:21:LEU:HD22	4:c:104:THR:HG21	1.91	0.52
4:c:28:ARG:HA	4:c:70:LEU:HD11	1.92	0.52
1:e:37:ASP:HB3	1:e:40:ALA:HB2	1.92	0.52
5:E:120:PRO:HD3	5:E:228:PRO:HB3	1.91	0.52
5:T:13:ALA:HB3	5:T:111:VAL:HG22	1.92	0.52
4:X:46:MET:HE3	5:Y:100:GLU:HG3	1.92	0.52
4:r:154:ILE:HG12	4:r:174:ALA:HB2	1.91	0.52
1:t:122:ASP:OD1	2:u:60:TRP:NE1	2.31	0.52
4:w:32:TYR:HE1	4:w:49:SER:HB2	1.74	0.52
4:w:34:TRP:CD1	4:w:46:MET:HE2	2.45	0.52
4:D:124:ASP:HA	5:E:126:PHE:HD1	1.74	0.52
2:a:37:VAL:HB	2:a:66:TYR:CE2	2.45	0.52
5:n:132:GLU:OE2	5:n:140:THR:OG1	2.23	0.52
1:t:37:ASP:HB3	1:t:40:ALA:HB2	1.92	0.52
5:x:120:PRO:HD3	5:x:228:PRO:HB3	1.89	0.52
2:G:37:VAL:HB	2:G:66:TYR:CE2	2.44	0.52
4:w:3:LYS:HD2	4:w:99:ILE:HD13	1.91	0.52
4:w:154:ILE:HG12	4:w:174:ALA:HB2	1.90	0.52
5:J:33:TYR:HB2	5:J:92:ALA:HB3	1.92	0.52
5:O:38:ASP:OD2	5:O:44:ARG:NH2	2.43	0.52
1:A:244:TRP:HZ3	1:A:246:ALA:HB2	1.75	0.52
1:F:244:TRP:HZ3	1:F:246:ALA:HB2	1.74	0.52
1:Z:249:VAL:HG21	1:Z:254:GLU:HG3	1.92	0.52
4:r:38:GLN:HB2	4:r:44:PRO:HB3	1.91	0.52
4:I:44:PRO:HG2	5:J:103:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:48:MET:HE1	4:X:58:GLU:HB2	1.92	0.51
4:m:117:PRO:HB2	4:m:196:THR:HG22	1.91	0.51
5:x:132:GLU:OE2	5:x:140:THR:OG1	2.21	0.51
1:P:253:GLN:HB3	1:P:256:ARG:HD3	1.90	0.51
1:Z:147:TRP:NE1	3:b:8:GLY:O	2.39	0.51
4:r:137:ASP:OD1	5:s:193:ARG:NH1	2.34	0.51
1:P:230:LEU:HD12	1:P:245:VAL:HG22	1.93	0.51
4:w:13:VAL:HG13	4:w:108:ILE:HG12	1.93	0.51
1:F:230:LEU:HD12	1:F:245:VAL:HG22	1.91	0.51
4:N:30:VAL:HG11	4:N:91:ALA:HB1	1.92	0.51
4:X:38:GLN:HB2	4:X:44:PRO:HB3	1.92	0.51
4:D:124:ASP:HB3	4:D:127:SER:O	2.11	0.51
4:S:48:MET:HG3	4:S:63:VAL:HG21	1.92	0.51
5:T:38:ASP:OD2	5:T:44:ARG:NH2	2.44	0.51
1:U:244:TRP:HZ3	1:U:246:ALA:HB2	1.76	0.51
4:h:13:VAL:HG13	4:h:108:ILE:HG12	1.92	0.51
4:S:21:LEU:HD22	4:S:104:THR:HG21	1.93	0.51
5:i:158:TRP:NE1	5:i:209:GLN:OE1	2.42	0.51
1:A:19:GLU:HG3	1:A:20:PRO:HD2	1.92	0.51
1:P:214:THR:HB	1:P:262:GLN:HB2	1.92	0.51
1:A:122:ASP:OD1	2:B:60:TRP:NE1	2.35	0.51
5:E:38:ASP:OD2	5:E:44:ARG:NH2	2.44	0.51
1:o:253:GLN:HB3	1:o:256:ARG:HD3	1.93	0.51
5:x:86:THR:HG23	5:x:110:THR:HA	1.92	0.51
4:D:21:LEU:HD22	4:D:104:THR:HG21	1.93	0.51
1:U:230:LEU:HD12	1:U:245:VAL:HG22	1.92	0.51
5:Y:33:TYR:HB2	5:Y:92:ALA:HB3	1.93	0.51
4:c:43:SER:OG	4:c:45:LYS:NZ	2.33	0.51
1:e:214:THR:HB	1:e:262:GLN:HB2	1.93	0.51
1:e:230:LEU:HD12	1:e:245:VAL:HG22	1.92	0.51
4:I:21:LEU:HD22	4:I:104:THR:HG21	1.93	0.50
5:O:6:GLN:HG3	5:O:105:PRO:HD2	1.94	0.50
5:i:38:ASP:OD2	5:i:44:ARG:NH2	2.44	0.50
4:D:3:LYS:HB3	4:D:99:ILE:HG21	1.93	0.50
4:I:13:VAL:HG13	4:I:108:ILE:HG12	1.94	0.50
1:U:202:ARG:NH1	2:V:98:ASP:O	2.43	0.50
4:m:28:ARG:HA	4:m:70:LEU:HD11	1.92	0.50
1:e:9:TYR:HB2	1:e:97:ILE:HB	1.92	0.50
1:e:244:TRP:HZ3	1:e:246:ALA:HB2	1.76	0.50
4:h:44:PRO:HG2	5:i:103:PHE:CD2	2.46	0.50
5:s:132:GLU:OE2	5:s:140:THR:OG1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ASP:OD1	2:G:60:TRP:NE1	2.34	0.50
2:f:37:VAL:HB	2:f:66:TYR:CE2	2.46	0.50
4:h:30:VAL:HG11	4:h:91:ALA:HB1	1.94	0.50
1:A:230:LEU:HD12	1:A:245:VAL:HG22	1.93	0.50
4:I:124:ASP:HA	5:J:126:PHE:HD1	1.77	0.50
4:N:48:MET:HG3	4:N:63:VAL:HG21	1.92	0.50
4:S:124:ASP:HB3	4:S:127:SER:O	2.12	0.50
4:X:43:SER:OG	4:X:45:LYS:NZ	2.35	0.50
5:d:171:ASP:OD2	5:d:189:SER:OG	2.27	0.50
4:r:110:PRO:HG3	4:r:159:VAL:HG11	1.94	0.50
1:j:235:PRO:HA	1:j:241:PHE:HD1	1.77	0.50
1:A:189:MET:HE3	1:A:272:LEU:HB3	1.93	0.50
1:F:32:GLN:NE2	2:G:53:ASP:OD2	2.44	0.50
4:N:38:GLN:HB2	4:N:44:PRO:HB3	1.92	0.50
4:X:34:TRP:CD1	4:X:46:MET:HE2	2.47	0.50
4:r:162:MET:HE1	5:s:138:LYS:HD3	1.92	0.50
4:m:13:VAL:HG13	4:m:108:ILE:HG12	1.94	0.50
4:N:48:MET:HE1	4:N:58:GLU:HB2	1.94	0.49
4:S:44:PRO:HG2	5:T:103:PHE:CD2	2.47	0.49
1:Z:244:TRP:HZ3	1:Z:246:ALA:HB2	1.76	0.49
5:d:33:TYR:HB2	5:d:92:ALA:HB3	1.93	0.49
5:d:38:ASP:OD2	5:d:44:ARG:NH2	2.45	0.49
5:J:14:VAL:HG22	5:J:115:LEU:HD21	1.93	0.49
1:K:32:GLN:NE2	2:L:53:ASP:OD2	2.43	0.49
4:N:21:LEU:HD22	4:N:104:THR:HG21	1.94	0.49
1:Z:224:GLN:O	1:Z:228:THR:OG1	2.23	0.49
4:r:160:LEU:HD13	5:s:193:ARG:HG3	1.93	0.49
5:x:6:GLN:HG3	5:x:105:PRO:HD2	1.93	0.49
4:D:43:SER:OG	4:D:45:LYS:NZ	2.37	0.49
5:J:222:THR:OG1	2:u:44:GLU:OE2	2.30	0.49
1:j:244:TRP:HZ3	1:j:246:ALA:HB2	1.76	0.49
1:j:253:GLN:HB3	1:j:256:ARG:HD3	1.92	0.49
4:m:38:GLN:HB2	4:m:44:PRO:HB3	1.95	0.49
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.95	0.49
1:K:202:ARG:HG2	1:K:246:ALA:HB2	1.94	0.49
4:N:124:ASP:HB3	4:N:127:SER:O	2.11	0.49
1:U:189:MET:HE3	1:U:272:LEU:HB3	1.93	0.49
5:T:189:SER:OG	5:T:191:ARG:NH1	2.45	0.49
1:o:235:PRO:HA	1:o:241:PHE:HD1	1.78	0.49
4:N:132:VAL:HG12	4:N:175:TRP:HB3	1.94	0.49
1:P:85:TYR:OH	1:P:137:ASP:OD2	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:28:ARG:HA	4:X:70:LEU:HD11	1.93	0.49
4:w:30:VAL:HG11	4:w:91:ALA:HB1	1.93	0.49
1:U:235:PRO:HA	1:U:241:PHE:HD1	1.77	0.49
1:Z:230:LEU:HD12	1:Z:245:VAL:HG22	1.93	0.49
4:r:15:GLU:OE2	4:r:168:LYS:NZ	2.46	0.49
1:P:224:GLN:O	1:P:228:THR:OG1	2.20	0.49
4:X:8:PRO:HG3	4:X:11:LEU:HD12	1.94	0.49
4:X:30:VAL:HG11	4:X:91:ALA:HB1	1.94	0.49
5:n:121:PRO:HB3	5:n:148:PHE:HB3	1.94	0.49
1:t:235:PRO:HA	1:t:241:PHE:HD1	1.78	0.49
4:D:32:TYR:HE1	4:D:49:SER:HB2	1.78	0.49
5:E:6:GLN:HG3	5:E:105:PRO:HD2	1.94	0.48
