



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:10 PM GMT

PDB ID : 3SJV  
Title : Crystal structure of the RL42 TCR in complex with HLA-B8-FLR  
Authors : Gras, S.; Wilmann, P.G.; Zhenjun, C.; Hanim, H.; Yu Chih, L.; Kjer-Nielsen, L.; Purcell, A.W.; Burrows, S.R.; Mccluskey, J.; Rossjohn, J.  
Deposited on : 2011-06-22  
Resolution : 3.10 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

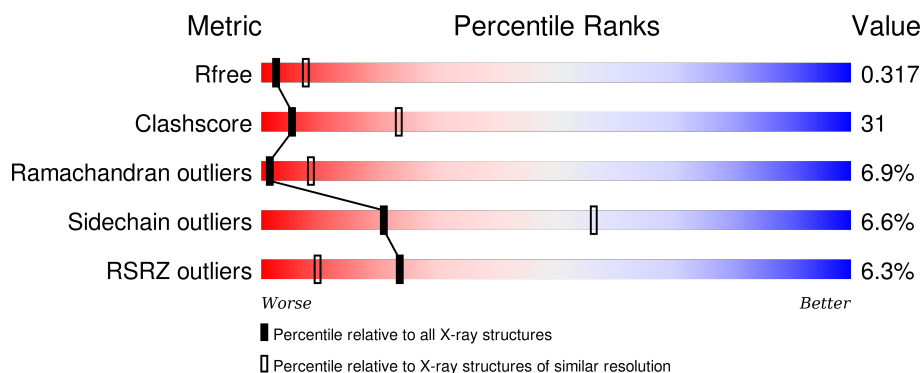
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	277	<div> <div>10%</div> <div> <div>43%</div> <div>46%</div> <div>10%</div> </div> </div>
1	F	277	<div> <div>13%</div> <div> <div>45%</div> <div>49%</div> <div>5%</div> </div> </div>
1	K	277	<div> <div>12%</div> <div> <div>49%</div> <div>45%</div> <div>6%</div> </div> </div>
1	P	277	<div> <div>5%</div> <div> <div>48%</div> <div>44%</div> <div>8%</div> </div> </div>
2	B	100	<div> <div>49%</div> <div>41%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	100	
2	L	100	
2	Q	100	
3	C	9	
3	H	9	
3	M	9	
3	R	9	
4	D	203	
4	I	203	
4	N	203	
4	S	203	
5	E	244	
5	J	244	
5	O	244	
5	T	244	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26455 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 HLA class I histocompatibility antigen, B-8 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2258	1398	412	441	7			
1	F	277	Total	C	N	O	S	0	0	0
			2258	1398	412	441	7			
1	K	277	Total	C	N	O	S	0	0	0
			2258	1398	412	441	7			
1	P	277	Total	C	N	O	S	0	0	0
			2258	1398	412	441	7			

- 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
			829	528	140	158	3			
2	G	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	L	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	Q	100	Total	C	N	O	S	0	0	0
			837	533	141	159	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 Epstein-Barr nuclear antigen 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			75	49	15	11			
3	H	9	Total	C	N	O	0	0	0
			75	49	15	11			
3	M	9	Total	C	N	O	0	0	0
			75	49	15	11			
3	R	9	Total	C	N	O	0	0	0
			75	49	15	11			

- Molecule 4 is a protein called RL42 T cell receptor, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	1	0	0
			1541	962	258	313	8			
4	I	197	Total	C	N	O	S	1	0	0
			1541	962	258	313	8			
4	N	197	Total	C	N	O	S	1	0	0
			1541	962	258	313	8			
4	S	197	Total	C	N	O	S	1	0	0
			1541	962	258	313	8			

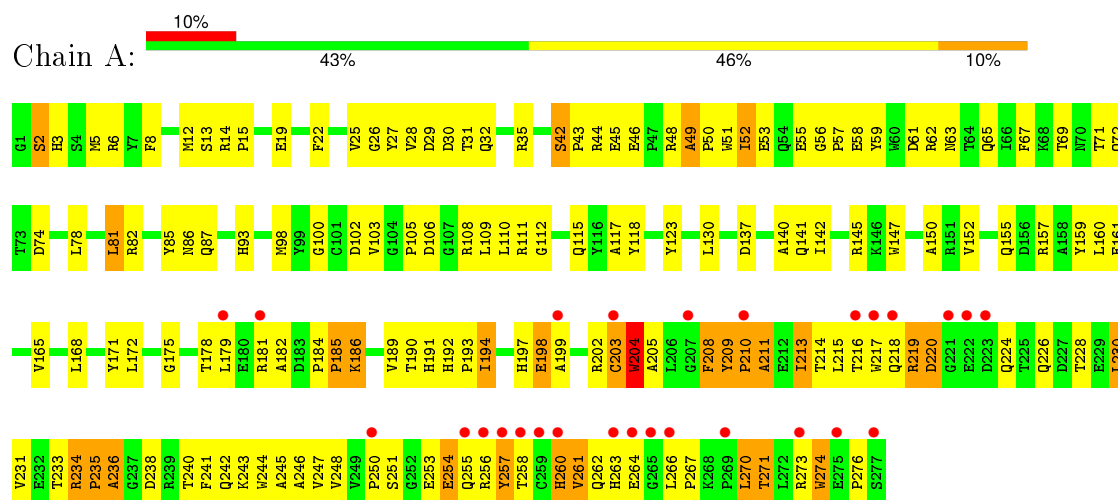
- Molecule 5 is a protein called RL42 T cell receptor, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	241	Total	C	N	O	S	2	0	0
			1908	1205	331	363	9			
5	J	240	Total	C	N	O	S	2	0	0
			1903	1202	330	362	9			
5	O	241	Total	C	N	O	S	2	0	0
			1908	1205	331	363	9			
5	T	241	Total	C	N	O	S	2	0	0
			1908	1205	331	363	9			

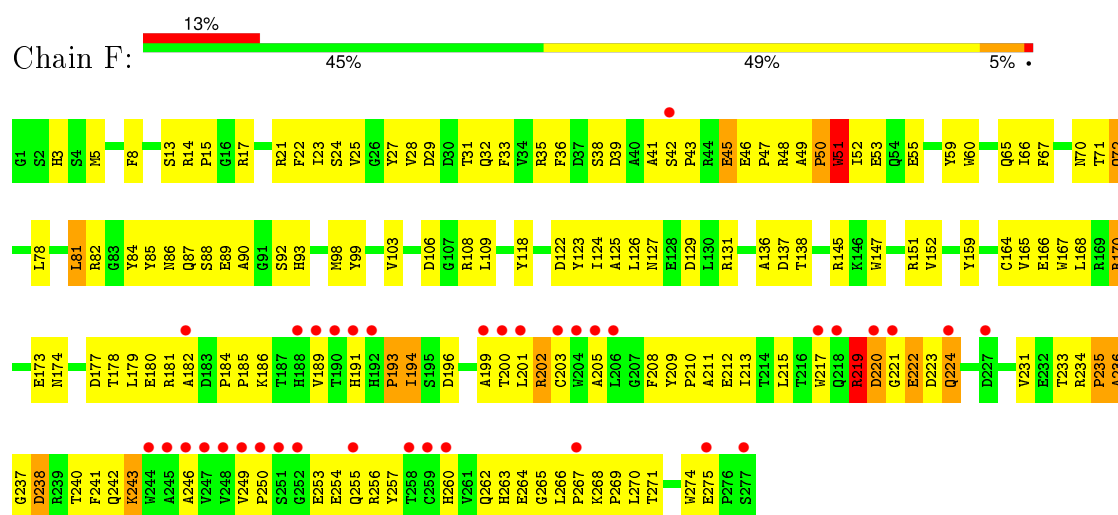
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: HLA class I histocompatibility antigen, B-8 alpha chain

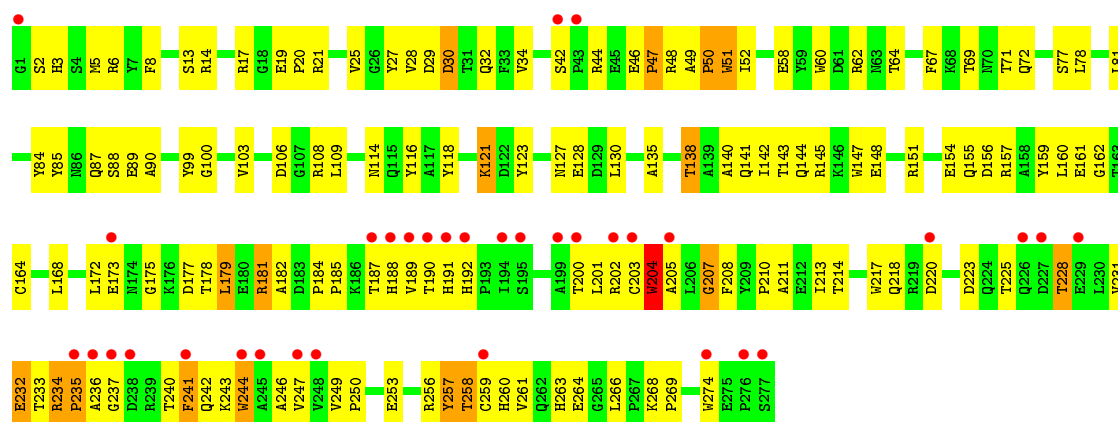


- Molecule 1: HLA class I histocompatibility antigen, B-8 alpha chain

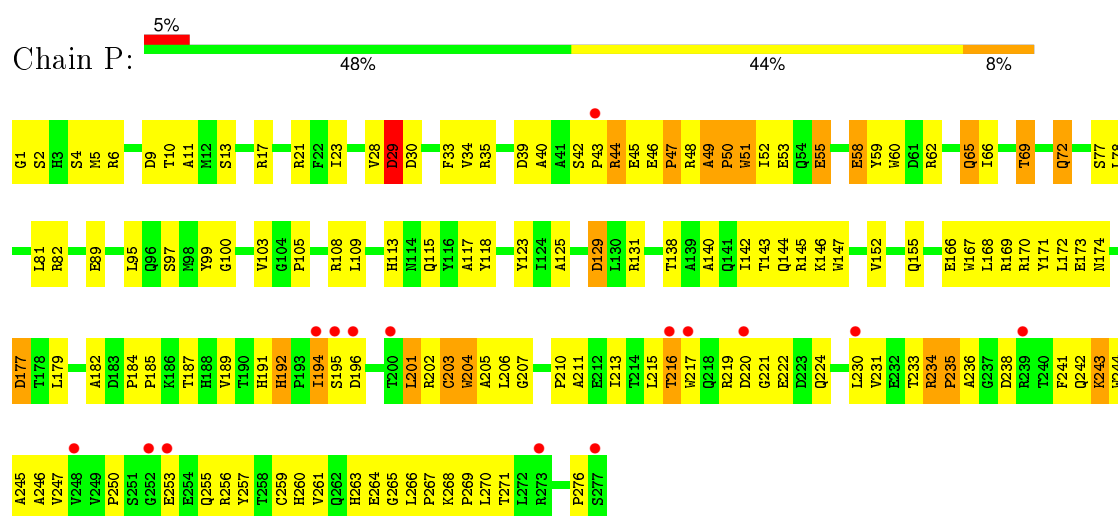


- Molecule 1: HLA class I histocompatibility antigen, B-8 alpha chain

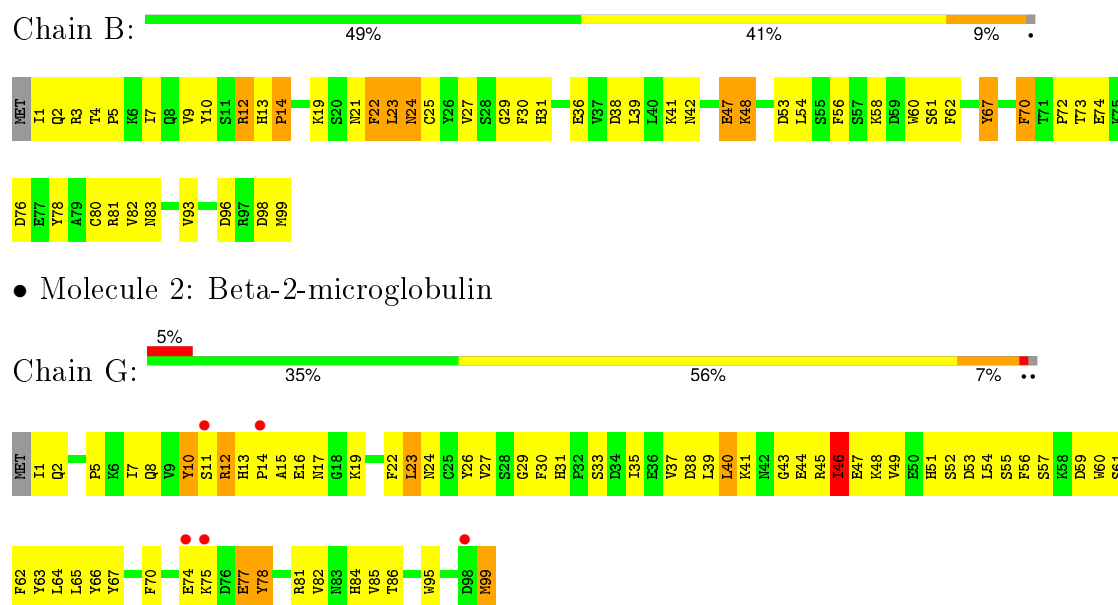




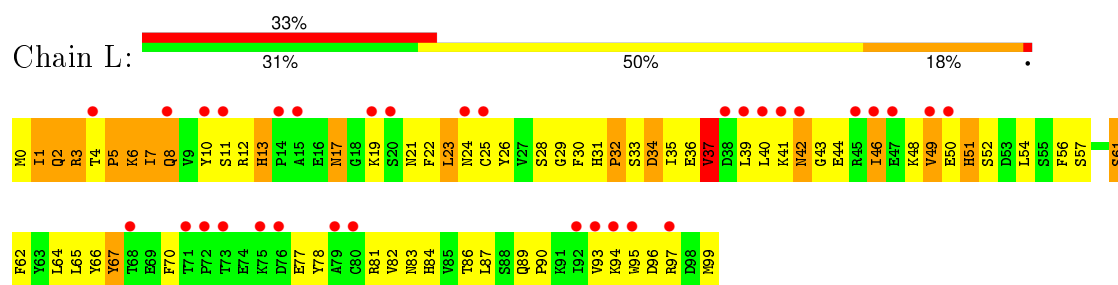
- Molecule 1: HLA class I histocompatibility antigen, B-8 alpha chain



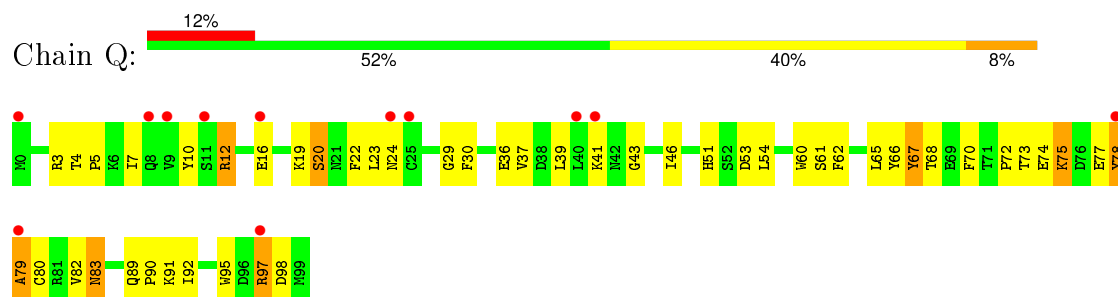
- Molecule 2: Beta-2-microglobulin



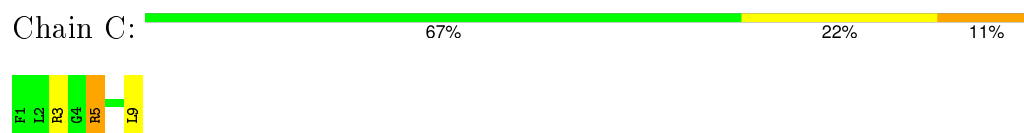
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



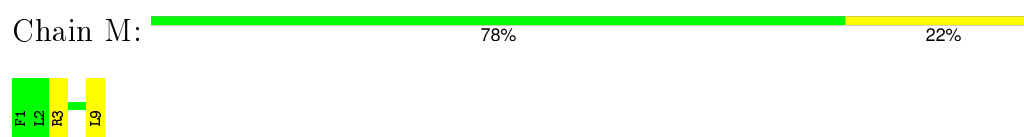
- Molecule 3: Epstein-Barr nuclear antigen 3



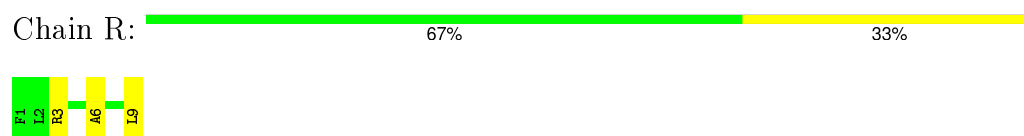
- Molecule 3: Epstein-Barr nuclear antigen 3



- Molecule 3: Epstein-Barr nuclear antigen 3



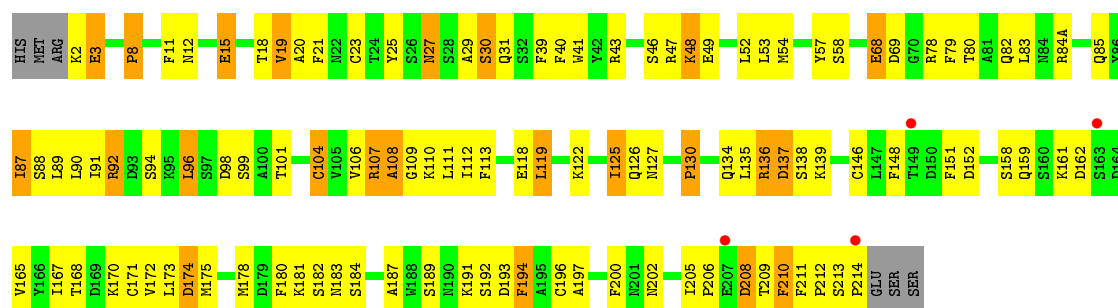
- Molecule 3: Epstein-Barr nuclear antigen 3



- Molecule 4: RL42 T cell receptor, alpha chain

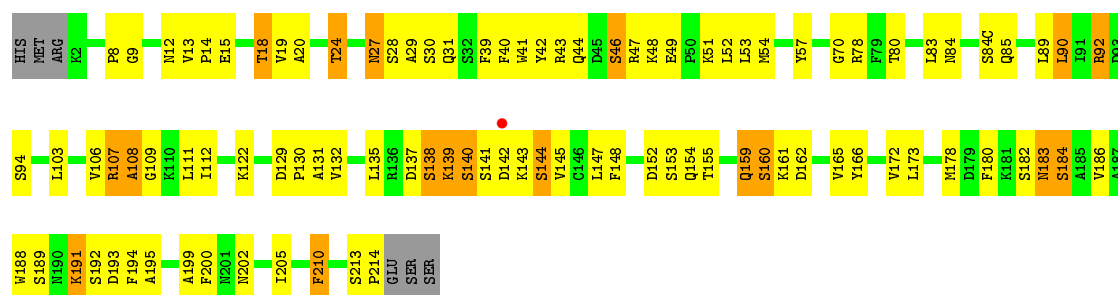






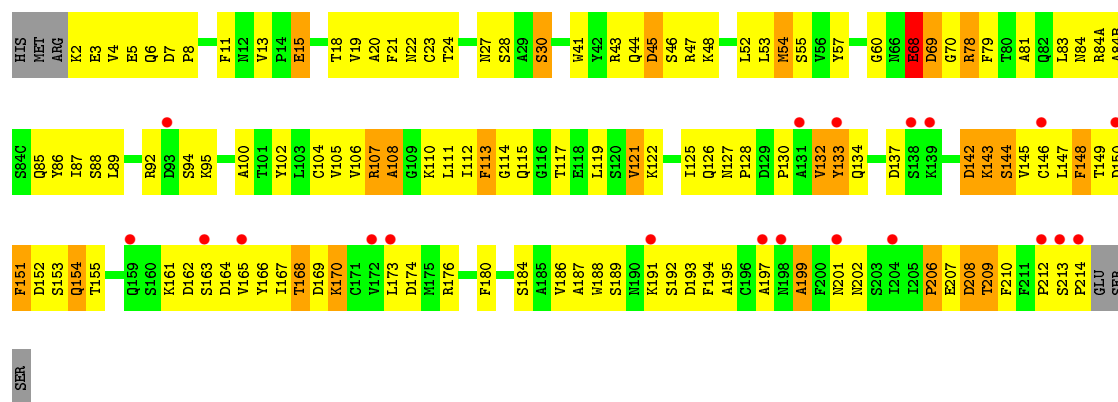
- Molecule 4: RL42 T cell receptor, alpha chain

Chain I: 49% 39% 9%



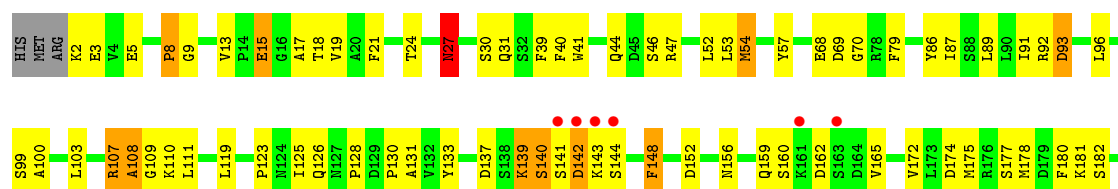
- Molecule 4: RL42 T cell receptor, alpha chain

