



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:09 AM GMT

PDB ID : 2ZCY  
Title : yeast 20S proteasome:syringolin A-complex  
Authors : Groll, M.; Dudler, R.; Kaiser, M.  
Deposited on : 2007-11-15  
Resolution : 2.90 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

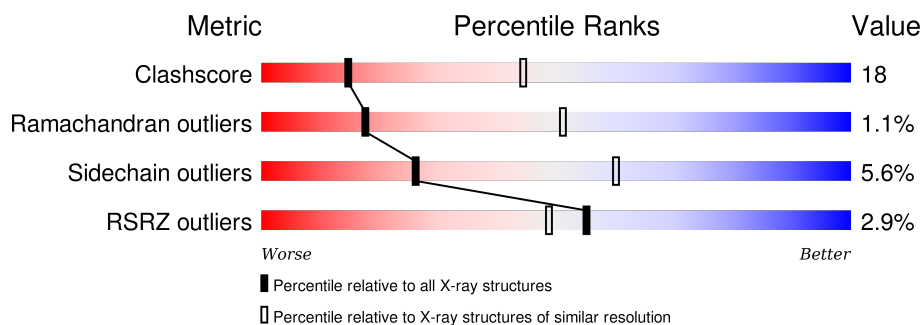
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	250	<div> <div>71%</div> <div>27%</div> <div>•</div> </div>
1	O	250	<div> <div>3%</div> <div>70%</div> <div>28%</div> <div>•</div> </div>
2	B	258	<div> <div>4%</div> <div>59%</div> <div>31%</div> <div>5%</div> <div>5%</div> </div>
2	P	258	<div> <div>6%</div> <div>59%</div> <div>31%</div> <div>5%</div> <div>5%</div> </div>
3	C	254	<div> <div>6%</div> <div>54%</div> <div>37%</div> <div>•</div> <div>5%</div> </div>
3	Q	254	<div> <div>10%</div> <div>55%</div> <div>36%</div> <div>•</div> <div>5%</div> </div>
4	D	260	<div> <div>5%</div> <div>63%</div> <div>27%</div> <div>•</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
4	R	260	
5	E	234	
5	S	234	
6	F	287	
6	T	287	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	241	
12	Z	241	
13	O	266	
13	M	266	
14	I	196	
14	N	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	SRG	I	7710	-	-	-	X
15	SRG	H	7710	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	SRG	N	7710	-	-	-	X
15	SRG	V	7710	-	-	-	X
15	SRG	Y	7710	-	-	-	X

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50766 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 Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1890	1181	331	374	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			
4	R	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			
6	T	244	Total	C	N	O	S	0	0	0
			1896	1205	330	357	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

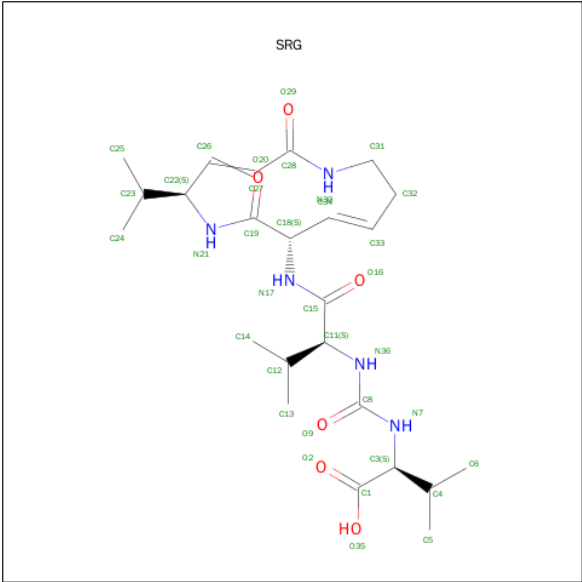
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	0	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	1	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is (2S)-2-[[[(2S)-1-[[[(5S,8S,9E)-2,7-DIOXO-5-PROPAN-2-YL-1,6-DIAZACYCLODODECA-3,9-DIEN-8-YL]AMINO]-3-METHYL-1-OXO-BUTAN-2-YL]CARBAMOYL]AMINO]-3-METHYL-BUTANOIC ACID (three-letter code: SRG) (formula: C<sub>24</sub>H<sub>39</sub>N<sub>5</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			35	24	5	6		
15	K	1	Total	C	N	O	0	0
			35	24	5	6		
15	N	1	Total	C	N	O	0	0
			35	24	5	6		
15	V	1	Total	C	N	O	0	0
			35	24	5	6		
15	Y	1	Total	C	N	O	0	0
			35	24	5	6		
15	1	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	38	Total	O	0	0
			38	38		
16	B	24	Total	O	0	0
			24	24		
16	C	33	Total	O	0	0
			33	33		
16	D	24	Total	O	0	0
			24	24		
16	E	17	Total	O	0	0
			17	17		
16	F	39	Total	O	0	0
			39	39		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	47	Total O 47 47	0	0
16	H	43	Total O 43 43	0	0
16	I	56	Total O 56 56	0	0
16	J	36	Total O 36 36	0	0
16	K	28	Total O 28 28	0	0
16	L	46	Total O 46 46	0	0
16	M	62	Total O 62 62	0	0
16	N	50	Total O 50 50	0	0
16	O	26	Total O 26 26	0	0
16	P	20	Total O 20 20	0	0
16	Q	21	Total O 21 21	0	0
16	R	19	Total O 19 19	0	0
16	S	16	Total O 16 16	0	0
16	T	30	Total O 30 30	0	0
16	U	50	Total O 50 50	0	0
16	V	41	Total O 41 41	0	0
16	W	37	Total O 37 37	0	0
16	X	33	Total O 33 33	0	0
16	Y	29	Total O 29 29	0	0
16	Z	38	Total O 38 38	0	0
16	0	60	Total O 60 60	0	0

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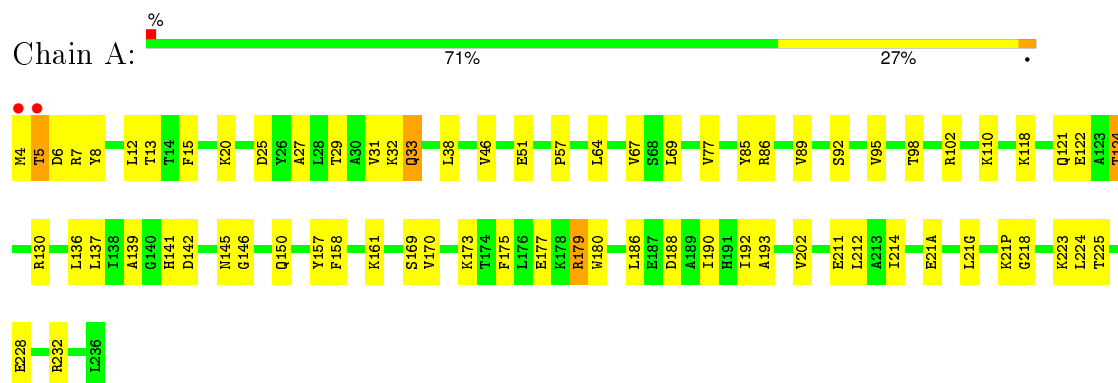
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	1	55	Total	O	0	0
			55	55		