1:P:37:ASP:HB3	1:P:40:ALA:HB2	1.95	0.48
2:Q:37:VAL:HG22	2:Q:82:VAL:HG22	1.94	0.48
5:n:176:LYS:HG2	5:n:186:TYR:CE1	2.48	0.48
1:o:244:TRP:HZ3	1:o:246:ALA:HB2	1.77	0.48
5:O:125:VAL:HG23	5:O:235:ALA:HB3	1.95	0.48
5:Y:115:LEU:HD22	5:Y:215:LEU:HD21	1.94	0.48
4:c:34:TRP:CD1	4:c:46:MET:HE2	2.48	0.48
4:c:44:PRO:HG2	5:d:103:PHE:CD2	2.48	0.48
1:e:202:ARG:HG2	1:e:246:ALA:HB2	1.95	0.48
4:m:34:TRP:HB2	4:m:90:ALA:HB3	1.96	0.48
1:t:214:THR:HB	1:t:262:GLN:HB2	1.94	0.48
4:D:46:MET:HE3	5:E:100:GLU:HG3	1.96	0.48
4:S:13:VAL:HG13	4:S:108:ILE:HG12	1.94	0.48
5:T:14:VAL:HG22	5:T:115:LEU:HD21	1.94	0.48
4:X:188:ASN:HB3	5:d:180:ALA:HA	1.95	0.48
5:x:176:LYS:HG2	5:x:186:TYR:CE1	2.48	0.48
4:I:124:ASP:HB3	4:I:127:SER:O	2.12	0.48
5:i:115:LEU:HD22	5:i:215:LEU:HD21	1.96	0.48
4:m:8:PRO:HG3	4:m:11:LEU:HD12	1.95	0.48
4:r:13:VAL:HG13	4:r:108:ILE:HG12	1.95	0.48
5:s:176:LYS:HG2	5:s:186:TYR:CE1	2.49	0.48
1:t:154:GLU:HG2	1:t:157:ARG:HH22	1.77	0.48
1:F:202:ARG:HH22	2:G:99:MET:HE2	1.79	0.48
4:N:135:PHE:HB2	4:N:187:PHE:CE2	2.49	0.48
5:O:176:LYS:HG2	5:O:186:TYR:CE1	2.47	0.48
4:h:3:LYS:HD2	4:h:99:ILE:HG12	1.94	0.48
4:h:48:MET:HG3	4:h:63:VAL:HG21	1.94	0.48
4:N:154:ILE:HG12	4:N:174:ALA:HB2	1.96	0.48
4:S:154:ILE:HG12	4:S:174:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:196:ASP:OD1	1:Z:196:ASP:N	2.47	0.48
4:c:124:ASP:HB3	4:c:127:SER:O	2.14	0.48
4:I:154:ILE:HG12	4:I:174:ALA:HB2	1.96	0.48
1:K:37:ASP:HB3	1:K:40:ALA:HB2	1.94	0.48
4:S:48:MET:HE1	4:S:58:GLU:HB2	1.95	0.48
5:d:126:PHE:HE2	5:d:144:LEU:HD12	1.78	0.48
1:j:193:PRO:HA	1:j:199:ALA:HA	1.96	0.48
1:P:38:SER:O	1:P:43:GLN:NE2	2.37	0.48
1:P:255:GLN:O	1:P:273:ARG:NH1	2.47	0.48
4:c:48:MET:HG3	4:c:63:VAL:HG21	1.95	0.48
5:d:158:TRP:NE1	5:d:209:GLN:OE1	2.47	0.48
5:i:126:PHE:HE2	5:i:144:LEU:HD12	1.78	0.48
4:w:48:MET:HG3	4:w:63:VAL:HG21	1.94	0.48
4:N:43:SER:OG	4:N:45:LYS:NZ	2.38	0.48
5:Y:189:SER:OG	5:Y:191:ARG:NH1	2.47	0.48
4:r:135:PHE:HB2	4:r:187:PHE:CE2	2.48	0.48
5:x:125:VAL:HG23	5:x:235:ALA:HB3	1.95	0.48
1:A:145:ARG:NH2	2:a:75:LYS:HD3	2.29	0.48
4:D:44:PRO:HG2	5:E:103:PHE:CD2	2.48	0.48
4:I:48:MET:HG3	4:I:63:VAL:HG21	1.94	0.48
1:P:109:PHE:HD1	1:P:165:VAL:HG11	1.79	0.48
4:S:30:VAL:HG11	4:S:91:ALA:HB1	1.95	0.48
4:X:154:ILE:HG12	4:X:174:ALA:HB2	1.94	0.48
5:d:176:LYS:HG2	5:d:186:TYR:CE1	2.49	0.48
1:j:230:LEU:HD12	1:j:245:VAL:HG22	1.94	0.48
1:o:249:VAL:HG12	1:o:257:TYR:CD2	2.49	0.48
4:r:28:ARG:HA	4:r:70:LEU:HD11	1.96	0.48
1:A:235:PRO:HA	1:A:241:PHE:HD1	1.79	0.47
3:l:5:VAL:HG12	3:l:7:VAL:HG13	1.96	0.47
5:n:158:TRP:NE1	5:n:209:GLN:OE1	2.46	0.47
4:w:160:LEU:HD21	5:x:191:ARG:HB3	1.95	0.47
5:T:158:TRP:NE1	5:T:209:GLN:OE1	2.47	0.47
1:U:109:PHE:HD1	1:U:165:VAL:HG11	1.78	0.47
1:U:253:GLN:HB3	1:U:256:ARG:HD3	1.94	0.47
4:m:124:ASP:HB3	4:m:127:SER:O	2.14	0.47
4:D:13:VAL:HG13	4:D:108:ILE:HG12	1.97	0.47
5:J:171:ASP:OD2	5:J:189:SER:OG	2.29	0.47
4:S:28:ARG:HA	4:S:70:LEU:HD11	1.97	0.47
1:U:171:TYR:OH	3:W:1:VAL:HG11	2.13	0.47
1:U:206:LEU:HD13	1:U:242:GLN:HG2	1.95	0.47
1:Z:229:GLU:HB3	1:Z:246:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:176:LYS:HG2	5:E:186:TYR:CE1	2.49	0.47
5:J:121:PRO:HB3	5:J:148:PHE:HB3	1.97	0.47
4:r:132:VAL:HG12	4:r:175:TRP:HB3	1.95	0.47
4:w:48:MET:HE1	4:w:58:GLU:HB2	1.95	0.47
5:J:125:VAL:HG23	5:J:235:ALA:HB3	1.96	0.47
1:Z:255:GLN:O	1:Z:273:ARG:NH1	2.47	0.47
4:D:154:ILE:HG12	4:D:174:ALA:HB2	1.95	0.47
5:J:180:ALA:HB2	4:N:188:ASN:HB3	1.97	0.47
5:O:13:ALA:HB3	5:O:111:VAL:HG22	1.96	0.47
5:O:14:VAL:HG22	5:O:115:LEU:HD21	1.95	0.47
1:P:234:ARG:HD2	2:Q:10:TYR:CE1	2.50	0.47
1:U:22:PHE:HE2	1:U:67:VAL:HG22	1.80	0.47
1:j:59:TYR:O	1:j:63:GLU:HG2	2.14	0.47
4:w:159:VAL:N	5:x:169:CYS:SG	2.88	0.47
1:A:9:TYR:OH	3:C:2:VAL:HG13	2.15	0.47
1:A:224:GLN:O	1:A:228:THR:OG1	2.27	0.47
4:I:8:PRO:HB3	4:N:11:LEU:HD21	1.97	0.47
1:K:196:ASP:OD1	1:K:196:ASP:N	2.44	0.47
1:P:189:MET:HE3	1:P:272:LEU:HB3	1.97	0.47
5:T:126:PHE:HE2	5:T:144:LEU:HD12	1.80	0.47
4:c:8:PRO:HG3	4:c:11:LEU:HD12	1.96	0.47
1:P:244:TRP:HZ3	1:P:246:ALA:HB2	1.80	0.47
4:X:48:MET:HG3	4:X:63:VAL:HG21	1.95	0.47
1:o:189:MET:HE3	1:o:272:LEU:HB3	1.97	0.47
4:I:135:PHE:HB2	4:I:187:PHE:CE2	2.50	0.47
5:s:33:TYR:HB2	5:s:92:ALA:HB3	1.96	0.47
3:C:5:VAL:HG12	3:C:7:VAL:HG23	1.97	0.47
1:F:202:ARG:HG2	1:F:246:ALA:HB2	1.96	0.47
4:N:28:ARG:HA	4:N:70:LEU:HD11	1.96	0.47
4:w:112:ILE:HG13	4:w:139:ASP:HA	1.97	0.47
5:x:115:LEU:HD22	5:x:215:LEU:HD21	1.97	0.47
5:O:189:SER:OG	5:O:191:ARG:NH1	2.47	0.46
1:P:235:PRO:HA	1:P:241:PHE:HD1	1.80	0.46
1:Z:109:PHE:HD1	1:Z:165:VAL:HG11	1.79	0.46
5:d:6:GLN:HG3	5:d:105:PRO:HD2	1.97	0.46
1:j:73:THR:HG23	5:n:30:ASN:ND2	2.31	0.46
5:O:126:PHE:HE2	5:O:144:LEU:HD12	1.79	0.46
4:S:132:VAL:HG12	4:S:175:TRP:HB3	1.97	0.46
5:T:121:PRO:HB3	5:T:148:PHE:HB3	1.97	0.46
5:Y:176:LYS:HG2	5:Y:186:TYR:CE1	2.50	0.46
5:d:125:VAL:HG23	5:d:235:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:189:MET:HE3	1:j:272:LEU:HB3	1.97	0.46
4:m:36:TYR:CE1	4:m:46:MET:HG3	2.50	0.46
1:K:244:TRP:HZ3	1:K:246:ALA:HB2	1.79	0.46
4:X:109:LYS:HD3	4:X:140:SER:HB3	1.97	0.46
5:Y:125:VAL:HG23	5:Y:235:ALA:HB3	1.97	0.46
5:i:176:LYS:HG2	5:i:186:TYR:CE1	2.50	0.46
4:m:160:LEU:HD13	5:n:193:ARG:HG3	1.96	0.46
