



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2025 – 10:39 AM JST

PDB ID : 9K2I / pdb\_00009k2i  
Title : Rac1 epitope specific TCR 5934 binding to Rac1P29S-HLA-A2  
Authors : Yang, D.D.; Wu, D.C.  
Deposited on : 2024-10-17  
Resolution : 3.05 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

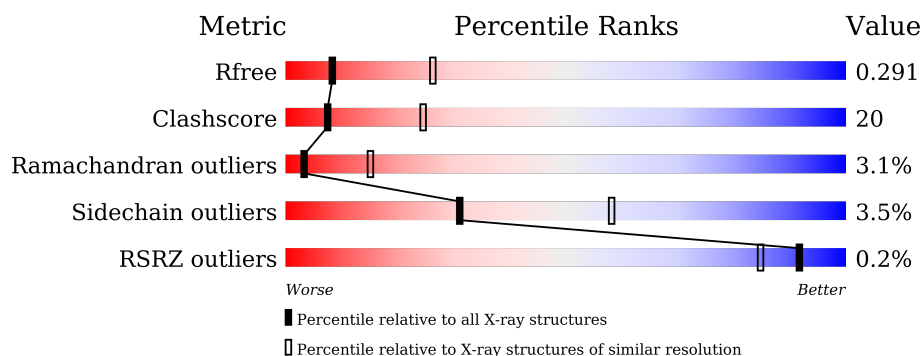
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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))
$R_{free}$	164625	2258 (3.10-3.02)
Clashscore	180529	2399 (3.10-3.02)
Ramachandran outliers	177936	2269 (3.10-3.02)
Sidechain outliers	177891	2268 (3.10-3.02)
RSRZ outliers	164620	2258 (3.10-3.02)

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  $\geq 3$ , 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	276	<div> <div>67%</div> <div>28%</div> <div>..</div> </div>
1	F	276	<div> <div>61%</div> <div>36%</div> <div>.</div> </div>
1	K	276	<div> <div>%</div> <div>57%</div> <div>33%</div> <div>7%</div> <div>.</div> </div>
1	P	276	<div> <div>70%</div> <div>26%</div> <div>..</div> </div>
2	B	100	<div> <div>70%</div> <div>27%</div> <div>.</div> </div>
2	G	100	<div> <div>79%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
2	L	100	 66% 32% .
2	Q	100	 79% 21%
3	C	9	 89% 11%
3	H	9	 44% 44% 11%
3	M	9	 67% 22% 11%
3	R	9	 56% 33% 11%
4	E	247	 61% 34% . .
4	J	247	 68% 28% . .
4	O	247	 64% 29% . .
4	T	247	 61% 34% . .
5	D	207	 53% 35% 5% . .
5	I	207	 % 46% 40% 7% . .
5	N	207	 50% 39% 5% . .
5	S	207	 57% 29% 8% . .

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26756 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			
1	F	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			
1	K	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			
1	P	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q8WLS4
F	0	MET	-	initiating methionine	UNP Q8WLS4
K	0	MET	-	initiating methionine	UNP Q8WLS4
P	0	MET	-	initiating methionine	UNP Q8WLS4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	4	3	0
			848	541	142	161	4			
2	G	100	Total	C	N	O	S	4	3	0
			848	541	142	161	4			
2	L	100	Total	C	N	O	S	3	3	0
			848	541	142	161	4			
2	Q	100	Total	C	N	O	S	4	3	0
			848	541	142	161	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
L	0	MET	-	initiating methionine	UNP P61769
Q	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called PHE-SER-GLY-GLU-TYR-ILE-PRO-THR-VAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			72	48	9	15			
3	H	9	Total	C	N	O	0	0	0
			72	48	9	15			
3	M	9	Total	C	N	O	0	0	0
			72	48	9	15			
3	R	9	Total	C	N	O	0	0	0
			72	48	9	15			

- Molecule 4 is a protein called T cell receptor 5934 chain beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	245	Total	C	N	O	S	0	0	0
			1962	1245	336	373	8			
4	E	245	Total	C	N	O	S	0	0	0
			1962	1245	336	373	8			
4	T	245	Total	C	N	O	S	0	0	0
			1962	1245	336	373	8			
4	O	245	Total	C	N	O	S	0	0	0
			1962	1245	336	373	8			

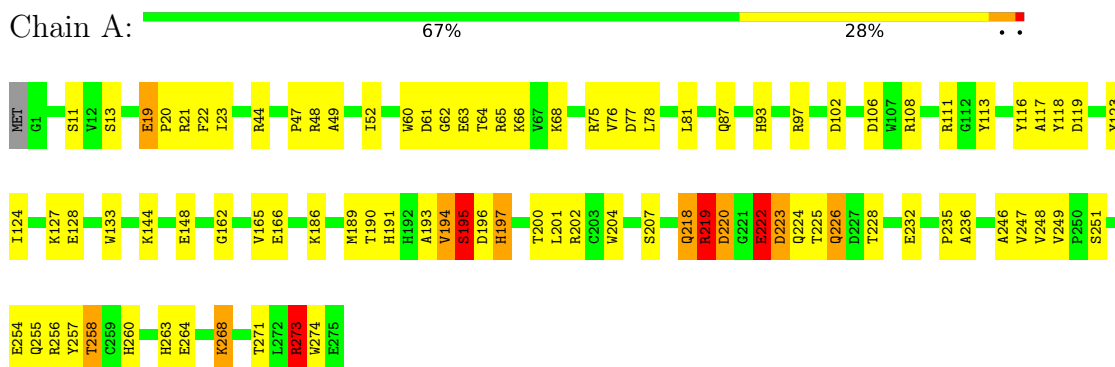
- Molecule 5 is a protein called T cell receptor5934 chain alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	200	Total	C	N	O	S	0	0	0
			1561	972	265	317	7			
5	D	200	Total	C	N	O	S	0	0	0
			1561	972	265	317	7			
5	S	200	Total	C	N	O	S	0	0	0
			1561	972	265	317	7			
5	N	200	Total	C	N	O	S	0	0	0
			1561	972	265	317	7			

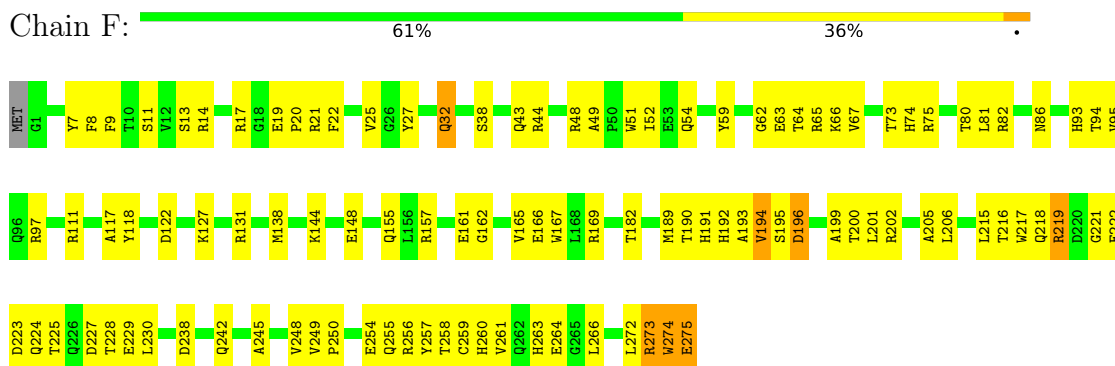
### 3 Residue-property plots

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.

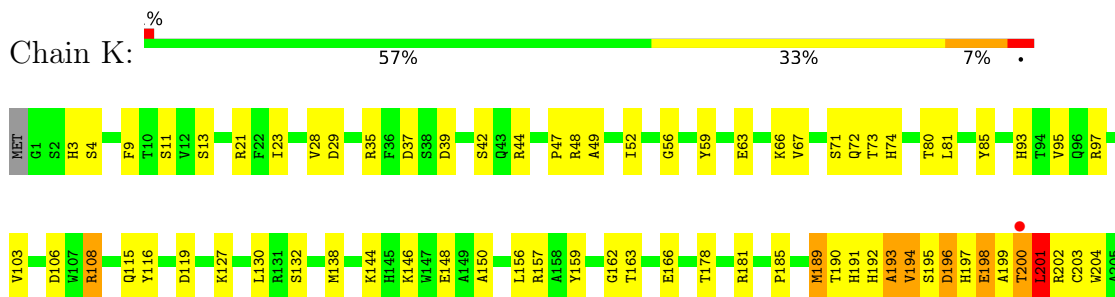
#### • Molecule 1: MHC class I antigen



#### • Molecule 1: MHC class I antigen



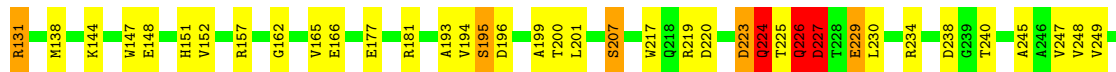
#### • Molecule 1: MHC class I antigen





- Molecule 1: MHC class I antigen

Chain P: 70% 26% ..



- Molecule 2: Beta-2-microglobulin

Chain B: 70% 27% .



- Molecule 2: Beta-2-microglobulin

Chain G: 79% 21%



- Molecule 2: Beta-2-microglobulin

Chain L: 66% 32% .



- Molecule 2: Beta-2-microglobulin

Chain Q: 79% 21%



- Molecule 3: PHE-SER-GLY-GLU-TYR-ILE-PRO-THR-VAL

Chain C: 89% 11%



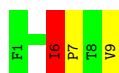
- Molecule 3: PHE-SER-GLY-GLU-TYR-ILE-PRO-THR-VAL

Chain H: 44% 44% 11%



- Molecule 3: PHE-SER-GLY-GLU-TYR-ILE-PRO-THR-VAL

Chain M: 67% 22% 11%



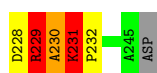
- Molecule 3: PHE-SER-GLY-GLU-TYR-ILE-PRO-THR-VAL

Chain R: 56% 33% 11%



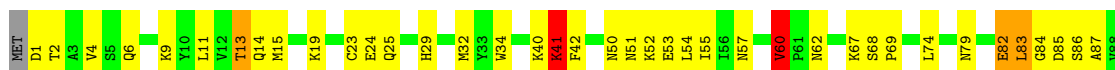
- Molecule 4: T cell receptor 5934 chain beta

Chain J: 68% 28% ...



- Molecule 4: T cell receptor 5934 chain beta

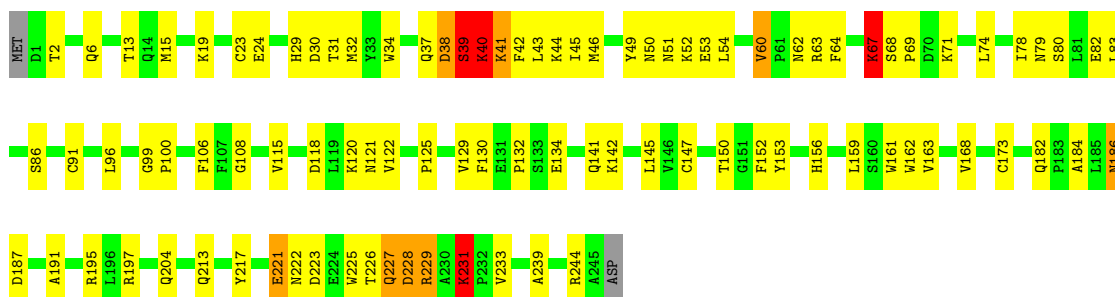
Chain E: 61% 34% ...





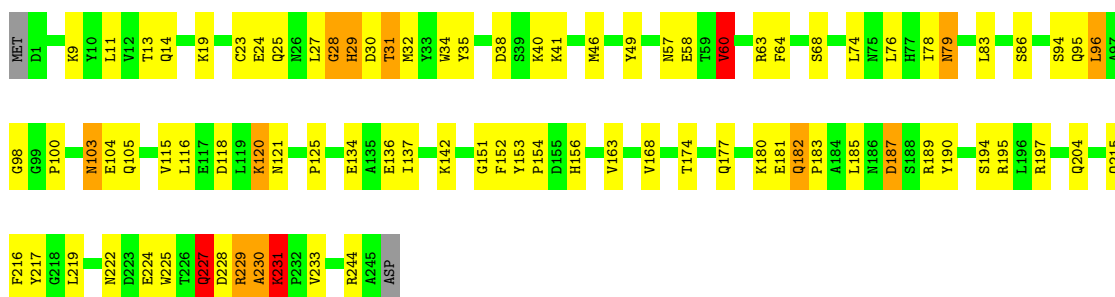
- Molecule 4: T cell receptor 5934 chain beta

Chain T:  61% 34%



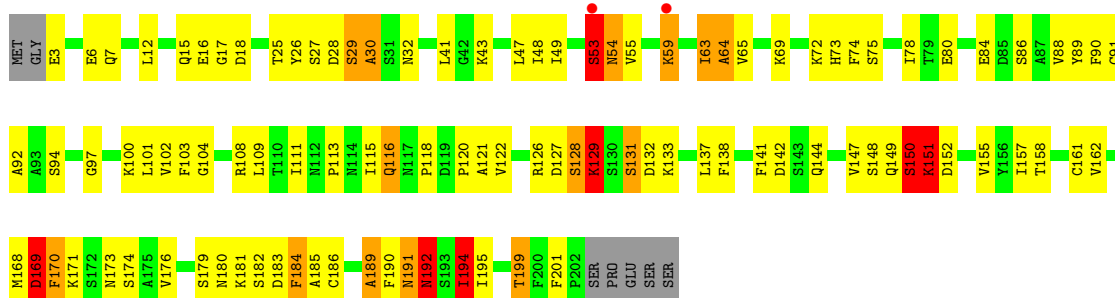
- Molecule 4: T cell receptor 5934 chain beta

Chain O:  64% 29%



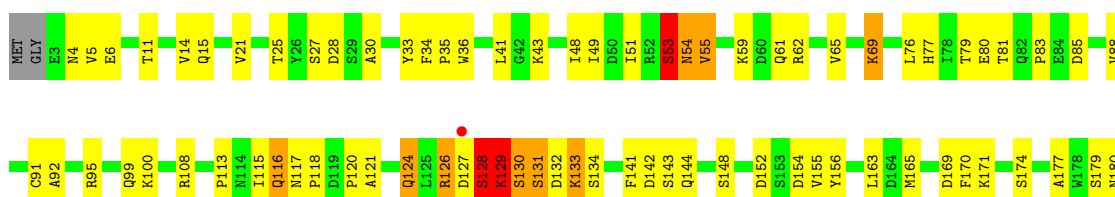
- Molecule 5: T cell receptor5934 chain alpha

Chain I:  % 46% 40% 7%



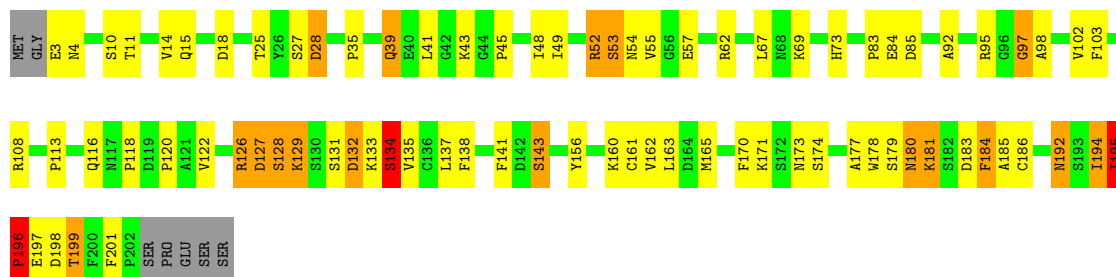
- Molecule 5: T cell receptor5934 chain alpha