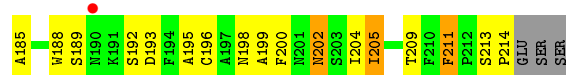
Chain N: 10% 34% 50% 12%



- Molecule 4: RL42 T cell receptor, alpha chain

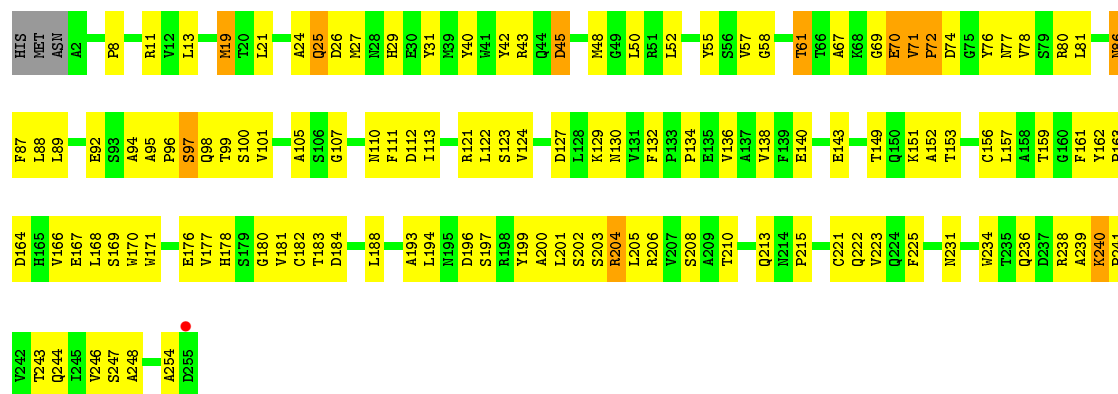
Chain S: 3% 52% 38% 6%





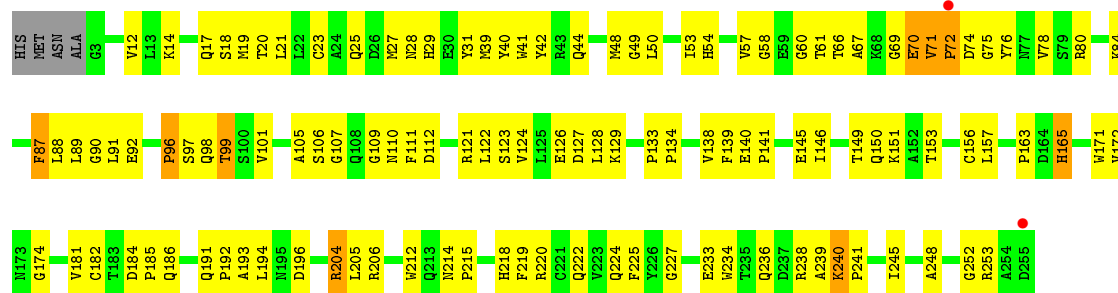
- Molecule 5: RL42 T cell receptor, beta chain

Chain E: 48% 46% 5%



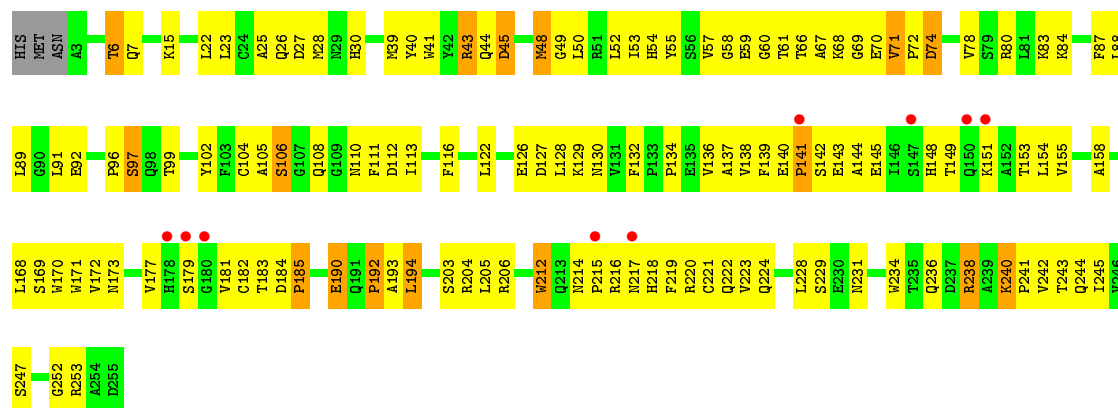
- Molecule 5: RL42 T cell receptor, beta chain

Chain J: 50% 45% 5%

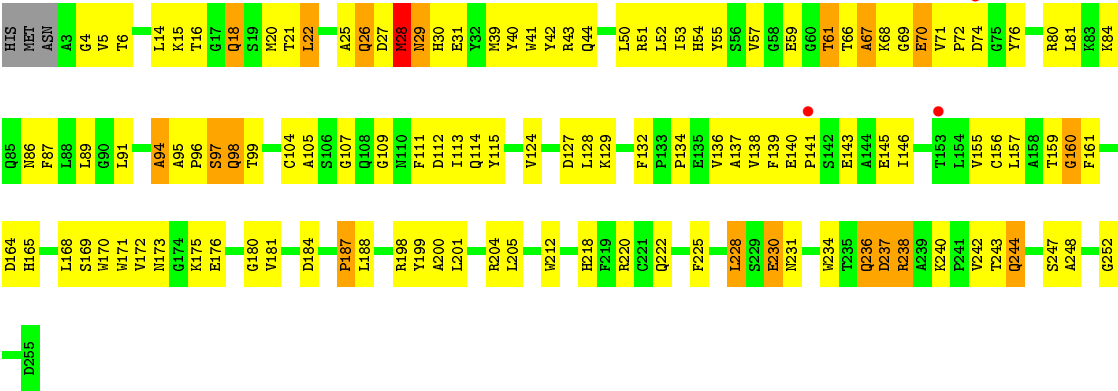


- Molecule 5: RL42 T cell receptor, beta chain

Chain O: 45% 47% 7%



- Molecule 5: RL42 T cell receptor, beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.08 Å   185.00 Å   217.68 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.99 – 3.10 19.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.7 (19.99-3.10) 99.9 (19.99-3.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 3.09 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.253   ,   0.321 0.260   ,   0.317	Depositor DCC
$R_{free}$ test set	3714 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.3	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	3 of 73724 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	26455	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/2320	0.40	0/3154
1	F	0.23	0/2320	0.40	0/3154
1	K	0.22	0/2320	0.40	0/3154
1	P	0.23	0/2320	0.40	0/3154
2	B	0.24	0/852	0.38	0/1152
2	G	0.22	0/852	0.41	0/1152
2	L	0.21	0/860	0.39	0/1162
2	Q	0.22	0/860	0.38	0/1162
3	C	0.23	0/76	0.43	0/98
3	H	0.31	0/76	0.35	0/98
3	M	0.28	0/76	0.45	0/98
3	R	0.28	0/76	0.36	0/98
4	D	0.26	0/1574	0.41	0/2132
4	I	0.26	0/1574	0.42	0/2132
4	N	0.24	0/1574	0.42	0/2132
4	S	0.27	0/1574	0.44	0/2132
5	E	0.25	0/1959	0.43	0/2662
5	J	0.28	0/1954	0.46	0/2655
5	O	0.24	0/1959	0.43	0/2662
5	T	0.25	0/1959	0.44	0/2662
All	All	0.24	0/27135	0.42	0/36805

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2258	0	2098	149	0
1	F	2258	0	2098	137	0
1	K	2258	0	2098	132	0
1	P	2258	0	2098	136	0
2	B	829	0	794	51	0
2	G	829	0	794	86	0
2	L	837	0	803	81	0
2	Q	837	0	803	48	0
3	C	75	0	79	3	0
3	H	75	0	79	8	0
3	M	75	0	79	4	0
3	R	75	0	79	5	0
4	D	1541	0	1466	109	0
4	I	1541	0	1464	83	0
4	N	1541	0	1464	148	0
4	S	1541	0	1464	83	0
5	E	1908	0	1819	109	0
5	J	1903	0	1814	95	0
5	O	1908	0	1819	138	0
5	T	1908	0	1819	109	0
All	All	26455	0	25031	1573	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 31.