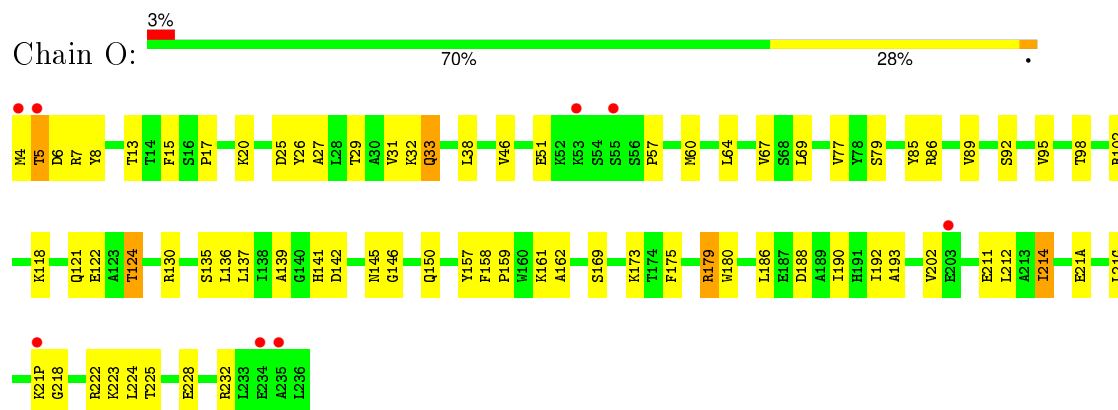
### 3 Residue-property plots

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.

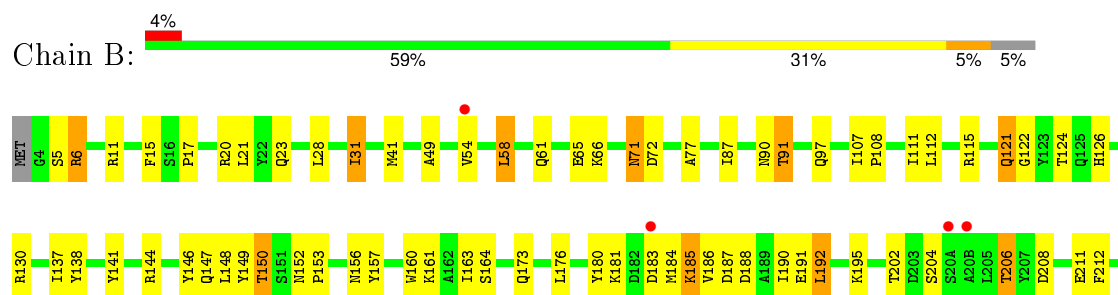
#### • Molecule 1: Proteasome component Y7