Chain D:  53% 35% 5%

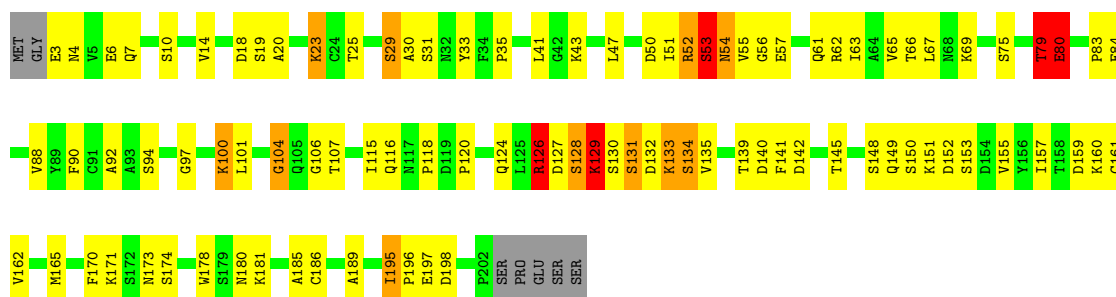




• Molecule 5: T cell receptor5934 chain alpha



• Molecule 5: T cell receptor5934 chain alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.30Å 147.50Å 122.17Å 90.00° 94.25° 90.00°	Depositor
Resolution (Å)	46.97 – 3.05 46.97 – 3.05	Depositor EDS
% Data completeness (in resolution range)	97.8 (46.97-3.05) 97.4 (46.97-3.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 3.06Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.222 , 0.290 0.227 , 0.291	Depositor DCC
$R_{free}$ test set	1978 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.6	Xtrriage
Anisotropy	0.524	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	26756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.82 % 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 9.9629e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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	0.72	0/2311	1.13	11/3137 (0.4%)
1	F	0.66	1/2311 (0.0%)	1.07	4/3137 (0.1%)
1	K	0.86	5/2311 (0.2%)	1.29	28/3137 (0.9%)
1	P	0.71	0/2311	1.17	7/3137 (0.2%)
2	B	0.52	0/884	0.94	0/1194
2	G	0.60	0/884	1.05	2/1194 (0.2%)
2	L	0.60	0/884	1.06	5/1194 (0.4%)
2	Q	0.57	0/884	1.01	0/1194
3	C	0.69	0/74	1.02	0/99
3	H	0.60	0/74	0.88	0/99
3	M	0.98	1/74 (1.4%)	1.03	0/99
3	R	0.82	0/74	0.94	0/99
4	E	0.67	1/2016 (0.0%)	1.14	14/2742 (0.5%)
4	J	0.62	0/2016	1.07	6/2742 (0.2%)
4	O	0.64	2/2016 (0.1%)	1.07	6/2742 (0.2%)
4	T	0.68	0/2016	1.14	13/2742 (0.5%)
5	D	0.77	2/1593 (0.1%)	1.37	19/2159 (0.9%)
5	I	0.74	0/1593	1.27	11/2159 (0.5%)
5	N	0.71	1/1593 (0.1%)	1.25	13/2159 (0.6%)
5	S	0.74	2/1593 (0.1%)	1.37	16/2159 (0.7%)
All	All	0.70	15/27512 (0.1%)	1.17	155/37324 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	K	0	5
1	P	0	1
2	G	0	1
2	L	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	T	0	1
5	D	0	5
5	I	0	6
5	N	0	6
5	S	0	5
All	All	0	33

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	258	THR	CA-C	9.75	1.63	1.52
1	K	218	GLN	CA-C	8.76	1.61	1.53
5	D	195	ILE	CA-C	7.50	1.60	1.52
5	S	127	ASP	CA-C	6.59	1.55	1.52
5	N	80	GLU	CA-C	6.38	1.61	1.52
1	K	217	TRP	CA-C	5.75	1.59	1.52
4	E	60	VAL	CA-CB	5.57	1.61	1.54
1	K	259	CYS	N-CA	5.45	1.52	1.46
1	K	257	TYR	CA-C	5.42	1.58	1.52
3	M	6	ILE	CA-CB	5.35	1.61	1.54
4	O	182	GLN	C-O	-5.26	1.20	1.25
5	D	194	ILE	CG1-CD1	5.22	1.72	1.51
5	S	195	ILE	CA-C	5.17	1.58	1.52
4	O	60	VAL	CA-CB	5.11	1.60	1.54
1	F	273	ARG	CG-CD	-5.02	1.37	1.52

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	195	ILE	CA-C-N	16.70	140.72	119.84
5	S	195	ILE	C-N-CA	16.70	140.72	119.84
1	A	218	GLN	N-CA-C	13.91	130.79	109.23
5	N	129	LYS	N-CA-C	12.11	127.44	108.67
5	D	195	ILE	CA-C-N	-11.99	104.85	119.84
5	D	195	ILE	C-N-CA	-11.99	104.85	119.84
1	F	273	ARG	N-CA-C	11.62	126.79	109.24
1	K	249	VAL	CA-C-N	11.43	132.15	119.92
1	K	249	VAL	C-N-CA	11.43	132.15	119.92
1	P	225	THR	N-CA-C	-11.12	97.09	110.44
5	N	134	SER	N-CA-C	10.85	124.72	109.31
4	T	38	ASP	N-CA-C	-10.72	96.90	110.19
5	I	152	ASP	N-CA-C	10.08	126.20	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	40	LYS	N-CA-C	-9.64	90.27	110.80
1	K	258	THR	N-CA-C	9.27	123.73	107.61
5	D	129	LYS	N-CA-C	9.26	124.33	109.24
5	D	192	ASN	N-CA-C	9.17	130.32	110.80
1	A	273	ARG	N-CA-C	9.04	122.44	108.96
5	I	189	ALA	N-CA-C	-8.97	102.92	114.04
1	K	219	ARG	CB-CG-CD	8.91	131.80	111.30
5	S	129	LYS	N-CA-C	8.68	123.18	109.65
5	N	189	ALA	N-CA-C	-8.64	103.32	114.04
4	J	40	LYS	N-CA-C	-8.28	102.44	112.54
2	L	73	THR	N-CA-C	-8.22	97.27	108.86
5	D	130	SER	N-CA-C	-8.19	96.55	109.50
1	K	222	GLU	N-CA-C	-8.06	100.49	110.41
4	J	79	ASN	N-CA-C	7.95	121.15	109.07
2	G	20	SER	N-CA-C	7.92	122.01	110.28
5	S	116	GLN	CA-C-N	-7.86	113.49	123.16
5	S	116	GLN	C-N-CA	-7.86	113.49	123.16
4	O	68	SER	CA-C-N	7.50	126.77	118.97
4	O	68	SER	C-N-CA	7.50	126.77	118.97
1	K	250	PRO	N-CA-C	7.38	122.78	111.34
2	G	1	ILE	N-CA-C	7.37	119.69	109.45
4	E	68	SER	CA-C-N	7.18	126.44	118.97
4	E	68	SER	C-N-CA	7.18	126.44	118.97
1	P	256	ARG	NE-CZ-NH1	-7.17	114.33	121.50
5	D	189	ALA	N-CA-C	-7.06	105.29	114.04
1	K	255	GLN	N-CA-C	7.05	121.60	112.92
4	O	187	ASP	N-CA-C	-7.03	104.70	113.28
4	T	38	ASP	CA-C-N	-7.02	111.02	122.81
4	T	38	ASP	C-N-CA	-7.02	111.02	122.81
1	A	19	GLU	CA-C-N	-6.95	113.50	120.31
1	A	19	GLU	C-N-CA	-6.95	113.50	120.31
5	N	130	SER	N-CA-C	-6.89	99.08	108.38
1	K	222	GLU	CA-CB-CG	6.87	127.83	114.10
5	S	195	ILE	C-N-CD	-6.86	96.87	125.00
1	K	256	ARG	N-CA-C	-6.83	102.96	112.25
5	D	79	THR	N-CA-C	-6.83	100.35	110.46
1	K	259	CYS	N-CA-C	6.77	120.04	110.23
5	D	115	ILE	N-CA-C	6.76	118.27	107.73
5	N	128	SER	N-CA-C	-6.75	96.42	110.80
5	I	192	ASN	N-CA-C	6.72	125.11	110.80
1	K	254	GLU	N-CA-C	6.71	120.34	111.75
1	K	222	GLU	N-CA-CB	6.70	119.56	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	227	ASP	N-CA-C	-6.59	96.77	110.80
5	S	53	SER	N-CA-C	6.57	122.20	111.37
1	K	220	ASP	N-CA-C	-6.55	105.83	113.88
1	K	217	TRP	CA-C-N	6.54	130.79	122.16
1	K	217	TRP	C-N-CA	6.54	130.79	122.16
5	S	127	ASP	N-CA-C	6.54	118.50	108.30
5	S	186	CYS	N-CA-C	-6.40	105.30	113.23
4	J	60	VAL	CA-C-N	-6.38	111.86	119.84
4	J	60	VAL	C-N-CA	-6.38	111.86	119.84
5	S	4	ASN	N-CA-C	6.38	124.39	110.80
5	D	194	ILE	CB-CA-C	6.38	121.75	111.29
1	A	195	SER	CB-CA-C	-6.35	107.51	115.89
4	E	94	SER	CA-C-N	-6.34	113.85	122.86
4	E	94	SER	C-N-CA	-6.34	113.85	122.86
5	I	64	ALA	N-CA-C	6.34	118.94	108.99
1	P	207	SER	N-CA-C	6.33	119.91	111.30
5	N	80	GLU	N-CA-C	6.24	124.08	110.80
1	A	251	SER	N-CA-C	6.16	119.89	112.38
1	K	226	GLN	N-CA-C	-6.16	103.51	111.02
5	D	182	SER	N-CA-C	-6.16	104.68	111.82
1	F	94	THR	N-CA-C	6.11	118.36	108.41
4	T	223	ASP	N-CA-C	-6.07	101.31	110.24
4	E	224	GLU	CA-C-N	-6.05	114.37	122.42
4	E	224	GLU	C-N-CA	-6.05	114.37	122.42
1	P	256	ARG	CA-CB-CG	5.98	126.06	114.10
5	N	126	ARG	N-CA-C	5.97	116.16	108.34
4	T	186	ASN	N-CA-C	-5.93	106.09	113.38
1	K	219	ARG	N-CA-C	-5.92	98.19	110.80
5	N	153	SER	N-CA-C	5.92	119.98	112.87
1	K	219	ARG	NE-CZ-NH1	-5.92	115.58	121.50
5	S	192	ASN	N-CA-C	5.87	123.31	110.80
1	P	227	ASP	CB-CA-C	-5.86	98.76	110.42
5	I	162	VAL	N-CA-C	5.86	116.44	107.77
5	D	80	GLU	CB-CA-C	-5.82	104.06	111.86
5	I	183	ASP	N-CA-C	-5.82	106.42	112.93
4	O	28	GLY	N-CA-C	-5.81	99.42	113.18
4	J	30	ASP	N-CA-C	-5.79	101.89	110.46
5	S	143	SER	N-CA-C	5.79	118.53	111.82
1	F	221	GLY	N-CA-C	-5.78	99.48	113.18
1	A	268	LYS	CA-C-N	5.76	125.77	119.89
1	A	268	LYS	C-N-CA	5.76	125.77	119.89
1	K	196	ASP	N-CA-C	-5.75	98.56	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	134	GLU	N-CA-C	-5.75	106.23	113.18
1	A	258	THR	N-CA-C	5.72	118.28	110.55
2	L	73	THR	CA-C-N	-5.72	113.47	122.79
2	L	73	THR	C-N-CA	-5.72	113.47	122.79
5	D	53	SER	N-CA-C	5.69	122.92	110.80
5	D	197	GLU	CA-CB-CG	-5.68	102.73	114.10
5	S	52	ARG	N-CA-C	5.68	117.85	108.48
5	D	183	ASP	CA-C-N	-5.63	110.78	121.54
5	D	183	ASP	C-N-CA	-5.63	110.78	121.54
5	D	194	ILE	N-CA-CB	-5.62	101.96	111.23
5	S	196	PRO	CA-N-CD	-5.61	104.15	112.00
5	N	100	LYS	N-CA-C	5.57	118.53	110.28
5	I	53	SER	N-CA-C	5.56	122.65	110.80
1	K	257	TYR	N-CA-C	5.56	117.42	107.80
1	K	258	THR	CA-C-N	5.56	128.60	120.71
1	K	258	THR	C-N-CA	5.56	128.60	120.71
4	E	185	LEU	N-CA-C	5.51	118.62	110.46
2	L	76	ASP	N-CA-C	5.51	118.52	109.76
4	O	224	GLU	CA-C-N	-5.47	115.72	122.84
4	O	224	GLU	C-N-CA	-5.47	115.72	122.84
5	I	100	LYS	N-CA-C	5.46	118.36	110.28
4	E	207	ARG	N-CA-C	-5.45	106.51	112.72
5	N	116	GLN	N-CA-C	5.45	117.30	111.36
1	K	56	GLY	CA-C-N	5.42	125.07	119.05
1	K	56	GLY	C-N-CA	5.42	125.07	119.05
5	N	126	ARG	CB-CG-CD	5.38	123.67	111.30
1	A	219	ARG	CA-C-N	5.37	131.80	121.54
1	A	219	ARG	C-N-CA	5.37	131.80	121.54
4	T	38	ASP	N-CA-CB	5.36	117.53	110.25
5	I	63	ILE	CB-CA-C	-5.35	102.26	110.50
5	I	170	PHE	N-CA-C	5.34	117.60	108.90
5	I	169	ASP	N-CA-C	5.33	122.14	110.80
5	D	191	ASN	CA-C-N	5.32	131.70	121.54
5	D	191	ASN	C-N-CA	5.32	131.70	121.54
5	N	104	GLY	N-CA-C	-5.29	104.08	112.66
5	N	126	ARG	CG-CD-NE	-5.29	100.36	112.00
1	K	201	LEU	CA-CB-CG	5.29	134.81	116.30
1	K	272	LEU	N-CA-C	5.28	116.94	107.80
4	T	2	THR	N-CA-C	5.26	118.65	110.17
4	E	41	LYS	N-CA-C	5.24	121.96	110.80
1	F	260	HIS	N-CA-CB	-5.24	101.89	110.68
4	T	108	GLY	CA-C-N	5.22	126.25	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	108	GLY	C-N-CA	5.22	126.25	120.45
4	E	82	GLU	CA-C-O	-5.20	115.08	120.70
5	S	134	SER	N-CA-C	5.18	121.83	110.80
1	P	229	GLU	N-CA-C	-5.17	101.53	109.76
4	E	96	LEU	N-CA-C	-5.15	102.07	110.20
4	E	121	ASN	N-CA-C	-5.13	106.87	112.72
5	S	52	ARG	CB-CA-C	-5.10	105.29	114.52
5	D	195	ILE	CB-CA-C	5.08	120.61	111.36
4	T	41	LYS	CA-C-N	5.06	127.95	120.82
4	T	41	LYS	C-N-CA	5.06	127.95	120.82
2	L	44	GLU	N-CA-C	5.04	117.78	109.72
1	K	248	VAL	N-CA-C	5.03	119.80	109.34
4	J	229	ARG	N-CA-C	5.02	118.14	110.20
4	E	108	GLY	CA-C-N	5.01	126.01	120.45
4	E	108	GLY	C-N-CA	5.01	126.01	120.45
1	K	193	ALA	N-CA-C	5.00	116.58	111.03

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	SER	Peptide
1	A	197	HIS	Peptide
5	D	126	ARG	Peptide
5	D	128	SER	Peptide
5	D	129	LYS	Peptide
5	D	133	LYS	Peptide
5	D	196	PRO	Peptide
2	G	19	LYS	Peptide
5	I	126	ARG	Peptide
5	I	131	SER	Peptide
5	I	148	SER	Peptide
5	I	150	SER	Peptide
5	I	151	LYS	Peptide
5	I	169	ASP	Peptide
1	K	108	ARG	Peptide
1	K	217	TRP	Peptide
1	K	219	ARG	Peptide
1	K	224	GLN	Peptide
1	K	226	GLN	Peptide
2	L	74	GLU	Peptide
5	N	126	ARG	Peptide