1:o:163:ARG:HG2	3:q:1:VAL:HG21	1.97	0.46
4:D:28:ARG:HA	4:D:70:LEU:HD11	1.97	0.46
2:G:24:ASN:HB3	2:G:65:LEU:HD11	1.97	0.46
4:I:132:VAL:HG12	4:I:175:TRP:HB3	1.96	0.46
1:U:202:ARG:HG2	1:U:246:ALA:HB2	1.98	0.46
5:n:128:PRO:HG2	5:n:139:ALA:HB1	1.97	0.46
5:O:121:PRO:HB3	5:O:148:PHE:HB3	1.98	0.46
1:U:77:ASP:CG	3:W:9:LYS:HG3	2.40	0.46
4:r:109:LYS:HD3	4:r:140:SER:HB3	1.98	0.46
4:S:21:LEU:HD11	4:S:87:TYR:HD2	1.79	0.46
4:c:46:MET:HE3	5:d:100:GLU:HG3	1.98	0.46
4:m:48:MET:HG3	4:m:63:VAL:HG21	1.97	0.46
4:r:124:ASP:HB3	4:r:127:SER:O	2.15	0.46
1:t:193:PRO:HA	1:t:199:ALA:HA	1.97	0.46
4:I:28:ARG:HA	4:I:70:LEU:HD11	1.96	0.46
4:S:135:PHE:HB2	4:S:187:PHE:CE2	2.51	0.46
4:m:132:VAL:HG12	4:m:175:TRP:HB3	1.98	0.46
1:F:189:MET:HE3	1:F:272:LEU:HB3	1.98	0.46
1:K:154:GLU:HG2	1:K:157:ARG:HH22	1.81	0.46
1:P:202:ARG:HG2	1:P:246:ALA:HB2	1.98	0.46
4:h:15:GLU:HG3	4:h:110:PRO:HA	1.98	0.46
4:m:112:ILE:HG13	4:m:139:ASP:HA	1.97	0.46
1:t:231:VAL:O	1:t:243:LYS:NZ	2.43	0.46
1:A:22:PHE:HE2	1:A:67:VAL:HG22	1.81	0.46
1:A:206:LEU:HD13	1:A:242:GLN:HG2	1.97	0.46
1:F:171:TYR:OH	3:H:1:VAL:HG11	2.16	0.46
1:K:189:MET:HE3	1:K:272:LEU:HB3	1.98	0.46
1:K:231:VAL:O	1:K:243:LYS:NZ	2.41	0.46
5:O:49:SER:HB3	5:O:68:ARG:HH11	1.81	0.46
5:T:33:TYR:HB2	5:T:92:ALA:HB3	1.98	0.46
5:T:176:LYS:HG2	5:T:186:TYR:CE1	2.51	0.46
1:U:196:ASP:OD1	1:U:196:ASP:N	2.46	0.46
4:X:124:ASP:HB3	4:X:127:SER:O	2.16	0.46
4:h:135:PHE:HB2	4:h:187:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:n:171:ASP:OD2	5:n:189:SER:OG	2.24	0.46
1:o:234:ARG:HD2	2:p:10:TYR:CE1	2.51	0.46
1:K:206:LEU:HD13	1:K:242:GLN:HG2	1.98	0.45
5:T:132:GLU:OE2	5:T:140:THR:OG1	2.27	0.45
1:t:196:ASP:OD1	1:t:196:ASP:N	2.49	0.45
4:D:34:TRP:CD1	4:D:46:MET:HE2	2.51	0.45
2:G:37:VAL:HG22	2:G:82:VAL:HG22	1.98	0.45
5:J:213:TYR:HA	5:J:230:THR:HG23	1.99	0.45
5:T:127:GLU:OE1	5:T:240:ARG:NH2	2.49	0.45
1:Z:22:PHE:HE2	1:Z:67:VAL:HG22	1.80	0.45
4:c:79:SER:HB3	4:c:108:ILE:HD13	1.98	0.45
5:d:128:PRO:HG2	5:d:139:ALA:HB1	1.98	0.45
5:i:125:VAL:HG23	5:i:235:ALA:HB3	1.97	0.45
4:r:8:PRO:HG3	4:r:11:LEU:HD12	1.99	0.45
4:w:135:PHE:HB2	4:w:187:PHE:CE2	2.51	0.45
4:c:112:ILE:HG13	4:c:139:ASP:HA	1.97	0.45
4:D:48:MET:HE1	4:D:58:GLU:HB2	1.98	0.45
2:a:37:VAL:HG22	2:a:82:VAL:HG22	1.98	0.45
4:h:28:ARG:HA	4:h:70:LEU:HD11	1.99	0.45
4:m:95:ASN:ND2	4:m:97:GLN:OE1	2.49	0.45
5:J:176:LYS:HG2	5:J:186:TYR:CE1	2.50	0.45
5:Y:57:LYS:HB3	5:Y:61:PRO:HG3	1.99	0.45
5:Y:108:ARG:HE	5:Y:152:HIS:HB3	1.81	0.45
5:d:115:LEU:HD22	5:d:215:LEU:HD21	1.99	0.45
1:e:171:TYR:OH	3:g:1:VAL:HG21	2.16	0.45
1:A:249:VAL:HG12	1:A:257:TYR:CD2	2.51	0.45
1:F:22:PHE:HE2	1:F:67:VAL:HG22	1.82	0.45
2:L:5:PRO:HB3	2:L:30:PHE:HB3	1.98	0.45
2:L:28:SER:HA	2:L:63:TYR:HA	1.99	0.45
5:d:189:SER:OG	5:d:191:ARG:NH1	2.48	0.45
4:m:48:MET:HE1	4:m:58:GLU:HB2	1.98	0.45
5:n:215:LEU:HD12	5:n:219:ASP:HB3	1.99	0.45
1:t:202:ARG:HG2	1:t:246:ALA:HB2	1.97	0.45
4:D:8:PRO:HG3	4:D:11:LEU:HD12	1.99	0.45
5:O:115:LEU:HD22	5:O:215:LEU:HD21	1.99	0.45
1:P:236:ALA:HB1	2:Q:12:ARG:HG3	1.98	0.45
1:U:59:TYR:O	1:U:63:GLU:HG2	2.16	0.45
5:n:47:HIS:CD2	5:n:57:LYS:HA	2.52	0.45
1:t:244:TRP:HZ3	1:t:246:ALA:HB2	1.81	0.45
2:u:5:PRO:HB3	2:u:30:PHE:HB3	1.99	0.45
1:P:22:PHE:HE2	1:P:67:VAL:HG22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:5:PRO:HB3	2:V:30:PHE:HB3	1.99	0.45
1:Z:249:VAL:HG12	1:Z:257:TYR:CD2	2.51	0.45
1:t:22:PHE:HE2	1:t:67:VAL:HG22	1.81	0.45
4:w:12:ILE:HA	4:w:107:ILE:O	2.17	0.45
5:E:125:VAL:HG23	5:E:235:ALA:HB3	1.98	0.45
4:N:79:SER:HB3	4:N:108:ILE:HD13	1.99	0.45
1:P:231:VAL:O	1:P:243:LYS:NZ	2.38	0.45
1:e:193:PRO:HA	1:e:199:ALA:HA	1.98	0.45
1:K:117:ALA:HB2	2:L:60:TRP:CE2	2.53	0.44
4:c:48:MET:HE1	4:c:58:GLU:HB2	1.98	0.44
4:r:46:MET:HE2	4:r:46:MET:HB3	1.90	0.44
4:w:124:ASP:HB3	4:w:127:SER:O	2.17	0.44
4:I:188:ASN:HB3	5:O:180:ALA:HB2	2.00	0.44
1:K:215:LEU:HB2	1:K:245:VAL:HG21	1.97	0.44
1:j:37:ASP:HB3	1:j:40:ALA:HB2	1.98	0.44
1:j:117:ALA:HB2	2:k:60:TRP:CE2	2.53	0.44
1:o:202:ARG:HG2	1:o:246:ALA:HB2	1.98	0.44
1:t:73:THR:HG21	3:v:6:GLY:HA3	1.99	0.44
5:x:126:PHE:HE2	5:x:144:LEU:HD12	1.83	0.44
4:I:48:MET:HE1	4:I:58:GLU:HB2	1.99	0.44
4:c:160:LEU:HD13	5:d:193:ARG:HG3	2.00	0.44
1:j:234:ARG:HD2	2:k:10:TYR:CE1	2.52	0.44
5:n:125:VAL:HG23	5:n:235:ALA:HB3	1.98	0.44
2:u:29:GLY:HA2	2:u:61:SER:HB2	2.00	0.44
5:E:213:TYR:HA	5:E:230:THR:HG23	2.00	0.44
1:K:193:PRO:HA	1:K:199:ALA:HA	1.99	0.44
4:N:8:PRO:HG3	4:N:11:LEU:HD12	2.00	0.44
4:S:46:MET:HE2	4:S:48:MET:HA	1.98	0.44
4:X:3:LYS:HD2	4:X:99:ILE:HG12	1.98	0.44
1:Z:9:TYR:HB2	1:Z:97:ILE:HB	1.99	0.44
1:Z:193:PRO:HA	1:Z:199:ALA:HA	1.99	0.44
4:h:132:VAL:HG12	4:h:175:TRP:HB3	2.00	0.44
1:A:28:VAL:HG11	1:A:179:LEU:HD13	2.00	0.44
4:D:132:VAL:HG12	4:D:175:TRP:HB3	2.00	0.44
5:E:92:ALA:HB2	5:E:103:PHE:CE1	2.53	0.44
1:F:249:VAL:HG12	1:F:257:TYR:CD2	2.52	0.44
4:I:11:LEU:HD21	4:N:8:PRO:HB3	1.98	0.44
5:J:145:ALA:HB2	5:J:210:VAL:HG21	2.00	0.44
2:V:37:VAL:HG22	2:V:82:VAL:HG22	1.98	0.44
2:a:5:PRO:HB3	2:a:30:PHE:HB3	2.00	0.44
1:e:196:ASP:OD1	1:e:196:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:151:ASP:HB3	5:J:186:TYR:CE2	2.52	0.44
1:Z:206:LEU:HD13	1:Z:242:GLN:HG2	1.99	0.44
1:e:22:PHE:HE2	1:e:67:VAL:HG22	1.82	0.44