#### • Molecule 1: Proteasome component Y7

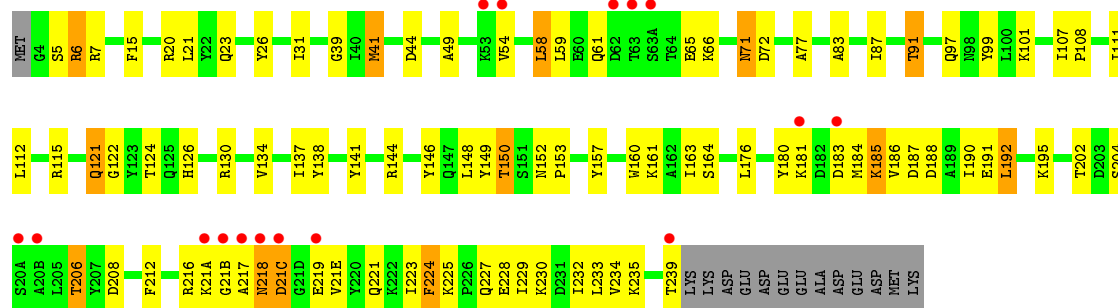


#### • Molecule 2: Proteasome component Y13

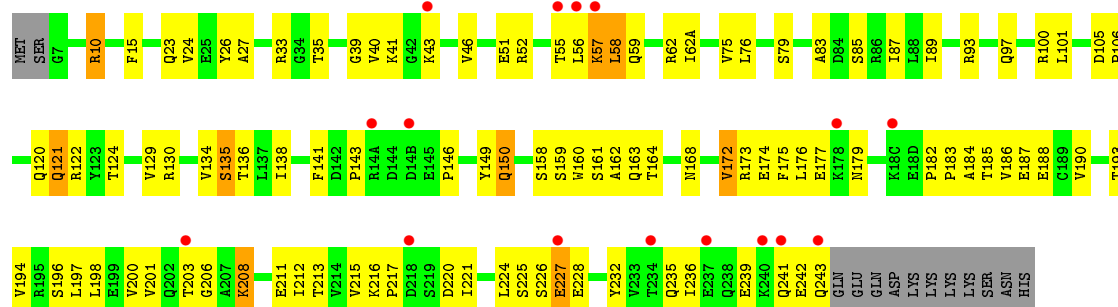




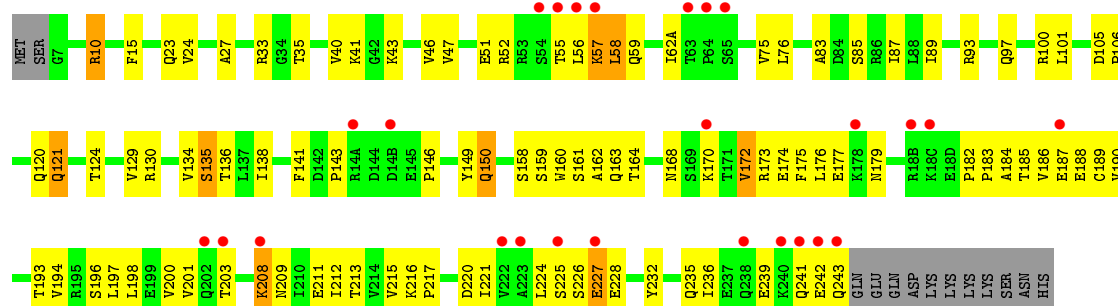
• Molecule 2: Proteasome component Y13



• Molecule 3: Proteasome component PRE6

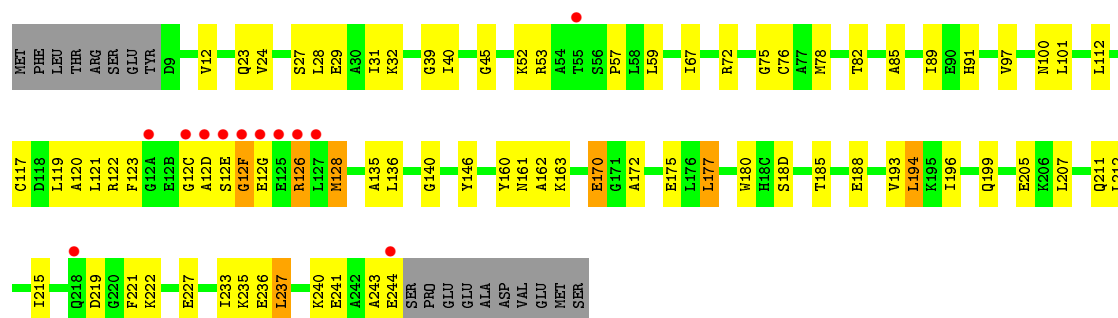


• Molecule 3: Proteasome component PRE6

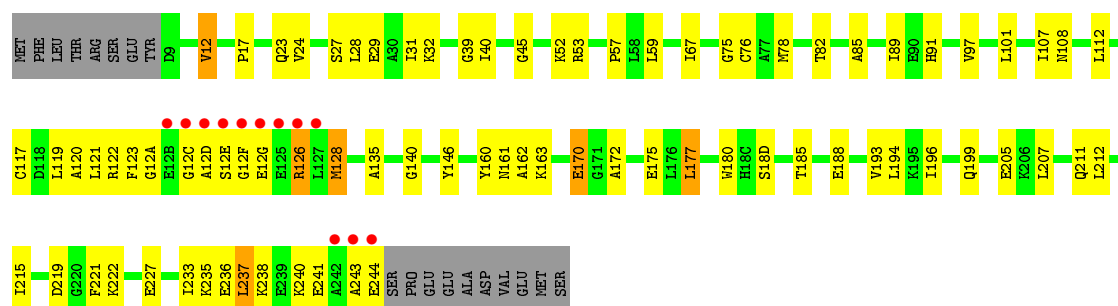


• Molecule 4: Proteasome component PUP2

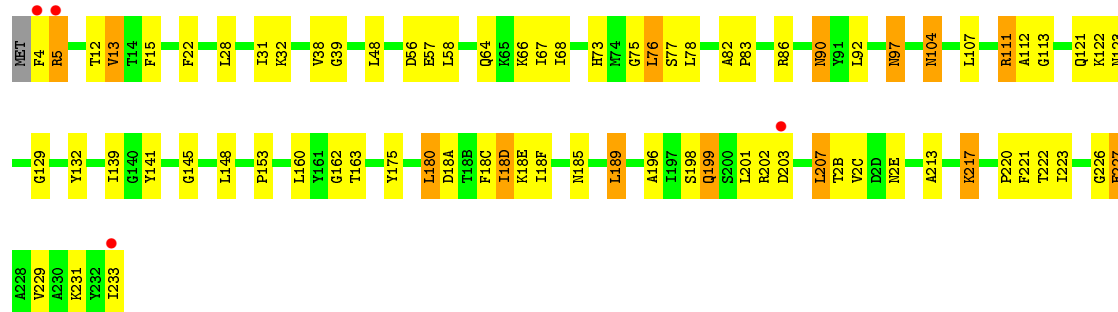




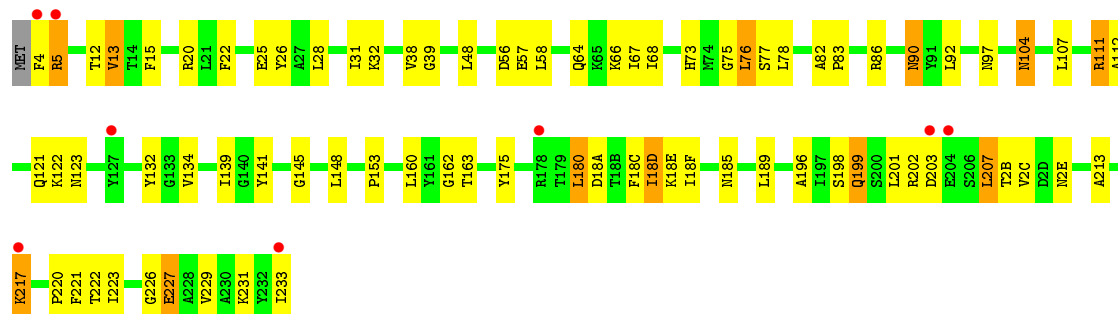
• Molecule 4: Proteasome component PUP2



• Molecule 5: Proteasome component PRE5



• Molecule 5: Proteasome component PRE5



Chain F:

3% 58% 25% 15%

THR SER ILE G5 T6 S11 V14 Q23 V28 E32 T35 T36 S37 I38 M43 V50 E51 K52 L53 I54 L59 V70 V77 I82 P83 R91 E95 S98 Y103 K104 T105 F106 I107 P108 I109 F112 R115 Y119 V120 Q121 A122 Y126 M127 S128 S135 T136 I137 D142 M150 Y157 A164 G168 A172 K173 A174 E175 L176 E177 K178 L179 V180 E18E G18F L184 S185 A186 R187 E188 A189 V190 R191 Q192 K195 I196 N197 Y198 L199 E203 D204 K205 K206 E20B K20C E209 L210 I212 S213 P214 G215 S216 E21A K225 Q237 I240 V241 G1Y ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP SER SER ASN VAL MET SER SER L179 ASP ASP ASP GLU ASN ASP ALA VAL VAL THR ASP ASP GLN GLU GLY ASP ILE HIS LEU GLU

Chain T: 

THR	SER	ILE	G5	T6	S11	N12	S13	V14	D18	Q23	V28	E32	T35	T36	S37	I38	M43	D44	G45	V50	E51	I54	L59	V69	V70	V77	I82	P83	R91	E95	S98	Y103	K104	T105	P106	I107	P108	I109	F112	P115							
Y119	V120	Q121	A122	M127	S128	T136	I137	D142	H147	M150	Y157	M158	ASP	ASP	A164	G168	R169	A172	K173	M174	E175	I176	E177	K178	L179	V180	P180	E181	L184	S185	A186	R187	E188	A189	V190	K191	Q192	K195	I196	G197	Y198	L199	E203	D204	S205	K206	E208

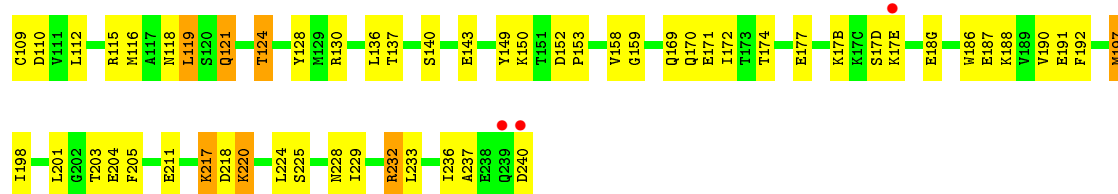
Chain G:

Sequence logo for Chain G. The y-axis represents frequency in bits. A color scale at the top indicates frequency percentages: 2% (red), 61% (green), and 31% (yellow). A legend on the left lists amino acids: MET, SER, GLY, ALA, ALA, ALA, SER, ALA, A6, G7, Y8, D9, R10, Y22, A30, Q33, T34, N34A, I35, L38, A39, V47, V48, I49, S50, Q51, L59, D60, P61, I67, R72, T73, I74, G75, V76, V77, T82, P83, R86, N87, A96, Y105, D106, M107, P108, C109, P110, Y111, L112, R115, H118, L119, S120, Q121, T124, Q125, R126, A127, Y128, L136, T137, S140, E143, Y149, K150, T151, D152, P153, Y157, V158, G159, P167, K168, Q169, Q170, E171, I172, T173, T174, E177, K178, K17C, S17D, K17E, M184, E186, V188, E187, K188, V189, E191, P192, D211, K217, D218, K220, F221, L224, S225, N228, I229, R232, L233, T236, A237, E238, Q239, D240.