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Mol	Chain	Res	Type	Group
5	N	129	LYS	Peptide
5	N	133	LYS	Peptide
5	N	195	ILE	Peptide
5	N	53	SER	Peptide
5	N	79	THR	Peptide
1	P	226	GLN	Peptide
5	S	126	ARG	Peptide
5	S	131	SER	Peptide
5	S	180	ASN	Peptide
5	S	196	PRO	Peptide
5	S	28	ASP	Peptide
4	T	39	SER	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2246	0	2096	105	0
1	F	2246	0	2096	97	1
1	K	2246	0	2096	141	1
1	P	2246	0	2096	95	0
2	B	848	0	817	26	0
2	G	848	0	817	15	0
2	L	848	0	817	27	0
2	Q	848	0	817	14	1
3	C	72	0	68	3	0
3	H	72	0	68	5	0
3	M	72	0	68	7	0
3	R	72	0	68	4	0
4	E	1962	0	1885	72	0
4	J	1962	0	1885	57	0
4	O	1962	0	1885	67	0
4	T	1962	0	1885	87	0
5	D	1561	0	1490	86	0
5	I	1561	0	1490	80	1
5	N	1561	0	1490	87	1
5	S	1561	0	1490	79	1
All	All	26756	0	25424	1044	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1044) 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)
4:E:211:ARG:NH1	4:E:213:GLN:OE1	1.87	1.08
1:K:219:ARG:HG3	1:K:220:ASP:H	1.12	1.06
1:K:217:TRP:CZ2	1:K:257:TYR:HA	1.94	1.03
5:I:59:LYS:HZ3	5:I:64:ALA:HB3	1.21	1.00
5:N:100:LYS:NZ	4:O:58:GLU:OE2	1.94	1.00
4:O:180:LYS:NZ	4:O:182:GLN:O	1.94	1.00
2:G:47:GLU:OE1	1:P:44:ARG:NH1	1.97	0.98
4:E:82:GLU:HG2	4:E:84:GLY:H	1.27	0.97
1:A:255:GLN:C	1:A:273:ARG:HH12	1.74	0.96
1:F:63:GLU:OE2	1:F:66:LYS:NZ	1.99	0.95
5:S:3:GLU:N	5:S:28:ASP:OD2	2.00	0.94
5:D:129:LYS:NZ	5:D:132:ASP:O	2.01	0.94
1:F:258:THR:HA	1:F:273:ARG:HD3	1.49	0.94
1:P:201:LEU:HB2	1:P:247:VAL:HG23	1.49	0.93
1:A:258:THR:HA	1:A:273:ARG:HG3	1.49	0.93
4:T:122:VAL:O	4:T:229:ARG:NH2	2.02	0.92
5:I:133:LYS:HZ2	5:I:180:ASN:HB2	1.34	0.92
5:D:83:PRO:HG2	5:D:171:LYS:NZ	1.85	0.92
1:K:255:GLN:NE2	1:K:274:TRP:O	2.03	0.91
1:K:218:GLN:HA	1:K:223:ASP:HA	1.51	0.91
1:P:219:ARG:HB2	1:P:256:ARG:HB2	1.52	0.91
1:P:226:GLN:HG2	1:P:227:ASP:N	1.86	0.91
1:A:224:GLN:HE22	1:A:226:GLN:HB2	1.36	0.90
5:S:179:SER:HB3	5:S:181:LYS:HE3	1.53	0.90
1:F:255:GLN:O	1:F:273:ARG:NH2	2.03	0.90
1:A:219:ARG:HB3	1:A:222:GLU:H	1.33	0.89
1:P:219:ARG:HH12	1:P:253:GLN:HG2	1.37	0.89
5:D:100:LYS:H	5:D:100:LYS:HD2	1.36	0.89
1:K:219:ARG:HG2	1:K:222:GLU:H	1.36	0.88
1:K:214:THR:HG21	1:K:262:GLN:HG2	1.54	0.88
1:A:232:GLU:OE1	2:B:6:LYS:NZ	2.06	0.88
4:T:40:LYS:HZ3	4:T:42:PHE:N	1.71	0.87
1:P:219:ARG:HD2	1:P:257:TYR:CE1	2.09	0.87
5:S:39:GLN:NE2	4:T:37:GLN:HE22	1.72	0.86
5:S:195:ILE:HB	5:S:196:PRO:HD3	1.55	0.86
1:F:258:THR:HA	1:F:273:ARG:CD	2.05	0.85
5:I:16:GLU:OE2	5:I:171:LYS:NZ	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:59:LYS:NZ	5:I:64:ALA:HB3	1.90	0.85
1:A:219:ARG:HH11	1:A:222:GLU:HB2	1.42	0.85
4:E:121:ASN:ND2	4:E:187:ASP:HB3	1.92	0.85
1:A:219:ARG:NH1	1:A:222:GLU:HB2	1.92	0.84
5:I:133:LYS:NZ	5:I:180:ASN:HB2	1.91	0.84
5:D:197:GLU:OE2	5:D:199:THR:HG23	1.77	0.84
1:K:231:VAL:O	1:K:243:LYS:NZ	2.11	0.84
4:E:82:GLU:HG2	4:E:84:GLY:N	1.92	0.84
5:S:127:ASP:CG	5:S:129:LYS:HD3	2.03	0.84
4:E:120:LYS:NZ	4:E:226:THR:OG1	2.10	0.83
1:K:219:ARG:CG	1:K:220:ASP:H	1.91	0.83
1:A:63:GLU:OE2	1:A:66:LYS:NZ	2.11	0.82
1:K:201:LEU:HG	1:K:247:VAL:HG21	1.60	0.82
2:Q:3:ARG:HD2	2:Q:61:SER:HB3	1.62	0.82
1:A:257:TYR:H	1:A:273:ARG:NH1	1.78	0.81
1:K:196:ASP:OD1	1:K:197:HIS:N	2.13	0.81
1:A:76:VAL:HG13	4:E:50:ASN:ND2	1.95	0.81
1:A:256:ARG:N	1:A:273:ARG:HH12	1.79	0.81
1:K:63:GLU:OE2	1:K:66:LYS:NZ	2.12	0.80
4:J:195:ARG:HH12	5:I:174:SER:N	1.80	0.79
5:S:28:ASP:HB3	5:S:95:ARG:HH21	1.47	0.79
1:P:226:GLN:NE2	1:P:247:VAL:HG12	1.99	0.78
5:S:195:ILE:CB	5:S:196:PRO:HD3	2.13	0.77
5:N:54:ASN:C	5:N:54:ASN:HD22	1.92	0.77
5:D:28:ASP:OD1	5:D:95:ARG:NH2	2.17	0.77
1:K:219:ARG:HB3	1:K:222:GLU:HG2	1.65	0.77
1:P:219:ARG:NH2	1:P:253:GLN:O	2.18	0.77
5:I:127:ASP:O	5:I:128:SER:OG	2.02	0.77
5:S:174:SER:N	4:T:195:ARG:HH12	1.83	0.77
4:J:38:ASP:OD2	4:J:40:LYS:HG3	1.85	0.76
1:K:191:HIS:NE2	1:K:199:ALA:HB1	2.00	0.76
5:I:168:MET:O	5:I:170:PHE:N	2.17	0.76
1:K:255:GLN:O	1:K:273:ARG:NH1	2.18	0.76
1:F:144:LYS:O	1:F:148:GLU:HG3	1.86	0.76
4:J:14:GLN:HE22	4:J:117:GLU:C	1.94	0.76
5:D:83:PRO:HG2	5:D:171:LYS:HZ2	1.51	0.76
2:B:45:ARG:HG2	2:B:45:ARG:HH11	1.48	0.76
1:K:191:HIS:CE1	1:K:199:ALA:HB1	2.20	0.75
1:P:219:ARG:CZ	1:P:256:ARG:HG2	2.15	0.75
1:P:63:GLU:OE2	1:P:66:LYS:NZ	2.19	0.75
5:D:132:ASP:OD1	5:D:133:LYS:N	2.14	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:121:ASN:HD22	4:E:187:ASP:HB3	1.47	0.75
4:O:30:ASP:O	4:O:31:THR:OG1	2.02	0.74
5:N:83:PRO:HG2	5:N:171:LYS:NZ	2.02	0.74
5:N:126:ARG:HH12	5:N:133:LYS:HD2	1.50	0.74
4:E:82:GLU:O	4:E:115:VAL:HG21	1.88	0.74
5:D:30:ALA:HB3	5:D:95:ARG:HH21	1.51	0.74
1:A:218:GLN:NE2	1:A:258:THR:OG1	2.21	0.74
5:D:59:LYS:NZ	5:D:61:GLN:O	2.21	0.74
1:K:258:THR:OG1	1:K:273:ARG:HD3	1.87	0.73
1:P:219:ARG:HH21	1:P:256:ARG:N	1.86	0.73
2:B:74:GLU:HG2	2:B:75:LYS:H	1.52	0.73
1:F:272:LEU:C	1:F:273:ARG:HG2	2.13	0.73
2:B:47:GLU:OE2	1:K:44:ARG:NH1	2.21	0.73
1:K:219:ARG:HG3	1:K:220:ASP:N	1.90	0.72
4:E:52:LYS:HE2	4:E:69:PRO:O	1.89	0.72
4:T:40:LYS:O	4:T:41:LYS:HG2	1.89	0.72
1:K:204:TRP:HE3	1:K:206:LEU:HD11	1.53	0.72
5:D:126:ARG:NH2	5:D:134:SER:OG	2.21	0.72
5:D:83:PRO:HG2	5:D:171:LYS:HZ3	1.54	0.71
1:K:217:TRP:CD2	1:K:218:GLN:N	2.58	0.71
1:A:61:ASP:OD1	2:L:45:ARG:NH2	2.23	0.71
4:T:52:LYS:HE2	4:T:69:PRO:O	1.91	0.71
1:A:255:GLN:C	1:A:273:ARG:NH1	2.49	0.71
1:A:201:LEU:HD12	1:A:249:VAL:HG21	1.72	0.70
5:I:48:ILE:HG13	5:I:49:ILE:HG22	1.74	0.70
5:N:124:GLN:HB2	5:N:186:CYS:SG	2.31	0.70
5:N:52:ARG:O	5:N:52:ARG:HG2	1.91	0.70
1:K:263:HIS:ND1	1:K:264:GLU:O	2.20	0.70
5:S:195:ILE:HD11	5:S:199:THR:HG23	1.73	0.70
5:N:97:GLY:HA2	4:O:100:PRO:HD3	1.73	0.70
5:N:132:ASP:OD1	5:N:133:LYS:N	2.18	0.70
1:K:191:HIS:HB2	1:K:201:LEU:HA	1.73	0.70
4:O:227:GLN:O	4:O:229:ARG:N	2.24	0.70
5:S:174:SER:OG	4:T:195:ARG:NH1	2.24	0.70
5:N:134:SER:OG	5:N:135:VAL:N	2.22	0.70
4:J:38:ASP:CG	4:J:40:LYS:HG3	2.16	0.70
1:K:219:ARG:HB3	1:K:222:GLU:CG	2.22	0.69
5:D:174:SER:OG	4:E:195:ARG:NH1	2.24	0.69
4:O:96:LEU:HA	4:O:100:PRO:HB3	1.75	0.69
1:A:102:ASP:OD2	1:A:113:TYR:OH	2.08	0.69
1:F:38:SER:O	1:F:43:GLN:NE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:40:LYS:NZ	4:T:42:PHE:N	2.40	0.69
1:P:219:ARG:NH2	1:P:256:ARG:H	1.91	0.69
1:K:47:PRO:O	1:K:48:ARG:HD3	1.93	0.68
1:F:255:GLN:C	1:F:273:ARG:HH22	2.01	0.68
1:A:263:HIS:ND1	1:A:264:GLU:O	2.25	0.68
5:D:116:GLN:OE1	5:D:117:ASN:N	2.26	0.68
4:J:211:ARG:NH1	4:J:213:GLN:OE1	2.26	0.68
1:K:106:ASP:CG	1:K:108:ARG:HG2	2.18	0.68
5:I:128:SER:O	5:I:129:LYS:HG2	1.93	0.68
2:B:48:LYS:HE2	1:K:47:PRO:HG2	1.74	0.67
1:F:218:GLN:HG3	1:F:258:THR:OG1	1.94	0.67
4:E:32:MET:HB2	4:E:74:LEU:HD22	1.75	0.67
1:K:258:THR:OG1	1:K:273:ARG:HA	1.94	0.67
5:I:94:SER:HB3	5:I:101:LEU:HD23	1.77	0.67
5:N:62:ARG:CZ	5:N:80:GLU:OE2	2.43	0.67
1:F:167:TRP:CG	3:H:1:PHE:HB2	2.29	0.67
1:K:106:ASP:OD2	1:K:108:ARG:HG2	1.93	0.67
5:S:132:ASP:OD2	5:S:180:ASN:HA	1.95	0.67
1:K:225:THR:HA	1:K:228:THR:HG23	1.75	0.67
4:O:31:THR:HA	4:O:49:TYR:O	1.95	0.67
1:A:257:TYR:O	1:A:273:ARG:HD3	1.96	0.66
1:A:44:ARG:NH1	2:L:47:GLU:OE2	2.29	0.66
1:A:256:ARG:HA	1:A:273:ARG:HH22	1.60	0.66
5:S:133:LYS:HB3	5:S:184:PHE:CZ	2.30	0.66
5:N:14:VAL:HG13	5:N:18:ASP:HB2	1.77	0.66
1:F:218:GLN:O	1:F:258:THR:N	2.27	0.66
1:P:219:ARG:HD2	1:P:257:TYR:CZ	2.30	0.66
1:P:230:LEU:HD12	1:P:245:ALA:HB2	1.76	0.66
5:D:62:ARG:NH2	5:D:85:ASP:OD2	2.19	0.66
5:N:7:GLN:HB2	5:N:104:GLY:HA3	1.77	0.66
1:F:195:SER:OG	1:F:196:ASP:N	2.23	0.66
5:D:124:GLN:HB2	5:D:186:CYS:SG	2.36	0.66
5:D:126:ARG:HG2	5:D:127:ASP:H	1.60	0.66
1:A:225:THR:HA	1:A:228:THR:HG22	1.77	0.66
4:E:40:LYS:O	4:E:42:PHE:N	2.29	0.66
5:N:126:ARG:HD2	5:N:134:SER:HB2	1.78	0.66
5:D:51:ILE:HD11	5:D:55:VAL:O	1.97	0.65
4:T:38:ASP:CB	4:T:40:LYS:HE3	2.26	0.65
1:K:204:TRP:CE3	1:K:206:LEU:HD11	2.30	0.65
2:L:3:ARG:NH2	2:L:59:ASP:O	2.29	0.65
5:I:59:LYS:HZ3	5:I:64:ALA:CB	2.06	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLN:HE21	2:B:0:MET:HE2	1.62	0.65
1:F:14:ARG:HH21	1:F:21:ARG:HD2	1.61	0.65
1:K:217:TRP:CE3	1:K:218:GLN:N	2.64	0.65
5:I:53:SER:OG	5:I:54:ASN:N	2.29	0.65
1:A:60:TRP:CG	2:L:47:GLU:HG3	2.32	0.65
1:A:76:VAL:HG13	4:E:50:ASN:HD21	1.61	0.65
5:I:63:ILE:HG22	5:I:78:ILE:HG12	1.78	0.65
5:N:126:ARG:HG2	5:N:127:ASP:H	1.60	0.64
2:L:39:LEU:O	2:L:46:ILE:HG13	1.98	0.64
5:N:165:MET:SD	4:O:197:ARG:HD3	2.37	0.64
1:K:250:PRO:HG2	1:K:253:GLN:HG2	1.80	0.64
1:K:256:ARG:NH1	1:K:257:TYR:OH	2.31	0.64
5:I:3:GLU:O	5:I:27:SER:OG	2.13	0.64
1:A:220:ASP:OD2	1:A:256:ARG:HB3	1.98	0.64
5:I:120:PRO:HB2	5:I:195:ILE:HG12	1.79	0.64
5:N:126:ARG:NH2	5:N:132:ASP:O	2.31	0.64
1:A:224:GLN:NE2	1:A:226:GLN:HB2	2.10	0.64
1:K:162:GLY:O	1:K:166:GLU:HG3	1.98	0.64
1:K:203:CYS:SG	1:K:272:LEU:HD21	2.37	0.64
1:F:272:LEU:O	1:F:273:ARG:HG2	1.98	0.64
4:J:83:LEU:HD12	4:J:83:LEU:H	1.61	0.64
1:K:272:LEU:HD12	1:K:272:LEU:O	1.98	0.64
5:D:127:ASP:HB3	5:D:129:LYS:HD3	1.78	0.64
1:P:201:LEU:N	1:P:247:VAL:O	2.28	0.64
1:P:238:ASP:HB3	2:Q:12:ARG:HD3	1.79	0.64
5:N:29:SER:OG	5:N:30:ALA:N	2.28	0.63
1:P:13:SER:OG	1:P:93:HIS:N	2.27	0.63
4:T:40:LYS:HZ3	4:T:42:PHE:H	1.45	0.63
1:F:258:THR:HG22	1:F:273:ARG:HD3	1.81	0.63
1:P:11:SER:HB3	1:P:22:PHE:HD1	1.63	0.63
1:P:219:ARG:NH2	1:P:256:ARG:N	2.47	0.63
1:A:111:ARG:NH2	1:A:128:GLU:OE2	2.31	0.63
5:D:144:GLN:N	5:D:144:GLN:OE1	2.32	0.63
5:N:23:LYS:HB3	5:N:75:SER:OG	1.99	0.63
5:N:115:ILE:HG13	5:N:142:ASP:HA	1.81	0.62
5:I:194:ILE:HG22	5:I:195:ILE:H	1.64	0.62
5:S:97:GLY:HA2	4:T:100:PRO:HD3	1.80	0.62
1:P:226:GLN:HE22	1:P:247:VAL:HG12	1.62	0.62
4:J:163:VAL:HB	4:J:168:VAL:HG21	1.80	0.62
5:S:83:PRO:HG2	5:S:171:LYS:NZ	2.14	0.62
4:J:35:TYR:OH	4:J:105:GLN:OE1	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:197:GLU:OE2	5:D:199:THR:CG2	2.47	0.62
4:T:82:GLU:O	4:T:115:VAL:HG21	2.00	0.62
4:O:163:VAL:HB	4:O:168:VAL:HG21	1.82	0.62
4:E:29:HIS:HE1	4:E:106:PHE:CD1	2.18	0.62
5:S:39:GLN:HE22	4:T:37:GLN:HE22	1.47	0.62
1:K:144:LYS:O	1:K:148:GLU:HG3	2.00	0.62
1:K:201:LEU:HG	1:K:247:VAL:CG2	2.29	0.62
1:K:159:TYR:HA	1:K:163:THR:HG22	1.82	0.62
5:S:11:THR:HG22	5:S:108:ARG:HB3	1.82	0.62
5:S:195:ILE:HD12	5:S:196:PRO:CD	2.30	0.62
5:N:84:GLU:OE1	5:N:84:GLU:N	2.26	0.61
1:A:21:ARG:NH1	1:A:23:ILE:HD11	2.15	0.61
4:O:174:THR:HG23	4:O:194:SER:HB2	1.82	0.61
1:A:62:GLY:O	1:A:65:ARG:HG2	2.01	0.61
4:E:163:VAL:HB	4:E:168:VAL:HG21	1.82	0.61
5:S:128:SER:C	5:S:129:LYS:HD2	2.25	0.61
5:S:194:ILE:HD12	5:S:194:ILE:H	1.64	0.61
1:P:70:HIS:HA	3:R:6:ILE:HD13	1.83	0.61
4:E:60:VAL:HG23	4:E:62:ASN:HB2	1.83	0.61
5:D:195:ILE:N	5:D:197:GLU:OE1	2.33	0.61
4:T:67:LYS:HD2	4:T:68:SER:H	1.66	0.61
1:A:256:ARG:HA	1:A:273:ARG:NH2	2.16	0.61
1:F:258:THR:CA	1:F:273:ARG:HD3	2.27	0.61
5:D:6:GLU:HB2	5:D:25:THR:OG1	2.01	0.61
1:F:219:ARG:HD2	1:F:256:ARG:HG2	1.82	0.61
1:F:263:HIS:ND1	1:F:264:GLU:O	2.30	0.61
1:F:201:LEU:HD12	1:F:249:VAL:HG21	1.83	0.61
4:E:180:LYS:HE3	4:E:183:PRO:HA	1.82	0.60
4:O:225:TRP:CG	4:O:231:LYS:HB2	2.36	0.60
1:P:226:GLN:CD	1:P:247:VAL:HG12	2.26	0.60
5:D:30:ALA:HB3	5:D:95:ARG:NH2	2.16	0.60
4:O:152:PHE:O	4:O:190:TYR:N	2.33	0.60
4:J:195:ARG:NH1	5:I:174:SER:OG	2.34	0.60
5:N:126:ARG:NH1	5:N:133:LYS:HD2	2.16	0.60
1:A:19:GLU:HG2	1:A:75:ARG:NH1	2.16	0.60
1:F:111:ARG:HB2	1:F:111:ARG:CZ	2.32	0.60
4:J:31:THR:HA	4:J:49:TYR:O	2.01	0.60
1:P:226:GLN:HE22	1:P:247:VAL:HA	1.66	0.60
1:P:227:ASP:O	1:P:229:GLU:N	2.35	0.60
1:F:20:PRO:HD3	1:F:75:ARG:HD3	1.84	0.60
5:I:115:ILE:HG13	5:I:142:ASP:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:229:ARG:O	4:T:231:LYS:N	2.31	0.60
1:F:162:GLY:O	1:F:166:GLU:HG3	2.01	0.59
4:J:225:TRP:CG	4:J:231:LYS:HB2	2.37	0.59
5:S:3:GLU:O	5:S:27:SER:OG	2.20	0.59
5:D:88:VAL:HG21	4:E:41:LYS:HE3	1.82	0.59
5:I:59:LYS:HA	5:I:64:ALA:HB2	1.85	0.59
4:T:29:HIS:HE1	4:T:106:PHE:CD1	2.21	0.59
5:S:127:ASP:OD1	5:S:129:LYS:HD3	2.02	0.59
4:T:64:PHE:CE1	4:T:78:ILE:HD13	2.37	0.59
1:K:219:ARG:CG	1:K:220:ASP:N	2.57	0.59
4:T:67:LYS:HD2	4:T:68:SER:N	2.17	0.59
4:O:14:GLN:HA	4:O:116:LEU:O	2.02	0.59
5:I:12:LEU:HD23	5:I:109:LEU:HD13	1.85	0.59
5:D:148:SER:HB2	5:D:192:ASN:ND2	2.17	0.59
1:A:189:MET:HE1	1:A:273:ARG:HG2	1.84	0.59
1:P:144:LYS:HE2	1:P:148:GLU:OE2	2.02	0.59
5:S:195:ILE:HD12	5:S:196:PRO:HD3	1.85	0.59
5:N:126:ARG:HH12	5:N:129:LYS:HZ1	1.50	0.59
1:P:219:ARG:NH1	1:P:253:GLN:HG2	2.13	0.59
1:A:254:GLU:O	1:A:273:ARG:NH1	2.35	0.59
1:P:200:THR:HA	1:P:248:VAL:HA	1.84	0.58
4:T:23:CYS:SG	4:T:24:GLU:N	2.77	0.58
5:N:29:SER:C	5:N:31:SER:H	2.09	0.58
5:D:36:TRP:CZ3	5:D:91:CYS:HB3	2.38	0.58
1:F:74:HIS:NE2	1:F:97:ARG:NH1	2.51	0.58
1:F:218:GLN:CB	1:F:223:ASP:HA	2.34	0.58
5:S:133:LYS:HD2	5:S:134:SER:H	1.68	0.58
1:A:223:ASP:OD1	1:A:224:GLN:N	2.35	0.58
2:G:41:LYS:HE3	2:G:78:TYR:OH	2.03	0.58
1:P:219:ARG:CB	1:P:256:ARG:HB2	2.31	0.58
4:J:6:GLN:NE2	4:J:89:TYR:O	2.36	0.58
1:K:217:TRP:HB2	1:K:259:CYS:HA	1.83	0.58
5:S:174:SER:CA	4:T:195:ARG:HH12	2.16	0.58
2:G:81:ARG:HG3	2:G:92:ILE:HG12	1.85	0.58
5:S:48:ILE:HG13	5:S:49:ILE:HG22	1.86	0.58
5:N:62:ARG:HB3	5:N:80:GLU:CD	2.28	0.58
5:N:162:VAL:HG22	5:N:173:ASN:OD1	2.03	0.58
1:A:77:ASP:CG	3:C:9:VAL:HG22	2.29	0.58
1:F:155:GLN:OE1	5:I:32:ASN:HB2	2.02	0.58
5:N:62:ARG:HH21	5:N:80:GLU:HG3	1.68	0.58
1:K:192:HIS:NE2	2:L:98:ASP:HB3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:226:GLN:NE2	1:P:247:VAL:HA	2.19	0.57
4:T:79:ASN:OD1	4:T:80:SER:N	2.37	0.57
4:T:38:ASP:CG	4:T:40:LYS:HE3	2.28	0.57
4:O:11:LEU:HD21	4:O:19:LYS:HD3	1.85	0.57
4:O:30:ASP:O	4:O:30:ASP:OD2	2.22	0.57
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.40	0.57
5:S:120:PRO:HB3	5:S:141:PHE:HB3	1.86	0.57
5:N:54:ASN:O	5:N:54:ASN:ND2	2.37	0.57
4:E:6:GLN:NE2	4:E:89:TYR:O	2.37	0.57
4:T:38:ASP:HB2	4:T:40:LYS:HG2	1.86	0.57
1:F:218:GLN:HB2	1:F:222:GLU:O	2.04	0.57
1:K:197:HIS:CD2	1:K:198:GLU:HB2	2.39	0.57
1:F:13:SER:HA	1:F:20:PRO:HB3	1.85	0.57
5:S:39:GLN:NE2	4:T:37:GLN:NE2	2.49	0.57
1:K:238:ASP:HB3	2:L:12:ARG:HD3	1.87	0.57
1:P:219:ARG:NE	1:P:256:ARG:HG2	2.20	0.57
5:S:199:THR:HB	5:S:201:PHE:CE1	2.39	0.57
1:F:264:GLU:C	1:F:266:LEU:H	2.13	0.56
1:K:258:THR:OG1	1:K:272:LEU:O	2.20	0.56
4:T:34:TRP:HB3	4:T:46:MET:HE3	1.88	0.56
5:N:53:SER:HB3	5:N:55:VAL:HG13	1.87	0.56
4:O:13:THR:OG1	4:O:19:LYS:HE2	2.05	0.56
4:O:83:LEU:HD22	4:O:83:LEU:H	1.69	0.56
4:O:94:SER:HB2	4:O:105:GLN:HG2	1.86	0.56
1:F:275:GLU:CD	1:F:275:GLU:H	2.11	0.56
1:K:219:ARG:NE	1:K:222:GLU:HG2	2.20	0.56
1:A:44:ARG:NH2	1:A:61:ASP:OD1	2.38	0.56
1:K:214:THR:HG22	1:K:262:GLN:H	1.71	0.56
1:K:259:CYS:O	1:K:272:LEU:HG	2.06	0.56
5:I:41:LEU:O	5:I:43:LYS:HG3	2.06	0.56
5:I:84:GLU:OE1	5:I:84:GLU:N	2.28	0.56
5:D:113:PRO:O	5:D:143:SER:OG	2.22	0.56
4:E:11:LEU:HD21	4:E:19:LYS:HD2	1.86	0.56
5:S:162:VAL:HG22	5:S:173:ASN:OD1	2.06	0.56
1:F:11:SER:HB3	1:F:22:PHE:HD1	1.71	0.56
1:K:258:THR:HG23	1:K:272:LEU:H	1.70	0.56
4:T:118:ASP:OD2	4:T:120:LYS:HE3	2.05	0.56
5:N:195:ILE:CD1	5:N:198:ASP:HB2	2.36	0.56
1:P:7:TYR:CE2	3:R:2:SER:HB3	2.41	0.56
4:T:225:TRP:CG	4:T:231:LYS:HB2	2.41	0.56
1:A:76:VAL:HG22	4:E:50:ASN:HD22	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3:HIS:HA	1:K:29:ASP:OD1	2.06	0.56
5:S:83:PRO:HG2	5:S:171:LYS:HZ2	1.71	0.56
5:S:174:SER:H	4:T:195:ARG:HH12	1.54	0.56
1:P:249:VAL:HB	1:P:257:TYR:CE2	2.41	0.55
5:S:113:PRO:O	5:S:143:SER:OG	2.21	0.55
4:T:118:ASP:OD1	4:T:120:LYS:HG3	2.06	0.55
5:N:62:ARG:NH2	5:N:80:GLU:HG3	2.21	0.55
1:P:195:SER:OG	1:P:196:ASP:N	2.37	0.55
5:I:144:GLN:N	5:I:144:GLN:OE1	2.39	0.55
5:S:181:LYS:HG2	5:S:184:PHE:HA	1.87	0.55
4:T:204:GLN:HA	4:T:244:ARG:O	2.06	0.55