1:F:196:ASP:OD1	1:F:196:ASP:N	2.44	0.44
1:P:122:ASP:OD1	2:Q:60:TRP:NE1	2.39	0.44
4:c:135:PHE:HB2	4:c:187:PHE:CE2	2.52	0.44
1:e:109:PHE:HD1	1:e:165:VAL:HG11	1.81	0.44
4:h:124:ASP:HB3	4:h:127:SER:O	2.18	0.44
4:m:154:ILE:HG12	4:m:174:ALA:HB2	1.99	0.44
2:u:37:VAL:HB	2:u:66:TYR:CE2	2.52	0.44
5:J:126:PHE:HE2	5:J:144:LEU:HD12	1.83	0.44
1:P:206:LEU:HD13	1:P:242:GLN:HG2	2.00	0.44
1:U:234:ARG:HD2	2:V:10:TYR:CE1	2.53	0.44
5:Y:128:PRO:HG2	5:Y:139:ALA:HB1	1.99	0.44
3:g:5:VAL:HG12	3:g:7:VAL:HG13	2.00	0.44
4:h:43:SER:OG	4:h:45:LYS:NZ	2.40	0.44
1:t:9:TYR:HB2	1:t:97:ILE:HB	2.00	0.44
1:A:154:GLU:HG2	1:A:157:ARG:HH22	1.82	0.44
1:K:235:PRO:HA	1:K:241:PHE:HD1	1.82	0.44
4:X:132:VAL:HG12	4:X:175:TRP:HB3	2.00	0.44
5:Y:92:ALA:HB2	5:Y:103:PHE:CE1	2.53	0.44
4:c:132:VAL:HG12	4:c:175:TRP:HB3	2.00	0.44
1:A:9:TYR:HB2	1:A:97:ILE:HB	1.99	0.43
1:K:22:PHE:HE2	1:K:67:VAL:HG22	1.82	0.43
1:o:22:PHE:HE2	1:o:67:VAL:HG22	1.83	0.43
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.54	0.43
1:F:234:ARG:HD2	2:G:10:TYR:CE1	2.53	0.43
5:O:112:LEU:HD11	5:O:150:PRO:HG3	2.00	0.43
5:T:125:VAL:HG23	5:T:235:ALA:HB3	1.99	0.43
4:X:8:PRO:HB3	4:c:11:LEU:HD21	2.00	0.43
1:e:159:TYR:OH	3:g:1:VAL:O	2.27	0.43
1:t:234:ARG:HD2	2:u:10:TYR:CE1	2.52	0.43
1:A:202:ARG:HG2	1:A:246:ALA:HB2	2.00	0.43
1:F:109:PHE:HD1	1:F:165:VAL:HG11	1.83	0.43
5:J:151:ASP:HB3	5:J:186:TYR:HE2	1.83	0.43
4:X:135:PHE:HB2	4:X:187:PHE:CE2	2.52	0.43
1:Z:117:ALA:HB2	2:a:60:TRP:CE2	2.54	0.43
1:j:196:ASP:OD1	1:j:196:ASP:N	2.48	0.43
1:o:217:TRP:HE1	1:o:245:VAL:HG12	1.82	0.43
5:s:92:ALA:HB2	5:s:103:PHE:CE1	2.54	0.43
5:x:151:ASP:HB3	5:x:186:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:112:LEU:HD11	5:J:150:PRO:HG3	1.99	0.43
1:K:249:VAL:HG12	1:K:257:TYR:CD2	2.53	0.43
1:P:202:ARG:HH22	2:Q:99:MET:HE2	1.83	0.43
5:T:213:TYR:HA	5:T:230:THR:HG23	2.00	0.43
1:U:249:VAL:HG12	1:U:257:TYR:CD2	2.53	0.43
5:d:13:ALA:HB3	5:d:111:VAL:HG22	2.00	0.43
5:d:132:GLU:OE2	5:d:140:THR:OG1	2.28	0.43
5:i:132:GLU:OE2	5:i:140:THR:OG1	2.31	0.43
4:m:12:ILE:HA	4:m:107:ILE:O	2.18	0.43
5:s:88:VAL:HG22	5:s:108:ARG:HG2	2.00	0.43
5:x:128:PRO:HG2	5:x:139:ALA:HB1	2.01	0.43
1:F:235:PRO:HA	1:F:241:PHE:HD1	1.82	0.43
1:K:147:TRP:NE1	3:M:8:GLY:O	2.43	0.43
4:N:36:TYR:CE1	4:N:46:MET:HG3	2.54	0.43
1:Z:33:PHE:CD2	1:Z:34:VAL:HG13	2.53	0.43
1:e:99:TYR:CE1	3:g:4:ALA:HB2	2.53	0.43
5:n:49:SER:HB3	5:n:68:ARG:HH11	1.82	0.43
4:D:135:PHE:HB2	4:D:187:PHE:CE2	2.53	0.43
5:Y:88:VAL:HG22	5:Y:108:ARG:HG2	2.00	0.43
1:t:147:TRP:CD1	3:v:7:VAL:HG23	2.53	0.43
4:w:15:GLU:HG3	4:w:110:PRO:HA	2.00	0.43
1:Z:81:LEU:HD12	1:Z:95:ILE:HD11	1.99	0.43
1:Z:235:PRO:O	2:a:10:TYR:OH	2.29	0.43
4:c:21:LEU:HD11	4:c:87:TYR:HD2	1.83	0.43
4:m:135:PHE:HB2	4:m:187:PHE:CE2	2.53	0.43
5:n:108:ARG:HE	5:n:152:HIS:HB3	1.84	0.43
1:A:234:ARG:HD2	2:B:10:TYR:CE1	2.53	0.43
1:P:196:ASP:OD1	1:P:196:ASP:N	2.46	0.43
5:T:92:ALA:HB2	5:T:103:PHE:CE1	2.54	0.43
4:X:160:LEU:HD13	5:Y:193:ARG:HG3	2.01	0.43
1:e:249:VAL:HG12	1:e:257:TYR:CD2	2.54	0.43
4:m:122:LEU:HB3	5:n:126:PHE:HB3	2.00	0.43
1:t:147:TRP:NE1	3:v:7:VAL:HG23	2.34	0.43
1:K:77:ASP:HB3	3:M:9:LYS:HD2	2.01	0.43
1:U:193:PRO:HA	1:U:199:ALA:HA	2.01	0.43
4:r:48:MET:HE1	4:r:58:GLU:HB2	2.01	0.43
5:s:49:SER:HB3	5:s:68:ARG:HH11	1.84	0.43
1:A:35:ARG:HH21	1:A:46:GLU:CD	2.27	0.42
1:F:207:GLY:HA2	1:F:240:THR:HB	2.00	0.42
1:Z:135:ALA:HB1	1:Z:140:ALA:HB3	2.00	0.42
4:w:37:ARG:HG3	4:w:87:TYR:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:171:ASP:OD2	5:O:189:SER:OG	2.28	0.42
1:e:234:ARG:HD2	2:f:10:TYR:CE1	2.54	0.42
4:h:8:PRO:HB3	4:m:11:LEU:HD21	2.01	0.42
5:i:92:ALA:HB2	5:i:103:PHE:CE1	2.53	0.42
1:o:109:PHE:HD1	1:o:165:VAL:HG11	1.84	0.42
1:e:255:GLN:O	1:e:273:ARG:NH1	2.53	0.42
1:j:202:ARG:HG2	1:j:246:ALA:HB2	2.02	0.42
5:E:128:PRO:HG2	5:E:139:ALA:HB1	2.01	0.42
1:e:135:ALA:HB1	1:e:140:ALA:HB3	2.01	0.42
1:j:23:ILE:HG21	2:k:54:LEU:HB3	2.01	0.42
5:n:221:TRP:CZ2	5:n:223:GLN:HB2	2.55	0.42
5:E:189:SER:OG	5:E:191:ARG:NH1	2.46	0.42
1:F:35:ARG:HH21	1:F:46:GLU:CD	2.28	0.42
4:N:12:ILE:HA	4:N:107:ILE:O	2.20	0.42
1:P:28:VAL:HG23	1:P:33:PHE:CE1	2.54	0.42
5:T:120:PRO:HD3	5:T:228:PRO:HB3	2.01	0.42
5:i:33:TYR:HB2	5:i:92:ALA:HB3	2.01	0.42
1:j:22:PHE:HE2	1:j:67:VAL:HG22	1.84	0.42
5:n:205:HIS:CE1	5:n:207:ARG:HB2	2.54	0.42
4:D:167:PHE:CE2	4:D:169:SER:HB3	2.55	0.42
5:O:33:TYR:HB2	5:O:92:ALA:HB3	2.02	0.42
5:O:205:HIS:HD2	5:O:238:TRP:CE2	2.37	0.42
1:P:65:ARG:HD2	5:T:48:TYR:OH	2.19	0.42
4:S:46:MET:HE3	4:S:49:SER:HB3	2.02	0.42
1:U:224:GLN:O	1:U:228:THR:OG1	2.21	0.42
4:h:154:ILE:HG12	4:h:174:ALA:HB2	2.00	0.42
1:j:249:VAL:HG12	1:j:257:TYR:CD2	2.54	0.42
5:s:152:HIS:CD2	5:s:213:TYR:HB2	2.54	0.42
1:t:253:GLN:HB3	1:t:256:ARG:HD3	2.01	0.42
1:A:127:ASN:OD1	1:A:134:THR:OG1	2.36	0.42
5:J:64:TYR:OH	5:J:89:TYR:OH	2.33	0.42
1:t:249:VAL:HG12	1:t:257:TYR:CD2	2.54	0.42
1:A:59:TYR:O	1:A:63:GLU:HG2	2.19	0.42
1:A:159:TYR:CE1	3:C:3:GLY:HA3	2.55	0.42
1:P:159:TYR:CE1	3:R:3:GLY:HA3	2.54	0.42
2:p:37:VAL:HG22	2:p:82:VAL:HG22	2.01	0.42
4:r:21:LEU:HD11	4:r:87:TYR:HD2	1.85	0.42
4:N:50:ILE:HG23	4:N:65:LEU:HD22	2.02	0.42
5:O:127:GLU:OE1	5:O:240:ARG:NH2	2.53	0.42
1:P:230:LEU:HD11	1:P:243:LYS:HE3	2.01	0.42