All (1573) 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:I:12:ASN:HB3	4:I:122:LYS:HE3	1.29	1.14
5:J:96:PRO:HB3	5:J:124:VAL:HB	1.32	1.07
5:O:142:SER:HB3	5:O:145:GLU:HB3	1.42	0.99
4:N:207:GLU:N	4:N:208:ASP:HB2	1.77	0.99
4:D:30:SER:HA	4:D:108:ALA:CB	1.92	0.99
1:A:238:ASP:HB3	2:B:12:ARG:HH22	1.26	0.98
4:D:192:SER:N	4:D:193:ASP:HA	1.79	0.96
1:F:234:ARG:HH11	2:G:10:TYR:HD2	1.08	0.96
4:I:31:GLN:H	4:I:108:ALA:HB2	1.31	0.96
4:N:192:SER:N	4:N:193:ASP:HA	1.81	0.95
1:F:238:ASP:H	2:G:12:ARG:HH21	1.07	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:30:SER:HA	4:S:108:ALA:CB	1.98	0.94
2:Q:12:ARG:HG3	2:Q:22:PHE:HB3	1.50	0.94
1:P:72:GLN:HG3	5:T:57:VAL:HG21	1.50	0.93
2:Q:79:ALA:HB1	2:Q:92:ILE:HD11	1.51	0.92
2:G:12:ARG:HB2	2:G:22:PHE:HB2	1.52	0.91
1:A:85:TYR:HB2	1:A:87:GLN:HE21	1.33	0.91
5:E:96:PRO:HA	5:E:97:SER:O	1.71	0.91
4:N:68:GLU:HG2	4:N:69:ASP:H	1.34	0.90
1:A:159:TYR:HD2	1:A:160:LEU:HD12	1.35	0.90
2:L:81:ARG:HH12	2:L:83:ASN:HB3	1.35	0.89
4:D:80:THR:HB	4:D:90:LEU:HB2	1.55	0.89
1:P:9:ASP:HB2	1:P:97:SER:HB3	1.55	0.89
2:L:29:GLY:HA2	2:L:61:SER:HB3	1.51	0.89
2:B:12:ARG:HE	2:B:22:PHE:HD2	1.17	0.88
1:F:28:VAL:HG11	1:F:179:LEU:HD21	1.55	0.88
4:D:12:ASN:HB3	4:D:122:LYS:HE3	1.52	0.88
2:L:12:ARG:HD3	2:L:22:PHE:HB2	1.55	0.88
1:P:115:GLN:HG3	1:P:125:ALA:HB2	1.54	0.87
5:O:136:VAL:HG21	5:O:223:VAL:HG11	1.55	0.87
4:I:30:SER:HA	4:I:108:ALA:CB	2.05	0.87
4:N:122:LYS:HE2	4:N:153:SER:HB2	1.57	0.86
4:S:107:ARG:HA	4:S:111:LEU:HA	1.57	0.86
5:T:160:GLY:HA2	5:T:198:ARG:HB3	1.56	0.86
1:K:202:ARG:HD2	1:K:246:ALA:HB2	1.57	0.86
4:N:133:TYR:HE2	5:O:144:ALA:HB3	1.40	0.86
4:D:23:CYS:HB3	4:D:87:ILE:HG23	1.55	0.86
5:T:96:PRO:HA	5:T:97:SER:O	1.77	0.85
4:S:30:SER:HA	4:S:108:ALA:HB1	1.55	0.85
1:K:204:TRP:N	1:K:204:TRP:HE3	1.74	0.85
1:A:258:THR:HB	1:A:273:ARG:HA	1.56	0.85
1:P:13:SER:HB3	1:P:78:LEU:HD13	1.58	0.85
5:O:72:PRO:HA	5:O:74:ASP:O	1.77	0.84
1:A:172:LEU:HD23	1:A:179:LEU:HD23	1.59	0.84
5:E:213:GLN:HB2	5:E:254:ALA:HA	1.58	0.84
5:E:13:LEU:HD11	5:E:19:MET:HG2	1.58	0.84
4:I:31:GLN:N	4:I:108:ALA:HB2	1.92	0.84
4:D:30:SER:HA	4:D:108:ALA:HB2	1.57	0.84
5:J:133:PRO:HD3	5:J:241:PRO:HB3	1.59	0.83
2:B:1:ILE:HG23	2:B:2:GLN:H	1.43	0.82
5:O:68:LYS:HG2	5:O:69:GLY:H	1.42	0.82
1:F:70:ASN:HB3	3:H:5:ARG:HH21	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:81:LEU:HD11	3:M:9:LEU:HD22	1.62	0.81
1:F:202:ARG:HE	1:F:246:ALA:HB2	1.44	0.81
1:P:167:TRP:HA	1:P:170:ARG:HB3	1.63	0.81
1:A:217:TRP:HE3	1:A:257:TYR:CE1	1.99	0.80
4:N:107:ARG:HA	4:N:111:LEU:HA	1.61	0.80
4:S:165:VAL:HG23	4:S:189:SER:HB2	1.64	0.80
1:K:253:GLU:HG2	1:K:256:ARG:HH22	1.46	0.80
4:N:81:ALA:HA	4:N:88:SER:O	1.81	0.80
4:S:213:SER:H	4:S:214:PRO:HD2	1.45	0.79
5:J:171:TRP:HB2	5:J:220:ARG:HB2	1.64	0.79
5:O:45:ASP:HB3	1:P:145:ARG:HH21	1.46	0.79
1:F:234:ARG:HD2	2:G:10:TYR:CD2	2.17	0.79
5:O:44:GLN:HB2	5:O:50:LEU:HD23	1.65	0.78
2:Q:36:GLU:HG2	2:Q:83:ASN:HB2	1.63	0.78
1:K:204:TRP:N	1:K:204:TRP:CE3	2.52	0.78
1:F:35:ARG:CZ	2:G:53:ASP:HB3	2.13	0.78
4:D:192:SER:H	4:D:193:ASP:HA	1.49	0.78
4:S:30:SER:CA	4:S:108:ALA:HB2	2.14	0.78
5:E:99:THR:HG23	5:E:123:SER:HA	1.65	0.78
1:P:233:THR:HB	1:P:243:LYS:HD3	1.64	0.77
4:N:133:TYR:HD1	4:N:134:GLN:N	1.82	0.77
2:G:13:HIS:HB3	2:G:14:PRO:HD2	1.67	0.77
5:J:71:VAL:H	5:J:72:PRO:HD2	1.48	0.77
2:G:24:ASN:HB3	2:G:67:TYR:HB3	1.65	0.77
4:I:191:LYS:HE2	4:I:191:LYS:HA	1.66	0.77
1:K:202:ARG:HE	1:K:244:TRP:HB2	1.50	0.77
4:N:19:VAL:HG12	4:N:20:ALA:H	1.49	0.77
5:O:68:LYS:HG2	5:O:69:GLY:N	1.99	0.76
4:N:122:LYS:NZ	4:N:153:SER:O	2.19	0.76
2:G:46:ILE:HG23	2:G:78:TYR:OH	1.85	0.76
4:N:194:PHE:CZ	4:N:199:ALA:HA	2.22	0.75
4:D:161:LYS:HG2	4:D:162:ASP:H	1.49	0.75
1:A:185:PRO:HB3	1:A:263:HIS:CD2	2.22	0.75
5:O:40:TYR:HB2	5:O:105:ALA:HB3	1.69	0.75
1:F:233:THR:HG22	1:F:243:LYS:HD2	1.66	0.74
4:N:176:ARG:HH21	5:O:179:SER:HB2	1.52	0.74
1:A:81:LEU:HD23	1:A:118:TYR:CD1	2.22	0.74
5:O:168:LEU:HA	5:O:222:GLN:O	1.86	0.74
5:E:78:VAL:HG23	5:E:88:LEU:O	1.86	0.74
1:F:31:THR:HG22	1:F:209:TYR:OH	1.88	0.74
1:A:217:TRP:HA	1:A:257:TYR:OH	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:136:ARG:O	4:D:137:ASP:HB3	1.87	0.74
1:F:222:GLU:HG2	1:F:224:GLN:H	1.52	0.74
4:N:133:TYR:CE2	5:O:144:ALA:HB3	2.23	0.74
2:Q:68:THR:HG21	2:Q:78:TYR:HE2	1.53	0.73
4:D:12:ASN:CB	4:D:122:LYS:HE3	2.18	0.73
4:I:27:ASN:HD22	4:I:27:ASN:C	1.91	0.73
2:L:81:ARG:HH12	2:L:83:ASN:CB	2.01	0.73
1:K:235:PRO:HA	1:K:241:PHE:CD1	2.23	0.73
4:S:192:SER:N	4:S:193:ASP:HA	2.01	0.73
5:J:25:GLN:HE21	5:J:29:HIS:H	1.36	0.73
2:L:7:ILE:HG12	2:L:8:GLN:H	1.54	0.73
5:O:182:CYS:O	5:O:204:ARG:HG2	1.88	0.73
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.70	0.73
1:A:159:TYR:CD2	1:A:160:LEU:HD12	2.22	0.73
4:N:122:LYS:CE	4:N:153:SER:HB2	2.18	0.73
5:O:96:PRO:HA	5:O:97:SER:O	1.89	0.73
5:J:71:VAL:O	5:J:74:ASP:N	2.22	0.72
4:S:30:SER:HA	4:S:108:ALA:HB2	1.70	0.72
4:S:13:VAL:HG11	4:S:19:VAL:HG12	1.70	0.72
1:P:182:ALA:HB1	1:P:265:GLY:HA2	1.70	0.72
5:O:190:GLU:O	5:O:192:PRO:HD3	1.89	0.72
4:N:132:VAL:H	4:N:209:THR:CG2	2.02	0.72
1:F:220:ASP:OD1	1:F:221:GLY:HA3	1.88	0.72
4:I:39:PHE:HD1	4:I:106:VAL:HG22	1.54	0.72
5:J:96:PRO:HB3	5:J:124:VAL:CB	2.14	0.72
2:G:39:LEU:HB2	2:G:46:ILE:HD11	1.72	0.72
1:F:202:ARG:HH12	2:G:99:MET:HG2	1.54	0.72
5:O:228:LEU:HD12	5:O:241:PRO:HD2	1.72	0.72
5:J:28:ASN:ND2	5:J:84:LYS:HE2	2.04	0.72
4:D:43:ARG:HH12	4:D:98:ASP:HA	1.55	0.71
5:T:222:GLN:HA	5:T:247:SER:HB3	1.72	0.71
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.73	0.71
5:J:21:LEU:HD13	5:J:89:LEU:HD23	1.72	0.71
5:T:31:GLU:HG2	5:T:84:LYS:HE3	1.72	0.71
1:P:222:GLU:HG3	1:P:224:GLN:HE22	1.55	0.71
1:F:234:ARG:HD2	2:G:10:TYR:HD2	1.55	0.71
5:E:71:VAL:HG13	5:E:72:PRO:HD3	1.73	0.71
1:A:217:TRP:O	1:A:224:GLN:HB3	1.90	0.71
4:I:49:GLU:OE2	4:I:51:LYS:HE3	1.91	0.71
4:S:213:SER:N	4:S:214:PRO:HD2	2.06	0.71
4:I:192:SER:HB3	4:I:193:ASP:HA	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:26:TYR:HB2	2:G:65:LEU:HD13	1.73	0.70
4:I:42:TYR:HB2	4:I:103:LEU:HB2	1.73	0.70
4:S:41:TRP:O	4:S:53:LEU:HB3	1.90	0.70
4:N:30:SER:HB3	4:N:108:ALA:HB2	1.74	0.70
2:L:11:SER:HB2	2:L:21:ASN:HD21	1.57	0.70
4:N:13:VAL:HG21	4:N:19:VAL:HG13	1.72	0.70
4:D:30:SER:CA	4:D:108:ALA:HB2	2.21	0.70
5:O:97:SER:HB3	1:P:142:ILE:HD11	1.73	0.70
4:N:68:GLU:CG	4:N:69:ASP:H	2.03	0.69
1:P:5:MET:HB2	1:P:168:LEU:HD13	1.74	0.69
4:N:161:LYS:HG3	4:N:202:ASN:CG	2.12	0.69
5:O:234:TRP:HZ2	5:O:238:ARG:HG3	1.58	0.69
2:Q:46:ILE:HB	2:Q:78:TYR:OH	1.92	0.69
2:L:7:ILE:HG21	2:L:93:VAL:HG21	1.75	0.69
1:P:219:ARG:NH1	1:P:256:ARG:HE	1.90	0.69
5:E:101:VAL:HG22	5:E:121:ARG:HG3	1.74	0.69
1:K:208:PHE:CE2	1:K:241:PHE:HB3	2.28	0.69
1:F:201:LEU:HD21	1:F:254:GLU:HG3	1.73	0.69
5:O:172:VAL:HG13	5:O:177:VAL:HG21	1.73	0.69
2:L:39:LEU:HB3	2:L:49:VAL:HG12	1.72	0.69
4:N:210:PHE:CZ	4:N:212:PRO:HG3	2.27	0.69
1:A:238:ASP:OD1	1:A:240:THR:HG22	1.93	0.69
4:N:4:VAL:HG11	4:N:113:PHE:O	1.93	0.69
1:K:14:ARG:HD2	1:K:17:ARG:NH2	2.08	0.69
4:D:79:PHE:CD1	4:D:91:ILE:HG22	2.28	0.69
1:A:217:TRP:HE3	1:A:257:TYR:HE1	1.40	0.69
5:E:138:VAL:HG23	5:E:248:ALA:HB3	1.75	0.68
5:E:11:ARG:HG2	5:E:19:MET:HE3	1.73	0.68
1:A:244:TRP:HZ3	1:A:246:ALA:HB2	1.57	0.68
2:L:81:ARG:HE	2:L:90:PRO:HB3	1.59	0.68
2:G:37:VAL:HG22	2:G:82:VAL:HG12	1.76	0.68
5:O:68:LYS:CG	5:O:69:GLY:H	2.05	0.68
4:N:133:TYR:HD1	4:N:134:GLN:H	1.42	0.67
2:G:12:ARG:CB	2:G:22:PHE:HB2	2.23	0.67
1:A:178:THR:HA	1:A:181:ARG:HD3	1.75	0.67
1:F:22:PHE:HB2	1:F:38:SER:HB3	1.74	0.67
5:E:71:VAL:O	5:E:74:ASP:N	2.27	0.67
4:D:96:LEU:HD23	4:D:181:LYS:HD3	1.75	0.67
2:G:46:ILE:H	2:G:46:ILE:HD12	1.58	0.67
1:A:184:PRO:HB2	1:A:186:LYS:HE3	1.76	0.67
1:P:166:GLU:O	1:P:169:ARG:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:45:ASP:HB2	5:E:48:MET:HG3	1.75	0.67
4:N:70:GLY:O	4:N:78:ARG:HG2	1.94	0.67
1:K:142:ILE:HA	1:K:145:ARG:NH1	2.10	0.67
4:N:168:THR:HG23	4:N:186:VAL:HB	1.75	0.67
4:D:52:LEU:HD22	5:E:113:ILE:HG23	1.75	0.67
1:P:202:ARG:HB3	1:P:246:ALA:HB2	1.77	0.67
4:S:30:SER:CA	4:S:108:ALA:CB	2.72	0.67
1:A:217:TRP:CE3	1:A:257:TYR:HE1	2.12	0.67
5:T:22:LEU:HD13	5:T:89:LEU:HD23	1.77	0.67
1:F:35:ARG:O	1:F:46:GLU:HB3	1.95	0.66
2:Q:24:ASN:HB3	2:Q:65:LEU:HD11	1.76	0.66
1:F:233:THR:HA	1:F:243:LYS:HB2	1.77	0.66
1:K:232:GLU:HG3	2:L:6:LYS:HD3	1.77	0.66
4:S:31:GLN:H	4:S:108:ALA:HB2	1.58	0.66
1:P:11:ALA:HB3	1:P:95:LEU:HB3	1.77	0.66
4:N:207:GLU:HB2	4:N:208:ASP:HA	1.78	0.66
2:L:24:ASN:HD21	2:L:65:LEU:HB3	1.60	0.66
1:A:234:ARG:HG2	1:A:234:ARG:O	1.96	0.66
2:B:1:ILE:HG23	2:B:2:GLN:N	2.11	0.66
1:P:50:PRO:HG2	1:P:51:TRP:CE3	2.30	0.66
4:S:27:ASN:C	4:S:27:ASN:HD22	1.98	0.66
4:I:213:SER:H	4:I:214:PRO:HD2	1.60	0.66
2:L:0:MET:HA	2:L:1:ILE:HD12	1.78	0.66
4:N:143:LYS:HG3	4:N:144:SER:H	1.61	0.65
1:K:5:MET:HB2	1:K:168:LEU:HD13	1.78	0.65
1:A:238:ASP:HB3	2:B:12:ARG:NH2	2.08	0.65
1:K:69:THR:HG23	5:O:110:ASN:ND2	2.11	0.65
4:D:134:GLN:HB2	4:D:196:CYS:SG	2.35	0.65
2:B:73:THR:OG1	2:B:76:ASP:HB2	1.95	0.65
5:J:174:GLY:HA2	5:J:220:ARG:HH12	1.61	0.65
2:B:12:ARG:NE	2:B:22:PHE:HD2	1.93	0.65
4:D:192:SER:N	4:D:193:ASP:CA	2.59	0.65
4:N:21:PHE:HB2	4:N:89:LEU:HB3	1.79	0.65
4:S:39:PHE:CD1	4:S:87:ILE:HD11	2.32	0.65
4:N:161:LYS:HG3	4:N:202:ASN:ND2	2.11	0.65
1:P:28:VAL:HG12	1:P:29:ASP:OD1	1.97	0.65
4:N:15:GLU:O	4:N:94:SER:HB2	1.97	0.65
1:P:147:TRP:CD1	1:P:152:VAL:HG21	2.32	0.65
1:A:242:GLN:O	1:A:243:LYS:HB3	1.97	0.65
2:G:45:ARG:HG2	2:G:46:ILE:H	1.61	0.65
4:N:167:ILE:HG12	4:N:187:ALA:HB1	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:4:THR:HG23	2:L:86:THR:HB	1.77	0.65
5:E:168:LEU:HD12	5:E:169:SER:H	1.61	0.65
4:D:30:SER:HA	4:D:108:ALA:HB1	1.79	0.64
1:K:244:TRP:CD1	1:K:244:TRP:N	2.64	0.64
4:I:15:GLU:O	4:I:94:SER:HB2	1.98	0.64
4:S:30:SER:CB	4:S:108:ALA:HB2	2.28	0.64
1:K:72:GLN:HG3	5:O:57:VAL:HG11	1.78	0.64
1:A:49:ALA:HB1	1:A:50:PRO:HD2	1.79	0.64
1:K:207:GLY:HA2	1:K:240:THR:OG1	1.97	0.64
4:I:52:LEU:HD12	4:I:53:LEU:H	1.62	0.64
5:J:141:PRO:HD2	5:J:212:TRP:CZ2	2.32	0.64
2:B:24:ASN:HB3	2:B:67:TYR:HB3	1.78	0.64
4:D:113:PHE:CE1	5:E:50:LEU:HD12	2.31	0.64
5:O:240:LYS:HG2	5:O:242:VAL:HG13	1.80	0.64
3:R:6:ALA:O	5:T:109:GLY:HA2	1.98	0.64
4:N:4:VAL:HG11	4:N:114:GLY:HA2	1.80	0.64
2:L:40:LEU:HD23	2:L:43:GLY:HA2	1.79	0.64
1:F:238:ASP:N	2:G:12:ARG:HH21	1.88	0.64
2:B:67:TYR:H	2:B:67:TYR:HD2	1.45	0.64
5:J:134:PRO:HD3	5:J:225:PHE:CD1	2.33	0.64
5:T:156:CYS:HB2	5:T:170:TRP:CH2	2.32	0.64
1:P:65:GLN:HE21	1:P:65:GLN:HA	1.63	0.64
4:D:8:PRO:HD2	4:D:11:PHE:HZ	1.63	0.64
4:N:210:PHE:O	4:N:212:PRO:HD3	1.98	0.63
4:I:30:SER:HA	4:I:108:ALA:HB2	1.79	0.63
4:N:28:SER:HA	4:N:85:GLN:NE2	2.13	0.63
4:N:70:GLY:C	4:N:79:PHE:H	1.99	0.63
2:L:2:GLN:OE1	2:L:31:HIS:HB2	1.98	0.63
5:J:78:VAL:HG23	5:J:88:LEU:O	1.98	0.63
1:K:225:THR:O	1:K:228:THR:HG22	1.98	0.63
5:J:25:GLN:HG2	5:J:27:MET:H	1.63	0.63
5:T:15:LYS:HE3	5:T:128:LEU:HD13	1.80	0.63
5:E:13:LEU:HD11	5:E:19:MET:CG	2.28	0.63
4:N:148:PHE:O	4:N:184:SER:HA	1.99	0.63
1:A:219:ARG:HB2	1:A:224:GLN:HB2	1.81	0.63
1:P:260:HIS:HA	1:P:271:THR:HG22	1.81	0.63
5:E:210:THR:HA	5:E:213:GLN:HE22	1.64	0.63
1:P:103:VAL:HG12	1:P:109:LEU:HA	1.80	0.63
5:E:98:GLN:O	5:E:122:LEU:HD23	1.99	0.63
5:O:170:TRP:CZ3	5:O:221:CYS:HB3	2.34	0.63
4:I:213:SER:N	4:I:214:PRO:HD2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:PRO:HB2	2:G:65:LEU:HD22	1.80	0.62
4:D:79:PHE:HD1	4:D:91:ILE:HG22	1.62	0.62
1:P:206:LEU:HD23	1:P:207:GLY:N	2.14	0.62
4:D:91:ILE:O	4:D:91:ILE:HG13	2.00	0.62
1:P:58:GLU:O	1:P:62:ARG:HG2	1.99	0.62
1:A:213:ILE:HG13	1:A:261:VAL:HG13	1.81	0.62
1:A:218:GLN:HB2	1:A:257:TYR:CD2	2.34	0.62
4:N:7:ASP:HB3	4:N:11:PHE:HZ	1.65	0.62
1:P:266:LEU:HD12	1:P:267:PRO:HD2	1.81	0.62
1:F:219:ARG:HD2	1:F:256:ARG:HB3	1.81	0.62
5:O:140:GLU:HB3	5:O:141:PRO:HD2	1.80	0.62
1:K:168:LEU:O	1:K:172:LEU:HG	2.00	0.62
2:G:29:GLY:HA2	2:G:61:SER:HB3	1.81	0.62
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.81	0.62
4:S:130:PRO:HG2	4:S:209:THR:HA	1.81	0.62
1:F:236:ALA:HB1	2:G:12:ARG:CZ	2.29	0.62
4:N:44:GLN:HE22	5:O:44:GLN:HE22	1.47	0.62
5:E:58:GLY:O	5:E:80:ARG:HG2	1.99	0.62
5:T:97:SER:O	5:T:99:THR:N	2.33	0.62
1:F:25:VAL:HG11	1:F:35:ARG:CZ	2.30	0.62
4:N:30:SER:HA	4:N:108:ALA:CB	2.30	0.62
1:K:204:TRP:H	1:K:204:TRP:HE3	1.47	0.62
4:N:145:VAL:HG13	4:N:187:ALA:H	1.63	0.62
1:A:72:GLN:HG3	5:E:57:VAL:HG21	1.80	0.62
5:J:31:TYR:CZ	5:J:110:ASN:HB2	2.34	0.61
5:T:16:THR:HG23	5:T:95:ALA:HA	1.80	0.61
1:P:182:ALA:HB1	1:P:265:GLY:CA	2.30	0.61
5:T:234:TRP:HZ2	5:T:238:ARG:HB2	1.63	0.61
4:N:137:ASP:OD1	5:O:139:PHE:HD1	1.83	0.61
4:I:145:VAL:HG12	4:I:188:TRP:HB3	1.81	0.61
1:K:202:ARG:CD	1:K:246:ALA:HB2	2.28	0.61
1:A:185:PRO:HB3	1:A:263:HIS:HD2	1.65	0.61
2:G:33:SER:HB2	2:G:54:LEU:HD11	1.83	0.61
1:P:21:ARG:NH2	1:P:23:ILE:HD11	2.14	0.61
5:E:45:ASP:HB3	1:F:145:ARG:HH21	1.66	0.61
4:D:27:ASN:HD22	4:D:27:ASN:C	2.03	0.61
5:T:188:LEU:HB3	5:T:200:ALA:HB3	1.81	0.61
1:A:103:VAL:HG12	1:A:109:LEU:HA	1.80	0.61
4:N:21:PHE:O	4:N:88:SER:HA	2.00	0.61
5:T:15:LYS:HB2	5:T:128:LEU:HD11	1.81	0.61
4:N:68:GLU:HG2	4:N:69:ASP:N	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:23:LEU:HD13	2:L:70:PHE:CZ	2.36	0.61
5:J:212:TRP:HE3	5:J:219:PHE:HE1	1.48	0.61
5:J:181:VAL:HG12	5:J:205:LEU:HD13	1.82	0.61
1:F:21:ARG:HE	1:F:23:ILE:HG13	1.66	0.61
4:N:206:PRO:HB2	4:N:208:ASP:HB2	1.83	0.61
4:D:12:ASN:HB3	4:D:122:LYS:CE	2.26	0.61
1:A:147:TRP:HB3	1:A:152:VAL:HB	1.83	0.61
5:O:154:LEU:HD11	5:O:205:LEU:HB3	1.81	0.61
4:D:126:GLN:HG3	4:D:127:ASN:N	2.16	0.60
1:A:35:ARG:CZ	2:B:53:ASP:HB3	2.30	0.60
2:L:23:LEU:HD23	2:L:78:TYR:HB3	1.82	0.60
1:P:211:ALA:HB2	1:P:241:PHE:CD2	2.36	0.60
4:N:30:SER:HA	4:N:108:ALA:HB1	1.82	0.60
2:G:5:PRO:HA	2:G:30:PHE:HB3	1.83	0.60
1:F:159:TYR:CE1	3:H:3:ARG:HB2	2.37	0.60
4:N:112:ILE:H	4:N:112:ILE:HD12	1.67	0.60
4:S:18:THR:HG22	4:S:93:ASP:H	1.66	0.60
5:O:128:LEU:HG	5:O:228:LEU:HD21	1.84	0.60
4:N:145:VAL:HG11	4:N:186:VAL:HG13	1.83	0.60
1:A:35:ARG:O	1:A:46:GLU:HB3	2.01	0.60
1:A:219:ARG:NH1	1:A:219:ARG:HA	2.17	0.60
5:T:57:VAL:HG22	5:T:61:THR:HG21	1.83	0.60
2:L:2:GLN:HE22	2:L:31:HIS:H	1.50	0.60
5:T:230:GLU:HG3	5:T:231:ASN:H	1.67	0.60
5:T:164:ASP:CB	5:T:187:PRO:HG2	2.32	0.60
1:K:187:THR:HB	1:K:204:TRP:CZ2	2.36	0.60
4:D:15:GLU:O	4:D:94:SER:HB2	2.02	0.60
4:N:148:PHE:CE2	4:N:151:PHE:HB2	2.37	0.60
5:O:136:VAL:HG12	5:O:137:ALA:H	1.66	0.60
1:K:69:THR:HA	1:K:72:GLN:OE1	2.01	0.60
1:K:51:TRP:CH2	1:K:178:THR:HB	2.37	0.60
1:K:257:TYR:N	1:K:257:TYR:HD2	2.00	0.60
1:K:188:HIS:H	1:K:204:TRP:HE1	1.49	0.60
1:A:217:TRP:CD2	1:A:247:VAL:HB	2.36	0.60
4:N:145:VAL:CG1	4:N:187:ALA:H	2.15	0.60
2:B:96:ASP:HB3	2:B:99:MET:HB3	1.83	0.59
5:T:43:ARG:HE	5:T:51:ARG:NH2	2.00	0.59
1:A:102:ASP:HB2	1:A:110:LEU:HD11	1.84	0.59
2:Q:68:THR:HG21	2:Q:78:TYR:CE2	2.36	0.59
4:N:30:SER:CB	4:N:108:ALA:HB2	2.31	0.59
4:I:80:THR:HB	4:I:90:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:97:SER:C	5:T:99:THR:H	2.04	0.59
5:E:11:ARG:HG2	5:E:19:MET:CE	2.33	0.59
2:Q:36:GLU:CG	2:Q:83:ASN:HB2	2.32	0.59
5:J:234:TRP:HZ2	5:J:238:ARG:HG3	1.68	0.59
1:A:214:THR:HG22	1:A:216:THR:HG23	1.83	0.59
1:F:129:ASP:O	1:F:131:ARG:HG3	2.03	0.59
5:T:6:THR:HG23	5:T:25:ALA:HB3	1.84	0.59
1:K:191:HIS:HE2	1:K:201:LEU:HG	1.67	0.59
2:G:23:LEU:HB2	2:G:70:PHE:CE2	2.37	0.59
1:P:51:TRP:CZ2	1:P:179:LEU:HD11	2.38	0.59
4:I:52:LEU:HD12	4:I:53:LEU:N	2.18	0.59
1:P:2:SER:H	1:P:105:PRO:HA	1.67	0.59
1:F:177:ASP:O	1:F:181:ARG:HB3	2.02	0.59
1:F:262:GLN:CD	1:F:262:GLN:H	2.06	0.59
5:O:170:TRP:HD1	5:O:181:VAL:HG23	1.67	0.59
1:P:81:LEU:HD12	1:P:118:TYR:CD2	2.38	0.59
1:A:255:GLN:CD	1:A:255:GLN:H	2.06	0.59
5:J:101:VAL:HG22	5:J:121:ARG:HG2	1.84	0.59
1:K:99:TYR:CE1	3:M:3:ARG:HB3	2.37	0.59
1:F:236:ALA:HB1	2:G:12:ARG:NH1	2.18	0.59
2:Q:41:LYS:HB2	2:Q:46:ILE:HD11	1.85	0.59
4:S:125:ILE:HG21	4:S:152:ASP:HA	1.85	0.59
4:N:194:PHE:CG	4:N:195:ALA:N	2.71	0.58
4:N:194:PHE:HZ	4:N:199:ALA:HA	1.66	0.58
1:A:198:GLU:HG3	1:A:248:VAL:HG12	1.85	0.58
1:K:241:PHE:HD1	1:K:242:GLN:H	1.52	0.58
5:E:193:ALA:HB1	5:J:27:MET:HE2	1.84	0.58
4:N:18:THR:HG22	4:N:92:ARG:HA	1.85	0.58
5:J:21:LEU:HD12	5:J:21:LEU:N	2.18	0.58
1:A:219:ARG:HH11	1:A:219:ARG:HA	1.67	0.58
4:I:70:GLY:O	4:I:78:ARG:HB3	2.02	0.58
1:A:209:TYR:HB3	1:A:210:PRO:HD3	1.85	0.58
4:I:195:ALA:O	4:I:199:ALA:HB2	2.03	0.58
4:I:18:THR:HB	4:I:92:ARG:HA	1.85	0.58
5:O:26:GLN:HG3	5:O:106:SER:HB2	1.85	0.58
1:A:203:CYS:HB2	1:A:215:LEU:HD11	1.86	0.58
4:N:21:PHE:HZ	4:N:119:LEU:HD13	1.69	0.58
1:K:257:TYR:CD2	1:K:257:TYR:N	2.69	0.58
4:D:58:SER:O	4:D:83:LEU:HD23	2.03	0.58
1:A:57:PRO:O	1:A:61:ASP:HB2	2.04	0.58
4:N:209:THR:O	4:N:210:PHE:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:91:LYS:HG3	2:Q:92:ILE:H	1.68	0.58
1:A:189:VAL:HG22	1:A:190:THR:N	2.18	0.58
2:G:7:ILE:HD12	2:G:82:VAL:HG21	1.84	0.58
2:L:2:GLN:HE22	2:L:31:HIS:N	2.01	0.58
5:T:5:VAL:HG22	5:T:26:GLN:HB2	1.85	0.58
1:K:233:THR:HG23	1:K:243:LYS:HG3	1.85	0.58
2:L:3:ARG:HG3	2:L:86:THR:HG21	1.86	0.58
1:P:269:PRO:O	1:P:271:THR:HG23	2.04	0.58
1:P:55:GLU:HB2	1:P:59:TYR:HB2	1.86	0.58
5:O:27:ASP:O	5:O:28:MET:HG3	2.03	0.58
2:G:47:GLU:O	2:G:48:LYS:HG2	2.04	0.58
1:K:191:HIS:NE2	1:K:201:LEU:HG	2.19	0.58
4:D:31:GLN:N	4:D:108:ALA:HB2	2.18	0.57
2:L:36:GLU:HG2	2:L:37:VAL:H	1.68	0.57
5:O:221:CYS:O	5:O:247:SER:HB3	2.03	0.57
2:G:17:ASN:HD21	2:G:19:LYS:HE3	1.69	0.57
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.86	0.57
4:I:165:VAL:HG12	4:I:189:SER:OG	2.04	0.57
4:N:133:TYR:CD1	4:N:134:GLN:N	2.68	0.57
5:J:42:TYR:HB3	5:J:50:LEU:HD22	1.86	0.57
2:B:70:PHE:CZ	2:B:72:PRO:HG3	2.38	0.57
4:N:206:PRO:HB2	4:N:208:ASP:CB	2.33	0.57
1:A:233:THR:OG1	1:A:243:LYS:HE3	2.05	0.57
1:K:188:HIS:C	1:K:204:TRP:HE1	2.08	0.57
4:D:52:LEU:HD22	5:E:113:ILE:CG2	2.34	0.57
4:S:137:ASP:HB2	5:T:139:PHE:CE2	2.39	0.57
5:O:216:ARG:HG3	5:O:216:ARG:O	2.04	0.57
4:N:133:TYR:CE2	4:N:212:PRO:HG2	2.40	0.57
5:E:99:THR:CG2	5:E:123:SER:HA	2.34	0.57
4:N:110:LYS:HG3	5:O:111:PHE:CE2	2.39	0.57
1:F:35:ARG:HB3	1:F:47:PRO:HG2	1.86	0.57
5:T:171:TRP:CZ3	5:T:176:GLU:HB2	2.39	0.57
1:A:74:ASP:HB3	3:C:5:ARG:NH1	2.19	0.57
5:O:138:VAL:HG22	5:O:139:PHE:H	1.68	0.57
1:A:142:ILE:HG12	1:A:145:ARG:HH12	1.69	0.57
5:E:149:THR:O	5:E:151:LYS:HG3	2.05	0.57
4:N:23:CYS:HB3	4:N:87:ILE:HG12	1.85	0.57
1:F:235:PRO:O	1:F:236:ALA:HB2	2.05	0.57
1:A:85:TYR:CB	1:A:87:GLN:HE21	2.13	0.57
1:K:203:CYS:O	1:K:204:TRP:HB3	2.04	0.57
2:L:12:ARG:HG3	2:L:13:HIS:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:ARG:HE	1:F:246:ALA:CB	2.16	0.57
1:F:99:TYR:CE1	3:H:3:ARG:HB3	2.38	0.57
2:B:54:LEU:HD11	2:B:62:PHE:HB3	1.87	0.57
4:S:205:ILE:HD12	4:S:205:ILE:H	1.69	0.57
1:F:215:LEU:HA	1:F:262:GLN:HE22	1.70	0.57
1:A:22:PHE:CD1	1:A:71:THR:HB	2.39	0.57
2:B:7:ILE:HD12	2:B:82:VAL:HG21	1.86	0.57
5:T:236:GLN:HG3	5:T:237:ASP:H	1.70	0.56
4:D:41:TRP:HB2	4:D:54:MET:HB2	1.87	0.56
4:S:52:LEU:HD22	5:T:113:ILE:HG23	1.86	0.56
1:F:220:ASP:CB	1:F:221:GLY:HA3	2.33	0.56
2:B:9:VAL:HG23	2:B:93:VAL:HG13	1.88	0.56
2:B:41:LYS:HG2	2:B:42:ASN:HD22	1.68	0.56
5:O:144:ALA:HB1	5:O:148:HIS:CE1	2.40	0.56
1:P:222:GLU:HG3	1:P:224:GLN:NE2	2.19	0.56
2:G:7:ILE:O	2:G:8:GLN:HG3	2.05	0.56
1:A:72:GLN:HE21	5:E:57:VAL:HG21	1.69	0.56
1:P:21:ARG:HH21	1:P:23:ILE:HD11	1.70	0.56
4:I:132:VAL:HG22	4:I:148:PHE:HB2	1.86	0.56
1:P:82:ARG:NH1	1:P:89:GLU:HG3	2.20	0.56
5:O:6:THR:HG23	5:O:25:ALA:HB3	1.87	0.56
5:T:138:VAL:HG23	5:T:248:ALA:HB3	1.87	0.56
2:G:11:SER:OG	2:G:15:ALA:HB2	2.05	0.56
2:Q:70:PHE:CE1	2:Q:72:PRO:HG3	2.40	0.56
2:L:96:ASP:HB2	2:L:99:MET:HB3	1.88	0.56
4:S:31:GLN:N	4:S:108:ALA:HB2	2.20	0.56
5:T:71:VAL:HB	5:T:72:PRO:HD3	1.88	0.56
4:S:39:PHE:HB3	4:S:87:ILE:HD13	1.87	0.56
1:P:66:ILE:HD13	4:S:109:GLY:HA2	1.87	0.56
4:N:52:LEU:HD22	5:O:113:ILE:HG23	1.87	0.56
1:A:217:TRP:CE3	1:A:257:TYR:CE1	2.86	0.56
5:J:54:HIS:CE1	5:J:71:VAL:HG21	2.40	0.56
2:L:3:ARG:HE	2:L:3:ARG:N	2.03	0.56
2:L:29:GLY:HA2	2:L:61:SER:CB	2.32	0.56
1:A:217:TRP:HA	1:A:257:TYR:CZ	2.40	0.56
1:A:208:PHE:CD1	1:A:210:PRO:HD2	2.39	0.56
1:F:191:HIS:CE1	1:F:193:PRO:HD3	2.41	0.56
5:J:224:GLN:HE22	5:J:245:ILE:HD11	1.69	0.56
5:E:234:TRP:CE2	5:E:236:GLN:HB2	2.40	0.56
1:P:72:GLN:HG3	5:T:57:VAL:CG2	2.31	0.56
5:J:19:MET:SD	5:J:122:LEU:HD13	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:21:PHE:HZ	4:D:119:LEU:HD22	1.71	0.56
1:A:218:GLN:HE22	1:A:260:HIS:CD2	2.24	0.56
5:O:45:ASP:HB3	1:P:145:ARG:NH2	2.18	0.56
1:P:219:ARG:HB3	1:P:224:GLN:NE2	2.20	0.56
1:P:217:TRP:CD1	1:P:259:CYS:HA	2.41	0.56
5:O:136:VAL:HG12	5:O:137:ALA:N	2.21	0.56
5:O:44:GLN:HB2	5:O:50:LEU:CD2	2.35	0.56
2:G:45:ARG:HG2	2:G:46:ILE:N	2.21	0.56
4:S:19:VAL:HG22	4:S:91:ILE:HB	1.87	0.56
5:O:26:GLN:HG3	5:O:106:SER:CB	2.35	0.56
1:P:55:GLU:HB2	1:P:59:TYR:CB	2.35	0.56
5:O:193:ALA:HB1	5:T:28:MET:HG2	1.86	0.56
1:K:67:PHE:O	1:K:71:THR:HG23	2.06	0.56
4:D:78:ARG:HG3	4:D:92:ARG:HD3	1.88	0.56
1:K:187:THR:HB	1:K:204:TRP:CH2	2.41	0.55
5:J:54:HIS:CE1	5:J:71:VAL:HG11	2.41	0.55
4:S:192:SER:H	4:S:193:ASP:HA	1.70	0.55
5:T:170:TRP:CD1	5:T:181:VAL:HG23	2.40	0.55
1:P:260:HIS:HA	1:P:271:THR:CG2	2.35	0.55
2:B:21:ASN:HB3	2:B:70:PHE:HE1	1.70	0.55
5:E:97:SER:C	5:E:99:THR:H	2.09	0.55
1:P:191:HIS:HD1	1:P:192:HIS:H	1.52	0.55
2:Q:22:PHE:HZ	2:Q:67:TYR:CD2	2.24	0.55
1:F:70:ASN:HB3	3:H:5:ARG:NH2	2.18	0.55
1:P:28:VAL:HG23	1:P:33:PHE:CD2	2.41	0.55
4:D:158:SER:HB2	4:D:202:ASN:O	2.06	0.55
5:O:173:ASN:HA	5:O:218:HIS:CE1	2.41	0.55
1:K:151:ARG:HD2	1:K:154:GLU:OE2	2.06	0.55
5:T:15:LYS:O	5:T:18:GLN:HB2	2.07	0.55
5:O:224:GLN:NE2	5:O:245:ILE:HD11	2.21	0.55
2:B:22:PHE:O	2:B:23:LEU:HB3	2.06	0.55
5:J:74:ASP:OD1	5:J:76:TYR:HD2	1.90	0.55
4:N:128:PRO:HB3	4:N:152:ASP:HB3	1.87	0.55
1:K:244:TRP:HD1	1:K:244:TRP:N	2.03	0.55
4:I:137:ASP:HA	5:J:139:PHE:HA	1.88	0.55
1:F:211:ALA:HB2	1:F:241:PHE:CE2	2.41	0.55
4:S:126:GLN:O	4:S:128:PRO:HD3	2.06	0.55
1:K:213:ILE:HG22	1:K:214:THR:N	2.21	0.55
2:L:12:ARG:HE	2:L:13:HIS:CE1	2.26	0.55
5:O:242:VAL:O	5:O:244:GLN:HG2	2.07	0.55
4:I:162:ASP:HB3	4:I:165:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:215:PRO:HA	5:O:252:GLY:HA3	1.89	0.55
1:A:28:VAL:O	1:A:29:ASP:HB2	2.06	0.55
4:N:132:VAL:H	4:N:209:THR:HG21	1.73	0.54
2:Q:41:LYS:HA	2:Q:78:TYR:HA	1.89	0.54
5:J:174:GLY:HA2	5:J:220:ARG:NH1	2.23	0.54
5:T:128:LEU:HD23	5:T:228:LEU:CD1	2.36	0.54
4:D:30:SER:CA	4:D:108:ALA:CB	2.77	0.54
1:F:72:GLN:HG3	5:J:57:VAL:HG21	1.89	0.54
1:K:211:ALA:O	1:K:213:ILE:HG13	2.08	0.54
2:L:3:ARG:N	2:L:3:ARG:NE	2.56	0.54
1:A:48:ARG:HB3	1:A:52:ILE:HD11	1.89	0.54
1:P:215:LEU:O	1:P:215:LEU:HD12	2.07	0.54
1:K:14:ARG:NH2	1:K:21:ARG:HB2	2.22	0.54
5:E:45:ASP:HB3	1:F:145:ARG:NH2	2.22	0.54
1:K:81:LEU:HD13	1:K:118:TYR:CD1	2.41	0.54
1:F:220:ASP:CG	1:F:221:GLY:HA3	2.28	0.54
5:O:66:THR:HG22	5:O:67:ALA:N	2.22	0.54
1:K:100:GLY:O	1:K:160:LEU:HD22	2.08	0.54
4:N:45:ASP:O	4:N:48:LYS:HG2	2.07	0.54
5:J:234:TRP:CD1	5:J:240:LYS:HB2	2.41	0.54
4:N:105:VAL:HG13	4:N:113:PHE:HA	1.90	0.54
5:O:130:ASN:HA	5:O:132:PHE:HE2	1.71	0.54
5:E:168:LEU:HD21	5:E:203:SER:HB2	1.89	0.54
1:A:110:LEU:HD12	1:A:111:ARG:N	2.23	0.54