5:I:59:LYS:NZ	5:I:64:ALA:CB	2.67	0.55
5:N:196:PRO:HD2	5:N:198:ASP:OD2	2.06	0.55
4:J:51:ASN:C	4:J:53:GLU:H	2.14	0.55
1:P:226:GLN:CG	1:P:227:ASP:N	2.65	0.55
5:I:138:PHE:HB2	5:I:190:PHE:CE2	2.41	0.55
1:K:21:ARG:HD2	1:K:39:ASP:OD2	2.07	0.55
5:S:120:PRO:HG3	5:S:141:PHE:HA	1.88	0.55
5:N:7:GLN:HE22	5:N:90:PHE:HA	1.72	0.55
1:P:226:GLN:HE22	1:P:247:VAL:CG1	2.19	0.55
5:I:92:ALA:HA	5:I:102:VAL:O	2.07	0.55
4:T:150:THR:HG22	4:T:191:ALA:HB1	1.89	0.55
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.07	0.55
1:A:258:THR:HA	1:A:273:ARG:CG	2.32	0.55
5:D:48:ILE:HG13	5:D:49:ILE:HG22	1.88	0.55
1:K:214:THR:CG2	1:K:262:GLN:HG2	2.31	0.55
1:A:258:THR:HG22	1:A:273:ARG:HE	1.72	0.55
1:K:195:SER:HB3	1:K:198:GLU:H	1.70	0.55
1:K:219:ARG:HG2	1:K:222:GLU:N	2.14	0.55
5:D:152:ASP:OD1	5:D:154:ASP:N	2.37	0.55
4:E:177:GLN:HG2	4:E:178:PRO:HD2	1.87	0.55
4:O:32:MET:HB2	4:O:74:LEU:HD22	1.89	0.55
5:I:29:SER:HB2	5:I:72:LYS:HD3	1.90	0.54
5:I:180:ASN:O	5:I:182:SER:N	2.40	0.54
4:E:150:THR:HG22	4:E:191:ALA:HB1	1.88	0.54
2:B:74:GLU:HG2	2:B:75:LYS:N	2.22	0.54
2:G:47:GLU:CD	1:P:44:ARG:HH12	2.15	0.54
5:I:65:VAL:HA	5:I:75:SER:O	2.08	0.54
5:I:149:GLN:HG2	5:I:150:SER:H	1.71	0.54
1:K:127:LYS:HZ3	1:K:132:SER:CB	2.20	0.54
2:Q:21:ASN:O	2:Q:69:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:40:LYS:HZ3	4:T:41:LYS:C	2.15	0.54
1:A:196:ASP:OD1	1:A:197:HIS:N	2.40	0.54
1:K:150:ALA:HA	5:N:52:ARG:HH21	1.73	0.54
1:K:219:ARG:CG	1:K:222:GLU:H	2.15	0.54
5:N:66:THR:OG1	5:N:75:SER:HB2	2.07	0.54
1:F:189:MET:SD	1:F:217:TRP:HH2	2.31	0.54
1:K:218:GLN:HG3	1:K:222:GLU:O	2.07	0.54
1:P:21:ARG:NH1	1:P:39:ASP:HB2	2.23	0.54
4:J:94:SER:HB2	4:J:105:GLN:HG2	1.90	0.54
4:E:82:GLU:HB3	4:E:85:ASP:OD2	2.07	0.54
5:S:67:LEU:HD21	5:S:69:LYS:HE3	1.89	0.54
5:S:195:ILE:CD1	5:S:196:PRO:HD3	2.37	0.54
4:E:85:ASP:O	4:E:87:ALA:N	2.41	0.54
5:S:45:PRO:HG2	4:T:43:LEU:HD21	1.90	0.54
1:A:13:SER:HG	1:A:93:HIS:H	1.54	0.54
5:N:141:PHE:CD1	5:N:145:THR:HB	2.43	0.54
1:A:106:ASP:OD1	1:A:106:ASP:N	2.40	0.54
1:P:151:HIS:ND1	5:S:53:SER:HB3	2.22	0.54
5:S:10:SER:O	5:S:108:ARG:N	2.33	0.54
5:S:163:LEU:HB3	4:T:173:CYS:HB2	1.89	0.54
1:F:27:TYR:CE1	1:F:32:GLN:HG3	2.43	0.53
1:F:215:LEU:HD22	1:F:261:VAL:HG22	1.91	0.53
1:P:177:GLU:O	1:P:181:ARG:HB3	2.08	0.53
1:P:234:ARG:HD2	2:Q:10:TYR:CE1	2.44	0.53
5:D:126:ARG:HH21	5:D:134:SER:HG	1.56	0.53
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.91	0.53
1:P:109:PHE:HD1	1:P:165:VAL:HG11	1.71	0.53
5:I:92:ALA:HB2	5:I:103:PHE:CD2	2.43	0.53
4:E:51:ASN:C	4:E:53:GLU:H	2.16	0.53
4:T:50:ASN:ND2	4:T:51:ASN:OD1	2.41	0.53
1:F:111:ARG:HB2	1:F:111:ARG:NH1	2.23	0.53
1:K:97:ARG:NH1	1:K:116:TYR:HE2	2.07	0.53
5:I:133:LYS:HZ1	5:I:180:ASN:N	2.06	0.53
5:D:127:ASP:CB	5:D:129:LYS:HD3	2.37	0.53
4:O:34:TRP:HE1	4:O:74:LEU:HG	1.73	0.53
1:F:275:GLU:OE1	1:F:275:GLU:N	2.36	0.53
5:N:83:PRO:HG2	5:N:171:LYS:HZ1	1.73	0.53
4:O:57:ASN:OD1	4:O:60:VAL:HG11	2.08	0.53
2:B:70:PHE:HD2	2:B:78:TYR:CZ	2.26	0.53
1:K:80:THR:HG21	3:M:9:VAL:OXT	2.07	0.53
5:I:186:CYS:HA	5:I:189:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:194:ILE:HG22	5:S:195:ILE:H	1.74	0.53
4:J:64:PHE:CD1	4:J:78:ILE:HG23	2.44	0.53
1:K:189:MET:HG3	1:K:272:LEU:HD13	1.91	0.53
4:J:141:GLN:C	4:J:200:ALA:HB2	2.34	0.53
1:K:73:THR:HG21	3:M:6:ILE:HG13	1.90	0.53
5:D:165:MET:SD	4:E:197:ARG:HD3	2.48	0.53
1:A:19:GLU:HG2	1:A:75:ARG:HH12	1.74	0.53
1:A:75:ARG:HH21	4:E:55:ILE:HD13	1.74	0.53
1:K:200:THR:O	1:K:201:LEU:HB3	2.08	0.53
5:I:6:GLU:HB2	5:I:25:THR:OG1	2.09	0.53
5:S:194:ILE:HG22	5:S:195:ILE:N	2.24	0.53
1:A:219:ARG:HD3	1:A:222:GLU:N	2.24	0.53
2:B:95:TRP:CD1	2:B:96:ASP:H	2.27	0.53
1:K:219:ARG:HG2	1:K:221:GLY:H	1.73	0.53
4:T:83:LEU:HD22	4:T:83:LEU:H	1.73	0.53
4:O:38:ASP:OD1	4:O:40:LYS:HG2	2.09	0.53
1:P:6:ARG:HG2	1:P:113:TYR:HE1	1.74	0.52
1:P:21:ARG:HH12	1:P:39:ASP:HB2	1.73	0.52
5:S:118:PRO:C	5:S:120:PRO:HD3	2.34	0.52
1:A:162:GLY:O	1:A:165:VAL:HG22	2.10	0.52
1:K:219:ARG:HE	1:K:222:GLU:HG2	1.75	0.52
5:S:120:PRO:HB2	5:S:195:ILE:HD11	1.90	0.52
4:T:40:LYS:HE2	4:T:42:PHE:HB3	1.91	0.52
4:O:38:ASP:CG	4:O:40:LYS:HG2	2.34	0.52
4:J:38:ASP:C	4:J:40:LYS:H	2.16	0.52
1:K:21:ARG:NH1	1:K:23:ILE:HD11	2.24	0.52
1:K:81:LEU:HD11	3:M:9:VAL:HG21	1.91	0.52
4:J:32:MET:HB2	4:J:74:LEU:HD22	1.90	0.52
2:Q:25:CYS:HB2	2:Q:39:LEU:HD21	1.91	0.52
5:I:120:PRO:HB3	5:I:141:PHE:HB3	1.92	0.52
1:A:162:GLY:O	1:A:166:GLU:HG3	2.10	0.52
4:J:18:ASP:HA	4:J:79:ASN:OD1	2.10	0.52
5:D:53:SER:O	5:D:54:ASN:HB2	2.09	0.52
4:O:219:LEU:O	4:O:233:VAL:HA	2.09	0.52
1:K:258:THR:HG22	1:K:258:THR:O	2.08	0.52
5:D:195:ILE:HG23	5:D:196:PRO:HD2	1.92	0.52
4:O:35:TYR:OH	4:O:105:GLN:OE1	2.26	0.52
1:A:44:ARG:NH1	2:L:47:GLU:CD	2.67	0.52
1:F:11:SER:HA	1:F:21:ARG:O	2.10	0.52
2:G:54:LEU:HD11	2:G:62:PHE:HB3	1.92	0.52
1:P:201:LEU:HD12	1:P:249:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:4:VAL:HG22	4:E:25:GLN:HB3	1.92	0.52
1:F:19:GLU:HG2	1:F:75:ARG:NH1	2.25	0.51
1:P:263:HIS:ND1	1:P:264:GLU:O	2.34	0.51
4:O:153:TYR:HB2	4:O:189:ARG:HA	1.92	0.51
4:O:230:ALA:O	4:O:231:LYS:HB3	2.09	0.51
4:J:76:LEU:HD21	4:J:78:ILE:HD11	1.92	0.51
1:K:216:THR:HG23	1:K:260:HIS:HB2	1.92	0.51
5:N:118:PRO:C	5:N:120:PRO:HD3	2.35	0.51
1:A:47:PRO:O	1:A:48:ARG:HD3	2.11	0.51
1:A:189:MET:SD	1:A:274:TRP:HB2	2.50	0.51
1:F:62:GLY:O	1:F:65:ARG:HB3	2.10	0.51
4:J:195:ARG:NH1	5:I:174:SER:CB	2.73	0.51
5:D:170:PHE:CD2	4:E:142:LYS:HE2	2.44	0.51
5:S:196:PRO:HD2	5:S:198:ASP:H	1.74	0.51
2:B:45:ARG:HG2	2:B:45:ARG:NH1	2.21	0.51
1:K:217:TRP:CE3	1:K:218:GLN:HB2	2.46	0.51
1:P:22:PHE:CE2	1:P:71:SER:HB3	2.45	0.51
5:I:28:ASP:O	5:I:30:ALA:N	2.39	0.51
4:J:34:TRP:HB3	4:J:46:MET:HE3	1.91	0.51
1:K:219:ARG:CB	1:K:222:GLU:HG2	2.40	0.51
5:D:127:ASP:O	5:D:128:SER:OG	2.24	0.51
5:D:191:ASN:OD1	5:D:192:ASN:N	2.43	0.51
5:N:47:LEU:HD22	4:O:104:GLU:HB2	1.90	0.51
1:K:250:PRO:HB2	1:K:253:GLN:HG2	1.91	0.51
4:T:221:GLU:O	4:T:222:ASN:ND2	2.44	0.51
5:N:135:VAL:HG12	5:N:178:TRP:HB3	1.93	0.51
1:A:144:LYS:O	1:A:148:GLU:HG3	2.10	0.51
1:F:249:VAL:HG12	1:F:250:PRO:O	2.11	0.51
1:K:3:HIS:HB2	1:K:103:VAL:HG22	1.93	0.51
5:D:192:ASN:ND2	5:D:192:ASN:H	2.09	0.51
4:T:231:LYS:HE3	4:T:233:VAL:HG22	1.91	0.51
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.93	0.51
5:I:121:ALA:HA	5:I:199:THR:HG22	1.92	0.51
1:A:186:LYS:HE2	1:A:207:SER:HB2	1.91	0.51
1:F:74:HIS:CD2	1:F:95:VAL:HG11	2.45	0.51
1:P:226:GLN:O	1:P:227:ASP:OD1	2.28	0.51
5:D:174:SER:CB	4:E:195:ARG:NH1	2.74	0.51
5:S:126:ARG:NE	5:S:133:LYS:HZ1	2.08	0.51
4:E:23:CYS:SG	4:E:24:GLU:N	2.83	0.51
4:E:120:LYS:NZ	4:E:226:THR:O	2.27	0.51
4:T:32:MET:HB2	4:T:74:LEU:HD22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:163:VAL:HB	4:T:168:VAL:HG21	1.93	0.51
5:N:159:ASP:OD1	5:N:160:LYS:N	2.44	0.51
5:I:122:VAL:HA	5:I:137:LEU:O	2.10	0.50
5:N:35:PRO:HG2	5:N:92:ALA:HB3	1.93	0.50
1:F:254:GLU:HB3	1:F:274:TRP:HD1	1.75	0.50
1:A:81:LEU:HD11	3:C:9:VAL:HG21	1.94	0.50
4:J:14:GLN:NE2	4:J:116:LEU:O	2.43	0.50
5:D:132:ASP:OD2	5:D:180:ASN:OD1	2.28	0.50
1:F:80:THR:HG21	3:H:9:VAL:OXT	2.11	0.50
5:I:15:GLN:HB2	5:I:18:ASP:OD2	2.12	0.50
5:I:194:ILE:HG22	5:I:195:ILE:N	2.26	0.50
5:D:194:ILE:HD13	5:D:197:GLU:HB2	1.93	0.50
1:F:217:TRP:CZ3	1:F:259:CYS:HB2	2.46	0.50
5:I:7:GLN:HE22	5:I:90:PHE:HA	1.76	0.50
4:T:38:ASP:HB2	4:T:40:LYS:HE3	1.92	0.50
1:K:191:HIS:CD2	1:K:192:HIS:N	2.80	0.50
5:N:33:TYR:CZ	4:O:103:ASN:HB3	2.47	0.50
1:A:255:GLN:O	1:A:273:ARG:NH2	2.44	0.50
1:K:119:ASP:HB3	2:L:0:MET:HA	1.93	0.50
3:M:6:ILE:HD12	3:M:7:PRO:HD2	1.92	0.50
5:S:129:LYS:HD2	5:S:129:LYS:N	2.25	0.50
1:F:194:VAL:HG23	1:F:195:SER:HB3	1.94	0.50
5:D:36:TRP:CE2	5:D:76:LEU:HB2	2.47	0.50
1:P:13:SER:HG	1:P:93:HIS:H	1.52	0.49
1:P:254:GLU:HB3	1:P:274:TRP:HD1	1.77	0.49
1:K:21:ARG:NH1	1:K:37:ASP:OD1	2.43	0.49
1:K:253:GLN:O	1:K:257:TYR:HD2	1.95	0.49
1:P:8:PHE:CE2	1:P:98:MET:HG3	2.47	0.49
5:D:194:ILE:HB	5:D:197:GLU:OE1	2.12	0.49
5:N:170:PHE:CD2	4:O:142:LYS:HE2	2.46	0.49
4:O:34:TRP:HB3	4:O:46:MET:HE3	1.94	0.49
4:O:118:ASP:OD1	4:O:120:LYS:HG2	2.13	0.49
1:F:230:LEU:HD12	1:F:245:ALA:HB2	1.94	0.49
2:Q:51:HIS:HA	2:Q:65:LEU:O	2.12	0.49
5:I:7:GLN:NE2	5:I:89:TYR:O	2.45	0.49
5:I:86:SER:HG	5:I:111:ILE:H	1.57	0.49
4:T:96:LEU:HA	4:T:100:PRO:HB3	1.95	0.49
1:A:256:ARG:O	1:A:257:TYR:HD1	1.95	0.49
5:I:7:GLN:HB2	5:I:104:GLY:HA3	1.93	0.49
4:T:83:LEU:HA	4:T:115:VAL:HG23	1.94	0.49
2:B:40:LEU:N	2:B:79:ALA:O	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:SER:OG	1:F:93:HIS:N	2.40	0.49
5:D:156:TYR:O	5:D:177:ALA:HA	2.13	0.49
4:E:50:ASN:O	4:E:53:GLU:HB2	2.12	0.49
4:T:125:PRO:HB3	4:T:152:PHE:HB3	1.94	0.49
5:N:83:PRO:HG2	5:N:171:LYS:HZ3	1.74	0.49
1:P:224:GLN:HG2	1:P:226:GLN:CB	2.43	0.49
1:P:226:GLN:CG	1:P:227:ASP:HB2	2.43	0.49
1:P:227:ASP:OD2	1:P:248:VAL:CG1	2.61	0.49
4:E:204:GLN:HA	4:E:244:ARG:O	2.12	0.49
5:S:126:ARG:CZ	5:S:133:LYS:NZ	2.76	0.49
4:O:34:TRP:NE1	4:O:74:LEU:HG	2.27	0.49
1:A:201:LEU:HB2	1:A:247:VAL:HG23	1.95	0.49
1:K:231:VAL:HG22	1:K:244:TRP:O	2.13	0.49
2:L:15:ALA:O	2:L:97:ARG:NH1	2.40	0.49
5:D:195:ILE:HG23	5:D:196:PRO:CD	2.43	0.49
5:N:47:LEU:HD22	4:O:104:GLU:CB	2.43	0.49
5:I:150:SER:O	5:I:151:LYS:HG3	2.13	0.49
5:D:183:ASP:OD1	5:D:183:ASP:O	2.31	0.49
5:S:195:ILE:CD1	5:S:199:THR:HG23	2.41	0.49
5:N:126:ARG:CZ	5:N:133:LYS:HA	2.43	0.49
4:O:25:GLN:HG2	4:O:27:LEU:H	1.78	0.49
1:A:219:ARG:HH11	1:A:222:GLU:CB	2.19	0.49
1:F:122:ASP:CG	2:G:60:TRP:HE1	2.21	0.49
1:K:4:SER:O	1:K:28:VAL:HA	2.13	0.49
1:F:64:THR:O	1:F:67:VAL:HG12	2.13	0.49
1:P:21:ARG:NH1	1:P:39:ASP:CG	2.71	0.49
4:T:51:ASN:ND2	4:T:71:LYS:HD3	2.28	0.49
4:O:64:PHE:CE1	4:O:78:ILE:HD13	2.46	0.49
1:F:273:ARG:HB3	1:F:273:ARG:NH1	2.28	0.48
2:G:47:GLU:CD	1:P:44:ARG:NH1	2.70	0.48
1:K:217:TRP:CH2	1:K:257:TYR:HA	2.46	0.48
5:S:156:TYR:O	5:S:177:ALA:HA	2.12	0.48
1:A:75:ARG:NH2	4:E:54:LEU:O	2.46	0.48
1:F:192:HIS:HB2	1:F:200:THR:CG2	2.42	0.48
2:G:36:GLU:HB3	2:G:83:ASN:HB3	1.95	0.48
5:I:150:SER:OG	5:I:157:ILE:HG13	2.13	0.48
5:D:163:LEU:HB3	4:E:173:CYS:HB2	1.94	0.48
4:T:31:THR:HA	4:T:49:TYR:O	2.13	0.48
4:T:156:HIS:HB3	4:T:217:TYR:HB2	1.94	0.48
5:N:126:ARG:CG	5:N:127:ASP:N	2.76	0.48
1:A:228:THR:HA	1:A:246:ALA:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:11:SER:HA	1:K:21:ARG:O	2.14	0.48
1:K:97:ARG:NH1	3:M:6:ILE:HD11	2.28	0.48
1:P:22:PHE:CD2	1:P:71:SER:HB3	2.49	0.48
2:Q:36:GLU:HB3	2:Q:83:ASN:HB3	1.95	0.48
1:A:228:THR:HG23	1:A:228:THR:O	2.13	0.48
4:J:60:VAL:O	4:J:62:ASN:ND2	2.46	0.48
1:K:219:ARG:HE	1:K:222:GLU:CD	2.22	0.48
5:I:120:PRO:HG3	5:I:141:PHE:HA	1.95	0.48
5:D:35:PRO:HD2	5:D:92:ALA:O	2.14	0.48
5:S:195:ILE:HD12	5:S:196:PRO:HD2	1.96	0.48
4:T:49:TYR:OH	4:T:54:LEU:HD12	2.13	0.48
5:N:132:ASP:OD2	5:N:180:ASN:HA	2.13	0.48
1:K:213:ILE:CG1	1:K:263:HIS:HD2	2.27	0.48
5:D:4:ASN:OD1	5:D:5:VAL:N	2.47	0.48
5:D:194:ILE:HB	5:D:197:GLU:CD	2.38	0.48
4:E:227:GLN:HG2	4:E:228:ASP:N	2.29	0.48
5:N:14:VAL:HG21	5:N:20:ALA:HB2	1.94	0.48
1:F:7:TYR:HB3	1:F:9:PHE:CE1	2.48	0.48
1:F:256:ARG:HG2	1:F:256:ARG:O	2.14	0.48
1:P:81:LEU:HD13	1:P:118:TYR:CD1	2.49	0.48
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.49	0.48
1:F:193:ALA:O	1:F:199:ALA:HA	2.14	0.48
4:J:154:PRO:HG2	4:J:156:HIS:CD2	2.48	0.48
5:N:29:SER:C	5:N:31:SER:N	2.72	0.48
1:F:75:ARG:NH1	4:J:53:GLU:OE2	2.47	0.48
5:D:126:ARG:CG	5:D:127:ASP:H	2.25	0.48
4:E:226:THR:O	4:E:227:GLN:HB2	2.14	0.48
5:S:39:GLN:HE22	4:T:37:GLN:NE2	2.10	0.48
1:A:235:PRO:O	2:B:10:TYR:OH	2.22	0.48
4:J:31:THR:OG1	4:J:50:ASN:ND2	2.46	0.48
5:N:7:GLN:NE2	5:N:106:GLY:HA2	2.28	0.48
5:N:54:ASN:C	5:N:54:ASN:ND2	2.66	0.48
5:N:126:ARG:NH2	5:N:129:LYS:HG3	2.29	0.48
1:A:219:ARG:N	1:A:223:ASP:O	2.34	0.47
1:A:236:ALA:O	2:B:24:ASN:ND2	2.44	0.47
4:J:14:GLN:NE2	4:J:117:GLU:C	2.68	0.47
4:J:16:GLY:HA2	4:J:80:SER:HA	1.96	0.47
4:J:76:LEU:HG	4:J:78:ILE:HG13	1.96	0.47
1:K:219:ARG:CG	1:K:221:GLY:H	2.27	0.47
1:A:21:ARG:CZ	1:A:23:ILE:HD11	2.43	0.47
2:B:19:LYS:HA	2:B:19:LYS:HD2	1.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:120:PRO:CB	5:I:195:ILE:HG12	2.43	0.47
5:D:34:PHE:HB2	5:D:51:ILE:HG22	1.95	0.47
4:E:122:VAL:HG13	4:E:153:TYR:O	2.13	0.47
5:N:23:LYS:HD2	5:N:75:SER:OG	2.14	0.47
1:A:62:GLY:O	1:A:66:LYS:HG3	2.14	0.47
1:A:257:TYR:N	1:A:273:ARG:NH1	2.56	0.47
1:F:49:ALA:O	1:F:52:ILE:HG22	2.14	0.47
5:D:41:LEU:O	5:D:43:LYS:HG3	2.13	0.47
4:O:154:PRO:HG2	4:O:156:HIS:CD2	2.49	0.47
1:F:218:GLN:HB3	1:F:223:ASP:HA	1.95	0.47
2:G:37:VAL:HG22	2:G:82:VAL:HG22	1.96	0.47
1:K:259:CYS:HB3	1:K:272:LEU:HD11	1.95	0.47
1:P:144:LYS:O	1:P:148:GLU:HG3	2.15	0.47
4:E:1:ASP:OD1	4:E:2:THR:N	2.47	0.47
4:T:60:VAL:HG22	4:T:62:ASN:HA	1.96	0.47
4:T:129:VAL:HG23	4:T:239:ALA:CB	2.45	0.47
4:J:156:HIS:HB3	4:J:217:TYR:HB2	1.96	0.47
4:E:177:GLN:HG2	4:E:178:PRO:CD	2.45	0.47
1:K:9:PHE:HE2	1:K:67:VAL:HG23	1.80	0.47
1:K:159:TYR:HA	1:K:163:THR:CG2	2.44	0.47
5:D:152:ASP:HB3	5:D:155:VAL:HB	1.97	0.47
5:N:3:GLU:O	5:N:4:ASN:HB3	2.13	0.47
4:O:25:GLN:NE2	4:O:28:GLY:O	2.48	0.47
1:A:186:LYS:HE2	1:A:207:SER:CB	2.45	0.47
1:A:254:GLU:HG2	1:A:274:TRP:CZ3	2.50	0.47
1:A:274:TRP:CZ2	1:F:274:TRP:CZ2	3.03	0.47
1:F:191:HIS:NE2	1:F:199:ALA:HB1	2.30	0.47
1:F:255:GLN:CA	1:F:273:ARG:HH22	2.28	0.47
1:K:35:ARG:HD2	2:L:53:ASP:OD1	2.15	0.47
2:L:51:HIS:HB3	2:L:66:TYR:CD2	2.50	0.47
1:P:74:HIS:NE2	1:P:97:ARG:NH1	2.62	0.47
5:I:194:ILE:H	5:I:194:ILE:HG13	1.44	0.47
5:D:179:SER:HB3	5:D:184:PHE:CD1	2.49	0.47
4:E:15:MET:HE3	4:E:117:GLU:HB2	1.96	0.47
4:T:44:LYS:HE3	4:T:45:ILE:O	2.14	0.47
4:O:204:GLN:HA	4:O:244:ARG:O	2.15	0.47
1:A:258:THR:HG22	1:A:273:ARG:HB2	1.97	0.47
2:B:95:TRP:CD1	2:B:96:ASP:N	2.82	0.47
5:D:121:ALA:N	5:D:199:THR:HG22	2.29	0.47
5:D:132:ASP:CG	5:D:133:LYS:H	2.15	0.47
2:L:95:TRP:CD1	2:L:96:ASP:H	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:25:THR:HG22	5:S:73:HIS:HB3	1.96	0.47
5:S:41:LEU:O	5:S:43:LYS:HG3	2.15	0.47
5:N:126:ARG:HH12	5:N:129:LYS:NZ	2.12	0.47
1:A:123:TYR:HD2	1:A:124:ILE:HG22	1.79	0.47
4:J:221:GLU:OE1	4:J:221:GLU:HA	2.15	0.47
5:D:120:PRO:HG2	5:D:195:ILE:HG21	1.96	0.47
4:E:225:TRP:HE1	4:E:229:ARG:HB2	1.79	0.47
2:B:48:LYS:CE	1:K:47:PRO:HG2	2.43	0.46
2:B:81:ARG:HG3	2:B:92:ILE:HG12	1.96	0.46
1:P:264:GLU:C	1:P:266:LEU:H	2.23	0.46
4:O:24:GLU:HG2	4:O:25:GLN:N	2.29	0.46
1:A:191:HIS:CD2	1:A:274:TRP:CH2	3.03	0.46
4:J:229:ARG:HG3	4:J:230:ALA:N	2.30	0.46
1:K:214:THR:O	1:K:215:LEU:HD23	2.15	0.46
1:K:260:HIS:CD2	1:K:271:THR:HG23	2.50	0.46
1:K:13:SER:OG	1:K:93:HIS:N	2.38	0.46
4:E:32:MET:HB3	4:E:32:MET:HE2	1.60	0.46
4:E:96:LEU:HA	4:E:100:PRO:HB3	1.96	0.46
5:S:35:PRO:HG2	5:S:92:ALA:HB3	1.98	0.46
5:N:120:PRO:HG3	5:N:141:PHE:HA	1.98	0.46
4:O:76:LEU:HD21	4:O:78:ILE:HD11	1.97	0.46
1:P:138:MET:HA	1:P:138:MET:HE2	1.97	0.46
4:T:147:CYS:HB2	4:T:161:TRP:CZ2	2.50	0.46
5:D:120:PRO:O	5:D:199:THR:HA	2.16	0.46
5:S:161:CYS:HB3	4:T:195:ARG:NH1	2.30	0.46
4:T:226:THR:O	4:T:227:GLN:HB2	2.16	0.46
1:A:255:GLN:CA	1:A:273:ARG:HH12	2.29	0.46
4:J:143:ALA:HB3	4:J:198:VAL:HG23	1.97	0.46
5:D:14:VAL:HG11	5:D:81:THR:HG21	1.97	0.46
1:F:21:ARG:HH11	1:F:21:ARG:HG3	1.81	0.46
1:F:227:ASP:O	1:F:229:GLU:N	2.49	0.46
4:J:19:LYS:HD3	4:J:19:LYS:HA	1.76	0.46
4:J:64:PHE:CE1	4:J:78:ILE:HD13	2.51	0.46
1:K:226:GLN:HB3	1:K:248:VAL:HG21	1.96	0.46
1:F:206:LEU:HG	1:F:242:GLN:HG2	1.98	0.46
1:K:74:HIS:CD2	1:K:95:VAL:HG11	2.49	0.46
1:P:223:ASP:O	1:P:224:GLN:HB2	2.15	0.46
1:A:65:ARG:NH1	5:D:95:ARG:CZ	2.79	0.46
1:F:75:ARG:NH1	4:J:53:GLU:OE1	2.49	0.46