2:Q:5:PRO:HB3	2:Q:30:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:230:LEU:HD11	1:Z:243:LYS:HE3	2.01	0.42
1:j:224:GLN:O	1:j:228:THR:OG1	2.28	0.42
1:t:109:PHE:HD1	1:t:165:VAL:HG11	1.85	0.42
5:E:151:ASP:HB3	5:E:186:TYR:CE2	2.55	0.42
5:J:115:LEU:HD22	5:J:215:LEU:HD21	2.01	0.42
1:K:59:TYR:O	1:K:63:GLU:HG2	2.20	0.42
1:K:59:TYR:OH	1:K:171:TYR:OH	2.24	0.42
1:U:35:ARG:HH21	1:U:46:GLU:CD	2.28	0.42
1:j:122:ASP:OD1	2:k:60:TRP:NE1	2.38	0.42
4:r:18:MET:HE2	4:r:77:ARG:HG2	2.01	0.42
1:t:217:TRP:HE1	1:t:245:VAL:HG12	1.85	0.42
5:O:151:ASP:HB3	5:O:186:TYR:CE2	2.55	0.41
1:P:215:LEU:HB2	1:P:245:VAL:HG21	2.02	0.41
5:T:116:LYS:HE2	5:T:223:GLN:NE2	2.35	0.41
4:r:46:MET:HB2	5:s:100:GLU:HG3	2.02	0.41
1:F:81:LEU:HD12	1:F:95:ILE:HD11	2.02	0.41
1:F:159:TYR:OH	3:H:1:VAL:O	2.29	0.41
2:G:28:SER:HA	2:G:63:TYR:HA	2.02	0.41
1:K:234:ARG:HD2	2:L:10:TYR:CE1	2.55	0.41
5:d:92:ALA:HB2	5:d:103:PHE:CE1	2.54	0.41
5:s:151:ASP:HB3	5:s:186:TYR:CE2	2.55	0.41
1:U:117:ALA:HB2	2:V:60:TRP:CE2	2.55	0.41
5:Y:3:ALA:N	5:Y:26:THR:HG1	2.18	0.41
1:Z:234:ARG:HD2	2:a:10:TYR:CE1	2.55	0.41
2:k:5:PRO:HB3	2:k:30:PHE:HB3	2.02	0.41
4:w:132:VAL:HG12	4:w:175:TRP:HB3	2.03	0.41
4:c:160:LEU:HD11	5:d:191:ARG:HB3	2.03	0.41
1:e:9:TYR:OH	3:g:2:VAL:HG13	2.20	0.41
1:j:206:LEU:HD13	1:j:242:GLN:HG2	2.02	0.41
5:E:14:VAL:HG22	5:E:115:LEU:HD21	2.02	0.41
1:F:193:PRO:HA	1:F:199:ALA:HA	2.03	0.41
5:J:92:ALA:HB2	5:J:103:PHE:CE1	2.56	0.41
5:O:88:VAL:HG22	5:O:108:ARG:HG2	2.03	0.41
1:P:35:ARG:NE	1:P:48:ARG:HH21	2.19	0.41
4:X:165:MET:SD	5:Y:195:SER:HB3	2.60	0.41
5:Y:151:ASP:HB3	5:Y:186:TYR:CE2	2.55	0.41
5:d:14:VAL:HG22	5:d:115:LEU:HD21	2.02	0.41
1:e:81:LEU:HD12	1:e:95:ILE:HD11	2.01	0.41
5:n:38:ASP:OD2	5:n:44:ARG:NH2	2.53	0.41
5:n:151:ASP:HB3	5:n:186:TYR:CE2	2.55	0.41
1:t:35:ARG:NE	1:t:48:ARG:HH21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t:117:ALA:HB2	2:u:60:TRP:CE2	2.56	0.41
1:A:215:LEU:HB2	1:A:245:VAL:HG21	2.02	0.41
4:S:18:MET:HE2	4:S:77:ARG:HG2	2.02	0.41
4:X:93:ASP:HB3	4:X:95:ASN:H	1.84	0.41
5:i:14:VAL:HG22	5:i:115:LEU:HD21	2.01	0.41
5:i:189:SER:OG	5:i:191:ARG:NH1	2.50	0.41
4:S:46:MET:SD	5:T:100:GLU:HB3	2.60	0.41
4:c:154:ILE:HG12	4:c:174:ALA:HB2	2.02	0.41
5:n:86:THR:HG23	5:n:110:THR:HA	2.02	0.41
4:w:8:PRO:HG3	4:w:11:LEU:HD12	2.03	0.41
1:F:106:ASP:OD1	1:F:106:ASP:N	2.52	0.41
2:G:96:ASP:HB3	2:G:99:MET:HB3	2.03	0.41
4:I:79:SER:HB3	4:I:108:ILE:HD13	2.02	0.41
1:Z:185:PRO:HB3	1:Z:208:PHE:HB3	2.03	0.41
1:j:109:PHE:HD1	1:j:165:VAL:HG11	1.86	0.41
5:n:33:TYR:HB2	5:n:92:ALA:HB3	2.02	0.41
1:A:196:ASP:OD1	1:A:196:ASP:N	2.48	0.41
4:D:8:PRO:HB3	4:r:11:LEU:HD21	2.03	0.41
2:Q:24:ASN:HB3	2:Q:65:LEU:HD11	2.02	0.41
4:S:79:SER:HB3	4:S:108:ILE:HD13	2.03	0.41
1:U:106:ASP:OD1	1:U:106:ASP:N	2.53	0.41
1:U:159:TYR:OH	3:W:1:VAL:O	2.35	0.41
1:Z:235:PRO:HG2	2:a:65:LEU:HD22	2.02	0.41
5:d:151:ASP:HB3	5:d:186:TYR:CE2	2.55	0.41
4:h:46:MET:HE3	4:h:48:MET:HA	2.02	0.41
4:h:160:LEU:HD13	5:i:193:ARG:HG3	2.03	0.41
1:j:249:VAL:HG21	1:j:254:GLU:HG3	2.02	0.41
4:r:124:ASP:HA	5:s:126:PHE:CD1	2.56	0.41
5:x:47:HIS:CD2	5:x:57:LYS:HA	2.55	0.41
1:A:191:HIS:CD2	1:A:193:PRO:HD3	2.55	0.41
4:D:11:LEU:HD21	4:r:8:PRO:HB3	2.03	0.41
2:L:96:ASP:HB3	2:L:99:MET:HB3	2.03	0.41
1:o:33:PHE:CD2	1:o:34:VAL:HG13	2.55	0.41
5:x:152:HIS:CD2	5:x:213:TYR:HB2	2.56	0.41
4:D:38:GLN:HB2	4:D:44:PRO:HB3	2.03	0.40
5:Y:157:TRP:HD1	5:Y:168:VAL:HG13	1.85	0.40
1:e:33:PHE:CD2	1:e:34:VAL:HG13	2.56	0.40
1:t:147:TRP:HE1	3:v:9:LYS:H	1.69	0.40
1:t:189:MET:HE3	1:t:272:LEU:HB3	2.02	0.40
1:A:217:TRP:HE1	1:A:245:VAL:HG12	1.87	0.40
1:P:35:ARG:HH21	1:P:46:GLU:CD	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:96:ASP:HB3	2:V:99:MET:HB3	2.03	0.40
5:Y:156:SER:OG	5:Y:158:TRP:NE1	2.51	0.40
1:Z:207:GLY:HA2	1:Z:240:THR:HB	2.03	0.40
5:i:128:PRO:HG2	5:i:139:ALA:HB1	2.02	0.40
1:o:9:TYR:CE2	1:o:70:GLN:HG2	2.57	0.40
1:o:69:ALA:HB2	5:s:50:TYR:CD2	2.57	0.40
1:t:28:VAL:HG23	1:t:33:PHE:CE1	2.56	0.40
1:t:77:ASP:HB3	3:v:9:LYS:HD2	2.03	0.40
5:E:151:ASP:HB3	5:E:186:TYR:HE2	1.86	0.40
4:I:12:ILE:HA	4:I:107:ILE:O	2.22	0.40
5:T:115:LEU:HD22	5:T:215:LEU:HD21	2.03	0.40
1:U:99:TYR:CE1	3:W:4:ALA:HB2	2.56	0.40
1:e:117:ALA:HB2	2:f:60:TRP:CE2	2.57	0.40
1:t:13:SER:HB3	1:t:78:LEU:HG	2.03	0.40
5:x:88:VAL:HG22	5:x:108:ARG:HG2	2.03	0.40
1:A:109:PHE:HD1	1:A:165:VAL:HG11	1.86	0.40
4:D:34:TRP:HH2	4:D:92:ARG:HD3	1.87	0.40
4:I:47:LEU:HD23	4:I:47:LEU:HA	1.94	0.40
1:K:106:ASP:OD1	1:K:106:ASP:N	2.52	0.40
4:N:36:TYR:CE2	4:N:100:TRP:HH2	2.40	0.40
1:e:206:LEU:HD13	1:e:242:GLN:HG2	2.03	0.40
1:e:217:TRP:HE1	1:e:245:VAL:HG12	1.87	0.40
5:i:180:ALA:HA	4:m:188:ASN:HB3	2.03	0.40
4:w:28:ARG:HA	4:w:70:LEU:HD11	2.03	0.40
1:A:202:ARG:NH1	2:B:98:ASP:O	2.51	0.40
4:D:148:LYS:HA	4:r:148:LYS:HA	2.04	0.40
5:O:92:ALA:HB2	5:O:103:PHE:CE1	2.57	0.40
1:P:231:VAL:HB	2:Q:8:GLN:HE22	1.87	0.40
5:Y:29:HIS:HB3	5:Y:94:GLY:O	2.21	0.40
4:h:12:ILE:HA	4:h:107:ILE:O	2.21	0.40
4:h:116:ASP:OD2	5:i:135:HIS:NE2	2.55	0.40
5:i:57:LYS:HB3	5:i:61:PRO:HG3	2.02	0.40
4:m:36:TYR:CE2	4:m:100:TRP:HH2	2.40	0.40
4:r:119:VAL:HA	4:r:134:LEU:O	2.22	0.40
5:s:120:PRO:HD3	5:s:228:PRO:HB3	2.03	0.40

There are no symmetry-related clashes.