4:S:21:PHE:HB2	4:S:89:LEU:HB3	1.90	0.54
5:E:74:ASP:OD1	5:E:76:TYR:HD2	1.90	0.54
2:L:40:LEU:HB2	2:L:78:TYR:CD1	2.43	0.54
5:T:228:LEU:HD22	5:T:228:LEU:H	1.71	0.54
1:K:51:TRP:HH2	1:K:178:THR:HB	1.72	0.54
1:F:182:ALA:HB1	1:F:265:GLY:HA2	1.88	0.54
1:A:8:PHE:HB3	2:B:56:PHE:CE1	2.43	0.54
5:O:48:MET:HG3	5:O:49:GLY:H	1.71	0.54
4:N:13:VAL:HG21	4:N:19:VAL:HG22	1.89	0.54
4:N:125:ILE:HG23	4:N:128:PRO:HG3	1.89	0.54
4:N:152:ASP:HB2	4:N:154:GLN:HE21	1.73	0.54
1:K:156:ASP:O	1:K:160:LEU:HG	2.07	0.54
5:O:194:LEU:H	5:O:194:LEU:HD12	1.72	0.54
1:F:220:ASP:CB	1:F:221:GLY:CA	2.86	0.54
5:E:166:VAL:CG1	5:E:223:VAL:HG13	2.38	0.54
4:D:25:TYR:CZ	4:D:85:GLN:HA	2.43	0.54
5:E:238:ARG:HG3	5:E:239:ALA:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:208:PHE:CZ	1:K:213:ILE:HD11	2.42	0.53
1:A:178:THR:HG23	1:A:179:LEU:HD13	1.90	0.53
1:P:2:SER:HB2	1:P:105:PRO:HG3	1.91	0.53
5:E:176:GLU:HG3	5:E:177:VAL:N	2.24	0.53
4:N:44:GLN:NE2	5:O:44:GLN:HE22	2.05	0.53
5:O:129:LYS:HE2	5:O:236:GLN:OE1	2.08	0.53
1:A:197:HIS:CE1	1:A:251:SER:H	2.25	0.53
1:K:233:THR:HG22	1:K:241:PHE:CE1	2.43	0.53
1:A:67:PHE:O	1:A:71:THR:HG23	2.08	0.53
2:Q:39:LEU:HB2	2:Q:78:TYR:CZ	2.43	0.53
1:A:217:TRP:HE3	1:A:257:TYR:CZ	2.27	0.53
2:G:39:LEU:HB2	2:G:46:ILE:CD1	2.38	0.53
1:P:266:LEU:HD21	1:P:270:LEU:HD22	1.91	0.53
5:T:55:TYR:CE2	5:T:67:ALA:HB3	2.43	0.53
1:F:13:SER:O	1:F:92:SER:HB2	2.08	0.53
4:N:210:PHE:HE1	5:O:148:HIS:CE1	2.25	0.53
1:A:6:ARG:HA	1:A:100:GLY:HA3	1.89	0.53
1:F:103:VAL:HG13	1:F:168:LEU:HD23	1.91	0.53
1:F:159:TYR:CE2	1:F:164:CYS:HB2	2.44	0.53
5:T:187:PRO:HB3	5:T:199:TYR:HB3	1.90	0.53
1:F:13:SER:HB2	1:F:78:LEU:HD13	1.89	0.53
2:B:38:ASP:HB2	2:B:81:ARG:HE	1.74	0.53
5:J:40:TYR:N	5:J:105:ALA:O	2.41	0.53
5:E:134:PRO:HB3	5:E:161:PHE:HB3	1.90	0.53
5:E:55:TYR:CE2	5:E:67:ALA:HB3	2.44	0.53
1:A:26:GLY:O	1:A:32:GLN:HA	2.09	0.53
1:P:263:HIS:CG	1:P:264:GLU:H	2.26	0.53
5:J:29:HIS:CE1	5:J:107:GLY:HA2	2.44	0.53
2:L:87:LEU:HD12	2:L:87:LEU:O	2.08	0.53
2:G:75:LYS:C	2:G:77:GLU:H	2.12	0.53
5:O:58:GLY:O	5:O:80:ARG:HG2	2.08	0.53
4:S:68:GLU:O	4:S:68:GLU:HG3	2.07	0.53
5:J:110:ASN:O	5:J:111:PHE:HB2	2.08	0.53
1:A:218:GLN:N	1:A:257:TYR:CE2	2.76	0.53
5:J:71:VAL:N	5:J:72:PRO:HD2	2.20	0.53
4:S:18:THR:HB	4:S:92:ARG:HA	1.89	0.53
1:F:15:PRO:C	1:F:17:ARG:H	2.11	0.53
5:J:58:GLY:O	5:J:80:ARG:HD3	2.09	0.53
4:D:12:ASN:CG	4:D:122:LYS:HE3	2.29	0.53
4:N:30:SER:CA	4:N:108:ALA:HB2	2.39	0.53
5:J:71:VAL:HG12	5:J:71:VAL:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:152:ASP:HB2	4:N:154:GLN:NE2	2.24	0.53
5:J:182:CYS:O	5:J:204:ARG:HD2	2.09	0.53
5:T:40:TYR:CD2	5:T:114:GLN:NE2	2.77	0.53
5:O:45:ASP:CB	1:P:145:ARG:HH21	2.20	0.53
4:D:161:LYS:HB3	4:D:161:LYS:NZ	2.24	0.53
1:A:155:GLN:HG2	4:D:57:TYR:HB3	1.91	0.53
4:I:159:GLN:O	4:I:160:SER:HB2	2.08	0.53
4:I:13:VAL:HG11	4:I:19:VAL:HG22	1.90	0.53
5:J:194:LEU:HG	5:J:196:ASP:H	1.74	0.53
1:P:170:ARG:HH11	1:P:174:ASN:ND2	2.08	0.52
5:O:154:LEU:O	5:O:204:ARG:HA	2.09	0.52
4:I:39:PHE:CD1	4:I:106:VAL:HG22	2.41	0.52
2:L:4:THR:HG21	2:L:87:LEU:HB3	1.91	0.52
2:B:24:ASN:HB3	2:B:67:TYR:CB	2.40	0.52
1:K:13:SER:HB2	1:K:78:LEU:HD13	1.91	0.52
4:S:2:LYS:O	4:S:3:GLU:HB2	2.09	0.52
5:E:162:TYR:CD1	5:E:163:PRO:HA	2.43	0.52
5:E:110:ASN:O	5:E:111:PHE:HB2	2.09	0.52
4:N:137:ASP:HB2	4:N:142:ASP:OD1	2.09	0.52
5:O:170:TRP:CD1	5:O:181:VAL:HG23	2.44	0.52
4:D:136:ARG:HA	4:D:136:ARG:NE	2.24	0.52
2:L:23:LEU:HD13	2:L:70:PHE:CE1	2.44	0.52
1:A:102:ASP:O	1:A:110:LEU:HG	2.10	0.52
5:T:180:GLY:O	5:T:205:LEU:HA	2.09	0.52
2:Q:29:GLY:HA2	2:Q:61:SER:CB	2.38	0.52
5:T:43:ARG:HB2	5:T:53:ILE:HD11	1.89	0.52
4:D:136:ARG:O	4:D:137:ASP:CB	2.57	0.52
4:N:145:VAL:HG11	4:N:186:VAL:HA	1.92	0.52
1:P:147:TRP:HZ2	3:R:9:LEU:HD12	1.73	0.52
2:L:81:ARG:NH2	2:L:90:PRO:HA	2.25	0.52
1:F:28:VAL:HG23	1:F:33:PHE:CD1	2.43	0.52
1:A:189:VAL:HG22	1:A:190:THR:H	1.74	0.52
1:P:77:SER:O	1:P:81:LEU:HD23	2.08	0.52
5:T:59:GLU:O	5:T:80:ARG:O	2.27	0.52
2:Q:37:VAL:HB	2:Q:66:TYR:CZ	2.44	0.52
4:S:141:SER:O	4:S:143:LYS:N	2.42	0.52
5:O:59:GLU:HG2	5:O:83:LYS:O	2.09	0.52
4:S:177:SER:O	4:S:178:MET:HG2	2.09	0.52
5:T:127:ASP:OD1	5:T:129:LYS:HG2	2.10	0.52
4:I:27:ASN:ND2	4:I:29:ALA:H	2.08	0.52
4:N:45:ASP:HA	4:N:100:ALA:HB1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:182:CYS:O	5:E:204:ARG:HD2	2.10	0.52
5:O:155:VAL:HG13	5:O:203:SER:O	2.09	0.52
4:N:4:VAL:HG13	4:N:4:VAL:O	2.09	0.52
4:S:79:PHE:CD1	4:S:91:ILE:HG12	2.45	0.52
4:I:70:GLY:O	4:I:78:ARG:CB	2.58	0.52
4:D:178:MET:CE	5:E:208:SER:HB3	2.40	0.52
4:I:107:ARG:HG2	4:I:108:ALA:N	2.25	0.52
4:N:122:LYS:HZ3	4:N:153:SER:HB2	1.74	0.52
2:L:95:TRP:CE2	2:L:97:ARG:HA	2.45	0.52
5:J:138:VAL:HG22	5:J:248:ALA:HB1	1.92	0.52
5:T:212:TRP:O	5:T:252:GLY:HA3	2.09	0.52
4:N:122:LYS:NZ	4:N:153:SER:HB2	2.23	0.52
1:P:66:ILE:CD1	4:S:109:GLY:HA2	2.40	0.52
1:K:60:TRP:CZ2	1:K:64:THR:HG21	2.45	0.52
5:T:27:ASP:O	5:T:29:ASN:N	2.35	0.52
1:F:220:ASP:OD1	1:F:220:ASP:N	2.42	0.52
5:E:42:TYR:CZ	5:E:52:LEU:HD13	2.44	0.52
4:S:139:LYS:HG3	4:S:140:SER:H	1.75	0.52
2:G:10:TYR:CD1	2:G:10:TYR:N	2.78	0.51
1:F:240:THR:HG22	2:G:12:ARG:HH22	1.75	0.51
1:K:244:TRP:HD1	1:K:244:TRP:H	1.57	0.51
1:P:215:LEU:HD11	1:P:230:LEU:HD13	1.92	0.51
2:Q:29:GLY:HA2	2:Q:61:SER:HB2	1.91	0.51
1:F:122:ASP:OD1	2:G:60:TRP:NE1	2.42	0.51
2:G:27:VAL:HG21	2:G:35:ILE:HD13	1.92	0.51
4:I:183:ASN:O	4:I:184:SER:HB2	2.10	0.51
4:N:207:GLU:HB2	4:N:208:ASP:CA	2.39	0.51
5:J:31:TYR:CE1	5:J:110:ASN:HB2	2.45	0.51
4:N:192:SER:H	4:N:193:ASP:HA	1.73	0.51
4:N:7:ASP:HB2	4:N:117:THR:HG21	1.92	0.51
4:N:44:GLN:HE22	5:O:44:GLN:NE2	2.07	0.51
5:O:182:CYS:HB3	5:O:204:ARG:CG	2.40	0.51
5:J:212:TRP:HE3	5:J:219:PHE:CE1	2.28	0.51
1:P:201:LEU:HD13	1:P:257:TYR:CZ	2.46	0.51
1:P:213:ILE:O	1:P:213:ILE:HD12	2.10	0.51
1:F:194:ILE:HG13	1:F:199:ALA:HA	1.92	0.51
1:F:236:ALA:HB1	2:G:12:ARG:NH2	2.25	0.51
4:D:113:PHE:CD1	5:E:50:LEU:HD12	2.46	0.51
5:T:143:GLU:O	5:T:146:ILE:HG12	2.11	0.51
1:K:103:VAL:HG23	1:K:108:ARG:C	2.29	0.51
2:G:40:LEU:HD11	2:G:81:ARG:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:70:GLY:C	4:N:79:PHE:N	2.63	0.51
1:F:266:LEU:HD12	1:F:267:PRO:HD2	1.91	0.51
4:I:12:ASN:CB	4:I:122:LYS:HE3	2.20	0.51
4:N:210:PHE:CE1	5:O:148:HIS:CE1	2.98	0.51
5:T:95:ALA:O	5:T:97:SER:O	2.28	0.51
5:E:80:ARG:O	5:E:81:LEU:C	2.49	0.51
1:F:159:TYR:CD1	3:H:3:ARG:HB2	2.46	0.51
1:A:209:TYR:H	1:A:210:PRO:HD2	1.75	0.51
1:P:217:TRP:CZ3	1:P:247:VAL:HG22	2.45	0.51
1:A:244:TRP:CZ3	1:A:246:ALA:HB2	2.42	0.51
2:L:6:LYS:O	2:L:7:ILE:HG22	2.10	0.51
4:N:143:LYS:O	4:N:144:SER:HB3	2.11	0.51
2:Q:54:LEU:HD11	2:Q:62:PHE:HB3	1.92	0.51
1:K:127:ASN:O	1:K:130:LEU:HD23	2.09	0.51
4:D:111:LEU:HD13	5:E:111:PHE:O	2.11	0.51
1:F:234:ARG:O	1:F:235:PRO:O	2.28	0.51
4:S:111:LEU:HB2	5:T:111:PHE:HB3	1.91	0.51
1:A:217:TRP:CE3	1:A:257:TYR:OH	2.64	0.51
1:P:49:ALA:HB1	1:P:50:PRO:HD2	1.93	0.51
1:K:141:GLN:O	1:K:144:GLN:HB3	2.10	0.51
4:N:107:ARG:NH1	5:O:110:ASN:O	2.44	0.51
4:S:139:LYS:CG	4:S:140:SER:H	2.23	0.51
1:F:3:HIS:CE1	1:F:180:GLU:HG2	2.46	0.51
4:D:82:GLN:HB3	4:D:88:SER:OG	2.11	0.51
2:L:28:SER:HA	2:L:62:PHE:O	2.11	0.51
5:T:42:TYR:CZ	5:T:52:LEU:HD13	2.45	0.51
4:N:2:LYS:O	4:N:3:GLU:HB2	2.11	0.51
2:L:8:GLN:O	2:L:10:TYR:HD1	1.94	0.51
2:L:39:LEU:CB	2:L:49:VAL:HG12	2.39	0.51
5:T:128:LEU:HD23	5:T:228:LEU:HD12	1.93	0.51
1:F:85:TYR:HE2	1:F:118:TYR:HD2	1.59	0.51
2:L:42:ASN:HA	2:L:77:GLU:O	2.11	0.51
2:B:4:THR:HG23	2:B:5:PRO:HD2	1.92	0.51
4:D:39:PHE:CD1	4:D:106:VAL:HG22	2.45	0.51
1:F:234:ARG:HG3	1:F:242:GLN:HB2	1.92	0.50
4:N:122:LYS:HE3	4:N:170:LYS:NZ	2.26	0.50
2:G:39:LEU:CB	2:G:46:ILE:HD11	2.40	0.50
2:L:40:LEU:HB2	2:L:78:TYR:HD1	1.76	0.50
5:E:168:LEU:HD12	5:E:169:SER:N	2.24	0.50
2:L:17:ASN:OD1	2:L:19:LYS:HG3	2.11	0.50
4:S:188:TRP:CD2	5:T:157:LEU:HD11	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:210:PHE:CG	4:D:212:PRO:HD3	2.46	0.50
1:F:151:ARG:HD2	4:I:57:TYR:HD2	1.75	0.50
4:N:132:VAL:H	4:N:209:THR:HG23	1.76	0.50
4:N:207:GLU:CA	4:N:208:ASP:HB2	2.41	0.50
1:A:217:TRP:HD1	1:A:228:THR:HG23	1.76	0.50
4:S:53:LEU:O	4:S:54:MET:HG2	2.11	0.50
4:N:145:VAL:HG22	4:N:187:ALA:C	2.31	0.50
1:P:65:GLN:OE1	4:S:110:LYS:HE3	2.11	0.50
1:A:137:ASP:O	1:A:141:GLN:HG3	2.10	0.50
5:E:43:ARG:HH22	5:E:98:GLN:N	2.10	0.50
5:E:43:ARG:NH2	5:E:97:SER:HB2	2.26	0.50
1:P:50:PRO:HG2	1:P:51:TRP:CZ3	2.46	0.50
5:E:223:VAL:O	5:E:223:VAL:HG12	2.11	0.50
4:D:130:PRO:O	4:D:209:THR:HA	2.11	0.50
4:D:135:LEU:HB3	5:E:140:GLU:O	2.11	0.50
4:S:133:TYR:CD2	5:T:145:GLU:HB2	2.46	0.50
1:F:89:GLU:OE1	1:F:89:GLU:N	2.42	0.50
1:F:65:GLN:OE1	1:F:65:GLN:HA	2.12	0.50
5:J:97:SER:O	5:J:99:THR:N	2.44	0.50
4:N:132:VAL:HG13	4:N:146:CYS:HB3	1.93	0.50
5:O:170:TRP:HZ2	5:O:203:SER:HG	1.59	0.50
1:K:234:ARG:H	1:K:234:ARG:HD2	1.77	0.50
5:O:132:PHE:HA	5:O:238:ARG:HH22	1.76	0.50
1:A:194:ILE:HG12	1:A:199:ALA:HA	1.93	0.50
5:O:183:THR:O	5:O:185:PRO:HD3	2.11	0.50
5:O:102:TYR:HE1	5:O:122:LEU:HB3	1.77	0.50
2:G:23:LEU:HD12	2:G:24:ASN:N	2.27	0.50
5:E:74:ASP:CG	5:E:76:TYR:HD2	2.14	0.50
1:A:109:LEU:HD23	1:A:161:GLU:HG2	1.94	0.50
5:T:164:ASP:HB3	5:T:187:PRO:HG2	1.92	0.50
2:Q:54:LEU:HD11	2:Q:62:PHE:CD2	2.46	0.50
5:T:172:VAL:O	5:T:175:LYS:HG2	2.11	0.50
1:F:48:ARG:O	1:F:49:ALA:HB3	2.11	0.50
1:K:208:PHE:CE2	1:K:213:ILE:HD11	2.47	0.50
1:P:170:ARG:HH11	1:P:174:ASN:HD21	1.60	0.50
4:N:110:LYS:HG2	4:N:110:LYS:O	2.12	0.50
1:F:25:VAL:HG11	1:F:35:ARG:NH2	2.27	0.50
5:O:132:PHE:HA	5:O:238:ARG:NH2	2.26	0.50
4:I:40:PHE:HZ	5:J:112:ASP:OD1	1.94	0.50
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.47	0.50
2:Q:97:ARG:HG2	2:Q:98:ASP:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:30:SER:HA	4:I:108:ALA:HB1	1.88	0.50
1:F:13:SER:HB3	1:F:93:HIS:H	1.77	0.50
5:T:157:LEU:CD2	5:T:159:THR:HG23	2.41	0.50
4:I:141:SER:HB3	4:I:143:LYS:HE2	1.92	0.50
4:D:20:ALA:HA	4:D:89:LEU:O	2.12	0.50
1:P:143:THR:O	1:P:146:LYS:HB3	2.12	0.50
2:L:36:GLU:HG2	2:L:83:ASN:OD1	2.11	0.50
1:K:228:THR:HA	1:K:246:ALA:O	2.11	0.50
2:B:73:THR:OG1	2:B:74:GLU:N	2.45	0.50
4:N:23:CYS:HB3	4:N:87:ILE:CG1	2.41	0.50
1:K:144:GLN:HE21	1:K:148:GLU:CD	2.15	0.50
1:A:250:PRO:O	1:A:254:GLU:HG3	2.12	0.50
5:E:156:CYS:O	5:E:202:SER:HA	2.11	0.50
1:K:19:GLU:HB3	1:K:20:PRO:HD2	1.94	0.50
5:O:72:PRO:HA	5:O:74:ASP:C	2.32	0.50
1:K:77:SER:HB3	3:M:9:LEU:HD13	1.92	0.50
2:L:40:LEU:C	2:L:46:ILE:HD11	2.32	0.50
1:K:44:ARG:HD3	1:K:48:ARG:HH22	1.77	0.50
5:J:12:VAL:HG22	5:J:123:SER:HB3	1.94	0.50
4:I:107:ARG:HG2	4:I:108:ALA:H	1.76	0.49
4:I:107:ARG:NH1	5:J:110:ASN:O	2.44	0.49
1:A:185:PRO:O	1:A:186:LYS:HB2	2.12	0.49
5:O:39:MET:HA	5:O:105:ALA:O	2.12	0.49
5:T:128:LEU:HD12	5:T:128:LEU:N	2.27	0.49
1:A:141:GLN:O	1:A:145:ARG:HG3	2.12	0.49
4:D:178:MET:HE3	5:E:208:SER:HB3	1.94	0.49
1:F:98:MET:HE3	2:G:60:TRP:CE3	2.47	0.49
5:E:69:GLY:O	5:E:70:GLU:HB2	2.12	0.49
5:J:156:CYS:C	5:J:157:LEU:HD12	2.32	0.49
2:L:23:LEU:O	2:L:67:TYR:HB2	2.11	0.49
1:F:21:ARG:HD3	1:F:39:ASP:CG	2.32	0.49
4:D:172:VAL:HG12	4:D:173:LEU:O	2.12	0.49
1:P:6:ARG:HD3	1:P:100:GLY:HA3	1.94	0.49
4:D:148:PHE:O	4:D:184:SER:HA	2.12	0.49
4:D:146:CYS:HB2	4:D:187:ALA:HB3	1.94	0.49
4:N:213:SER:HB3	4:N:214:PRO:HD3	1.93	0.49
5:O:136:VAL:HG22	5:O:158:ALA:HB2	1.94	0.49
1:A:215:LEU:HD22	1:A:245:ALA:HB3	1.93	0.49
1:P:263:HIS:CG	1:P:264:GLU:N	2.81	0.49
1:K:103:VAL:HG23	1:K:108:ARG:O	2.12	0.49
2:L:48:LYS:HG2	2:L:50:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:LEU:HD12	1:F:84:TYR:HD2	1.76	0.49
5:E:178:HIS:O	5:E:181:VAL:HG22	2.13	0.49
1:K:44:ARG:HD3	1:K:48:ARG:NH2	2.27	0.49
5:E:25:GLN:HG2	5:E:26:ASP:N	2.26	0.49
5:J:18:SER:HB2	5:J:92:GLU:O	2.12	0.49
3:H:6:ALA:O	5:J:109:GLY:HA2	2.12	0.49
5:E:225:PHE:O	5:E:243:THR:HG23	2.11	0.49
5:E:171:TRP:CZ3	5:E:222:GLN:HB3	2.47	0.49
5:T:95:ALA:O	5:T:98:GLN:HB2	2.13	0.49
4:N:70:GLY:O	4:N:78:ARG:CG	2.60	0.49
5:E:166:VAL:CG1	5:E:167:GLU:N	2.75	0.49
5:E:171:TRP:HZ3	5:E:222:GLN:HB3	1.77	0.49
5:T:136:VAL:HG12	5:T:137:ALA:N	2.28	0.49
4:D:208:ASP:HA	1:P:108:ARG:HB3	1.93	0.49
5:J:39:MET:HA	5:J:106:SER:HA	1.93	0.49
5:T:20:MET:HG2	5:T:91:LEU:HD12	1.94	0.49
1:P:35:ARG:CZ	2:Q:53:ASP:HB3	2.43	0.49
4:S:148:PHE:HB3	4:S:185:ALA:HB3	1.93	0.49
4:D:107:ARG:HG2	4:D:108:ALA:N	2.27	0.49
4:N:21:PHE:CZ	4:N:119:LEU:HD13	2.48	0.49
4:D:25:TYR:OH	4:D:85:GLN:HA	2.11	0.49
1:K:201:LEU:HD12	1:K:201:LEU:N	2.28	0.49
1:K:159:TYR:CE2	1:K:164:CYS:HB2	2.47	0.49
5:E:94:ALA:O	5:E:95:ALA:HB2	2.12	0.49
3:H:9:LEU:N	3:H:9:LEU:HD12	2.27	0.49
4:D:159:GLN:H	4:D:159:GLN:CD	2.16	0.49
2:L:81:ARG:NH1	2:L:83:ASN:HB3	2.15	0.49
2:L:7:ILE:HA	2:L:26:TYR:O	2.12	0.49
5:O:182:CYS:HB3	5:O:204:ARG:HG3	1.93	0.49
2:G:39:LEU:HD12	2:G:39:LEU:N	2.28	0.49
5:J:29:HIS:ND1	5:J:107:GLY:HA2	2.28	0.49
4:I:47:ARG:HD3	5:J:186:GLN:HE22	1.77	0.49
4:I:27:ASN:HD22	4:I:29:ALA:H	1.60	0.49
1:F:262:GLN:NE2	1:F:262:GLN:H	2.10	0.49
5:O:214:ASN:ND2	5:O:216:ARG:HB3	2.28	0.49
5:O:59:GLU:HG2	5:O:84:LYS:HB2	1.95	0.49
1:F:123:TYR:HD2	1:F:124:ILE:HG22	1.78	0.49
5:T:95:ALA:C	5:T:124:VAL:HG11	2.33	0.49
1:K:142:ILE:HA	1:K:145:ARG:HH11	1.76	0.49
5:O:40:TYR:N	5:O:105:ALA:O	2.46	0.49
2:B:29:GLY:HA2	2:B:61:SER:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:40:PHE:HZ	5:T:112:ASP:OD1	1.96	0.49
1:K:109:LEU:HD22	1:K:161:GLU:HA	1.94	0.49
1:A:6:ARG:HG2	1:A:100:GLY:HA3	1.94	0.48
4:N:167:ILE:HG23	4:N:187:ALA:HB2	1.96	0.48
1:F:203:CYS:H	1:F:217:TRP:HZ2	1.59	0.48
4:S:211:PHE:C	4:S:211:PHE:HD2	2.16	0.48
1:P:115:GLN:HG3	1:P:125:ALA:CB	2.37	0.48
4:N:147:LEU:CD2	4:N:149:THR:HB	2.43	0.48
5:O:78:VAL:HG23	5:O:88:LEU:O	2.12	0.48
5:O:78:VAL:HG23	5:O:89:LEU:HA	1.95	0.48
1:K:8:PHE:HB2	1:K:25:VAL:HG13	1.95	0.48
5:J:172:VAL:HG22	5:J:219:PHE:HD2	1.78	0.48
5:O:224:GLN:HE22	5:O:245:ILE:HD11	1.77	0.48
5:O:54:HIS:CE1	5:O:71:VAL:HG12	2.48	0.48
5:O:54:HIS:HE1	5:O:71:VAL:HG12	1.78	0.48
4:D:68:GLU:O	4:D:69:ASP:HB3	2.13	0.48
5:T:225:PHE:O	5:T:243:THR:HG23	2.13	0.48
4:S:44:GLN:HE22	5:T:44:GLN:HE22	1.61	0.48
1:A:2:SER:H	1:A:105:PRO:HG3	1.79	0.48
1:K:249:VAL:CG2	1:K:250:PRO:HD2	2.44	0.48
4:I:27:ASN:ND2	4:I:27:ASN:C	2.63	0.48
1:K:121:LYS:HG2	2:L:1:ILE:CD1	2.42	0.48
1:K:217:TRP:CE3	1:K:247:VAL:HB	2.48	0.48
4:S:211:PHE:C	4:S:211:PHE:CD2	2.87	0.48
4:I:161:LYS:HE3	4:I:202:ASN:OD1	2.13	0.48
1:P:129:ASP:OD2	1:P:131:ARG:HB2	2.13	0.48
5:T:54:HIS:CE1	5:T:71:VAL:HG22	2.49	0.48
2:G:40:LEU:HD12	2:G:40:LEU:N	2.29	0.48
1:P:266:LEU:HD21	1:P:270:LEU:HB2	1.94	0.48
1:P:189:VAL:HG11	1:P:203:CYS:HA	1.95	0.48
1:F:50:PRO:C	1:F:52:ILE:H	2.17	0.48
4:D:148:PHE:HB2	4:D:200:PHE:CE2	2.49	0.48
5:E:8:PRO:HD2	5:E:21:LEU:HD22	1.96	0.48
4:I:138:SER:O	4:I:139:LYS:C	2.52	0.48
1:A:217:TRP:HZ2	1:A:245:ALA:O	1.97	0.48
5:J:239:ALA:O	5:J:240:LYS:HB3	2.14	0.48
5:T:132:PHE:O	5:T:161:PHE:HA	2.14	0.48
2:Q:19:LYS:O	2:Q:20:SER:HB2	2.13	0.48
1:F:67:PHE:O	1:F:71:THR:HG23	2.14	0.48
2:B:27:VAL:O	2:B:27:VAL:HG23	2.14	0.48
1:K:27:TYR:CE2	1:K:32:GLN:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:ARG:HB2	2:G:10:TYR:CE2	2.49	0.48
1:P:72:GLN:HG3	5:T:57:VAL:HG11	1.95	0.48
5:O:223:VAL:O	5:O:223:VAL:HG13	2.14	0.48
2:G:46:ILE:HB	2:G:47:GLU:H	1.41	0.48
4:D:25:TYR:HD2	4:D:27:ASN:O	1.97	0.48
1:P:211:ALA:HB2	1:P:241:PHE:CG	2.48	0.48
1:F:123:TYR:CE2	3:H:9:LEU:HD23	2.49	0.48
2:B:47:GLU:O	2:B:48:LYS:C	2.52	0.48
1:A:242:GLN:HE22	2:B:12:ARG:HA	1.79	0.48
1:F:201:LEU:HD22	1:F:274:TRP:CD1	2.49	0.48
5:T:139:PHE:HB2	5:T:155:VAL:HG13	1.96	0.48
5:T:157:LEU:HD21	5:T:159:THR:HG23	1.96	0.48
5:O:60:GLY:C	5:O:61:THR:HG23	2.34	0.48
4:N:95:LYS:O	4:N:121:VAL:HG11	2.13	0.48
1:F:55:GLU:CG	1:F:170:ARG:HH22	2.26	0.48
4:D:168:THR:HB	5:E:184:ASP:OD2	2.14	0.48
1:F:147:TRP:CD1	1:F:152:VAL:HG21	2.48	0.48
2:Q:80:CYS:H	2:Q:92:ILE:CD1	2.27	0.48
5:O:155:VAL:HG13	5:O:203:SER:H	1.79	0.48
1:P:206:LEU:HG	1:P:242:GLN:HE22	1.79	0.48
4:N:126:GLN:C	4:N:128:PRO:HD3	2.33	0.48
5:J:149:THR:HG23	5:J:151:LYS:H	1.79	0.48
4:D:194:PHE:HD2	4:D:194:PHE:H	1.62	0.48
5:E:99:THR:HG23	5:E:124:VAL:H	1.79	0.48
4:N:11:PHE:N	4:N:11:PHE:CD2	2.82	0.48
4:S:213:SER:N	4:S:214:PRO:CD	2.77	0.48
4:N:19:VAL:HG12	4:N:20:ALA:N	2.24	0.48
5:E:45:ASP:HB2	5:E:48:MET:CG	2.43	0.48
1:A:67:PHE:CE2	1:A:71:THR:HG21	2.49	0.48
1:F:211:ALA:HB2	1:F:241:PHE:HE2	1.79	0.48
4:N:166:TYR:HD2	4:N:188:TRP:NE1	2.12	0.48
4:I:111:LEU:HD13	5:J:111:PHE:O	2.14	0.47
2:Q:12:ARG:HG2	2:Q:24:ASN:HD21	1.79	0.47
4:N:113:PHE:CE1	5:O:50:LEU:HD12	2.48	0.47
4:S:41:TRP:HA	4:S:103:LEU:O	2.14	0.47
4:N:112:ILE:N	4:N:112:ILE:HD12	2.29	0.47
5:T:80:ARG:HD2	5:T:86:ASN:O	2.13	0.47
4:N:83:LEU:HD21	4:N:84(A):ARG:HH11	1.79	0.47
1:F:72:GLN:HE21	5:J:57:VAL:HG21	1.79	0.47
1:A:82:ARG:HG3	1:A:87:GLN:HB2	1.95	0.47
4:D:21:PHE:CZ	4:D:119:LEU:HD22	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PHE:HD1	1:A:209:TYR:N	2.12	0.47
5:E:151:LYS:HD3	5:E:206:ARG:HD3	1.95	0.47
4:S:96:LEU:HD21	4:S:172:VAL:HG11	1.96	0.47
1:P:250:PRO:HG2	1:P:253:GLU:HB2	1.96	0.47
4:N:6:GLN:NE2	4:N:102:TYR:O	2.47	0.47
2:L:40:LEU:H	2:L:78:TYR:HE1	1.59	0.47
1:F:249:VAL:HB	1:F:250:PRO:HD2	1.95	0.47
5:E:80:ARG:HG3	5:E:80:ARG:O	2.15	0.47
1:K:3:HIS:HB3	1:K:29:ASP:OD2	2.14	0.47
4:I:162:ASP:HB3	4:I:165:VAL:CG2	2.44	0.47
1:A:253:GLU:HB3	1:A:256:ARG:HD3	1.96	0.47
4:S:162:ASP:HB3	4:S:165:VAL:HG12	1.95	0.47
1:F:231:VAL:HG13	2:G:8:GLN:HE21	1.79	0.47
5:T:230:GLU:HG3	5:T:231:ASN:N	2.27	0.47
4:N:115:GLN:HE21	5:O:48:MET:HA	1.80	0.47
4:I:200:PHE:O	4:I:205:ILE:HD11	2.14	0.47
5:E:40:TYR:N	5:E:105:ALA:O	2.46	0.47
5:E:127:ASP:OD1	5:E:129:LYS:HG3	2.15	0.47
1:P:231:VAL:HG11	1:P:244:TRP:CE2	2.49	0.47
4:D:125:ILE:HG13	4:D:152:ASP:HA	1.97	0.47
5:E:193:ALA:HB1	5:J:27:MET:CE	2.44	0.47
5:T:41:TRP:CD1	5:T:89:LEU:HB2	2.49	0.47
1:K:172:LEU:HD12	1:K:173:GLU:N	2.30	0.47
5:J:140:GLU:HG2	5:J:212:TRP:HH2	1.79	0.47
1:A:198:GLU:HG3	1:A:248:VAL:CG1	2.43	0.47
5:T:171:TRP:HB2	5:T:220:ARG:HB3	1.97	0.47
5:T:67:ALA:HB1	5:T:68:LYS:HG2	1.97	0.47
4:S:44:GLN:O	4:S:100:ALA:HB1	2.14	0.47
1:F:165:VAL:C	1:F:167:TRP:H	2.18	0.47
2:Q:73:THR:O	2:Q:74:GLU:HB2	2.14	0.47
1:A:53:GLU:N	1:A:53:GLU:OE1	2.47	0.47
1:F:36:PHE:HA	1:F:46:GLU:OE2	2.15	0.47
5:T:164:ASP:HB2	5:T:187:PRO:HG2	1.94	0.47
1:K:218:GLN:HB2	1:K:258:THR:OG1	2.14	0.47
4:D:41:TRP:CZ3	4:D:104:CYS:HB2	2.50	0.47
2:B:9:VAL:CG2	2:B:93:VAL:HG13	2.45	0.47
5:J:96:PRO:HA	5:J:97:SER:C	2.35	0.47
2:B:13:HIS:O	2:B:14:PRO:C	2.53	0.47
1:F:240:THR:CG2	2:G:12:ARG:HH22	2.28	0.47
4:S:107:ARG:O	4:S:108:ALA:C	2.52	0.47
5:T:99:THR:HB	5:T:124:VAL:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:189:VAL:N	1:K:204:TRP:CZ2	2.82	0.47
1:F:220:ASP:HB2	1:F:221:GLY:CA	2.44	0.47
1:P:191:HIS:ND1	1:P:192:HIS:N	2.63	0.47
1:P:123:TYR:OH	1:P:140:ALA:HA	2.14	0.47
1:P:50:PRO:O	1:P:51:TRP:C	2.53	0.47
1:P:147:TRP:CZ2	3:R:9:LEU:HD12	2.49	0.47
1:A:211:ALA:C	1:A:213:ILE:H	2.18	0.47
5:T:4:GLY:HA2	5:T:28:MET:CE	2.45	0.47
5:T:66:THR:HG22	5:T:67:ALA:N	2.30	0.47
1:F:123:TYR:O	1:F:136:ALA:HB3	2.14	0.47
1:F:59:TYR:HE1	1:F:167:TRP:CZ3	2.32	0.47
5:E:27:MET:HB2	5:E:29:HIS:CE1	2.49	0.47
2:B:36:GLU:HB2	2:B:83:ASN:HB3	1.97	0.47
2:Q:80:CYS:H	2:Q:92:ILE:HD11	1.80	0.47
1:A:258:THR:CB	1:A:273:ARG:HA	2.37	0.47
1:K:256:ARG:O	1:K:256:ARG:HG3	2.15	0.47
4:N:11:PHE:HB2	4:N:119:LEU:CD1	2.45	0.47
5:O:96:PRO:HA	5:O:97:SER:C	2.34	0.47
5:T:15:LYS:HB2	5:T:128:LEU:CD1	2.43	0.47
5:J:14:LYS:HB3	5:J:17:GLN:HG3	1.96	0.47
1:P:171:TYR:C	1:P:173:GLU:H	2.17	0.47
5:O:223:VAL:HG12	5:O:247:SER:OG	2.15	0.47
5:E:71:VAL:N	5:E:72:PRO:CD	2.77	0.47
1:P:65:GLN:O	1:P:69:THR:HB	2.15	0.47
4:D:27:ASN:ND2	4:D:29:ALA:H	2.12	0.47
4:D:39:PHE:HD1	4:D:106:VAL:HG22	1.80	0.47
2:G:55:SER:HB2	2:G:63:TYR:CZ	2.49	0.47
2:Q:23:LEU:CD2	2:Q:78:TYR:HB3	2.45	0.47
5:O:134:PRO:HB2	5:O:158:ALA:HB1	1.97	0.47
5:J:71:VAL:HA	5:J:74:ASP:OD1	2.15	0.47
1:K:121:LYS:HZ3	2:L:1:ILE:HD11	1.80	0.47
1:A:14:ARG:NE	1:A:19:GLU:O	2.48	0.47
1:P:184:PRO:HA	1:P:185:PRO:HD3	1.77	0.47
1:A:189:VAL:HG23	1:A:203:CYS:HA	1.96	0.46
4:N:107:ARG:HG2	4:N:108:ALA:N	2.30	0.46
4:N:13:VAL:HG11	4:N:19:VAL:HG22	1.96	0.46
4:I:44:GLN:HE22	5:J:44:GLN:HE22	1.62	0.46
5:O:83:LYS:HG3	5:O:84:LYS:H	1.79	0.46
1:P:35:ARG:O	1:P:46:GLU:HB3	2.14	0.46
4:D:46:SER:HA	4:D:47:ARG:HA	1.63	0.46
1:F:126:LEU:HD12	1:F:127:ASN:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:81:ARG:HG3	2:L:81:ARG:HH11	1.81	0.46
5:O:172:VAL:HG12	5:O:219:PHE:HD2	1.80	0.46
2:G:17:ASN:ND2	2:G:19:LYS:HE3	2.30	0.46
5:E:238:ARG:HG3	5:E:239:ALA:N	2.29	0.46
4:D:197:ALA:HA	4:D:211:PHE:CE1	2.50	0.46
2:Q:75:LYS:HB2	2:Q:75:LYS:HE2	1.70	0.46
2:Q:89:GLN:O	2:Q:89:GLN:HG3	2.15	0.46
4:S:142:ASP:C	4:S:144:SER:H	2.19	0.46
1:P:33:PHE:HB3	1:P:51:TRP:HZ2	1.81	0.46
1:K:34:VAL:HA	1:K:47:PRO:O	2.16	0.46
4:I:24:THR:HG22	4:I:85:GLN:O	2.15	0.46
5:J:127:ASP:C	5:J:129:LYS:H	2.18	0.46
2:G:1:ILE:HG23	2:G:2:GLN:N	2.29	0.46
1:F:8:PHE:HB3	2:G:56:PHE:CE1	2.50	0.46
1:F:235:PRO:HG2	2:G:26:TYR:CE1	2.50	0.46
4:S:30:SER:HB3	4:S:108:ALA:HB2	1.97	0.46
4:S:27:ASN:C	4:S:27:ASN:ND2	2.67	0.46
1:P:203:CYS:O	1:P:204:TRP:CD1	2.67	0.46
4:D:40:PHE:HZ	5:E:112:ASP:OD1	1.98	0.46
4:D:101:THR:HA	4:D:118:GLU:HA	1.97	0.46
1:A:266:LEU:HD13	1:A:270:LEU:HD23	1.97	0.46
1:K:155:GLN:HG2	4:N:57:TYR:CD1	2.50	0.46
5:O:138:VAL:HG22	5:O:139:PHE:N	2.30	0.46
5:T:94:ALA:O	5:T:95:ALA:HB2	2.15	0.46
1:P:266:LEU:CD2	1:P:270:LEU:HB2	2.45	0.46
2:B:3:ARG:O	2:B:30:PHE:HA	2.15	0.46
1:K:143:THR:O	1:K:144:GLN:C	2.54	0.46
5:T:14:LEU:HD11	5:T:20:MET:HB3	1.97	0.46
4:I:83:LEU:HD12	4:I:84:ASN:H	1.81	0.46
5:E:157:LEU:HD12	5:E:201:LEU:O	2.16	0.46
2:Q:10:TYR:HA	2:Q:95:TRP:CZ3	2.50	0.46
1:F:255:GLN:O	1:F:255:GLN:HG3	2.16	0.46
1:A:217:TRP:HE3	1:A:257:TYR:OH	1.99	0.46
2:L:40:LEU:HD23	2:L:43:GLY:CA	2.45	0.46
1:P:217:TRP:HZ3	1:P:247:VAL:HG22	1.81	0.46
4:D:205:ILE:HG23	4:D:206:PRO:HD2	1.97	0.46
2:L:5:PRO:HG3	2:L:30:PHE:HB3	1.98	0.46
5:T:105:ALA:HA	5:T:115:TYR:O	2.14	0.46
1:K:266:LEU:O	1:K:266:LEU:HD12	2.15	0.46
5:E:97:SER:C	5:E:99:THR:N	2.68	0.46
5:O:220:ARG:CZ	5:O:222:GLN:NE2	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:41:LYS:HB2	2:G:78:TYR:CZ	2.51	0.46
2:L:7:ILE:HG12	2:L:8:GLN:N	2.28	0.46
5:J:41:TRP:CD1	5:J:89:LEU:HB2	2.51	0.46
4:D:126:GLN:HG3	4:D:127:ASN:H	1.81	0.46
1:K:218:GLN:HA	1:K:223:ASP:HA	1.98	0.46
4:I:28:SER:HA	4:I:85:GLN:NE2	2.31	0.46
4:S:200:PHE:C	4:S:202:ASN:H	2.18	0.46
4:N:54:MET:HE1	4:N:55:SER:H	1.80	0.46
1:A:44:ARG:HB2	1:A:48:ARG:HH21	1.80	0.46
1:K:130:LEU:HB2	1:K:157:ARG:HG3	1.98	0.46
5:E:24:ALA:HB2	5:E:86:ASN:HB3	1.96	0.46
4:N:132:VAL:HG22	4:N:146:CYS:HB3	1.98	0.46
1:P:219:ARG:HH11	1:P:256:ARG:HE	1.60	0.46
1:A:130:LEU:HB3	1:A:157:ARG:HG3	1.98	0.46
5:E:159:THR:HG22	5:E:200:ALA:HB1	1.97	0.46
5:O:234:TRP:CZ2	5:O:238:ARG:HG3	2.45	0.46
5:E:168:LEU:HD13	5:E:223:VAL:HG23	1.98	0.46
5:E:134:PRO:O	5:E:246:VAL:HG11	2.15	0.46
5:T:40:TYR:O	5:T:104:CYS:HA	2.16	0.46
1:K:128:GLU:C	1:K:130:LEU:H	2.18	0.46
1:K:123:TYR:CZ	1:K:140:ALA:HA	2.51	0.46
4:I:107:ARG:O	4:I:108:ALA:HB3	2.16	0.45
5:J:234:TRP:HZ2	5:J:238:ARG:CG	2.28	0.45
1:P:170:ARG:NH1	1:P:174:ASN:HD21	2.13	0.45
4:N:11:PHE:HB2	4:N:119:LEU:HD11	1.98	0.45
4:N:60:GLY:HA2	4:N:81:ALA:O	2.16	0.45