1:F:257:TYR:O	1:F:273:ARG:NH1	2.48	0.46
4:T:30:ASP:HB3	4:T:31:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:THR:HG22	1:F:273:ARG:CD	2.46	0.46
2:G:5:PRO:HA	2:G:30:PHE:HB3	1.98	0.46
4:J:142:LYS:HE2	5:I:170:PHE:CD2	2.51	0.46
5:I:92:ALA:HB2	5:I:103:PHE:CE2	2.51	0.46
4:O:121:ASN:ND2	4:O:187:ASP:HB3	2.31	0.46
1:K:116:TYR:CE1	3:M:9:VAL:HG11	2.50	0.45
5:S:165:MET:SD	4:T:197:ARG:HD3	2.56	0.45
5:N:97:GLY:HA2	4:O:100:PRO:CD	2.43	0.45
5:N:152:ASP:OD1	5:N:155:VAL:N	2.49	0.45
1:A:60:TRP:CD1	2:L:47:GLU:HG3	2.51	0.45
4:J:46:MET:HE1	4:J:89:TYR:HD2	1.82	0.45
1:K:260:HIS:HA	1:K:270:LEU:O	2.16	0.45
1:K:264:GLU:C	1:K:266:LEU:H	2.25	0.45
1:P:270:LEU:HA	1:P:270:LEU:HD12	1.56	0.45
5:S:174:SER:C	4:T:195:ARG:NH1	2.74	0.45
4:T:162:TRP:NE1	4:T:213:GLN:OE1	2.49	0.45
1:A:116:TYR:CE1	3:C:9:VAL:HG11	2.52	0.45
1:F:238:ASP:HB3	2:G:12:ARG:HD3	1.99	0.45
1:P:219:ARG:HD2	1:P:257:TYR:CD1	2.50	0.45
5:I:182:SER:C	5:I:184:PHE:H	2.23	0.45
4:O:23:CYS:SG	4:O:24:GLU:N	2.89	0.45
4:O:215:GLN:HG2	4:O:217:TYR:CE1	2.51	0.45
4:O:229:ARG:O	4:O:231:LYS:N	2.41	0.45
1:A:254:GLU:HG2	1:A:274:TRP:HZ3	1.81	0.45
1:F:75:ARG:NH1	4:J:53:GLU:CD	2.74	0.45
2:G:95:TRP:CD1	2:G:96:ASP:H	2.34	0.45
1:K:138:MET:HA	1:K:138:MET:HE2	1.97	0.45
1:K:185:PRO:HG2	1:K:266:LEU:HD11	1.98	0.45
5:D:33:TYR:CZ	4:E:103:ASN:HB3	2.51	0.45
5:D:118:PRO:HB3	5:D:142:ASP:HB3	1.98	0.45
4:T:6:GLN:NE2	4:T:91:CYS:H	2.14	0.45
4:J:83:LEU:HA	4:J:115:VAL:HG23	1.99	0.45
5:S:62:ARG:NH2	5:S:85:ASP:OD2	2.38	0.45
1:F:273:ARG:HB3	1:F:273:ARG:CZ	2.46	0.45
1:P:217:TRP:CG	1:P:247:VAL:HG13	2.52	0.45
5:D:11:THR:HG22	5:D:108:ARG:HB3	1.98	0.45
4:O:118:ASP:CG	4:O:120:LYS:HG2	2.41	0.45
4:O:181:GLU:OE2	4:O:189:ARG:HB2	2.17	0.45
1:A:13:SER:HA	1:A:20:PRO:HB3	1.99	0.45
1:A:200:THR:HA	1:A:248:VAL:HA	1.97	0.45
1:F:191:HIS:HB2	1:F:274:TRP:CZ2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:156:LEU:O	1:K:159:TYR:HB3	2.16	0.45
1:K:185:PRO:HD2	1:K:266:LEU:HG	1.97	0.45
1:K:202:ARG:HG2	1:K:204:TRP:CD1	2.51	0.45
1:P:219:ARG:HE	1:P:257:TYR:N	2.15	0.45
5:S:92:ALA:HA	5:S:102:VAL:O	2.16	0.45
5:N:19:SER:OG	5:N:79:THR:HA	2.16	0.45
1:P:66:LYS:O	1:P:70:HIS:ND1	2.27	0.45
1:P:129:ASP:O	1:P:131:ARG:NE	2.49	0.45
1:P:130:LEU:O	1:P:157:ARG:HD2	2.17	0.45
1:P:162:GLY:O	1:P:166:GLU:HG3	2.16	0.45
2:Q:5:PRO:CA	2:Q:30:PHE:HB3	2.47	0.45
1:A:111:ARG:NH2	1:A:128:GLU:CD	2.75	0.45
1:A:225:THR:HG22	1:A:225:THR:O	2.17	0.45
4:J:159:LEU:C	4:J:159:LEU:HD23	2.42	0.45
1:K:217:TRP:HZ2	1:K:257:TYR:HA	1.71	0.45
2:Q:51:HIS:HB3	2:Q:66:TYR:CD2	2.52	0.45
5:S:174:SER:O	4:T:195:ARG:NH1	2.49	0.45
4:T:39:SER:C	4:T:40:LYS:HG2	2.42	0.45
1:F:20:PRO:CD	1:F:75:ARG:HD3	2.45	0.45
1:F:66:LYS:HE2	3:H:1:PHE:CZ	2.52	0.45
1:F:258:THR:HA	1:F:273:ARG:HD2	1.93	0.45
2:L:55:SER:HB3	2:L:63:TYR:CZ	2.52	0.45
1:F:8:PHE:HB2	1:F:25:VAL:HG22	1.98	0.44
1:F:157:ARG:NH1	1:F:161:GLU:OE1	2.50	0.44
5:I:59:LYS:CG	5:I:64:ALA:HB2	2.47	0.44
5:I:127:ASP:C	5:I:128:SER:HG	2.17	0.44
4:E:156:HIS:HB3	4:E:217:TYR:HB2	1.98	0.44
5:S:92:ALA:HB2	5:S:103:PHE:CE1	2.52	0.44
4:T:227:GLN:OE1	4:T:228:ASP:N	2.50	0.44
5:N:196:PRO:CD	5:N:198:ASP:OD2	2.65	0.44
3:R:5:TYR:C	3:R:6:ILE:HG13	2.41	0.44
5:I:113:PRO:HG2	5:I:115:ILE:HD11	1.99	0.44
5:D:155:VAL:HA	5:D:179:SER:HB2	1.99	0.44
4:O:83:LEU:HA	4:O:115:VAL:HG23	2.00	0.44
4:O:125:PRO:HB3	4:O:152:PHE:CD1	2.52	0.44
4:O:180:LYS:HE3	4:O:183:PRO:HA	1.99	0.44
1:K:130:LEU:O	1:K:157:ARG:HD2	2.16	0.44
1:P:74:HIS:HD2	1:P:95:VAL:HG11	1.83	0.44
5:I:74:PHE:CZ	5:I:91:CYS:HB2	2.51	0.44
5:D:95:ARG:HD3	5:D:99:GLN:OE1	2.18	0.44
5:D:174:SER:HB3	4:E:195:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:133:SER:O	4:E:137:ILE:HG13	2.17	0.44
4:T:51:ASN:C	4:T:53:GLU:H	2.24	0.44
4:O:32:MET:HE2	4:O:32:MET:HB3	1.77	0.44
1:K:236:ALA:HB3	1:K:238:ASP:OD1	2.18	0.44
5:I:149:GLN:CG	5:I:150:SER:H	2.30	0.44
4:O:156:HIS:HB3	4:O:217:TYR:HB2	1.99	0.44
1:A:11:SER:HB3	1:A:22:PHE:HD1	1.82	0.44
1:A:194:VAL:HG22	1:A:195:SER:H	1.83	0.44
1:K:193:ALA:O	1:K:194:VAL:HG22	2.18	0.44
5:N:50:ASP:OD1	5:N:50:ASP:N	2.50	0.44
4:O:34:TRP:CD1	4:O:74:LEU:HD21	2.52	0.44
1:A:111:ARG:HH21	1:A:128:GLU:CD	2.22	0.44
2:B:74:GLU:CD	2:B:74:GLU:H	2.25	0.44
1:F:205:ALA:C	1:F:206:LEU:HD12	2.43	0.44
5:D:120:PRO:HG3	5:D:141:PHE:HA	2.00	0.44
5:S:174:SER:CA	4:T:195:ARG:NH1	2.79	0.44
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.98	0.44
2:B:27[A]:VAL:HG23	2:B:64:LEU:HB2	1.99	0.44
3:H:4:GLU:HB2	5:I:30:ALA:HB1	2.00	0.44
1:P:6:ARG:HG2	1:P:113:TYR:CE1	2.53	0.44
4:T:19:LYS:HD3	4:T:19:LYS:HA	1.72	0.44
5:N:139:THR:HG23	5:N:140:ASP:CG	2.43	0.44
4:O:63:ARG:HB3	4:O:79:ASN:O	2.18	0.44
4:J:38:ASP:OD1	4:J:40:LYS:HG3	2.17	0.44
1:P:219:ARG:CZ	1:P:257:TYR:CE2	3.01	0.44
5:D:118:PRO:C	5:D:120:PRO:HD3	2.43	0.44
4:T:63:ARG:CZ	4:T:82:GLU:OE2	2.65	0.44
5:N:126:ARG:HG2	5:N:127:ASP:N	2.29	0.44
4:J:231:LYS:HA	4:J:232:PRO:HD3	1.86	0.44
1:K:217:TRP:CE3	1:K:258:THR:O	2.71	0.44
1:P:128:GLU:N	1:P:128:GLU:OE1	2.50	0.44
5:D:130:SER:O	5:D:131:SER:CB	2.66	0.44
4:E:57:ASN:HD21	4:E:60:VAL:HG11	1.82	0.44
4:E:83:LEU:O	4:E:83:LEU:HG	2.17	0.44
5:N:132:ASP:OD2	5:N:180:ASN:CG	2.61	0.44
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.53	0.43
4:J:6:GLN:HE22	4:J:110:GLY:HA2	1.83	0.43
1:K:250:PRO:CG	1:K:253:GLN:HG2	2.46	0.43
5:D:196:PRO:HD2	5:D:198:ASP:H	1.82	0.43
5:N:62:ARG:HB2	5:N:80:GLU:OE2	2.17	0.43
5:N:94:SER:HB2	5:N:101:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:29:HIS:HA	4:O:95:GLN:OE1	2.17	0.43
1:A:260:HIS:CD2	1:A:271:THR:HG23	2.53	0.43
1:F:217:TRP:HE1	1:F:245:ALA:C	2.27	0.43
4:J:38:ASP:C	4:J:40:LYS:N	2.76	0.43
1:K:178:THR:O	1:K:181:ARG:NH1	2.45	0.43
1:K:202:ARG:HG2	1:K:204:TRP:NE1	2.33	0.43
1:K:214:THR:HG21	1:K:262:GLN:CG	2.36	0.43
5:D:21:VAL:HG22	5:D:77:HIS:ND1	2.33	0.43
4:T:40:LYS:CE	4:T:42:PHE:HB3	2.48	0.43
5:N:131:SER:O	5:N:132:ASP:HB3	2.17	0.43
1:F:191:HIS:CB	1:F:274:TRP:CZ2	3.01	0.43
1:K:217:TRP:CZ3	1:K:218:GLN:HB2	2.53	0.43
5:N:88:VAL:HA	5:N:107:THR:O	2.18	0.43
1:K:254:GLU:HB3	1:K:274:TRP:CZ3	2.53	0.43
5:I:86:SER:HA	5:I:109:LEU:O	2.19	0.43
5:S:170:PHE:CD2	4:T:142:LYS:HE2	2.54	0.43
5:S:174:SER:CB	4:T:195:ARG:NH1	2.81	0.43
4:T:121:ASN:ND2	4:T:187:ASP:O	2.47	0.43
5:N:52:ARG:O	5:N:52:ARG:CG	2.64	0.43
5:N:62:ARG:CB	5:N:80:GLU:OE2	2.67	0.43
1:F:165:VAL:O	1:F:169:ARG:HG3	2.18	0.43
1:K:258:THR:HG1	1:K:273:ARG:HA	1.82	0.43
1:P:44:ARG:NH2	1:P:61:ASP:OD1	2.51	0.43
5:D:14:VAL:HG12	5:D:15:GLN:O	2.18	0.43
4:E:163:VAL:HB	4:E:168:VAL:CG2	2.49	0.43
1:A:194:VAL:HG13	1:A:195:SER:N	2.34	0.43
1:F:73:THR:HG23	3:H:8:THR:HG22	2.00	0.43
1:F:193:ALA:O	1:F:194:VAL:HG22	2.19	0.43
1:K:194:VAL:HG23	1:K:195:SER:N	2.34	0.43
1:K:214:THR:CG2	1:K:262:GLN:H	2.31	0.43
1:K:218:GLN:CG	1:K:222:GLU:O	2.66	0.43
1:K:250:PRO:CB	1:K:253:GLN:HG2	2.49	0.43
1:P:21:ARG:HH11	1:P:39:ASP:CG	2.27	0.43
1:P:27:TYR:CE1	1:P:32:GLN:HB2	2.53	0.43
5:I:158:THR:HG23	5:I:176:VAL:O	2.18	0.43
4:J:64:PHE:CE1	4:J:78:ILE:HG23	2.54	0.43
1:K:228:THR:O	1:K:228:THR:OG1	2.34	0.43
2:Q:5:PRO:HA	2:Q:30:PHE:HB3	2.01	0.43
5:N:62:ARG:HE	5:N:80:GLU:HG3	1.84	0.43
1:K:3:HIS:HB2	1:K:103:VAL:CG2	2.49	0.43
1:P:80:THR:HG21	3:R:9:VAL:OXT	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:198:ASP:O	5:D:199:THR:C	2.60	0.43
4:E:1:ASP:CG	4:E:2:THR:H	2.26	0.43
5:N:67:LEU:HD21	5:N:69:LYS:HE2	2.01	0.43
1:F:81:LEU:HD13	1:F:118:TYR:CD1	2.53	0.42
1:P:147:TRP:CG	1:P:152:VAL:HG21	2.54	0.42
1:P:226:GLN:HG2	1:P:227:ASP:CA	2.47	0.42
1:P:227:ASP:OD2	1:P:248:VAL:HG12	2.19	0.42
4:E:182:GLN:OE1	4:E:182:GLN:N	2.52	0.42
4:T:159:LEU:C	4:T:159:LEU:HD23	2.44	0.42
4:T:40:LYS:HG3	4:T:41:LYS:N	2.33	0.42
4:O:40:LYS:HD3	4:O:40:LYS:N	2.34	0.42
4:J:133:SER:O	4:J:137:ILE:HG13	2.19	0.42
2:L:75:LYS:HE2	2:L:76:ASP:OD1	2.20	0.42
5:S:160:LYS:HG2	5:S:161:CYS:N	2.34	0.42
5:N:174:SER:OG	4:O:195:ARG:NH1	2.51	0.42
4:O:120:LYS:HG2	4:O:120:LYS:H	1.68	0.42
1:A:258:THR:CG2	1:A:273:ARG:HE	2.33	0.42
1:F:227:ASP:CG	1:F:248:VAL:HG12	2.45	0.42
1:K:71:SER:O	1:K:72:GLN:C	2.62	0.42
1:K:218:GLN:HA	1:K:222:GLU:O	2.18	0.42
5:D:49:ILE:HD13	5:D:65:VAL:HG23	2.02	0.42
5:D:130:SER:O	5:D:131:SER:HB2	2.19	0.42
4:E:6:GLN:HE22	4:E:90:PHE:HA	1.84	0.42
4:E:19:LYS:HA	4:E:19:LYS:HD3	1.64	0.42
4:E:82:GLU:HG2	4:E:84:GLY:CA	2.48	0.42
4:T:40:LYS:HD2	4:T:42:PHE:HB3	2.02	0.42
4:O:180:LYS:HZ2	4:O:182:GLN:C	2.16	0.42
2:B:40:LEU:HB2	2:B:79:ALA:HB3	2.01	0.42
1:P:219:ARG:CZ	1:P:257:TYR:CD2	3.03	0.42
5:I:26:TYR:OH	5:I:69:LYS:HB2	2.20	0.42
5:S:133:LYS:HB3	5:S:184:PHE:HZ	1.83	0.42
4:T:34:TRP:NE1	4:T:74:LEU:HG	2.34	0.42
5:N:149:GLN:C	5:N:157:ILE:HD12	2.44	0.42
5:N:160:LYS:HG2	5:N:161:CYS:N	2.34	0.42
2:L:81:ARG:HG3	2:L:92:ILE:HG12	2.02	0.42
1:P:199:ALA:O	1:P:248:VAL:HA	2.20	0.42
4:E:34:TRP:NE1	4:E:74:LEU:HG	2.35	0.42
5:S:122:VAL:HA	5:S:137:LEU:O	2.19	0.42
1:F:51:TRP:O	1:F:54:GLN:HG3	2.20	0.42
4:J:138:SER:OG	4:J:139:HIS:N	2.52	0.42
1:P:74:HIS:CD2	1:P:95:VAL:HG11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:226:GLN:HG3	1:P:227:ASP:CG	2.45	0.42
5:D:69:LYS:HB2	5:D:69:LYS:HE3	1.86	0.42
4:E:29:HIS:HE1	4:E:106:PHE:CE1	2.37	0.42
5:S:98:ALA:HB2	4:T:96:LEU:HD13	2.02	0.42
1:A:64:THR:O	1:A:68:LYS:HG3	2.18	0.42
1:A:108:ARG:HG3	1:A:108:ARG:HH11	1.83	0.42
1:A:193:ALA:O	1:A:194:VAL:HG12	2.20	0.42
1:K:244:TRP:CZ3	1:K:246:ALA:HB2	2.55	0.42
1:P:21:ARG:HH11	1:P:21:ARG:HG3	1.85	0.42
1:P:207:SER:HA	1:P:240:THR:OG1	2.20	0.42
5:I:155:VAL:HA	5:I:179:SER:HB2	2.00	0.42
4:T:15:MET:HE3	4:T:15:MET:HB2	1.97	0.42
4:T:129:VAL:HG23	4:T:239:ALA:HB1	2.02	0.42
1:F:257:TYR:O	1:F:273:ARG:HD2	2.19	0.42
5:D:126:ARG:NH2	5:D:134:SER:HG	2.13	0.42
4:E:13:THR:O	4:E:115:VAL:HA	2.20	0.42
4:E:51:ASN:O	4:E:53:GLU:N	2.53	0.42
5:N:126:ARG:HH12	5:N:133:LYS:CD	2.26	0.42
1:A:204:TRP:HZ2	2:B:98:ASP:O	2.03	0.42
1:F:202:ARG:NH1	2:G:98:ASP:O	2.53	0.42
5:S:135:VAL:HG13	4:T:130:PHE:CE2	2.55	0.42
4:T:99:GLY:HA3	4:T:100:PRO:C	2.44	0.42
4:T:182:GLN:C	4:T:184:ALA:H	2.27	0.42
5:N:41:LEU:C	5:N:43:LYS:H	2.28	0.42
1:F:190:THR:OG1	1:F:202:ARG:HB3	2.20	0.41
4:J:4:VAL:HG22	4:J:25:GLN:HB3	2.02	0.41
1:P:122:ASP:OD1	2:Q:60:TRP:NE1	2.35	0.41
5:I:59:LYS:CD	5:I:64:ALA:HB2	2.50	0.41
5:D:195:ILE:HG22	5:D:197:GLU:OE2	2.20	0.41
1:A:97:ARG:NH1	1:A:116:TYR:HE2	2.18	0.41
1:A:201:LEU:N	1:A:247:VAL:O	2.50	0.41
1:F:44:ARG:NH1	2:Q:47:GLU:OE2	2.53	0.41
1:K:207:SER:HA	1:K:240:THR:OG1	2.20	0.41
5:I:128:SER:O	5:I:129:LYS:CG	2.66	0.41
5:D:197:GLU:HG3	5:D:199:THR:H	1.84	0.41
5:S:52:ARG:HB2	5:S:53:SER:H	1.71	0.41
4:T:132:PRO:HD3	4:T:145:LEU:HG	2.02	0.41
1:F:82:ARG:O	1:F:86:ASN:N	2.53	0.41
2:L:51:HIS:HD2	2:L:66:TYR:CE2	2.38	0.41
1:P:11:SER:HA	1:P:21:ARG:O	2.20	0.41
5:D:116:GLN:HG3	5:D:170:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:GLN:HA	1:F:273:ARG:HH22	1.86	0.41
2:G:5:PRO:CA	2:G:30:PHE:HB3	2.50	0.41
4:J:166:LYS:HA	4:J:166:LYS:HD3	1.76	0.41
1:K:226:GLN:OE1	1:K:248:VAL:HG21	2.21	0.41
2:L:19:LYS:O	2:L:72:PRO:HD2	2.21	0.41
5:S:84:GLU:CD	5:S:84:GLU:H	2.27	0.41
1:F:59:TYR:CZ	1:F:63:GLU:HG3	2.56	0.41
1:F:138:MET:HE3	1:F:138:MET:HB3	1.88	0.41
1:F:264:GLU:C	1:F:266:LEU:N	2.76	0.41
4:J:91:CYS:SG	4:J:92:ALA:N	2.94	0.41
1:K:23:ILE:HG21	2:L:54:LEU:HB3	2.03	0.41
1:P:275:GLU:H	1:P:275:GLU:HG3	1.29	0.41
5:D:116:GLN:HG3	5:D:170:PHE:CE1	2.55	0.41
1:A:218:GLN:HE21	1:A:258:THR:C	2.29	0.41
1:F:218:GLN:HB3	1:F:223:ASP:CG	2.45	0.41
1:K:42:SER:O	1:K:44:ARG:HG3	2.20	0.41
1:K:106:ASP:OD2	1:K:108:ARG:CG	2.66	0.41
1:K:146:LYS:HD3	4:O:98:GLY:HA3	2.02	0.41
5:I:118:PRO:C	5:I:120:PRO:HD3	2.45	0.41
5:I:161:CYS:O	5:I:173:ASN:HA	2.21	0.41
5:S:181:LYS:O	5:S:184:PHE:CZ	2.73	0.41
1:F:258:THR:CG2	1:F:273:ARG:HD3	2.49	0.41
1:K:97:ARG:CZ	3:M:6:ILE:HD11	2.51	0.41
1:K:234:ARG:HD3	2:L:8:GLN:OE1	2.21	0.41
1:K:255:GLN:NE2	1:K:274:TRP:C	2.76	0.41
1:P:234:ARG:HD3	2:Q:8:GLN:OE1	2.20	0.41
5:N:6:GLU:HB2	5:N:25:THR:OG1	2.20	0.41
5:N:126:ARG:NH1	5:N:129:LYS:NZ	2.68	0.41
1:K:59:TYR:CE2	1:K:63:GLU:HG3	2.55	0.41
1:P:193:ALA:O	1:P:199:ALA:HA	2.21	0.41
1:P:226:GLN:CG	1:P:227:ASP:CB	2.99	0.41
5:I:147:VAL:HA	5:I:192:ASN:OD1	2.21	0.41
4:E:94:SER:HB2	4:E:105:GLN:HG2	2.03	0.41
4:E:137:ILE:HG23	4:E:200:ALA:HB1	2.03	0.41
4:T:122:VAL:HG13	4:T:153:TYR:O	2.20	0.41
1:A:49:ALA:O	1:A:52:ILE:HG22	2.21	0.41
1:A:65:ARG:NH1	5:D:95:ARG:NH2	2.68	0.41
1:F:264:GLU:O	1:F:266:LEU:N	2.51	0.41
1:K:219:ARG:HG2	1:K:221:GLY:N	2.35	0.41
1:K:253:GLN:O	1:K:257:TYR:CD2	2.73	0.41
2:L:51:HIS:CD2	2:L:66:TYR:CE2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:49:ALA:O	1:P:52:ILE:HG22	2.21	0.41
5:I:17:GLY:O	5:I:80:GLU:HA	2.21	0.41
5:I:116:GLN:OE1	5:I:170:PHE:HD1	2.04	0.41
5:D:148:SER:HB2	5:D:192:ASN:HD21	1.86	0.41
4:E:14:GLN:HB3	4:E:119:LEU:HD13	2.02	0.41
4:E:82:GLU:HB3	4:E:85:ASP:CG	2.45	0.41
4:T:32:MET:HE2	4:T:32:MET:HB3	1.74	0.41
4:T:39:SER:C	4:T:40:LYS:CG	2.93	0.41
5:N:4:ASN:OD1	5:N:4:ASN:C	2.64	0.41
5:N:62:ARG:NE	5:N:80:GLU:HG3	2.36	0.41
5:N:132:ASP:OD2	5:N:180:ASN:CB	2.68	0.41
4:O:151:GLY:N	4:O:190:TYR:O	2.54	0.41
4:J:195:ARG:HH12	5:I:174:SER:H	1.66	0.41
1:K:218:GLN:CA	1:K:222:GLU:O	2.69	0.41
5:I:25:THR:HG22	5:I:73:HIS:HB3	2.03	0.41
4:E:150:THR:HG22	4:E:191:ALA:CB	2.51	0.41
4:E:230:ALA:O	4:E:231:LYS:HB3	2.21	0.41
5:S:120:PRO:HB2	5:S:195:ILE:CD1	2.49	0.41
4:T:38:ASP:H	4:T:40:LYS:HE3	1.86	0.41
5:N:51:ILE:HB	5:N:65:VAL:HG21	2.02	0.41
5:N:174:SER:HB3	4:O:195:ARG:NH1	2.36	0.41
4:O:134:GLU:HA	4:O:137:ILE:HD12	2.03	0.41
1:A:44:ARG:HH11	2:L:47:GLU:CD	2.28	0.40
4:J:61:PRO:HB2	4:J:63:ARG:HH21	1.86	0.40
1:P:227:ASP:OD2	1:P:248:VAL:HG13	2.21	0.40
2:Q:95:TRP:CD1	2:Q:96:ASP:H	2.39	0.40
5:I:88:VAL:HG22	5:I:108:ARG:HG3	2.03	0.40
4:O:30:ASP:OD2	4:O:95:GLN:O	2.39	0.40
4:O:125:PRO:HD3	4:O:216:PHE:CD1	2.56	0.40
1:K:213:ILE:HG13	1:K:263:HIS:HD2	1.86	0.40
2:L:39:LEU:HD23	2:L:39:LEU:HA	1.86	0.40
5:I:191:ASN:O	5:I:192:ASN:O	2.39	0.40
5:D:129:LYS:HE2	5:D:131:SER:HB2	2.02	0.40
5:N:62:ARG:O	5:N:80:GLU:OE1	2.39	0.40
5:N:126:ARG:HH22	5:N:129:LYS:HE3	1.86	0.40
4:O:136:GLU:HG3	4:O:142:LYS:O	2.22	0.40
2:B:45:ARG:HH11	2:B:45:ARG:CG	2.27	0.40
1:F:182:THR:O	1:F:182:THR:HG23	2.21	0.40
5:I:199:THR:O	5:I:201:PHE:HD1	2.04	0.40
5:D:4:ASN:HB3	5:D:27:SER:OG	2.22	0.40
4:E:231:LYS:O	4:E:233:VAL:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:VAL:HG22	1:A:257:TYR:CE2	2.56	0.40
4:J:100:PRO:HD3	5:I:97:GLY:HA2	2.04	0.40
4:J:104:GLU:CB	5:I:47:LEU:HD22	2.52	0.40
1:K:219:ARG:HE	1:K:222:GLU:CG	2.34	0.40
2:L:5:PRO:HB3	2:L:30:PHE:HB3	2.03	0.40
2:L:7:ILE:HD12	2:L:91[B]:LYS:HD2	2.03	0.40
5:I:59:LYS:HG2	5:I:64:ALA:HB2	2.03	0.40
4:E:101:LEU:HG	4:E:102:TYR:CE2	2.56	0.40
4:E:219:LEU:O	4:E:233:VAL:HA	2.22	0.40
5:S:135:VAL:HG12	5:S:178:TRP:HB3	2.02	0.40
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.91	0.40
1:A:127:LYS:HE2	1:A:133:TRP:O	2.22	0.40
1:A:225:THR:HG23	1:A:228:THR:HG22	2.04	0.40
2:B:31:HIS:CD2	2:B:62:PHE:CE2	3.09	0.40
4:J:200:ALA:O	4:J:204:GLN:HG2	2.22	0.40
1:K:49:ALA:O	1:K:52:ILE:HG22	2.22	0.40
1:K:71:SER:O	1:K:74:HIS:N	2.54	0.40
4:E:231:LYS:O	4:E:233:VAL:HG23	2.22	0.40
5:S:14:VAL:HG13	5:S:18:ASP:HB2	2.02	0.40
5:S:15:GLN:HB2	5:S:18:ASP:OD2	2.21	0.40
5:S:92:ALA:HB2	5:S:103:PHE:CD1	2.56	0.40
5:S:138:PHE:O	5:S:174:SER:HA	2.21	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	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:MET:SD	5:I:151:LYS:NZ[2_647]	2.15	0.05
2:Q:89:GLN:NE2	5:N:197:GLU:OE2[2_556]	2.15	0.05
1:K:85:TYR:O	5:S:183:ASP:OD2[2_656]	2.19	0.01