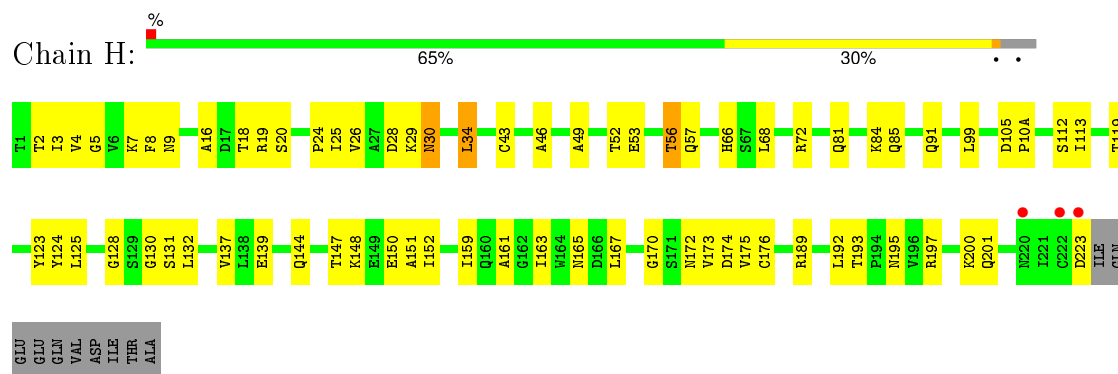
Chain U:

63% 29% 2%

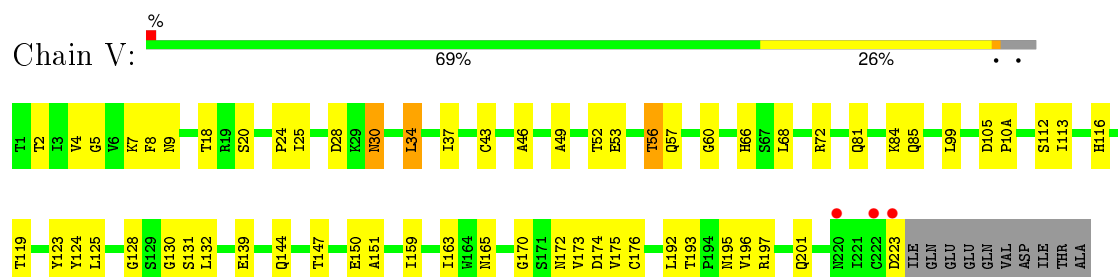
MET SER GLY ALA ALA ALA SER ALA ALA A6 C7 Y8 R10 P17 Y22 A30 Q33 I35 L38 A39 V47 V48 I49 S50 Q51 L59 D60 P61 V64 I67 R72 T73 I74 V77 I82 P83 R86 I87 A96 Y105 D106 M107 M109