1:K:14:ARG:HD2	1:K:17:ARG:HH21	1.78	0.45
1:A:209:TYR:HB3	1:A:210:PRO:CD	2.46	0.45
1:F:151:ARG:HD2	4:I:57:TYR:CD2	2.50	0.45
4:I:205:ILE:HD12	4:I:205:ILE:N	2.31	0.45
5:J:69:GLY:O	5:J:70:GLU:CB	2.63	0.45
4:S:196:CYS:HA	4:S:199:ALA:HB2	1.96	0.45
1:F:72:GLN:CG	5:J:57:VAL:HG11	2.47	0.45
1:A:150:ALA:HB3	1:A:152:VAL:HG23	1.99	0.45
2:B:41:LYS:O	2:B:42:ASN:HB2	2.16	0.45
1:K:181:ARG:HD2	1:K:182:ALA:N	2.31	0.45
4:I:135:LEU:HD21	5:J:153:THR:O	2.16	0.45
5:E:130:ASN:HA	5:E:132:PHE:CE2	2.51	0.45
4:S:69:ASP:HA	4:S:70:GLY:HA2	1.57	0.45
4:S:175:MET:HB3	4:S:175:MET:HE2	1.72	0.45
2:G:24:ASN:HB3	2:G:67:TYR:CB	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TRP:HE1	1:A:246:ALA:N	2.15	0.45
4:I:44:GLN:OE1	4:I:103:LEU:HD11	2.16	0.45
5:E:100:SER:OG	5:E:101:VAL:N	2.49	0.45
4:D:68:GLU:HG2	4:D:69:ASP:N	2.30	0.45
4:I:41:TRP:CE2	4:I:89:LEU:HB2	2.52	0.45
5:T:184:ASP:HB2	5:T:201:LEU:HD12	1.98	0.45
1:P:155:GLN:HG2	4:S:57:TYR:CD1	2.51	0.45
1:A:234:ARG:O	1:A:235:PRO:C	2.53	0.45
5:T:234:TRP:CZ2	5:T:236:GLN:HB3	2.52	0.45
5:T:127:ASP:OD1	5:T:129:LYS:HE3	2.17	0.45
4:S:110:LYS:O	4:S:110:LYS:HG2	2.16	0.45
1:A:72:GLN:CG	5:E:57:VAL:HG21	2.47	0.45
1:P:21:ARG:HD3	1:P:39:ASP:OD2	2.17	0.45
1:K:106:ASP:OD2	1:K:108:ARG:HG2	2.16	0.45
1:F:124:ILE:HG12	1:F:125:ALA:N	2.32	0.45
4:N:132:VAL:HG22	4:N:146:CYS:O	2.17	0.45
4:N:208:ASP:C	4:N:210:PHE:H	2.20	0.45
5:J:74:ASP:O	5:J:76:TYR:N	2.49	0.45
1:P:62:ARG:O	1:P:65:GLN:HB3	2.17	0.45
5:O:59:GLU:O	5:O:80:ARG:O	2.34	0.45
5:E:222:GLN:HA	5:E:247:SER:HB3	1.98	0.45
5:J:70:GLU:O	5:J:70:GLU:CD	2.54	0.45
5:J:146:ILE:O	5:J:150:GLN:HA	2.16	0.45
2:Q:91:LYS:HG3	2:Q:92:ILE:N	2.32	0.45
5:E:166:VAL:HG13	5:E:223:VAL:HG13	1.98	0.45
1:F:253:GLU:HA	1:F:256:ARG:HH11	1.82	0.45
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.52	0.45
5:O:104:CYS:O	5:O:116:PHE:HA	2.16	0.45
1:A:160:LEU:O	1:A:165:VAL:HG23	2.16	0.45
2:B:3:ARG:HH21	2:B:61:SER:HB3	1.81	0.45
1:P:45:GLU:O	1:P:46:GLU:C	2.55	0.45
4:N:5:GLU:HB2	4:N:24:THR:OG1	2.15	0.45
4:D:79:PHE:HA	4:D:90:LEU:O	2.16	0.45
2:B:1:ILE:HG13	2:B:2:GLN:N	2.32	0.45
4:I:27:ASN:HD22	4:I:29:ALA:N	2.15	0.45
4:I:192:SER:CB	4:I:193:ASP:HA	2.36	0.45
1:A:234:ARG:HG3	2:B:10:TYR:CD2	2.52	0.45
5:E:166:VAL:HG11	5:E:223:VAL:HG13	1.99	0.45
1:F:103:VAL:CG1	1:F:168:LEU:HD23	2.47	0.45
5:O:184:ASP:HA	5:O:185:PRO:HD2	1.88	0.45
5:J:145:GLU:O	5:J:149:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:49:GLU:N	4:D:49:GLU:OE1	2.48	0.45
4:S:107:ARG:HA	4:S:111:LEU:CA	2.40	0.45
5:O:128:LEU:O	5:O:234:TRP:HZ3	1.99	0.45
1:F:274:TRP:O	1:F:275:GLU:HB3	2.17	0.45
5:E:168:LEU:CD2	5:E:203:SER:HB2	2.47	0.45
1:K:218:GLN:OE1	1:K:260:HIS:HB2	2.17	0.45
4:D:41:TRP:O	4:D:53:LEU:HB3	2.16	0.45
1:A:69:THR:HG21	4:D:109:GLY:O	2.17	0.45
4:N:68:GLU:CD	4:N:68:GLU:H	2.21	0.44
2:G:47:GLU:C	2:G:48:LYS:HG2	2.38	0.44
4:N:199:ALA:C	4:N:201:ASN:H	2.20	0.44
4:N:143:LYS:O	4:N:144:SER:CB	2.65	0.44
2:G:31:HIS:CD2	2:G:62:PHE:CE1	3.05	0.44
2:B:70:PHE:HD2	2:B:78:TYR:CZ	2.34	0.44
1:P:44:ARG:HB3	1:P:48:ARG:HH21	1.82	0.44
1:F:201:LEU:HD21	1:F:254:GLU:CG	2.44	0.44
4:I:213:SER:N	4:I:214:PRO:CD	2.80	0.44
1:F:98:MET:HE3	2:G:60:TRP:CZ3	2.53	0.44
4:D:148:PHE:HB2	4:D:200:PHE:CZ	2.52	0.44
2:G:1:ILE:HG23	2:G:2:GLN:H	1.82	0.44
4:N:180:PHE:CD2	5:O:206:ARG:NH1	2.85	0.44
4:N:180:PHE:HD2	5:O:206:ARG:NH1	2.14	0.44
2:L:35:ILE:HD13	2:L:84:HIS:HD2	1.83	0.44
4:N:206:PRO:C	4:N:208:ASP:HB2	2.37	0.44
1:K:188:HIS:N	1:K:204:TRP:CZ2	2.86	0.44
1:A:219:ARG:CB	1:A:224:GLN:HB2	2.47	0.44
1:A:274:TRP:CG	1:A:274:TRP:O	2.70	0.44
5:E:238:ARG:CG	5:E:239:ALA:H	2.30	0.44
1:P:203:CYS:HB2	1:P:217:TRP:HZ2	1.82	0.44
5:J:138:VAL:HG13	5:J:248:ALA:HB3	1.99	0.44
1:F:48:ARG:NH1	1:F:60:TRP:CD2	2.86	0.44
1:F:203:CYS:N	1:F:217:TRP:HZ2	2.15	0.44
5:T:39:MET:HA	5:T:105:ALA:O	2.17	0.44
5:J:60:GLY:O	5:J:61:THR:OG1	2.32	0.44
4:S:5:GLU:HB3	4:S:24:THR:OG1	2.17	0.44
5:J:90:GLY:C	5:J:91:LEU:HD23	2.37	0.44
1:K:220:ASP:OD1	1:K:256:ARG:HB2	2.18	0.44
1:A:235:PRO:HA	1:A:241:PHE:HD1	1.82	0.44
4:D:180:PHE:CZ	4:D:182:SER:HB3	2.53	0.44
1:F:66:ILE:HD11	4:I:109:GLY:H	1.83	0.44
5:O:155:VAL:HG22	5:O:203:SER:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:202:ARG:NE	1:K:244:TRP:CE3	2.85	0.44
5:T:43:ARG:HH12	5:T:98:GLN:HA	1.83	0.44
1:A:226:GLN:C	1:A:228:THR:H	2.21	0.44
1:A:260:HIS:NE2	1:A:271:THR:HG23	2.33	0.44
2:L:31:HIS:ND1	2:L:32:PRO:HA	2.33	0.44
1:A:255:GLN:HB3	1:A:274:TRP:NE1	2.33	0.44
1:A:3:HIS:HA	1:A:29:ASP:OD1	2.18	0.44
1:F:87:GLN:OE1	1:F:93:HIS:NE2	2.51	0.44
1:A:42:SER:OG	1:A:45:GLU:HG3	2.17	0.44
4:D:167:ILE:HD12	4:D:167:ILE:C	2.37	0.44
5:O:240:LYS:HA	5:O:241:PRO:HD3	1.81	0.44
4:D:27:ASN:ND2	4:D:27:ASN:C	2.69	0.44
1:K:259:CYS:O	1:K:261:VAL:HG23	2.17	0.44
2:L:94:LYS:HG3	2:L:95:TRP:N	2.33	0.44
4:N:84:ASN:C	4:N:84(B):ALA:H	2.21	0.44
5:O:212:TRP:CZ2	5:O:253:ARG:HB3	2.53	0.44
5:T:242:VAL:O	5:T:244:GLN:HG2	2.17	0.44
2:G:84:HIS:CE1	2:G:86:THR:HG1	2.36	0.44
4:D:151:PHE:CZ	4:D:183:ASN:HB3	2.53	0.44
1:K:84:TYR:CD1	1:K:142:ILE:HD12	2.53	0.44
4:S:19:VAL:CG2	4:S:91:ILE:HB	2.47	0.44
1:P:28:VAL:O	1:P:30:ASP:N	2.51	0.44
1:F:249:VAL:HG11	1:F:257:TYR:CE2	2.53	0.44
1:A:255:GLN:HA	1:A:274:TRP:HE1	1.83	0.44
1:K:135:ALA:HB3	1:K:141:GLN:HG2	2.00	0.44
4:S:131:ALA:HB1	4:S:133:TYR:CE1	2.53	0.44
1:F:50:PRO:HG2	1:F:51:TRP:HD1	1.83	0.44
4:D:47:ARG:C	4:D:48:LYS:HG2	2.35	0.44
4:S:180:PHE:CE2	4:S:182:SER:HB3	2.53	0.44
5:J:23:CYS:HB3	5:J:87:PHE:HB3	1.99	0.44
2:Q:23:LEU:HD22	2:Q:78:TYR:HB3	2.00	0.44
1:P:117:ALA:HA	1:P:123:TYR:H	1.83	0.44
2:L:0:MET:N	2:L:1:ILE:HA	2.31	0.44
5:J:140:GLU:HA	5:J:141:PRO:HD3	1.85	0.44
5:E:234:TRP:HZ2	5:E:238:ARG:HB3	1.82	0.44
1:P:201:LEU:O	1:P:217:TRP:HH2	2.01	0.44
5:T:4:GLY:HA2	5:T:28:MET:HE1	2.00	0.44
4:D:210:PHE:CD1	4:D:212:PRO:HD3	2.53	0.44
1:F:82:ARG:CZ	1:F:89:GLU:HG3	2.48	0.44
1:F:170:ARG:O	1:F:173:GLU:HB3	2.18	0.44
5:T:168:LEU:HD23	5:T:169:SER:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:180:PHE:CE2	4:I:182:SER:HB3	2.53	0.44
1:K:268:LYS:HB3	1:K:269:PRO:HD2	2.00	0.44
1:F:88:SER:C	1:F:90:ALA:H	2.20	0.44
4:I:30:SER:CA	4:I:108:ALA:HB2	2.46	0.44
5:E:43:ARG:HH22	5:E:98:GLN:H	1.65	0.44
5:T:54:HIS:NE2	5:T:71:VAL:HG13	2.33	0.44
5:O:41:TRP:CD1	5:O:89:LEU:HB2	2.53	0.44
4:D:2:LYS:O	4:D:3:GLU:HB2	2.18	0.44
2:L:33:SER:O	2:L:34:ASP:C	2.55	0.44
2:G:23:LEU:HB2	2:G:70:PHE:CZ	2.53	0.43
2:L:56:PHE:HB2	2:L:61:SER:O	2.18	0.43
1:P:219:ARG:O	1:P:220:ASP:HB3	2.18	0.43
5:E:71:VAL:H	5:E:72:PRO:CD	2.31	0.43
5:J:172:VAL:HG22	5:J:219:PHE:CD2	2.53	0.43
4:I:145:VAL:HG12	4:I:188:TRP:CB	2.46	0.43
4:I:20:ALA:HA	4:I:90:LEU:HD12	1.99	0.43
1:P:215:LEU:O	1:P:216:THR:HG23	2.18	0.43
1:P:234:ARG:HG3	2:Q:10:TYR:CG	2.53	0.43
2:Q:4:THR:HA	2:Q:5:PRO:HD3	1.87	0.43
1:K:58:GLU:O	1:K:62:ARG:HG2	2.18	0.43
5:E:31:TYR:HB2	5:E:107:GLY:O	2.18	0.43
5:E:180:GLY:O	5:E:205:LEU:HA	2.18	0.43
5:T:30:HIS:CE1	5:T:107:GLY:HA2	2.53	0.43
4:N:43:ARG:HB2	4:N:53:LEU:HD22	2.00	0.43
1:A:217:TRP:CD1	1:A:228:THR:HG23	2.53	0.43
2:G:41:LYS:C	2:G:43:GLY:H	2.20	0.43
2:G:64:LEU:HD13	2:G:66:TYR:HE1	1.83	0.43
4:N:143:LYS:HG3	4:N:144:SER:N	2.32	0.43
1:P:234:ARG:H	1:P:234:ARG:HD2	1.84	0.43
4:N:173:LEU:HD23	4:N:174:ASP:N	2.33	0.43
2:B:25:CYS:HB2	2:B:39:LEU:HD21	2.00	0.43
5:O:53:ILE:O	5:O:68:LYS:O	2.36	0.43
1:P:266:LEU:HD21	1:P:270:LEU:HD13	2.00	0.43
1:F:81:LEU:HA	1:F:81:LEU:HD12	1.81	0.43
4:S:156:ASN:H	4:S:204:ILE:HD11	1.82	0.43
5:J:214:ASN:HA	5:J:215:PRO:HD3	1.85	0.43
2:B:22:PHE:HA	2:B:22:PHE:HD1	1.75	0.43
3:R:6:ALA:HB2	4:S:107:ARG:CZ	2.48	0.43
2:Q:39:LEU:HA	2:Q:80:CYS:HA	2.00	0.43
5:O:110:ASN:O	5:O:111:PHE:HB2	2.18	0.43
1:F:221:GLY:O	1:F:222:GLU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:51:TRP:NE1	1:P:52:ILE:HG12	2.33	0.43
1:K:217:TRP:NE1	1:K:259:CYS:SG	2.92	0.43
2:L:94:LYS:HG3	2:L:95:TRP:H	1.83	0.43
1:P:143:THR:O	1:P:144:GLN:C	2.56	0.43
1:P:185:PRO:O	1:P:187:THR:HG23	2.18	0.43
1:A:230:LEU:HG	1:A:231:VAL:N	2.31	0.43
5:T:173:ASN:HA	5:T:218:HIS:HB3	2.00	0.43
4:I:152:ASP:OD2	4:I:154:GLN:HG2	2.18	0.43
1:K:263:HIS:ND1	1:K:264:GLU:N	2.64	0.43
2:G:10:TYR:N	2:G:10:TYR:HD1	2.14	0.43
4:D:91:ILE:CD1	4:D:119:LEU:HD21	2.48	0.43
4:S:192:SER:N	4:S:193:ASP:CA	2.75	0.43
1:P:219:ARG:HB3	1:P:224:GLN:HE22	1.83	0.43
1:K:159:TYR:CZ	3:M:3:ARG:HB2	2.53	0.43
1:P:203:CYS:O	1:P:204:TRP:HD1	2.01	0.43
5:O:55:TYR:CE2	5:O:67:ALA:HB3	2.53	0.43
1:F:49:ALA:HB1	1:F:50:PRO:CD	2.48	0.43
1:F:55:GLU:CD	1:F:170:ARG:HH22	2.21	0.43
1:A:130:LEU:CB	1:A:157:ARG:HG3	2.48	0.43
4:I:153:SER:C	4:I:155:THR:H	2.22	0.43
1:A:62:ARG:O	1:A:65:GLN:HB3	2.17	0.43
5:J:240:LYS:HA	5:J:241:PRO:HD3	1.77	0.43
4:N:41:TRP:CE2	4:N:89:LEU:HB2	2.54	0.43
4:I:192:SER:HA	4:I:194:PHE:H	1.82	0.43
5:J:88:LEU:HD12	5:J:88:LEU:N	2.33	0.43
4:D:78:ARG:HG3	4:D:92:ARG:CD	2.48	0.43
5:E:161:PHE:CE1	5:E:199:TYR:HB2	2.52	0.43
1:P:34:VAL:HG22	1:P:35:ARG:N	2.33	0.43
5:T:44:GLN:NE2	5:T:50:LEU:HD21	2.33	0.43
4:I:161:LYS:HG3	4:I:202:ASN:ND2	2.34	0.43
2:Q:12:ARG:HG3	2:Q:22:PHE:HD2	1.84	0.43
1:P:72:GLN:CG	5:T:57:VAL:HG11	2.49	0.43
2:Q:91:LYS:CG	2:Q:92:ILE:H	2.30	0.43
5:O:169:SER:HB3	5:O:222:GLN:HB2	2.01	0.43
5:T:74:ASP:O	5:T:76:TYR:N	2.52	0.43
5:T:97:SER:C	5:T:99:THR:N	2.71	0.43
5:J:171:TRP:HE1	5:J:222:GLN:HB3	1.82	0.43
4:N:164:ASP:O	4:N:189:SER:HB2	2.19	0.43
1:F:23:ILE:HG22	1:F:24:SER:N	2.34	0.43
4:D:173:LEU:O	4:D:174:ASP:HB2	2.18	0.43
2:G:63:TYR:CD1	2:G:63:TYR:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:138:SER:HA	4:D:139:LYS:HA	1.48	0.43
1:A:236:ALA:O	2:B:12:ARG:HD2	2.19	0.43
1:F:205:ALA:HB3	1:F:242:GLN:O	2.17	0.43
1:A:112:GLY:CA	1:A:160:LEU:HD23	2.48	0.43
1:F:25:VAL:HG12	1:F:35:ARG:HG3	1.99	0.43
5:E:168:LEU:HD23	5:E:183:THR:CG2	2.49	0.43
1:K:46:GLU:O	1:K:48:ARG:HG3	2.19	0.43
4:I:131:ALA:CB	4:I:210:PHE:HB3	2.49	0.43
1:A:204:TRP:O	1:A:205:ALA:HB2	2.19	0.43
1:K:89:GLU:HG2	1:K:89:GLU:O	2.19	0.43
5:E:143:GLU:CD	5:E:143:GLU:H	2.22	0.43
5:O:141:PRO:HB2	5:O:142:SER:H	1.69	0.43
1:P:233:THR:CB	1:P:243:LYS:HD3	2.44	0.43
2:G:37:VAL:HG22	2:G:82:VAL:CG1	2.47	0.43
1:F:219:ARG:HB2	1:F:257:TYR:HA	2.00	0.43
5:O:218:HIS:O	5:O:218:HIS:CG	2.72	0.43
4:D:112:ILE:N	4:D:112:ILE:HD12	2.34	0.43
2:G:13:HIS:HB3	2:G:14:PRO:CD	2.45	0.43
2:L:23:LEU:HD12	2:L:23:LEU:HA	1.82	0.43
1:P:10:THR:HB	1:P:23:ILE:HB	2.01	0.43
4:D:25:TYR:OH	4:D:84(A):ARG:HA	2.19	0.43
1:A:208:PHE:CD1	1:A:209:TYR:N	2.86	0.43
4:I:13:VAL:HG23	4:I:14:PRO:O	2.18	0.43
1:F:27:TYR:CE2	1:F:32:GLN:HB2	2.54	0.43
4:S:30:SER:CB	4:S:108:ALA:CB	2.95	0.42
2:G:41:LYS:HA	2:G:78:TYR:CD1	2.53	0.42
1:A:186:LYS:NZ	1:A:186:LYS:HB2	2.33	0.42
4:N:145:VAL:HG22	4:N:187:ALA:O	2.18	0.42
1:P:1:GLY:HA3	1:P:105:PRO:HA	2.01	0.42
2:Q:97:ARG:HG2	2:Q:98:ASP:H	1.84	0.42
5:T:134:PRO:HA	5:T:161:PHE:HB3	2.00	0.42
4:N:22:ASN:OD1	4:N:86:TYR:HD1	2.02	0.42
2:Q:7:ILE:HD12	2:Q:82:VAL:HG21	2.01	0.42
4:I:172:VAL:HG12	4:I:173:LEU:O	2.19	0.42
4:S:99:SER:HA	4:S:119:LEU:O	2.19	0.42
2:B:12:ARG:O	2:B:13:HIS:C	2.57	0.42
1:K:242:GLN:HE22	2:L:12:ARG:HA	1.83	0.42
2:G:39:LEU:HB2	2:G:46:ILE:CG1	2.49	0.42
2:G:47:GLU:O	2:G:49:VAL:HG13	2.19	0.42
2:Q:29:GLY:CA	2:Q:61:SER:HB2	2.49	0.42
5:O:23:LEU:HD13	5:O:88:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:138:SER:HA	4:D:139:LYS:HD3	1.99	0.42
4:D:107:ARG:O	4:D:108:ALA:O	2.36	0.42
5:O:171:TRP:CD2	5:O:222:GLN:NE2	2.87	0.42
2:G:38:ASP:C	2:G:39:LEU:HD12	2.39	0.42
1:F:209:TYR:O	1:F:263:HIS:HE1	2.03	0.42
5:O:97:SER:C	5:O:99:THR:N	2.72	0.42
5:O:228:LEU:N	5:O:241:PRO:O	2.52	0.42
2:L:67:TYR:CD1	2:L:67:TYR:N	2.85	0.42
1:P:123:TYR:CZ	1:P:140:ALA:HA	2.54	0.42
5:T:44:GLN:HB2	5:T:50:LEU:CD2	2.49	0.42
4:D:167:ILE:O	4:D:167:ILE:HD12	2.20	0.42
1:F:268:LYS:HA	1:F:269:PRO:HD3	1.82	0.42
2:G:23:LEU:HD12	2:G:24:ASN:H	1.85	0.42
2:G:24:ASN:OD1	2:G:24:ASN:N	2.52	0.42
5:E:43:ARG:HH22	5:E:97:SER:HB2	1.83	0.42
4:D:99:SER:HA	4:D:119:LEU:O	2.19	0.42
2:L:57:SER:OG	2:L:61:SER:HB2	2.20	0.42
1:A:257:TYR:CD2	1:A:258:THR:N	2.88	0.42
5:O:127:ASP:C	5:O:129:LYS:H	2.21	0.42
1:P:266:LEU:HG	1:P:268:LYS:O	2.20	0.42
1:K:257:TYR:O	1:K:258:THR:HG23	2.20	0.42
2:G:77:GLU:HB2	2:G:95:TRP:HE3	1.84	0.42
4:D:208:ASP:N	1:P:108:ARG:HH11	2.17	0.42
5:T:30:HIS:CG	5:T:107:GLY:H	2.36	0.42
4:D:107:ARG:NH1	5:E:110:ASN:O	2.46	0.42
2:L:12:ARG:HH21	2:L:13:HIS:CE1	2.37	0.42
1:A:191:HIS:CD2	1:A:193:PRO:HG3	2.54	0.42
1:F:35:ARG:NH2	2:G:53:ASP:HB3	2.34	0.42
5:O:154:LEU:CD1	5:O:205:LEU:HB3	2.47	0.42
4:N:167:ILE:HG12	4:N:187:ALA:CB	2.47	0.42
1:P:117:ALA:HB2	2:Q:60:TRP:CE2	2.55	0.42
1:A:46:GLU:O	1:A:48:ARG:HG3	2.19	0.42
1:K:3:HIS:HE1	1:K:179:LEU:O	2.03	0.42
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.53	0.42
5:T:68:LYS:HB2	5:T:69:GLY:H	1.51	0.42
4:I:139:LYS:O	4:I:140:SER:HB2	2.19	0.42
4:S:160:SER:HA	4:S:202:ASN:HD22	1.83	0.42
1:A:51:TRP:HZ3	1:A:171:TYR:CD1	2.37	0.42
2:L:52:SER:O	2:L:64:LEU:HD11	2.20	0.42
2:G:26:TYR:HB2	2:G:65:LEU:CD1	2.46	0.42
1:A:181:ARG:HG3	1:A:182:ALA:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PRO:CB	1:A:186:LYS:HE3	2.48	0.42
1:K:234:ARG:HG3	2:L:10:TYR:CG	2.53	0.42
4:N:168:THR:CG2	4:N:186:VAL:HB	2.46	0.42
5:T:128:LEU:HD23	5:T:228:LEU:HD11	2.01	0.42
4:S:188:TRP:CE2	5:T:157:LEU:HD11	2.55	0.42
5:T:140:GLU:HA	5:T:141:PRO:HD3	1.90	0.42
1:A:55:GLU:HB3	1:A:59:TYR:HB3	2.01	0.42
5:E:170:TRP:CZ3	5:E:221:CYS:HB2	2.54	0.42
1:A:238:ASP:H	2:B:12:ARG:NH1	2.18	0.42
5:O:169:SER:O	5:O:221:CYS:HA	2.20	0.42
1:K:202:ARG:HH22	1:K:231:VAL:HG22	1.84	0.42
1:A:190:THR:HG22	1:A:191:HIS:N	2.35	0.42
1:K:81:LEU:HD23	1:K:84:TYR:HD2	1.85	0.42
5:T:22:LEU:HD12	5:T:89:LEU:O	2.19	0.42
1:K:78:LEU:HD23	1:K:78:LEU:HA	1.84	0.42
1:K:138:THR:HA	1:K:141:GLN:HG3	2.01	0.42
2:L:48:LYS:HB3	2:L:48:LYS:HE2	1.87	0.42
5:E:222:GLN:HA	5:E:247:SER:CB	2.50	0.42
4:S:148:PHE:CD1	4:S:148:PHE:C	2.91	0.42
2:L:51:HIS:HB3	2:L:66:TYR:CD2	2.54	0.42
1:A:106:ASP:OD1	1:A:108:ARG:HG2	2.19	0.42
4:N:137:ASP:OD1	5:O:139:PHE:HA	2.19	0.42
2:G:5:PRO:HB2	2:G:7:ILE:HD11	2.02	0.42
1:P:202:ARG:HA	1:P:245:ALA:O	2.19	0.42
2:L:31:HIS:CG	2:L:32:PRO:HA	2.55	0.42
5:E:153:THR:HG1	5:E:206:ARG:HE	1.68	0.42
5:O:52:LEU:HD21	5:O:55:TYR:CD2	2.54	0.42
1:K:6:ARG:HA	1:K:100:GLY:HA3	2.01	0.42
4:S:178:MET:CE	4:S:178:MET:HA	2.50	0.42
4:I:142:ASP:O	4:I:143:LYS:HD3	2.20	0.42
5:E:127:ASP:OD1	5:E:129:LYS:HE2	2.20	0.42
4:D:31:GLN:H	4:D:108:ALA:HB2	1.84	0.42
2:G:10:TYR:CE1	2:G:24:ASN:CG	2.93	0.42
1:K:173:GLU:C	1:K:175:GLY:H	2.23	0.42
5:E:166:VAL:HG12	5:E:167:GLU:N	2.35	0.42
5:T:69:GLY:O	5:T:70:GLU:HB2	2.20	0.42
1:P:46:GLU:O	1:P:47:PRO:C	2.58	0.42
4:D:47:ARG:HG3	4:D:47:ARG:O	2.20	0.42
2:Q:75:LYS:HD3	2:Q:75:LYS:O	2.20	0.42
1:K:263:HIS:CG	1:K:264:GLU:H	2.36	0.42
1:A:242:GLN:NE2	2:B:12:ARG:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:165:VAL:HA	4:N:189:SER:HB3	2.01	0.42
1:P:51:TRP:CH2	1:P:179:LEU:HD11	2.55	0.42
1:K:200:THR:C	1:K:201:LEU:HD12	2.40	0.42
4:N:46:SER:HA	4:N:47:ARG:HA	1.60	0.42
5:O:43:ARG:HD3	5:O:70:GLU:OE1	2.20	0.42
1:P:238:ASP:HB3	2:Q:12:ARG:CZ	2.50	0.41
4:D:19:VAL:HB	4:D:91:ILE:HD11	2.01	0.41
5:T:74:ASP:C	5:T:76:TYR:N	2.73	0.41
1:A:219:ARG:O	1:A:220:ASP:HB2	2.20	0.41
4:N:150:ASP:O	4:N:151:PHE:C	2.58	0.41
1:K:192:HIS:O	1:K:200:THR:HB	2.19	0.41
1:K:217:TRP:CD1	1:K:259:CYS:HA	2.55	0.41
1:A:98:MET:HE3	2:B:60:TRP:CZ3	2.55	0.41
1:K:184:PRO:HA	1:K:185:PRO:HD3	1.83	0.41
4:I:147:LEU:HD13	4:I:186:VAL:HG22	2.02	0.41
5:E:240:LYS:HA	5:E:241:PRO:HD3	1.82	0.41
5:O:22:LEU:HD12	5:O:22:LEU:N	2.35	0.41
5:O:220:ARG:NH1	5:O:222:GLN:HE21	2.19	0.41
5:O:130:ASN:HA	5:O:132:PHE:CE2	2.54	0.41
4:N:145:VAL:HG21	4:N:186:VAL:HG13	2.02	0.41
4:N:143:LYS:HA	4:N:143:LYS:HD2	1.77	0.41
1:F:21:ARG:HE	1:F:23:ILE:CG1	2.33	0.41
4:I:46:SER:HA	4:I:47:ARG:HA	1.55	0.41
5:O:149:THR:O	5:O:151:LYS:HG3	2.19	0.41
1:K:88:SER:C	1:K:90:ALA:H	2.24	0.41
1:P:78:LEU:O	1:P:81:LEU:HB2	2.19	0.41
2:G:39:LEU:H	2:G:46:ILE:HD11	1.86	0.41
2:G:40:LEU:C	2:G:78:TYR:CD2	2.94	0.41
2:L:41:LYS:N	2:L:46:ILE:HD11	2.35	0.41
1:K:50:PRO:HG2	1:K:51:TRP:CE3	2.55	0.41
5:O:153:THR:HA	5:O:206:ARG:HB3	2.02	0.41
1:K:190:THR:HA	1:K:274:TRP:CZ3	2.55	0.41
1:A:27:TYR:HA	1:A:31:THR:O	2.20	0.41
4:S:46:SER:HA	4:S:47:ARG:HA	1.50	0.41
1:A:87:GLN:OE1	1:A:93:HIS:NE2	2.52	0.41
5:T:43:ARG:NH1	5:T:76:TYR:OH	2.54	0.41
1:K:253:GLU:H	1:K:253:GLU:CD	2.23	0.41
4:N:7:ASP:HB3	4:N:11:PHE:CZ	2.51	0.41
1:P:242:GLN:O	1:P:243:LYS:HB3	2.20	0.41
2:G:39:LEU:O	2:G:45:ARG:HA	2.20	0.41
5:O:15:LYS:HD2	5:O:128:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:192:HIS:CE1	1:P:202:ARG:HG2	2.54	0.41
5:J:225:PHE:HE2	5:J:227:GLY:HA3	1.84	0.41
1:P:261:VAL:H	1:P:271:THR:HG22	1.85	0.41
1:A:74:ASP:HB3	3:C:5:ARG:HH12	1.82	0.41
4:S:123:PRO:HG3	4:S:172:VAL:CG1	2.50	0.41
5:J:214:ASN:O	5:J:252:GLY:HA3	2.20	0.41
4:S:15:GLU:O	4:S:17:ALA:N	2.54	0.41
4:I:112:ILE:HD12	4:I:112:ILE:N	2.35	0.41
5:O:143:GLU:H	5:O:143:GLU:CD	2.24	0.41
5:J:191:GLN:C	5:J:193:ALA:H	2.23	0.41
1:K:188:HIS:N	1:K:204:TRP:HE1	2.16	0.41
2:L:39:LEU:HD22	2:L:49:VAL:HA	2.02	0.41
2:G:37:VAL:HB	2:G:66:TYR:CE1	2.55	0.41
4:D:15:GLU:OE1	4:D:181:LYS:HE3	2.20	0.41
5:E:136:VAL:HG21	5:E:223:VAL:HB	2.03	0.41
1:K:49:ALA:HB1	1:K:50:PRO:HD2	2.02	0.41
1:K:201:LEU:HD13	1:K:247:VAL:O	2.20	0.41
5:E:234:TRP:CZ2	5:E:236:GLN:HB2	2.55	0.41
1:P:213:ILE:HG22	1:P:263:HIS:ND1	2.35	0.41
4:I:84(C):SER:O	4:I:85:GLN:HB2	2.21	0.41
1:A:51:TRP:CG	1:A:175:GLY:HA3	2.54	0.41
1:F:184:PRO:HA	1:F:185:PRO:HD3	1.84	0.41
5:J:184:ASP:HA	5:J:185:PRO:HD3	1.91	0.41
1:P:194:ILE:HG22	1:P:195:SER:N	2.36	0.41
5:T:72:PRO:HA	5:T:74:ASP:HA	1.35	0.41
2:G:41:LYS:HB2	2:G:78:TYR:CE1	2.55	0.41
2:B:73:THR:HG1	2:B:76:ASP:HB2	1.86	0.41
1:K:28:VAL:O	1:K:29:ASP:HB2	2.20	0.41
2:L:54:LEU:HD11	2:L:62:PHE:HD1	1.86	0.41
1:K:48:ARG:O	1:K:52:ILE:HB	2.20	0.41
5:O:78:VAL:HG23	5:O:88:LEU:C	2.41	0.41
1:A:189:VAL:CG2	1:A:190:THR:N	2.83	0.41
4:N:27:ASN:HB3	4:N:30:SER:OG	2.21	0.41
5:O:99:THR:HG23	5:O:99:THR:O	2.21	0.41
1:P:95:LEU:HD12	1:P:117:ALA:O	2.20	0.41
1:P:51:TRP:CD1	1:P:52:ILE:HG12	2.55	0.41
2:L:2:GLN:NE2	2:L:31:HIS:N	2.68	0.41
4:I:166:TYR:HD2	4:I:188:TRP:NE1	2.17	0.41
4:S:8:PRO:HB2	4:S:9:GLY:H	1.50	0.41
1:F:174:ASN:HD22	1:F:174:ASN:H	1.69	0.41
4:N:210:PHE:O	4:N:210:PHE:CG	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASP:CG	2:B:12:ARG:HH12	2.24	0.41
1:A:257:TYR:CG	1:A:258:THR:N	2.86	0.41
2:L:7:ILE:HD11	2:L:25:CYS:HB3	2.03	0.41
2:L:39:LEU:HG	2:L:46:ILE:HD12	2.03	0.41
1:P:147:TRP:CG	1:P:152:VAL:HG21	2.56	0.41
5:J:172:VAL:HA	5:J:218:HIS:O	2.21	0.41
2:B:9:VAL:HG22	2:B:80:CYS:HB2	2.02	0.41
4:D:208:ASP:HA	1:P:108:ARG:CB	2.50	0.41
1:F:45:GLU:HA	1:F:45:GLU:OE2	2.20	0.41
4:D:165:VAL:HA	4:D:189:SER:HB2	2.02	0.41
5:J:31:TYR:CE1	5:J:57:VAL:HG12	2.56	0.41
1:F:72:GLN:HG3	5:J:57:VAL:HG11	2.03	0.41
2:Q:12:ARG:HG3	2:Q:22:PHE:CD2	2.55	0.41
5:O:170:TRP:C	5:O:171:TRP:HD1	2.24	0.41
1:K:189:VAL:HB	1:K:204:TRP:CZ2	2.55	0.41
1:A:5:MET:O	1:A:100:GLY:HA3	2.21	0.41
5:O:234:TRP:CZ2	5:O:236:GLN:HB2	2.56	0.41
4:S:125:ILE:HD13	4:S:181:LYS:O	2.21	0.41
5:O:27:ASP:C	5:O:28:MET:HG3	2.41	0.41
2:L:95:TRP:CD1	2:L:96:ASP:N	2.89	0.41
2:Q:3:ARG:HG2	2:Q:29:GLY:O	2.21	0.41
1:F:194:ILE:HD11	1:F:200:THR:HG23	2.01	0.41
4:D:135:LEU:HD12	4:D:135:LEU:H	1.85	0.41
1:P:6:ARG:NH1	1:P:113:HIS:HB2	2.35	0.41
4:S:160:SER:HA	4:S:202:ASN:ND2	2.35	0.41
2:Q:5:PRO:HA	2:Q:30:PHE:HB3	2.01	0.41
1:K:116:TYR:CE2	1:K:147:TRP:CH2	3.09	0.41
2:G:57:SER:HB2	2:G:59:ASP:OD1	2.21	0.41
5:E:77:ASN:O	5:E:89:LEU:HD12	2.21	0.41
5:J:71:VAL:H	5:J:72:PRO:CD	2.23	0.41
2:G:46:ILE:HD13	2:G:49:VAL:HG21	2.02	0.41
1:A:49:ALA:HB1	1:A:50:PRO:CD	2.50	0.41
5:T:15:LYS:HE3	5:T:128:LEU:CD1	2.49	0.41
5:E:152:ALA:O	5:E:206:ARG:HA	2.21	0.41
4:D:18:THR:HG22	4:D:92:ARG:HA	2.02	0.41
4:I:137:ASP:HB3	5:J:139:PHE:CE2	2.55	0.41
1:A:8:PHE:HB2	1:A:25:VAL:CG1	2.51	0.41
1:F:85:TYR:HB3	1:F:87:GLN:HE21	1.85	0.41
1:F:14:ARG:HA	1:F:15:PRO:HD3	1.83	0.41
4:I:143:LYS:HB2	4:I:144:SER:H	1.70	0.41
5:J:163:PRO:HB2	5:J:165:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:97:SER:OG	5:E:98:GLN:N	2.50	0.40
1:A:263:HIS:HB3	1:A:264:GLU:H	1.67	0.40
2:L:7:ILE:HD12	2:L:82:VAL:CG2	2.50	0.40
4:N:145:VAL:HG13	4:N:187:ALA:N	2.34	0.40
1:P:46:GLU:OE1	1:P:60:TRP:HZ2	2.03	0.40
4:I:84:ASN:ND2	4:I:84(C):SER:OG	2.54	0.40
5:J:153:THR:OG1	5:J:206:ARG:HB2	2.21	0.40
4:D:213:SER:HB3	4:D:214:PRO:HD3	2.02	0.40
1:P:99:TYR:CZ	3:R:3:ARG:HB3	2.56	0.40
5:O:30:HIS:CD2	5:O:108:GLN:N	2.89	0.40
1:F:208:PHE:CE2	1:F:242:GLN:O	2.74	0.40
1:P:205:ALA:O	1:P:206:LEU:HB2	2.20	0.40
5:J:53:ILE:HG22	5:J:54:HIS:CD2	2.56	0.40
4:D:27:ASN:HD22	4:D:29:ALA:N	2.19	0.40
1:K:51:TRP:CH2	1:K:179:LEU:HD13	2.56	0.40
1:F:178:THR:HA	1:F:181:ARG:HH11	1.87	0.40
2:L:96:ASP:CB	2:L:99:MET:HB3	2.51	0.40
5:T:115:TYR:CD2	5:T:115:TYR:N	2.88	0.40
1:K:203:CYS:O	1:K:204:TRP:CB	2.69	0.40
1:A:202:ARG:HA	1:A:245:ALA:O	2.21	0.40
1:K:69:THR:HG23	5:O:110:ASN:HD21	1.83	0.40
1:K:121:LYS:HA	1:K:121:LYS:HD3	1.89	0.40
2:B:67:TYR:CD2	2:B:67:TYR:N	2.84	0.40
2:G:33:SER:HB3	2:G:62:PHE:CE2	2.55	0.40
4:N:87:ILE:HD11	4:N:104:CYS:SG	2.61	0.40
1:F:50:PRO:HA	1:F:53:GLU:OE1	2.21	0.40
5:O:7:GLN:HB3	5:O:104:CYS:SG	2.61	0.40
1:F:268:LYS:O	1:F:270:LEU:HD12	2.20	0.40
1:F:260:HIS:CD2	1:F:271:THR:HB	2.56	0.40
5:O:139:PHE:HB2	5:O:155:VAL:O	2.22	0.40
4:N:30:SER:CA	4:N:108:ALA:CB	2.97	0.40
4:N:165:VAL:O	4:N:167:ILE:HG13	2.22	0.40
2:L:96:ASP:O	2:L:97:ARG:C	2.60	0.40
5:T:42:TYR:CE2	5:T:52:LEU:HB2	2.56	0.40
4:D:197:ALA:HA	4:D:211:PHE:CD1	2.57	0.40
1:P:235:PRO:HG2	2:Q:10:TYR:OH	2.21	0.40
4:I:129:ASP:HA	4:I:130:PRO:HD2	1.84	0.40
1:K:85:TYR:HB2	1:K:87:GLN:NE2	2.35	0.40
3:C:9:LEU:HD12	3:C:9:LEU:N	2.37	0.40
2:Q:77:GLU:H	2:Q:77:GLU:CD	2.25	0.40
2:L:81:ARG:HG3	2:L:81:ARG:NH1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:VAL:O	1:F:29:ASP:HB2	2.21	0.40
5:E:176:GLU:HG2	5:E:178:HIS:HE1	1.87	0.40
2:B:4:THR:HG23	2:B:5:PRO:CD	2.52	0.40
2:G:44:GLU:HA	2:G:44:GLU:OE1	2.22	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	275/277 (99%)	193 (70%)	54 (20%)	28 (10%)	1	4
1	F	275/277 (99%)	196 (71%)	57 (21%)	22 (8%)	1	6
1	K	275/277 (99%)	196 (71%)	62 (22%)	17 (6%)	2	10
1	P	275/277 (99%)	210 (76%)	43 (16%)	22 (8%)	1	6
2	B	97/100 (97%)	77 (79%)	15 (16%)	5 (5%)	2	15
2	G	97/100 (97%)	75 (77%)	16 (16%)	6 (6%)	2	10
2	L	98/100 (98%)	70 (71%)	17 (17%)	11 (11%)	0	3
2	Q	98/100 (98%)	72 (74%)	20 (20%)	6 (6%)	2	11
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	M	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	R	7/9 (78%)	7 (100%)	0	0	100	100
4	D	195/203 (96%)	139 (71%)	39 (20%)	17 (9%)	1	5
4	I	195/203 (96%)	140 (72%)	42 (22%)	13 (7%)	1	9
4	N	195/203 (96%)	120 (62%)	54 (28%)	21 (11%)	0	3
4	S	195/203 (96%)	146 (75%)	37 (19%)	12 (6%)	2	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	239/244 (98%)	192 (80%)	40 (17%)	7 (3%)	6	29
5	J	238/244 (98%)	191 (80%)	35 (15%)	12 (5%)	3	16
5	O	239/244 (98%)	172 (72%)	54 (23%)	13 (5%)	2	14
5	T	239/244 (98%)	196 (82%)	31 (13%)	12 (5%)	3	16
All	All	3253/3332 (98%)	2409 (74%)	620 (19%)	224 (7%)	1	8