## 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	273/276 (99%)	240 (88%)	28 (10%)	5 (2%)	7	25
1	F	273/276 (99%)	241 (88%)	26 (10%)	6 (2%)	5	20
1	K	273/276 (99%)	234 (86%)	35 (13%)	4 (2%)	8	29
1	P	273/276 (99%)	240 (88%)	28 (10%)	5 (2%)	7	25
2	B	101/100 (101%)	96 (95%)	5 (5%)	0	100	100
2	G	101/100 (101%)	96 (95%)	5 (5%)	0	100	100
2	L	101/100 (101%)	96 (95%)	5 (5%)	0	100	100
2	Q	101/100 (101%)	97 (96%)	4 (4%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	M	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	R	7/9 (78%)	7 (100%)	0	0	100	100
4	E	243/247 (98%)	207 (85%)	32 (13%)	4 (2%)	8	27
4	J	243/247 (98%)	207 (85%)	29 (12%)	7 (3%)	3	16
4	O	243/247 (98%)	205 (84%)	28 (12%)	10 (4%)	2	11
4	T	243/247 (98%)	209 (86%)	27 (11%)	7 (3%)	3	16
5	D	198/207 (96%)	159 (80%)	26 (13%)	13 (7%)	1	5
5	I	198/207 (96%)	154 (78%)	26 (13%)	18 (9%)	0	2
5	N	198/207 (96%)	154 (78%)	35 (18%)	9 (4%)	2	9
5	S	198/207 (96%)	157 (79%)	28 (14%)	13 (7%)	1	5
All	All	3288/3356 (98%)	2818 (86%)	369 (11%)	101 (3%)	3	15