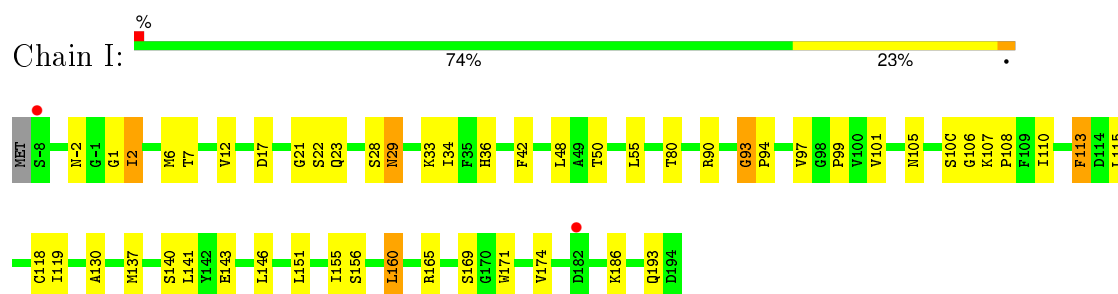
• Molecule 8: Proteasome component PUP1



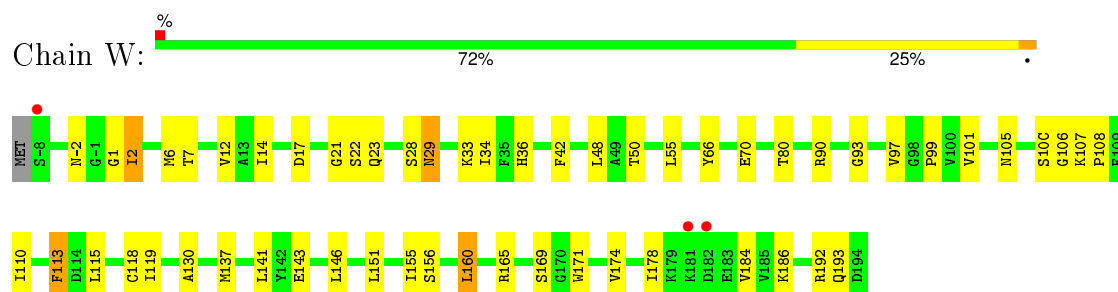
• Molecule 8: Proteasome component PUP1



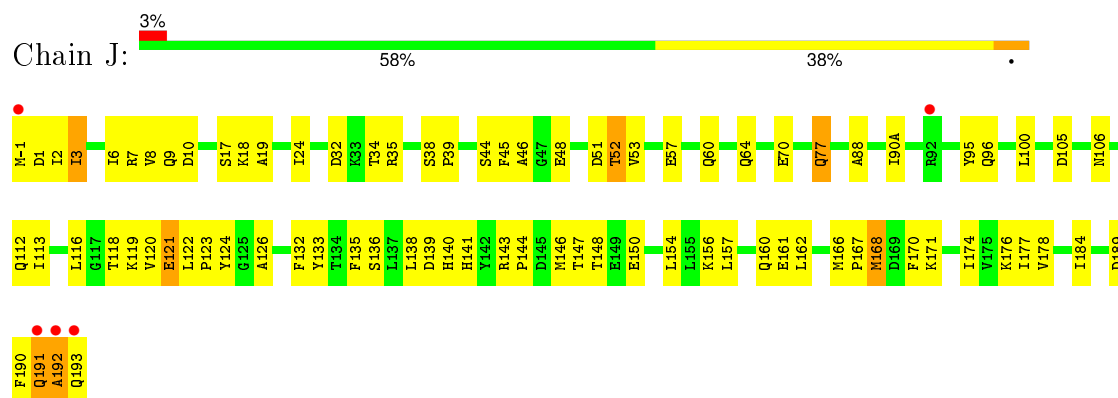
• Molecule 9: Proteasome component PUP3



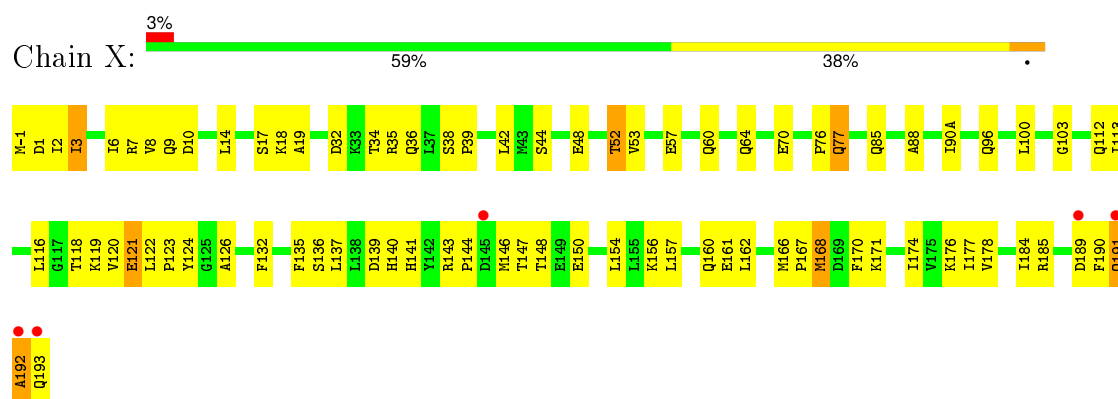
• Molecule 9: Proteasome component PUP3



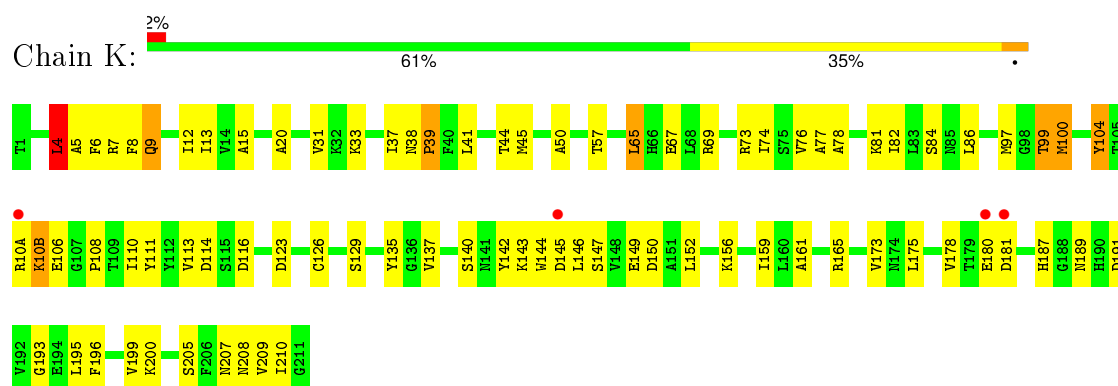
- Molecule 10: Proteasome component C11



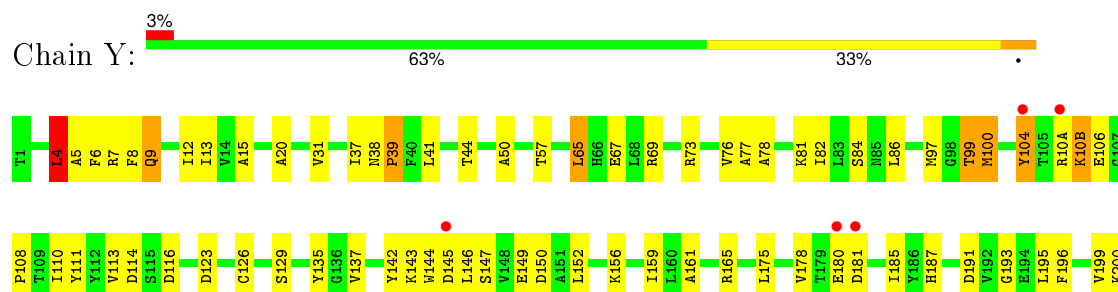
- Molecule 10: Proteasome component C11

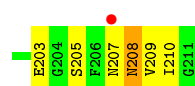


- Molecule 11: Proteasome component PRE2

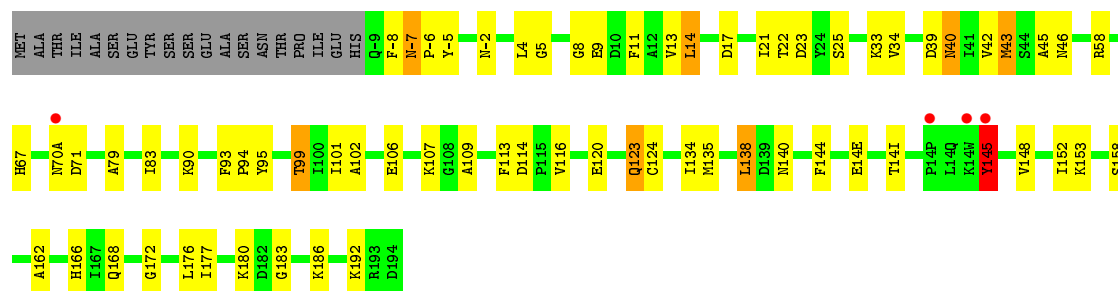


- Molecule 11: Proteasome component PRE2

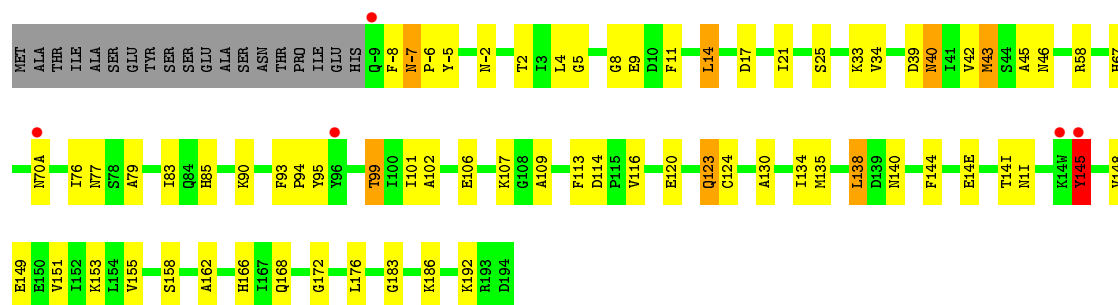




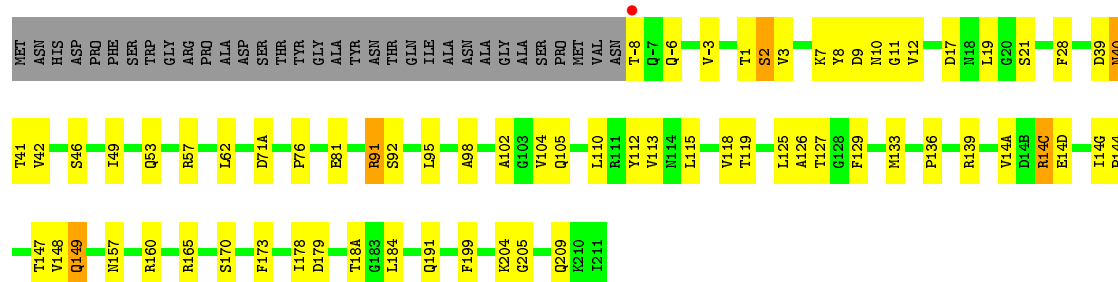
• Molecule 12: Proteasome component C5



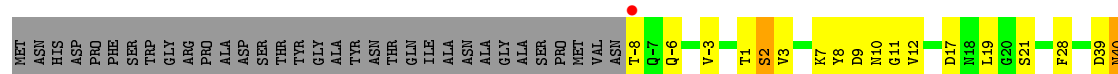
• Molecule 12: Proteasome component C5

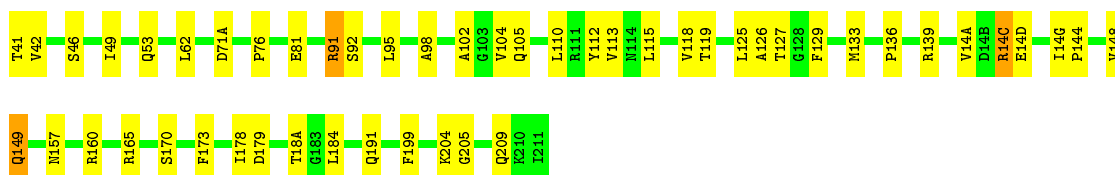


• Molecule 13: Proteasome component PRE4

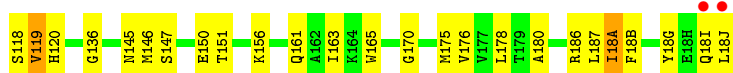


• Molecule 13: Proteasome component PRE4

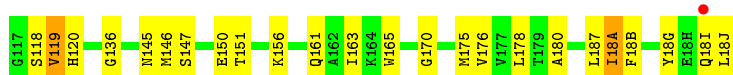
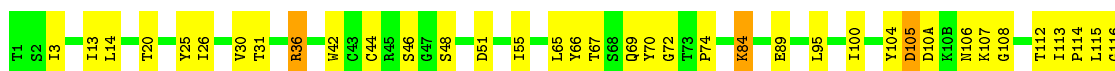




• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.05Å 301.96Å 143.84Å 90.00° 112.87° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 20.02 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.6 (15.00-2.90) 99.2 (20.02-2.82)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.83Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.215 , 0.245 0.226 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 65.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 252502 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	50766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SRG

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	0.38	0/1952	0.64	0/2642
1	O	0.38	0/1952	0.64	0/2642
2	B	0.36	0/1934	0.63	0/2618
2	P	0.38	0/1934	0.63	0/2618
3	C	0.35	0/1919	0.61	0/2598
3	Q	0.36	0/1919	0.61	0/2598
4	D	0.35	0/1886	0.62	0/2541
4	R	0.35	0/1886	0.62	0/2541
5	E	0.35	0/1823	0.62	0/2463
5	S	0.36	0/1823	0.62	0/2463
6	F	0.36	0/1936	0.61	0/2614
6	T	0.38	0/1936	0.62	0/2614
7	G	0.41	0/1959	0.63	0/2652