All (224) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	211	ALA
1	A	235	PRO
1	A	267	PRO
2	B	14	PRO
4	D	8	PRO
4	D	108	ALA
4	D	136	ARG
4	D	137	ASP
5	E	70	GLU
5	E	97	SER
1	F	106	ASP
1	F	235	PRO
1	F	236	ALA
2	G	12	ARG
4	I	8	PRO
4	I	139	LYS
4	I	159	GLN
5	J	70	GLU
5	J	96	PRO
1	K	210	PRO
1	K	235	PRO
1	K	236	ALA
2	L	5	PRO
2	L	6	LYS
2	L	7	ILE
2	L	34	ASP
2	L	37	VAL
4	N	15	GLU
4	N	30	SER
4	N	68	GLU
4	N	107	ARG

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Mol	Chain	Res	Type
4	N	162	ASP
1	P	29	ASP
1	P	43	PRO
1	P	47	PRO
1	P	50	PRO
1	P	177	ASP
1	P	196	ASP
2	Q	12	ARG
2	Q	20	SER
4	S	142	ASP
5	T	70	GLU
5	T	97	SER
5	T	98	GLN
1	A	185	PRO
1	A	194	ILE
1	A	203	CYS
1	A	208	PHE
1	A	210	PRO
1	A	236	ALA
1	A	254	GLU
2	B	48	LYS
4	D	125	ILE
4	D	170	LYS
4	D	174	ASP
4	D	208	ASP
5	E	61	THR
5	E	72	PRO
1	F	213	ILE
2	G	16	GLU
4	I	107	ARG
4	I	138	SER
4	I	140	SER
4	I	144	SER
4	I	160	SER
4	I	178	MET
4	I	184	SER
5	J	98	GLN
1	K	30	ASP
1	K	207	GLY
2	L	8	GLN
2	L	42	ASN
4	N	8	PRO