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ASP
1	A	222	GLU
1	F	194	VAL
1	F	228	THR
4	J	227	GLN
4	J	230	ALA
1	K	201	LEU
1	P	194	VAL
1	P	220	ASP

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Mol	Chain	Res	Type
1	P	224	GLN
1	P	227	ASP
5	I	53	SER
5	I	116	GLN
5	I	128	SER
5	I	129	LYS
5	I	132	ASP
5	I	150	SER
5	I	169	ASP
5	I	192	ASN
5	I	194	ILE
5	D	53	SER
5	D	128	SER
5	D	131	SER
5	D	185	ALA
5	D	191	ASN
5	D	192	ASN
5	D	194	ILE
5	D	195	ILE
4	E	41	LYS
4	E	97	ALA
5	S	54	ASN
5	S	55	VAL
5	S	128	SER
5	S	132	ASP
5	S	134	SER
5	S	181	LYS
5	S	185	ALA
5	S	192	ASN
5	S	194	ILE
5	S	196	PRO
4	T	40	LYS
5	N	56	GLY
5	N	128	SER
5	N	131	SER
5	N	150	SER
5	N	185	ALA
4	O	29	HIS
4	O	31	THR
4	O	96	LEU
4	O	227	GLN
4	O	228	ASP

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Mol	Chain	Res	Type
1	A	194	VAL
1	F	224	GLN
1	F	225	THR
1	F	274	TRP
1	K	194	VAL
1	P	223	ASP
5	I	29	SER
5	I	54	ASN
5	I	131	SER
5	I	181	LYS
5	I	191	ASN
5	D	54	ASN
5	D	55	VAL
5	D	116	GLN
5	S	184	PHE
4	T	227	GLN
4	T	228	ASP
4	T	229	ARG
5	N	29	SER
4	O	229	ARG
4	J	86	SER
1	K	224	GLN
5	I	185	ALA
4	E	86	SER
4	E	231	LYS
5	S	97	GLY
5	N	53	SER
5	N	57	GLU
4	O	230	ALA
4	O	231	LYS
1	A	219	ARG
1	A	223	ASP
1	F	219	ARG
4	J	31	THR
4	J	228	ASP
4	J	231	LYS
4	T	86	SER
4	T	231	LYS
4	O	86	SER
5	I	30	ALA
5	I	55	VAL
5	D	169	ASP