7	U	0.41	0/1959	0.63	0/2652
8	H	0.37	0/1715	0.66	0/2326
8	V	0.37	0/1715	0.66	0/2326
9	I	0.39	0/1611	0.65	0/2174
9	W	0.41	0/1611	0.66	0/2174
10	J	0.38	0/1613	0.64	0/2173
10	X	0.39	0/1613	0.64	0/2173
11	K	0.39	0/1681	0.65	1/2274 (0.0%)
11	Y	0.39	0/1681	0.65	1/2274 (0.0%)
12	L	0.40	0/1795	0.67	0/2420
12	Z	0.39	0/1795	0.67	0/2420
13	0	0.39	0/1855	0.67	1/2514 (0.0%)
13	M	0.39	0/1855	0.67	1/2514 (0.0%)
14	1	0.41	0/1541	0.66	0/2087
14	N	0.42	0/1541	0.66	0/2087
All	All	0.38	0/50440	0.64	4/68192 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
12	Z	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	0	95	LEU	N-CA-C	-5.83	95.27	111.00
13	M	95	LEU	N-CA-C	-5.78	95.39	111.00
11	K	4	LEU	CA-CB-CG	5.06	126.94	115.30
11	Y	4	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
12	Z	145	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	65	0
1	O	1915	0	1926	73	0
2	B	1904	0	1901	99	0
2	P	1904	0	1901	96	0
3	C	1890	0	1900	104	0
3	Q	1890	0	1900	94	0
4	D	1861	0	1836	63	0
4	R	1861	0	1836	63	0
5	E	1795	0	1797	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	S	1795	0	1797	69	0
6	F	1896	0	1886	68	0
6	T	1896	0	1886	79	0
7	G	1921	0	1910	77	0
7	U	1921	0	1910	75	0
8	H	1684	0	1687	52	0
8	V	1684	0	1687	47	0
9	I	1581	0	1574	40	0
9	W	1581	0	1574	41	0
10	J	1585	0	1590	87	0
10	X	1585	0	1590	89	0
11	K	1644	0	1594	77	0
11	Y	1644	0	1594	77	0
12	L	1757	0	1711	53	0
12	Z	1757	0	1711	56	0
13	O	1824	0	1832	57	0
13	M	1824	0	1832	58	0
14	1	1512	0	1480	51	0
14	N	1512	0	1480	51	0
15	1	35	0	37	3	0
15	H	35	0	37	3	0
15	K	35	0	37	2	0
15	N	35	0	37	3	0
15	V	35	0	37	3	0
15	Y	35	0	37	2	0
16	O	60	0	0	2	0
16	1	55	0	0	1	0
16	A	38	0	0	2	0
16	B	24	0	0	5	0
16	C	33	0	0	6	0
16	D	24	0	0	3	0
16	E	17	0	0	1	0
16	F	39	0	0	1	0
16	G	47	0	0	2	0
16	H	43	0	0	1	0
16	I	56	0	0	3	0
16	J	36	0	0	3	0
16	K	28	0	0	4	0
16	L	46	0	0	3	0
16	M	62	0	0	4	0
16	N	50	0	0	3	0
16	O	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	20	0	0	3	0
16	Q	21	0	0	4	0
16	R	19	0	0	3	0
16	S	16	0	0	1	0
16	T	30	0	0	4	0
16	U	50	0	0	3	0
16	V	41	0	0	4	0
16	W	37	0	0	1	0
16	X	33	0	0	3	0
16	Y	29	0	0	8	0
16	Z	38	0	0	2	0
All	All	50766	0	49470	1761	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 18.