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	272/274 (99%)	270 (99%)	2 (1%)	0	100	100
1	F	272/274 (99%)	271 (100%)	1 (0%)	0	100	100
1	K	272/274 (99%)	271 (100%)	1 (0%)	0	100	100
1	P	272/274 (99%)	270 (99%)	2 (1%)	0	100	100
1	U	272/274 (99%)	269 (99%)	3 (1%)	0	100	100
1	Z	272/274 (99%)	271 (100%)	1 (0%)	0	100	100
1	e	272/274 (99%)	269 (99%)	3 (1%)	0	100	100
1	j	272/274 (99%)	269 (99%)	3 (1%)	0	100	100
1	o	272/274 (99%)	269 (99%)	3 (1%)	0	100	100
1	t	272/274 (99%)	269 (99%)	3 (1%)	0	100	100
2	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	G	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
2	L	97/99 (98%)	97 (100%)	0	0	100	100
2	Q	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	V	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	a	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	f	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	k	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
2	p	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	u	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	7 (100%)	0	0	100	100
3	M	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	R	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	W	7/9 (78%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	b	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	g	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	l	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	q	7/9 (78%)	7 (100%)	0	0	100	100
3	v	7/9 (78%)	7 (100%)	0	0	100	100
4	D	196/199 (98%)	193 (98%)	3 (2%)	0	100	100
4	I	196/199 (98%)	193 (98%)	3 (2%)	0	100	100
4	N	196/199 (98%)	192 (98%)	4 (2%)	0	100	100
4	S	196/199 (98%)	190 (97%)	6 (3%)	0	100	100
4	X	196/199 (98%)	194 (99%)	2 (1%)	0	100	100
4	c	196/199 (98%)	194 (99%)	2 (1%)	0	100	100
4	h	196/199 (98%)	193 (98%)	3 (2%)	0	100	100
4	m	196/199 (98%)	193 (98%)	3 (2%)	0	100	100
4	r	196/199 (98%)	192 (98%)	4 (2%)	0	100	100
4	w	196/199 (98%)	192 (98%)	4 (2%)	0	100	100
5	E	238/242 (98%)	237 (100%)	1 (0%)	0	100	100
5	J	238/242 (98%)	234 (98%)	4 (2%)	0	100	100
5	O	238/242 (98%)	236 (99%)	2 (1%)	0	100	100
5	T	238/242 (98%)	233 (98%)	5 (2%)	0	100	100
5	Y	238/242 (98%)	236 (99%)	2 (1%)	0	100	100
5	d	238/242 (98%)	236 (99%)	2 (1%)	0	100	100
5	i	238/242 (98%)	237 (100%)	1 (0%)	0	100	100
5	n	238/242 (98%)	233 (98%)	5 (2%)	0	100	100
5	s	238/242 (98%)	235 (99%)	3 (1%)	0	100	100
5	x	238/242 (98%)	233 (98%)	5 (2%)	0	100	100
All	All	8099/8230 (98%)	7985 (99%)	114 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	F	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	K	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	P	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	U	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	Z	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	e	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	j	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	o	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	t	232/232 (100%)	231 (100%)	1 (0%)	84	83
2	B	94/94 (100%)	94 (100%)	0	100	100
2	G	94/94 (100%)	94 (100%)	0	100	100
2	L	94/94 (100%)	94 (100%)	0	100	100
2	Q	94/94 (100%)	94 (100%)	0	100	100
2	V	94/94 (100%)	94 (100%)	0	100	100
2	a	94/94 (100%)	94 (100%)	0	100	100
2	f	94/94 (100%)	94 (100%)	0	100	100
2	k	94/94 (100%)	94 (100%)	0	100	100
2	p	94/94 (100%)	94 (100%)	0	100	100
2	u	93/94 (99%)	93 (100%)	0	100	100
3	C	5/5 (100%)	5 (100%)	0	100	100
3	H	5/5 (100%)	5 (100%)	0	100	100
3	M	5/5 (100%)	5 (100%)	0	100	100
3	R	5/5 (100%)	5 (100%)	0	100	100
3	W	5/5 (100%)	5 (100%)	0	100	100
3	b	5/5 (100%)	5 (100%)	0	100	100
3	g	5/5 (100%)	5 (100%)	0	100	100
3	l	5/5 (100%)	5 (100%)	0	100	100
3	q	5/5 (100%)	5 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	v	5/5 (100%)	5 (100%)	0	100	100
4	D	180/181 (99%)	180 (100%)	0	100	100
4	I	180/181 (99%)	180 (100%)	0	100	100
4	N	180/181 (99%)	180 (100%)	0	100	100
4	S	180/181 (99%)	180 (100%)	0	100	100
4	X	180/181 (99%)	180 (100%)	0	100	100
4	c	180/181 (99%)	180 (100%)	0	100	100
4	h	180/181 (99%)	180 (100%)	0	100	100
4	m	180/181 (99%)	180 (100%)	0	100	100
4	r	180/181 (99%)	180 (100%)	0	100	100
4	w	180/181 (99%)	180 (100%)	0	100	100
5	E	205/206 (100%)	205 (100%)	0	100	100
5	J	205/206 (100%)	205 (100%)	0	100	100
5	O	205/206 (100%)	205 (100%)	0	100	100
5	T	205/206 (100%)	205 (100%)	0	100	100
5	Y	205/206 (100%)	205 (100%)	0	100	100
5	d	205/206 (100%)	205 (100%)	0	100	100
5	i	205/206 (100%)	205 (100%)	0	100	100
5	n	205/206 (100%)	205 (100%)	0	100	100
5	s	205/206 (100%)	205 (100%)	0	100	100
5	x	205/206 (100%)	205 (100%)	0	100	100
All	All	7159/7180 (100%)	7149 (100%)	10 (0%)	88	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	259	CYS
1	F	259	CYS
1	K	259	CYS
1	P	259	CYS
1	U	259	CYS
1	Z	259	CYS
1	e	259	CYS
1	j	259	CYS
1	o	259	CYS

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Mol	Chain	Res	Type
1	t	259	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	17	ASN
4	D	146	GLN
5	E	47	HIS
5	E	173	GLN
4	I	146	GLN
5	J	71	GLN
5	J	173	GLN
1	K	180	GLN
1	K	191	HIS
4	N	6	GLN
4	N	71	HIS
4	N	95	ASN
4	N	97	GLN
5	O	30	ASN
1	P	188	HIS