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Mol	Chain	Res	Type
5	D	196	PRO
5	S	199	THR
5	N	79	THR
1	K	200	THR
5	I	184	PHE
4	T	67	LYS
4	O	222	ASN
4	J	205	ASN

### 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	231/232 (100%)	226 (98%)	5 (2%)	47	68
1	F	231/232 (100%)	223 (96%)	8 (4%)	31	58
1	K	231/232 (100%)	219 (95%)	12 (5%)	19	45
1	P	231/232 (100%)	223 (96%)	8 (4%)	31	58
2	B	98/95 (103%)	91 (93%)	7 (7%)	12	35
2	G	98/95 (103%)	98 (100%)	0	100	100
2	L	98/95 (103%)	97 (99%)	1 (1%)	73	85
2	Q	98/95 (103%)	98 (100%)	0	100	100
3	C	8/8 (100%)	8 (100%)	0	100	100
3	H	8/8 (100%)	6 (75%)	2 (25%)	0	1
3	M	8/8 (100%)	7 (88%)	1 (12%)	3	13
3	R	8/8 (100%)	7 (88%)	1 (12%)	3	13
4	E	217/219 (99%)	210 (97%)	7 (3%)	34	60
4	J	217/219 (99%)	209 (96%)	8 (4%)	29	56
4	O	217/219 (99%)	207 (95%)	10 (5%)	23	49
4	T	217/219 (99%)	209 (96%)	8 (4%)	29	56
5	D	178/184 (97%)	174 (98%)	4 (2%)	47	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	178/184 (97%)	172 (97%)	6 (3%)	32	59
5	N	178/184 (97%)	168 (94%)	10 (6%)	17	43
5	S	178/184 (97%)	174 (98%)	4 (2%)	47	68
All	All	2928/2952 (99%)	2826 (96%)	102 (4%)	31	58

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	SER
1	A	222	GLU
1	A	226	GLN
1	A	268	LYS
1	A	273	ARG
2	B	0	MET
2	B	4	THR
2	B	27[A]	VAL
2	B	27[B]	VAL
2	B	75	LYS
2	B	94	LYS
2	B	99	MET
1	F	17	ARG
1	F	32	GLN
1	F	48	ARG
1	F	127	LYS
1	F	131	ARG
1	F	196	ASP
1	F	216	THR
1	F	275	GLU
3	H	4	GLU
3	H	6	ILE
4	J	18	ASP
4	J	41	LYS
4	J	82	GLU
4	J	101	LEU
4	J	180	LYS
4	J	189	ARG
4	J	229	ARG
4	J	231	LYS
1	K	115	GLN
1	K	189	MET
1	K	190	THR

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Mol	Chain	Res	Type
1	K	198	GLU
1	K	213	ILE
1	K	214	THR
1	K	218	GLN
1	K	223	ASP
1	K	254	GLU
1	K	255	GLN
1	K	258	THR
1	K	264	GLU
2	L	75	LYS
3	M	6	ILE
1	P	115	GLN
1	P	131	ARG
1	P	195	SER
1	P	224	GLN
1	P	226	GLN
1	P	256	ARG
1	P	268	LYS
1	P	275	GLU
3	R	6	ILE
5	I	59	LYS
5	I	129	LYS
5	I	151	LYS
5	I	169	ASP
5	I	194	ILE
5	I	199	THR
5	D	69	LYS
5	D	124	GLN
5	D	194	ILE
5	D	195	ILE
4	E	9	LYS
4	E	13	THR
4	E	60	VAL
4	E	67	LYS
4	E	79	ASN
4	E	83	LEU
4	E	186	ASN
5	S	39	GLN
5	S	57	GLU
5	S	195	ILE
5	S	197	GLU
4	T	13	THR

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Mol	Chain	Res	Type
4	T	39	SER
4	T	60	VAL
4	T	67	LYS
4	T	141	GLN
4	T	186	ASN
4	T	221	GLU
4	T	231	LYS
5	N	10	SER
5	N	23	LYS
5	N	52	ARG
5	N	54	ASN
5	N	61	GLN
5	N	63	ILE
5	N	80	GLU
5	N	148	SER
5	N	151	LYS
5	N	181	LYS
4	O	9	LYS
4	O	41	LYS
4	O	60	VAL
4	O	79	ASN
4	O	103	ASN
4	O	120	LYS
4	O	177	GLN
4	O	185	LEU
4	O	227	GLN
4	O	231	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	HIS
1	A	192	HIS
1	A	218	GLN
1	A	260	HIS
1	F	86	ASN
1	F	93	HIS
1	F	96	GLN
1	F	180	GLN
1	F	218	GLN
1	F	224	GLN
1	F	262	GLN

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Mol	Chain	Res	Type
2	G	13	HIS
4	J	14	GLN
4	J	37	GLN
4	J	62	ASN
4	J	103	ASN
4	J	227	GLN
1	K	32	GLN
1	K	43	GLN
1	K	141	GLN
1	K	197	HIS
1	K	255	GLN
1	P	32	GLN
1	P	224	GLN
1	P	262	GLN
5	I	73	HIS
5	D	73	HIS
5	D	117	ASN
5	D	124	GLN
5	D	192	ASN
4	E	37	GLN
4	E	50	ASN
4	E	121	ASN
4	E	227	GLN
5	S	39	GLN
4	T	6	GLN
4	T	103	ASN
4	T	139	HIS
4	T	222	ASN
5	N	8	HIS
5	N	54	ASN
5	N	77	HIS
4	O	25	GLN
4	O	51	ASN
4	O	156	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	275/276 (99%)	-0.31	0 100 100	44, 66, 127, 184	0
1	F	275/276 (99%)	-0.42	0 100 100	43, 62, 118, 164	0
1	K	275/276 (99%)	-0.16	2 (0%) 84 69	46, 71, 155, 172	0
1	P	275/276 (99%)	-0.39	0 100 100	43, 60, 117, 133	0
2	B	100/100 (100%)	-0.33	0 100 100	47, 77, 103, 117	3 (3%)
2	G	100/100 (100%)	-0.43	0 100 100	44, 64, 87, 113	3 (3%)
2	L	100/100 (100%)	-0.39	0 100 100	46, 68, 93, 116	3 (3%)
2	Q	100/100 (100%)	-0.45	0 100 100	44, 65, 93, 99	3 (3%)
3	C	9/9 (100%)	-0.58	0 100 100	51, 55, 63, 63	0
3	H	9/9 (100%)	-0.31	0 100 100	52, 56, 66, 66	0
3	M	9/9 (100%)	-0.20	0 100 100	52, 54, 57, 60	0
3	R	9/9 (100%)	-0.37	0 100 100	49, 53, 57, 58	0
4	E	245/247 (99%)	-0.39	0 100 100	41, 66, 106, 119	0
4	J	245/247 (99%)	-0.28	0 100 100	46, 72, 115, 131	0
4	O	245/247 (99%)	-0.33	0 100 100	47, 71, 106, 129	0
4	T	245/247 (99%)	-0.42	0 100 100	47, 65, 98, 123	0
5	D	200/207 (96%)	-0.16	1 (0%) 87 74	50, 78, 123, 154	0
5	I	200/207 (96%)	-0.12	2 (1%) 79 63	52, 81, 133, 157	0
5	N	200/207 (96%)	-0.15	0 100 100	52, 82, 137, 159	0
5	S	200/207 (96%)	-0.21	0 100 100	45, 74, 123, 154	0
All	All	3316/3356 (98%)	-0.30	5 (0%) 92 85	41, 70, 121, 184	12 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	247	VAL	2.4
5	I	53	SER	2.3
5	I	59	LYS	2.3
5	D	127	ASP	2.2
1	K	200	THR	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no 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.