All (1761) 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)
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.12	1.14
14:N:107:LYS:HG2	14:N:108:GLY:H	1.15	1.11
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.12	1.10
14:1:107:LYS:HG2	14:1:108:GLY:H	1.13	1.09
7:U:96:ALA:HA	7:U:107:MET:HE2	1.35	1.09
7:G:96:ALA:HA	7:G:107:MET:HE2	1.33	1.09
10:X:-1:MET:HG2	10:X:1:ASP:H	1.14	1.08
14:N:136:GLY:HA2	14:1:161:GLN:HE21	1.18	1.07
10:J:-1:MET:HG2	10:J:1:ASP:H	1.15	1.05
14:N:161:GLN:HE21	14:1:136:GLY:HA2	1.20	1.05
2:P:202:THR:HG22	2:P:204:SER:H	1.22	1.03
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.77	1.00
1:O:15:PHE:H	2:P:23:GLN:HE22	1.09	0.99
13:O:157:ASN:HD22	13:O:160:ARG:HH11	1.03	0.98
14:N:107:LYS:HG2	14:N:108:GLY:N	1.79	0.97
3:C:100:ARG:NH1	3:C:106:PRO:HB3	1.77	0.97
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.29	0.97
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.29	0.97
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.25	0.96
2:B:202:THR:HG22	2:B:204:SER:H	1.26	0.96
2:P:71:ASN:ND2	2:P:72:ASP:H	1.65	0.94
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:107:LYS:HG2	14:1:108:GLY:N	1.78	0.94
3:C:163:GLN:HE21	3:C:164:THR:H	0.97	0.94
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.33	0.93
2:B:15:PHE:H	3:C:23:GLN:HE22	1.12	0.93
2:B:71:ASN:ND2	2:B:72:ASP:H	1.66	0.93
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.31	0.93
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.51	0.93
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.50	0.93
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.00	0.92
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.13	0.91
14:N:20:THR:HG22	15:N:7710:SRG:H25B	1.52	0.91
5:S:15:PHE:H	6:T:23:GLN:HE22	1.14	0.91
14:1:20:THR:HG22	15:1:7710:SRG:H25B	1.51	0.91
3:C:15:PHE:H	4:D:23:GLN:HE22	1.16	0.90
5:E:207:LEU:HD23	5:E:207:LEU:H	1.35	0.90
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.51	0.90
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.35	0.90
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.54	0.90
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.55	0.89
1:A:15:PHE:H	2:B:23:GLN:HE22	1.15	0.89
5:S:207:LEU:HD23	5:S:207:LEU:H	1.36	0.89
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	1.85	0.89
3:Q:163:GLN:HE21	3:Q:164:THR:H	0.99	0.88
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.37	0.88
14:1:107:LYS:CG	14:1:108:GLY:H	1.87	0.87
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.20	0.87
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.54	0.87
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.37	0.87
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.56	0.87
3:C:185:THR:HB	3:C:188:GLU:HG2	1.57	0.87
12:L:123:GLN:HG3	12:L:145:TYR:OH	1.75	0.86
10:X:-1:MET:HG2	10:X:1:ASP:N	1.90	0.86
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	1.76	0.86
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.41	0.85
10:J:-1:MET:HG2	10:J:1:ASP:N	1.91	0.85
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.59	0.85
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.56	0.85
3:C:185:THR:HG22	3:C:187:GLU:H	1.41	0.85
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.39	0.84
2:P:185:LYS:HD3	2:P:186:VAL:N	1.93	0.84
5:E:15:PHE:H	6:F:23:GLN:HE22	1.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.58	0.84
2:B:185:LYS:HD3	2:B:186:VAL:N	1.93	0.84
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.42	0.83
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.22	0.83
5:E:18(D):ILE:O	5:E:18(D):ILE:HD13	1.79	0.83
14:N:136:GLY:HA2	14:1:161:GLN:NE2	1.94	0.83
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.22	0.83
3:Q:52:ARG:HH21	3:Q:211:GLU:HB3	1.40	0.83
13:M:149:GLN:NE2	13:M:149:GLN:H	1.77	0.82
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.85	0.82
14:N:107:LYS:CG	14:N:108:GLY:H	1.87	0.82
11:Y:143:LYS:O	11:Y:146:LEU:HD13	1.79	0.82
3:C:52:ARG:HH21	3:C:211:GLU:HB3	1.42	0.82
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.60	0.82
5:S:18(D):ILE:HD13	5:S:18(D):ILE:O	1.80	0.81
3:C:101:LEU:HD11	10:J:57:GLU:HB3	1.61	0.81
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.62	0.81
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.79	0.80
14:1:36:ARG:HG3	14:1:42:TRP:CE2	2.15	0.80
2:P:202:THR:HG22	2:P:204:SER:N	1.96	0.80
13:0:149:GLN:H	13:0:149:GLN:NE2	1.80	0.80
3:Q:101:LEU:HD11	10:X:57:GLU:HB3	1.64	0.80
14:N:161:GLN:NE2	14:1:136:GLY:HA2	1.96	0.80
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.45	0.80
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.82	0.80
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.62	0.80
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.93	0.80
5:E:227:GLU:CD	5:E:227:GLU:H	1.86	0.80
7:G:198:ILE:HG23	7:G:203:THR:O	1.82	0.79
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.81	0.79
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.62	0.79
2:B:202:THR:HG22	2:B:204:SER:N	1.98	0.79
11:K:99:THR:HG22	11:K:113:VAL:O	1.82	0.79
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.30	0.79
2:P:71:ASN:HD22	2:P:72:ASP:H	1.29	0.78
11:K:143:LYS:O	11:K:146:LEU:HD13	1.83	0.78
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.18	0.78
5:S:227:GLU:CD	5:S:227:GLU:H	1.86	0.77
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.97	0.77
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.15	0.77
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:20:THR:HG23	14:N:31:THR:OG1	1.85	0.77
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.85	0.77
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.14	0.76
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.15	0.76
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.81	0.76
7:U:198:ILE:HG23	7:U:203:THR:O	1.86	0.76
2:B:71:ASN:HD22	2:B:72:ASP:H	1.32	0.75
14:1:20:THR:HG23	14:1:31:THR:OG1	1.86	0.75
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.49	0.75
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.68	0.75
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.00	0.75
8:V:53:GLU:O	8:V:56:THR:HG22	1.87	0.74
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.99	0.74
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.69	0.74