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Mol	Chain	Res	Type
4	N	78	ARG
4	N	108	ALA
4	N	121	VAL
4	N	142	ASP
4	N	151	PHE
4	N	199	ALA
5	O	74	ASP
5	O	97	SER
5	O	141	PRO
5	O	229	SER
1	P	17	ARG
1	P	40	ALA
1	P	51	TRP
1	P	235	PRO
1	P	255	GLN
4	S	8	PRO
4	S	108	ALA
4	S	139	LYS
5	T	28	MET
1	A	204	TRP
1	A	209	TYR
1	A	276	PRO
2	B	19	LYS
4	D	15	GLU
4	D	191	LYS
1	F	51	TRP
1	F	86	ASN
1	F	219	ARG
1	F	222	GLU
1	F	243	LYS
2	G	52	SER
2	G	74	GLU
2	G	77	GLU
4	I	108	ALA
4	I	183	ASN
5	J	67	ALA
5	J	72	PRO
5	J	233	GLU
1	K	177	ASP
1	K	204	TRP
1	K	205	ALA
1	K	232	GLU

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Mol	Chain	Res	Type
2	L	61	SER
4	N	143	LYS
4	N	144	SER
4	N	170	LYS
4	N	191	LYS
4	N	197	ALA
4	N	206	PRO
4	N	208	ASP
5	O	106	SER
5	O	240	LYS
1	P	42	SER
1	P	194	ILE
1	P	221	GLY
1	P	236	ALA
4	S	159	GLN
4	S	195	ALA
5	T	18	GLN
5	T	94	ALA
1	A	2	SER
1	A	86	ASN
1	A	220	ASP
1	A	262	GLN
1	A	271	THR
4	D	3	GLU
4	D	107	ARG
4	D	119	LEU
5	E	92	GLU
5	E	240	LYS
1	F	41	ALA
1	F	166	GLU
1	F	196	ASP
1	F	202	ARG
1	F	212	GLU
1	F	224	GLN
5	J	66	THR
5	J	75	GLY
5	J	240	LYS
1	K	2	SER
1	K	51	TRP
1	K	114	ASN
1	K	162	GLY
1	K	237	GLY