1	P	191	HIS
4	S	6	GLN
5	T	30	ASN
2	V	17	ASN
4	X	22	ASN
4	X	146	GLN
5	Y	71	GLN
5	Y	173	GLN
1	Z	188	HIS
2	a	17	ASN
4	c	95	ASN
4	c	188	ASN
5	d	30	ASN
5	d	73	ASN
5	d	173	GLN
1	e	180	GLN
2	f	17	ASN
4	h	22	ASN
4	h	146	GLN
2	k	17	ASN
4	m	71	HIS
4	m	95	ASN

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Mol	Chain	Res	Type
4	m	146	GLN
1	o	72	GLN
1	o	192	HIS
4	r	64	HIS
4	r	66	ASN
5	s	73	ASN
5	s	173	GLN
1	t	180	GLN
1	t	191	HIS
2	u	17	ASN
5	x	73	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	274/274 (100%)	-0.08	0 100 100	38, 61, 98, 129	0
1	F	274/274 (100%)	0.03	1 (0%) 88 80	46, 66, 101, 127	0
1	K	274/274 (100%)	0.10	3 (1%) 78 62	41, 68, 105, 130	0
1	P	274/274 (100%)	-0.05	1 (0%) 88 80	39, 61, 100, 136	0
1	U	274/274 (100%)	0.12	4 (1%) 72 53	42, 71, 113, 151	0
1	Z	274/274 (100%)	0.24	3 (1%) 78 62	50, 73, 108, 155	0
1	e	274/274 (100%)	0.26	3 (1%) 78 62	49, 80, 110, 128	0
1	j	274/274 (100%)	0.18	0 100 100	50, 75, 111, 142	0
1	o	274/274 (100%)	0.54	22 (8%) 18 14	48, 83, 175, 197	0
1	t	274/274 (100%)	0.60	24 (8%) 15 13	52, 91, 175, 192	0
2	B	99/99 (100%)	-0.06	0 100 100	45, 66, 97, 122	0
2	G	99/99 (100%)	0.12	2 (2%) 65 47	54, 76, 111, 126	0
2	L	99/99 (100%)	0.17	1 (1%) 79 64	50, 77, 109, 120	0
2	Q	99/99 (100%)	0.01	0 100 100	44, 65, 97, 120	0
2	V	99/99 (100%)	0.19	1 (1%) 79 64	59, 87, 116, 131	0
2	a	99/99 (100%)	0.20	0 100 100	59, 82, 111, 120	0
2	f	99/99 (100%)	0.83	9 (9%) 15 12	63, 102, 142, 148	0
2	k	99/99 (100%)	0.22	1 (1%) 79 64	62, 86, 111, 138	0
2	p	99/99 (100%)	0.47	2 (2%) 65 47	64, 96, 136, 143	0
2	u	98/99 (98%)	0.56	4 (4%) 41 27	67, 108, 133, 153	0
3	C	9/9 (100%)	0.34	0 100 100	47, 52, 58, 66	0
3	H	9/9 (100%)	0.42	0 100 100	54, 60, 64, 64	0
3	M	9/9 (100%)	0.65	0 100 100	47, 58, 66, 69	0
3	R	9/9 (100%)	0.61	1 (11%) 10 10	41, 55, 58, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	W	9/9 (100%)	0.67	0 100 100	52, 60, 65, 69	0
3	b	9/9 (100%)	0.66	0 100 100	52, 67, 70, 74	0
3	g	9/9 (100%)	0.71	0 100 100	59, 69, 80, 81	0
3	l	9/9 (100%)	0.77	0 100 100	58, 67, 73, 80	0
3	q	9/9 (100%)	0.07	0 100 100	58, 60, 62, 63	0
3	v	9/9 (100%)	1.21	1 (11%) 10 10	62, 74, 78, 95	0
4	D	198/199 (99%)	0.48	12 (6%) 27 19	42, 81, 160, 177	0
4	I	198/199 (99%)	0.52	11 (5%) 30 21	41, 78, 144, 176	0
4	N	198/199 (99%)	0.53	11 (5%) 30 21	36, 77, 143, 187	0
4	S	198/199 (99%)	0.53	9 (4%) 38 25	43, 79, 154, 174	0
4	X	198/199 (99%)	0.86	33 (16%) 4 4	46, 86, 169, 190	0
4	c	198/199 (99%)	0.73	18 (9%) 15 12	48, 92, 177, 198	0
4	h	198/199 (99%)	0.88	23 (11%) 9 9	56, 92, 176, 196	0
4	m	198/199 (99%)	0.86	32 (16%) 4 5	49, 93, 164, 196	0
4	r	198/199 (99%)	0.72	18 (9%) 15 12	44, 86, 151, 197	0
4	w	198/199 (99%)	0.70	17 (8%) 16 13	45, 85, 161, 195	0
5	E	240/242 (99%)	0.12	4 (1%) 69 51	47, 74, 117, 143	0
5	J	240/242 (99%)	0.09	2 (0%) 82 69	41, 65, 114, 136	0
5	O	240/242 (99%)	0.12	3 (1%) 75 57	41, 66, 113, 135	0
5	T	240/242 (99%)	0.11	2 (0%) 82 69	43, 73, 118, 155	0
5	Y	240/242 (99%)	0.57	11 (4%) 37 25	47, 93, 145, 182	0
5	d	240/242 (99%)	0.85	14 (5%) 29 19	56, 131, 176, 190	0
5	i	240/242 (99%)	0.94	24 (10%) 12 11	66, 136, 181, 198	0
5	n	240/242 (99%)	0.94	32 (13%) 7 7	46, 94, 151, 186	0
5	s	240/242 (99%)	0.35	5 (2%) 63 45	48, 78, 125, 151	0
5	x	240/242 (99%)	0.91	20 (8%) 17 13	54, 98, 147, 180	0
All	All	8199/8230 (99%)	0.42	384 (4%) 36 25	36, 79, 156, 198	0

All (384) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	o	257	TYR	5.0
4	D	147	SER	4.9

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Mol	Chain	Res	Type	RSRZ
4	N	147	SER	4.5
4	r	131	SER	4.5
4	m	191	ILE	4.1
4	h	197	PHE	4.1
4	X	5	GLN	4.0
5	n	161	GLY	4.0
4	X	199	PRO	4.0
4	c	131	SER	4.0
5	x	120	PRO	4.0
1	o	203	CYS	3.8
1	o	259	CYS	3.8
1	Z	16	GLY	3.8
4	X	129	ASP	3.8
4	N	130	LYS	3.8
4	h	130	LYS	3.8
4	r	189	ASN	3.7
1	o	250	PRO	3.6
1	t	16	GLY	3.6
5	i	180	ALA	3.6
1	e	138	MET	3.6
5	x	221	TRP	3.6
4	c	191	ILE	3.6
4	c	199	PRO	3.6
1	t	257	TYR	3.6
5	n	186	TYR	3.6
4	r	116	ASP	3.6
4	X	130	LYS	3.5
5	x	218	ASN	3.5
1	e	141	GLN	3.5
5	x	241	ALA	3.5
4	X	191	ILE	3.5
5	n	168	VAL	3.4
4	r	129	ASP	3.4
4	X	167	PHE	3.4
1	t	203	CYS	3.4
5	n	120	PRO	3.4
5	n	179	PRO	3.4
4	N	187	PHE	3.3
4	m	187	PHE	3.3
5	i	226	ALA	3.3
1	t	224	GLN	3.3
4	c	197	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
4	h	128	SER	3.3
1	o	224	GLN	3.3
4	h	131	SER	3.3
5	n	195	SER	3.3
4	r	130	LYS	3.3
1	t	259	CYS	3.2
4	m	152	VAL	3.2
1	t	251	SER	3.2
4	m	197	PHE	3.2
4	S	147	SER	3.2
5	T	201	ASP	3.2
2	f	24	ASN	3.2
4	I	150	SER	3.2
2	f	69	GLU	3.2
4	S	187	PHE	3.2
4	m	153	TYR	3.2
2	u	98	ASP	3.1
4	w	197	PHE	3.1
4	I	130	LYS	3.1
4	I	147	SER	3.1
5	Y	222	THR	3.1
4	X	197	PHE	3.1
4	m	199	PRO	3.1
2	p	98	ASP	3.1
4	m	148	LYS	3.1
5	n	71	GLN	3.1
4	X	138	PHE	3.1
4	w	130	LYS	3.0
4	r	128	SER	3.0
5	x	217	GLU	3.0
4	S	191	ILE	3.0
5	n	202	PRO	3.0
4	S	183	CYS	3.0
4	X	118	ALA	3.0
4	r	197	PHE	3.0
4	m	168	LYS	3.0
1	o	249	VAL	3.0
4	m	115	PRO	2.9
5	n	196	ALA	2.9
4	r	150	SER	2.9
1	o	261	VAL	2.9
4	I	128	SER	2.9

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Mol	Chain	Res	Type	RSRZ
4	w	128	SER	2.9
5	n	180	ALA	2.9
4	c	153	TYR	2.9
4	I	187	PHE	2.9
4	X	160	LEU	2.9