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Mol	Chain	Res	Type
2	L	32	PRO
4	N	130	PRO
5	O	112	ASP
5	O	217	ASN
1	P	210	PRO
2	Q	43	GLY
2	Q	79	ALA
4	S	15	GLU
4	S	27	ASN
4	S	93	ASP
4	S	140	SER
4	S	174	ASP
5	T	67	ALA
5	T	238	ARG
5	T	240	LYS
1	A	42	SER
2	B	23	LEU
2	B	47	GLU
4	D	30	SER
4	D	110	LYS
1	F	43	PRO
1	F	264	GLU
2	G	46	ILE
1	K	47	PRO
2	L	46	ILE
4	N	163	SER
5	O	92	GLU
5	O	190	GLU
5	O	243	THR
1	P	4	SER
1	P	58	GLU
1	P	172	LEU
1	P	243	LYS
1	A	58	GLU
1	A	192	HIS
4	D	175	MET
1	F	237	GLY
5	J	71	VAL
5	J	192	PRO
2	Q	16	GLU
4	S	107	ARG
5	T	236	GLN

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Mol	Chain	Res	Type
1	A	56	GLY
4	D	130	PRO
1	F	193	PRO
1	K	42	SER
1	K	50	PRO
2	L	49	VAL
5	T	187	PRO
1	A	213	ILE
1	P	49	ALA
1	P	276	PRO
2	Q	90	PRO
5	T	160	GLY
1	F	50	PRO
4	I	9	GLY
5	O	185	PRO
1	A	15	PRO
1	A	261	VAL
1	F	194	ILE
5	J	49	GLY
1	A	43	PRO
1	A	49	ALA
5	E	215	PRO
5	O	192	PRO
1	F	210	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/236 (100%)	221 (94%)	15 (6%)	22	57
1	F	236/236 (100%)	220 (93%)	16 (7%)	20	55
1	K	236/236 (100%)	224 (95%)	12 (5%)	29	66
1	P	236/236 (100%)	220 (93%)	16 (7%)	20	55
2	B	94/95 (99%)	86 (92%)	8 (8%)	13	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	94/95 (99%)	86 (92%)	8 (8%)	13	45
2	L	95/95 (100%)	84 (88%)	11 (12%)	7	27
2	Q	95/95 (100%)	89 (94%)	6 (6%)	22	58
3	C	6/6 (100%)	4 (67%)	2 (33%)	0	0
3	H	6/6 (100%)	5 (83%)	1 (17%)	3	11
3	M	6/6 (100%)	6 (100%)	0	100	100
3	R	6/6 (100%)	6 (100%)	0	100	100
4	D	177/183 (97%)	166 (94%)	11 (6%)	23	59
4	I	177/183 (97%)	166 (94%)	11 (6%)	23	59
4	N	177/183 (97%)	162 (92%)	15 (8%)	13	45
4	S	177/183 (97%)	169 (96%)	8 (4%)	34	70
5	E	205/208 (99%)	190 (93%)	15 (7%)	17	52
5	J	205/208 (99%)	195 (95%)	10 (5%)	31	68
5	O	205/208 (99%)	193 (94%)	12 (6%)	24	60
5	T	205/208 (99%)	191 (93%)	14 (7%)	20	55
All	All	2874/2912 (99%)	2683 (93%)	191 (7%)	21	56

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	52	ILE
1	A	63	ASN
1	A	81	LEU
1	A	115	GLN
1	A	186	LYS
1	A	198	GLU
1	A	204	TRP
1	A	219	ARG
1	A	230	LEU
1	A	234	ARG
1	A	257	TYR
1	A	260	HIS
1	A	270	LEU
1	A	274	TRP
2	B	12	ARG
2	B	22	PHE

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Mol	Chain	Res	Type
2	B	24	ASN
2	B	31	HIS
2	B	58	LYS
2	B	67	TYR
2	B	70	PHE
2	B	98	ASP
3	C	3	ARG
3	C	5	ARG
4	D	19	VAL
4	D	27	ASN
4	D	48	LYS
4	D	68	GLU
4	D	87	ILE
4	D	92	ARG
4	D	96	LEU
4	D	104	CYS
4	D	171	CYS
4	D	194	PHE
4	D	210	PHE
5	E	19	MET
5	E	25	GLN
5	E	45	ASP
5	E	61	THR
5	E	71	VAL
5	E	86	ASN
5	E	87	PHE
5	E	164	ASP
5	E	188	LEU
5	E	194	LEU
5	E	196	ASP
5	E	197	SER
5	E	204	ARG
5	E	231	ASN
5	E	244	GLN
1	F	42	SER
1	F	45	GLU
1	F	51	TRP
1	F	72	GLN
1	F	81	LEU
1	F	108	ARG
1	F	109	LEU
1	F	137	ASP

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Mol	Chain	Res	Type
1	F	138	THR
1	F	170	ARG
1	F	186	LYS
1	F	189	VAL
1	F	219	ARG
1	F	220	ASP
1	F	223	ASP
1	F	238	ASP
2	G	10	TYR
2	G	23	LEU
2	G	40	LEU
2	G	46	ILE
2	G	51	HIS
2	G	78	TYR
2	G	85	VAL
2	G	99	MET
3	H	5	ARG
4	I	18	THR
4	I	24	THR
4	I	27	ASN
4	I	43	ARG
4	I	46	SER
4	I	48	LYS
4	I	54	MET
4	I	90	LEU
4	I	92	ARG
4	I	191	LYS
4	I	210	PHE
5	J	20	THR
5	J	48	MET
5	J	87	PHE
5	J	99	THR
5	J	126	GLU
5	J	128	LEU
5	J	165	HIS
5	J	204	ARG
5	J	236	GLN
5	J	253	ARG
1	K	30	ASP
1	K	121	LYS
1	K	138	THR
1	K	179	LEU

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Mol	Chain	Res	Type
1	K	181	ARG
1	K	204	TRP
1	K	228	THR
1	K	234	ARG
1	K	241	PHE
1	K	244	TRP
1	K	257	TYR
1	K	258	THR
2	L	1	ILE
2	L	2	GLN
2	L	3	ARG
2	L	13	HIS
2	L	17	ASN
2	L	23	LEU
2	L	37	VAL
2	L	44	GLU
2	L	51	HIS
2	L	67	TYR
2	L	89	GLN
4	N	45	ASP
4	N	54	MET
4	N	68	GLU
4	N	69	ASP
4	N	106	VAL
4	N	113	PHE
4	N	127	ASN
4	N	132	VAL
4	N	133	TYR
4	N	148	PHE
4	N	154	GLN
4	N	155	THR
4	N	168	THR
4	N	169	ASP
4	N	209	THR
5	O	6	THR
5	O	43	ARG
5	O	45	ASP
5	O	48	MET
5	O	71	VAL
5	O	87	PHE
5	O	91	LEU
5	O	126	GLU

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Mol	Chain	Res	Type
5	O	194	LEU
5	O	212	TRP
5	O	231	ASN
5	O	238	ARG
1	P	29	ASP
1	P	44	ARG
1	P	53	GLU
1	P	55	GLU
1	P	65	GLN
1	P	69	THR
1	P	72	GLN
1	P	129	ASP
1	P	138	THR
1	P	177	ASP
1	P	192	HIS
1	P	201	LEU
1	P	203	CYS
1	P	204	TRP
1	P	216	THR
1	P	234	ARG
2	Q	51	HIS
2	Q	67	TYR
2	Q	75	LYS
2	Q	78	TYR
2	Q	83	ASN
2	Q	97	ARG
4	S	27	ASN
4	S	54	MET
4	S	86	TYR
4	S	148	PHE
4	S	198	ASN
4	S	202	ASN
4	S	205	ILE
4	S	211	PHE
5	T	21	THR
5	T	22	LEU
5	T	26	GLN
5	T	28	MET
5	T	29	ASN
5	T	61	THR
5	T	81	LEU
5	T	87	PHE

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Mol	Chain	Res	Type
5	T	165	HIS
5	T	204	ARG
5	T	228	LEU
5	T	230	GLU
5	T	237	ASP
5	T	244	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	72	GLN
1	A	87	GLN
1	A	115	GLN
1	A	197	HIS
1	A	218	GLN
1	A	263	HIS
2	B	42	ASN
4	D	27	ASN
4	D	134	GLN
5	E	25	GLN
5	E	98	GLN
5	E	178	HIS
5	E	213	GLN
5	E	231	ASN
5	E	244	GLN
1	F	115	GLN
1	F	174	ASN
1	F	191	HIS
1	F	260	HIS
1	F	262	GLN
2	G	8	GLN
4	I	27	ASN
4	I	84	ASN
4	I	183	ASN
5	J	25	GLN
5	J	28	ASN
5	J	44	GLN
5	J	86	ASN
5	J	98	GLN
5	J	114	GLN
5	J	224	GLN

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Mol	Chain	Res	Type
1	K	3	HIS
1	K	65	GLN
1	K	93	HIS
1	K	144	GLN
1	K	174	ASN
1	K	226	GLN
1	K	242	GLN
1	K	262	GLN
2	L	13	HIS
2	L	51	HIS
4	N	44	GLN
4	N	85	GLN
4	N	115	GLN
4	N	154	GLN
5	O	44	GLN
5	O	54	HIS
5	O	98	GLN
5	O	110	ASN
5	O	148	HIS
5	O	213	GLN
5	O	218	HIS
5	O	222	GLN
5	O	224	GLN
1	P	3	HIS
1	P	65	GLN
1	P	141	GLN
1	P	144	GLN
1	P	174	ASN
1	P	262	GLN
2	Q	2	GLN
2	Q	24	ASN
4	S	27	ASN
4	S	84	ASN
4	S	85	GLN
4	S	202	ASN
5	T	44	GLN
5	T	86	ASN
5	T	98	GLN
5	T	191	GLN
5	T	244	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	277/277 (100%)	0.31	27 (9%) 10 3	21, 78, 193, 223	0
1	F	277/277 (100%)	0.40	36 (12%) 5 2	30, 82, 214, 249	0
1	K	277/277 (100%)	0.41	34 (12%) 5 2	31, 93, 215, 245	0
1	P	277/277 (100%)	0.15	15 (5%) 29 12	25, 87, 200, 220	0
2	B	99/100 (99%)	-0.14	0 100 100	34, 67, 116, 130	0
2	G	99/100 (99%)	0.35	5 (5%) 32 13	49, 100, 159, 188	0
2	L	100/100 (100%)	1.57	33 (33%) 0 0	66, 193, 228, 236	0
2	Q	100/100 (100%)	0.70	12 (12%) 6 2	45, 136, 184, 191	0
3	C	9/9 (100%)	-0.86	0 100 100	27, 31, 41, 48	0
3	H	9/9 (100%)	-0.83	0 100 100	22, 34, 43, 45	0
3	M	9/9 (100%)	-0.62	0 100 100	29, 34, 52, 62	0
3	R	9/9 (100%)	-0.83	0 100 100	22, 27, 46, 54	0
4	D	197/203 (97%)	0.09	4 (2%) 68 46	31, 78, 133, 162	0
4	I	197/203 (97%)	-0.31	1 (0%) 91 83	20, 46, 116, 143	0
4	N	197/203 (97%)	0.65	20 (10%) 9 3	35, 97, 178, 201	0
4	S	197/203 (97%)	-0.13	7 (3%) 46 23	21, 51, 132, 166	0
5	E	241/244 (98%)	-0.25	1 (0%) 93 85	28, 64, 113, 133	2 (0%)
5	J	240/244 (98%)	-0.44	2 (0%) 87 75	20, 41, 90, 137	2 (0%)
5	O	241/244 (98%)	0.02	9 (3%) 45 22	27, 61, 177, 189	2 (0%)
5	T	241/244 (98%)	-0.30	3 (1%) 81 64	20, 52, 114, 145	2 (0%)
All	All	3293/3332 (98%)	0.12	209 (6%) 23 9	20, 72, 193, 249	8 (0%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	GLN	10.3
1	K	237	GLY	8.4
1	A	217	TRP	7.4
1	F	249	VAL	7.1
1	F	199	ALA	6.8
1	A	221	GLY	6.6
1	A	265	GLY	6.3
1	F	255	GLN	6.2
1	F	277	SER	6.2
1	A	258	THR	6.2
4	N	214	PRO	6.1
1	F	190	THR	5.9
2	Q	0	MET	5.9
1	A	255	GLN	5.9
2	L	68	THR	5.7
2	Q	79	ALA	5.5
1	A	259	CYS	5.4
1	F	252	GLY	5.3
1	P	220	ASP	5.2
1	K	191	HIS	5.2
5	O	179	SER	5.1
1	K	199	ALA	5.0
1	A	256	ARG	5.0
2	L	45	ARG	4.9
1	K	236	ALA	4.9
5	J	255	ASP	4.9
1	K	188	HIS	4.8
1	K	227	ASP	4.8
1	K	195	SER	4.8
1	K	194	ILE	4.8
4	I	142	ASP	4.8
4	N	213	SER	4.7
1	P	277	SER	4.6
1	A	223	ASP	4.4
2	L	25	CYS	4.4
1	F	220	ASP	4.4
2	L	95	TRP	4.4
1	K	190	THR	4.4
2	L	79	ALA	4.2
2	L	41	LYS	4.1
1	A	257	TYR	4.1
2	G	14	PRO	4.0
2	L	76	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
2	L	80	CYS	4.0
1	K	192	HIS	3.9
2	L	46	ILE	3.9
1	A	210	PRO	3.9
2	L	92	ILE	3.9
4	D	207	GLU	3.9
1	K	203	CYS	3.9
4	D	214	PRO	3.9
4	S	141	SER	3.8
1	K	277	SER	3.8
1	F	200	THR	3.7
2	L	24	ASN	3.7
2	L	20	SER	3.7
1	A	266	LEU	3.7
2	Q	16	GLU	3.7
2	L	39	LEU	3.7
4	N	201	ASN	3.7
1	A	264	GLU	3.7
1	F	246	ALA	3.5
1	A	260	HIS	3.5
2	Q	11	SER	3.4
1	F	218	GLN	3.4
1	K	226	GLN	3.3
1	K	244	TRP	3.3
1	A	273	ARG	3.3
4	N	173	LEU	3.3
2	Q	78	TYR	3.3
1	F	191	HIS	3.2
2	Q	24	ASN	3.2
4	D	163	SER	3.2
4	N	133	TYR	3.2
1	A	179	LEU	3.2
2	L	42	ASN	3.2
2	L	71	THR	3.2
4	N	150	ASP	3.2
1	A	277	SER	3.2
5	O	217	ASN	3.2
1	A	216	THR	3.1
2	Q	25	CYS	3.1
4	N	198	ASN	3.1
1	A	250	PRO	3.1
1	F	259	CYS	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	N	172	VAL	3.1
1	A	269	PRO	3.1
1	F	227	ASP	3.1
2	L	94	LYS	3.0
4	S	142	ASP	3.0
1	A	199	ALA	3.0
1	K	238	ASP	3.0
5	O	151	LYS	3.0
4	N	163	SER	3.0
1	P	195	SER	3.0
4	S	144	SER	3.0
5	T	141	PRO	3.0
2	L	40	LEU	2.9
1	F	203	CYS	2.9
4	N	146	CYS	2.9
1	P	230	LEU	2.9
1	F	267	PRO	2.9
1	F	205	ALA	2.9
1	A	207	GLY	2.9
1	K	187	THR	2.8
1	F	258	THR	2.8
5	O	141	PRO	2.8
1	K	43	PRO	2.8
2	L	49	VAL	2.8
1	F	250	PRO	2.8
2	Q	40	LEU	2.7
4	N	131	ALA	2.7
1	F	244	TRP	2.7
1	K	259	CYS	2.7
1	A	181	ARG	2.7
1	F	248	VAL	2.7
5	O	178	HIS	2.7
1	P	252	GLY	2.6
1	K	189	VAL	2.6
4	N	191	LYS	2.6
1	F	204	TRP	2.6
1	K	241	PHE	2.6
2	G	98	ASP	2.6
2	Q	8	GLN	2.6
1	F	189	VAL	2.6
1	F	221	GLY	2.6
5	O	180	GLY	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	N	93	ASP	2.6
1	K	205	ALA	2.6
1	F	224	GLN	2.6
1	K	42	SER	2.6
1	K	235	PRO	2.6
2	L	93	VAL	2.6
1	F	188	HIS	2.5
4	S	143	LYS	2.5
1	F	275	GLU	2.5
1	F	42	SER	2.5
4	N	212	PRO	2.5
1	A	203	CYS	2.5
4	N	165	VAL	2.5
1	K	202	ARG	2.5
1	P	239	ARG	2.5
1	F	217	TRP	2.5
1	K	276	PRO	2.5
1	P	196	ASP	2.5
5	E	255	ASP	2.5
2	Q	41	LYS	2.5
1	K	245	ALA	2.4
4	N	139	LYS	2.4
1	F	251	SER	2.4
2	L	38	ASP	2.4
2	L	4	THR	2.4
2	L	11	SER	2.4
1	K	248	VAL	2.4
2	G	75	LYS	2.4
2	L	8	GLN	2.4
2	L	10	TYR	2.4
5	T	74	ASP	2.4
1	P	273	ARG	2.4
2	G	74	GLU	2.3
1	F	245	ALA	2.3
2	Q	9	VAL	2.3
1	A	222	GLU	2.3
1	K	200	THR	2.3
4	N	204	ILE	2.3
4	S	163	SER	2.3
5	O	215	PRO	2.3
4	D	149	THR	2.3
2	L	97	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	G	11	SER	2.3
1	F	260	HIS	2.3
1	P	217	TRP	2.3
4	N	159	GLN	2.3
1	P	248	VAL	2.3
1	P	200	THR	2.3
2	L	72	PRO	2.3
1	F	206	LEU	2.3
1	K	1	GLY	2.3
2	L	73	THR	2.2
1	A	263	HIS	2.2
1	A	275	GLU	2.2
2	L	75	LYS	2.2
2	L	14	PRO	2.2
5	O	147	SER	2.2
1	F	192	HIS	2.2
1	F	247	VAL	2.2
2	L	47	GLU	2.2
1	F	182	ALA	2.2
1	K	220	ASP	2.1
1	K	229	GLU	2.1
1	P	253	GLU	2.1
1	F	201	LEU	2.1
5	O	150	GLN	2.1
1	P	216	THR	2.1
5	T	153	THR	2.1
2	L	50	GLU	2.1
1	P	194	ILE	2.1
2	Q	97	ARG	2.1
2	L	19	LYS	2.1
1	K	173	GLU	2.1
1	K	274	TRP	2.0
4	N	138	SER	2.0
4	S	161	LYS	2.0
1	K	247	VAL	2.0
4	S	190	ASN	2.0
5	J	72	PRO	2.0
4	N	197	ALA	2.0
1	P	43	PRO	2.0
2	L	15	ALA	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 carbohydrates 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.