4	X	162	MET	2.9
4	m	150	SER	2.9
5	n	129	SER	2.9
5	n	166	SER	2.9
5	E	183	ASP	2.9
4	w	118	ALA	2.9
1	t	248	VAL	2.9
4	r	153	TYR	2.9
2	k	98	ASP	2.8
4	N	199	PRO	2.8
4	D	167	PHE	2.8
1	o	258	THR	2.8
4	X	161	ASP	2.8
1	t	272	LEU	2.8
4	X	187	PHE	2.8
4	m	184	ALA	2.8
5	i	202	PRO	2.8
1	o	248	VAL	2.8
4	h	119	VAL	2.8
4	m	160	LEU	2.8
5	x	226	ALA	2.8
4	I	199	PRO	2.8
4	D	191	ILE	2.8
4	w	138	PHE	2.7
1	t	197	HIS	2.7
4	D	184	ALA	2.7
1	K	230	LEU	2.7
2	u	1	ILE	2.7
4	X	117	PRO	2.7
4	S	197	PHE	2.7
4	N	191	ILE	2.7
4	h	187	PHE	2.7
4	r	187	PHE	2.7
4	X	148	LYS	2.7
4	X	128	SER	2.7
4	r	118	ALA	2.7
1	o	272	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
5	i	151	ASP	2.7
5	Y	160	ASN	2.7
4	c	168	LYS	2.6
5	x	239	GLY	2.6
2	f	80	CYS	2.6
5	d	233	VAL	2.6
4	X	116	ASP	2.6
1	t	255	GLN	2.6
4	c	130	LYS	2.6
5	n	160	ASN	2.6
1	o	274	TRP	2.6
4	h	191	ILE	2.6
4	S	199	PRO	2.6
4	m	193	PRO	2.6
5	n	24	ASN	2.6
4	h	118	ALA	2.6
5	n	139	ALA	2.6
5	i	115	LEU	2.6
5	d	226	ALA	2.6
5	n	158	TRP	2.6
5	x	216	SER	2.6
4	r	111	ASP	2.6
5	x	180	ALA	2.6
5	s	96	THR	2.6
2	u	90	PRO	2.5
4	w	125	SER	2.5
4	c	116	ASP	2.5
4	m	130	LYS	2.5
4	r	152	VAL	2.5
5	d	239	GLY	2.5
4	h	157	LYS	2.5
4	m	157	LYS	2.5
1	o	194	ILE	2.5
4	w	153	TYR	2.5
5	n	203	ARG	2.5
1	o	255	GLN	2.5
4	h	146	GLN	2.5
1	t	128	GLU	2.5
2	V	34	ASP	2.5
5	n	140	THR	2.5
4	r	199	PRO	2.5
5	d	202	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
5	n	174	PRO	2.5
1	U	230	LEU	2.5
1	Z	17	ARG	2.5
5	d	164	VAL	2.5
5	n	164	VAL	2.5
4	D	193	PRO	2.5
5	n	205	HIS	2.5
5	E	180	ALA	2.4
5	i	195	SER	2.4
1	P	128	GLU	2.4
1	Z	128	GLU	2.4
4	c	187	PHE	2.4
4	S	93	ASP	2.4
4	X	163	ARG	2.4
5	x	138	LYS	2.4
1	t	270	LEU	2.4
5	x	128	PRO	2.4
5	n	131	ALA	2.4
4	c	128	SER	2.4
5	i	166	SER	2.4
4	h	148	LYS	2.4
5	d	199	TRP	2.4
1	t	260	HIS	2.4
2	f	78	TYR	2.4
5	d	125	VAL	2.4
4	N	126	LYS	2.4
4	m	125	SER	2.4
4	m	134	LEU	2.4
1	t	204	TRP	2.4
5	i	199	TRP	2.4
4	m	149	ASP	2.4
5	x	207	ARG	2.4
4	m	167	PHE	2.4
1	F	128	GLU	2.4
1	o	247	VAL	2.4
1	t	269	PRO	2.4
2	u	14	PRO	2.4
5	Y	168	VAL	2.4
1	t	79	GLY	2.4
5	s	201	ASP	2.4
4	m	118	ALA	2.4
5	n	137	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
4	X	171	SER	2.4
5	d	128	PRO	2.4
1	t	94	THR	2.3
4	r	177	ASN	2.3
2	G	78	TYR	2.3
5	n	133	ILE	2.3
4	c	129	ASP	2.3
1	o	201	LEU	2.3
4	h	134	LEU	2.3
5	i	137	GLN	2.3
1	o	269	PRO	2.3
4	h	182	ALA	2.3
5	n	208	CYS	2.3
4	I	137	ASP	2.3
4	w	137	ASP	2.3
1	U	19	GLU	2.3
1	o	128	GLU	2.3
4	X	168	LYS	2.3
1	t	217	TRP	2.3
4	I	131	SER	2.3
4	I	191	ILE	2.3
5	x	110	THR	2.3
1	e	230	LEU	2.3
1	o	19	GLU	2.3
4	D	136	THR	2.3
4	X	131	SER	2.3
4	m	171	SER	2.3
4	X	139	ASP	2.3
4	w	129	ASP	2.3
4	X	159	VAL	2.3
4	h	179	SER	2.3
4	N	5	GLN	2.3
4	X	93	ASP	2.3
4	X	119	VAL	2.3
4	w	119	VAL	2.3
5	i	125	VAL	2.3
5	i	164	VAL	2.3
5	i	194	VAL	2.3
5	Y	217	GLU	2.2
4	r	186	ALA	2.2
5	J	180	ALA	2.2
2	p	95	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
4	X	198	PHE	2.2
4	w	198	PHE	2.2
4	N	128	SER	2.2
4	S	157	LYS	2.2
5	Y	166	SER	2.2
4	X	143	ASN	2.2
4	h	95	ASN	2.2
5	Y	223	GLN	2.2
4	m	133	CYS	2.2
5	O	201	ASP	2.2
5	Y	120	PRO	2.2
4	h	122	LEU	2.2
5	O	152	HIS	2.2
4	c	146	GLN	2.2
5	x	71	GLN	2.2
5	n	130	GLU	2.2
4	D	162	MET	2.2
4	X	134	LEU	2.2
4	h	93	ASP	2.2
4	X	184	ALA	2.2
4	h	117	PRO	2.2
5	i	92	ALA	2.2
5	i	128	PRO	2.2
5	x	179	PRO	2.2
4	w	187	PHE	2.2
5	Y	221	TRP	2.2
1	t	249	VAL	2.2
1	t	261	VAL	2.2
4	c	127	SER	2.2
4	w	176	SER	2.2
4	h	5	GLN	2.2
1	t	194	ILE	2.2
4	D	95	ASN	2.2
4	N	160	LEU	2.2
5	i	241	ALA	2.2
5	x	97	GLY	2.2
4	S	130	LYS	2.2
4	w	148	LYS	2.2
5	x	151	ASP	2.2
1	o	190	THR	2.2
5	O	222	THR	2.2
4	h	120	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	194	ILE	2.2
4	X	125	SER	2.2
4	m	154	ILE	2.2
5	i	234	SER	2.2
4	c	122	LEU	2.2
4	h	184	ALA	2.2
4	w	177	ASN	2.2
5	d	131	ALA	2.2
5	i	237	ALA	2.2
3	v	8	GLY	2.2
2	f	76	ASP	2.2
4	m	129	ASP	2.2
4	m	137	ASP	2.2
5	x	183	ASP	2.2
4	m	136	THR	2.1
4	c	134	LEU	2.1
4	c	157	LYS	2.1
4	m	178	LYS	2.1
2	L	69	GLU	2.1
5	s	214	GLY	2.1
1	o	86	ASN	2.1
4	c	117	PRO	2.1
4	D	137	ASP	2.1
4	h	183	CYS	2.1
4	m	156	ASP	2.1
5	i	91	CYS	2.1
5	d	168	VAL	2.1
1	t	225	THR	2.1
4	X	120	TYR	2.1
5	d	71	GLN	2.1
1	t	236	ALA	2.1
4	N	131	SER	2.1
5	i	152	HIS	2.1
5	n	135	HIS	2.1
5	E	96	THR	2.1
4	D	48	MET	2.1
4	D	5	GLN	2.1
4	I	121	GLN	2.1
4	w	199	PRO	2.1
5	d	130	GLU	2.1
5	s	128	PRO	2.1
4	D	197	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	X	150	SER	2.1
4	m	131	SER	2.1
5	i	129	SER	2.1
4	I	126	LYS	2.1
2	f	1	ILE	2.1
5	d	232	ILE	2.1
5	n	183	ASP	2.1
5	x	140	THR	2.1
4	m	117	PRO	2.1
4	r	127	SER	2.1
5	E	166	SER	2.1
4	c	132	VAL	2.1
5	i	159	VAL	2.1
5	i	233	VAL	2.1
2	f	42	ASN	2.1
4	r	148	LYS	2.1
2	f	23	LEU	2.1
5	Y	152	HIS	2.1
5	n	199	TRP	2.1
4	X	111	ASP	2.1
5	Y	219	ASP	2.1
5	d	114	ASP	2.1
5	J	50	TYR	2.1
1	U	18	GLY	2.1
1	t	252	GLY	2.1
2	G	2	GLN	2.1
4	h	167	PHE	2.1
5	i	150	PRO	2.1
5	s	166	SER	2.0
1	o	270	LEU	2.0
4	N	189	ASN	2.0
1	o	217	TRP	2.0
4	w	111	ASP	2.0
5	T	183	ASP	2.0
5	x	219	ASP	2.0
1	U	259	CYS	2.0
3	R	8	GLY	2.0
5	n	162	LYS	2.0
4	m	189	ASN	2.0
1	K	217	TRP	2.0
5	i	157	TRP	2.0
4	m	120	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
2	f	75	LYS	2.0
5	n	228	PRO	2.0
5	Y	185	ARG	2.0
5	n	185	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.