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.35	0.74
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.69	0.74
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.03	0.74
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.68	0.74
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.87	0.74
8:H:52:THR:O	8:H:56:THR:HB	1.88	0.74
7:U:121:GLN:O	7:U:124:THR:HB	1.88	0.73
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.02	0.73
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.69	0.73
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.68	0.73
3:C:163:GLN:NE2	3:C:164:THR:H	1.81	0.73
3:C:185:THR:HG22	3:C:187:GLU:N	2.02	0.73
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.03	0.73
11:Y:99:THR:HG22	11:Y:113:VAL:O	1.89	0.73
2:B:181:LYS:O	2:B:184:MET:HG3	1.89	0.72
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.71	0.72
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.71	0.72
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.70	0.72
3:C:41:LYS:HG2	3:C:161:SER:O	1.89	0.72
13:O:157:ASN:HD22	13:O:160:ARG:NH1	1.83	0.72
11:Y:114:ASP:OD1	11:Y:116:ASP:HB2	1.90	0.72
4:D:52:LYS:HE3	4:D:211:GLN:HB2	1.72	0.72
6:F:35:THR:HG21	6:F:51:GLU:O	1.88	0.72
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.72	0.72
11:Y:10(B):LYS:N	11:Y:10(B):LYS:HD2	1.96	0.71
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.72	0.71
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.83	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:52:LYS:HE3	4:R:211:GLN:HB2	1.73	0.71
10:X:156:LYS:O	10:X:160:GLN:HG3	1.90	0.71
2:P:71:ASN:HD22	2:P:72:ASP:N	1.86	0.71
5:S:207:LEU:H	5:S:207:LEU:CD2	2.03	0.71
2:P:181:LYS:O	2:P:184:MET:HG3	1.89	0.71
7:G:121:GLN:O	7:G:124:THR:HB	1.90	0.71
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.83	0.71
5:S:132:TYR:O	5:S:153:PRO:HB3	1.91	0.71
1:O:159:PRO:O	2:P:59:LEU:HD12	1.91	0.71
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.92	0.70
5:E:132:TYR:O	5:E:153:PRO:HB3	1.91	0.70
8:V:52:THR:O	8:V:56:THR:HB	1.90	0.70
8:H:53:GLU:O	8:H:56:THR:HG22	1.91	0.70
2:P:121:GLN:O	2:P:124:THR:HB	1.91	0.70
10:J:156:LYS:O	10:J:160:GLN:HG3	1.92	0.70
3:Q:85:SER:O	3:Q:89:ILE:HD12	1.90	0.70
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.56	0.70
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.92	0.70
2:B:121:GLN:O	2:B:124:THR:HB	1.92	0.69
8:V:81:GLN:O	8:V:85:GLN:HG3	1.92	0.69
5:E:207:LEU:CD2	5:E:207:LEU:H	2.03	0.69
6:T:35:THR:HG21	6:T:51:GLU:O	1.92	0.69
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.23	0.69
2:P:71:ASN:ND2	2:P:72:ASP:N	2.40	0.69
2:B:71:ASN:HD22	2:B:72:ASP:N	1.89	0.69
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.57	0.69
14:N:106:ASN:O	14:N:107:LYS:HB3	1.90	0.69
1:O:57:PRO:HG3	7:U:177:GLU:CD	2.12	0.69
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.22	0.69
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.40	0.69
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.84	0.68
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.04	0.68
14:1:106:ASN:O	14:1:107:LYS:HB3	1.92	0.68
10:J:52:THR:HG22	10:J:53:VAL:N	2.07	0.68
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.76	0.68
3:C:85:SER:O	3:C:89:ILE:HD12	1.94	0.68
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.74	0.68
11:K:143:LYS:HB2	11:K:146:LEU:HD11	1.76	0.68
2:B:41:MET:HE1	3:C:62:ARG:HH21	1.57	0.68
8:H:165:ASN:HD22	13:O:139:ARG:HH11	1.40	0.68
8:V:34:LEU:HB2	16:V:7725:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.93	0.68
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.59	0.68
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	1.96	0.68
11:Y:143:LYS:HB2	11:Y:146:LEU:HD11	1.74	0.68
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	1.92	0.68
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.76	0.67
8:H:81:GLN:O	8:H:85:GLN:HG3	1.93	0.67
7:U:233:LEU:O	7:U:236:ILE:HG13	1.94	0.67
3:C:163:GLN:HE21	3:C:164:THR:N	1.82	0.67
7:G:233:LEU:O	7:G:236:ILE:HG13	1.93	0.67
13:O:41:THR:OG1	13:O:76:PRO:HG3	1.94	0.67
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.09	0.67
6:T:127:ASN:HD22	6:T:128:SER:N	1.93	0.67
6:F:192:GLN:O	6:F:196:ILE:HG12	1.94	0.67
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.92	0.67
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.30	0.67
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.77	0.67
4:D:72:ARG:HG3	16:D:268:HOH:O	1.94	0.67
10:X:52:THR:HG22	10:X:53:VAL:N	2.10	0.67
13:O:40:ASN:H	13:O:40:ASN:HD22	1.43	0.67
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.25	0.66
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.60	0.66
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.76	0.66
2:B:71:ASN:ND2	2:B:72:ASP:N	2.42	0.66
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	1.92	0.66
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.39	0.66
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.10	0.66
12:L:166:HIS:HD2	12:L:168:GLN:H	1.41	0.66
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.77	0.66
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.60	0.66
2:B:15:PHE:H	3:C:23:GLN:NE2	1.91	0.66
13:M:149:GLN:HE21	13:M:149:GLN:H	1.44	0.66
6:F:127:ASN:HD22	6:F:128:SER:N	1.93	0.66
13:O:157:ASN:ND2	13:O:160:ARG:HH11	1.86	0.66
6:F:109:ILE:HD12	6:F:109:ILE:N	2.11	0.66
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.62	0.65
1:A:7:ARG:HB2	2:B:5:SER:OG	1.96	0.65
2:B:15:PHE:N	3:C:23:GLN:HE22	1.91	0.65
13:M:40:ASN:H	13:M:40:ASN:HD22	1.43	0.65
14:1:112:THR:HG22	14:1:120:HIS:HB2	1.77	0.65
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:107:LYS:NZ	14:N:145:ASN:HD21	1.95	0.65
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.79	0.65
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.61	0.65
11:K:99:THR:HG22	11:K:113:VAL:HB	1.78	0.65
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.78	0.65
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.79	0.65
5:S:227:GLU:N	5:S:227:GLU:CD	2.50	0.65
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.27	0.65
6:T:109:ILE:HD12	6:T:109:ILE:N	2.11	0.64
10:J:133:TYR:CD1	16:Y:7726:HOH:O	2.50	0.64
11:K:114:ASP:OD1	11:K:116:ASP:HB2	1.96	0.64
7:U:96:ALA:HA	7:U:107:MET:CE	2.21	0.64
12:Z:134:ILE:HD11	12:Z:162:ALA:HB2	1.80	0.64
13:O:149:GLN:H	13:O:149:GLN:HE21	1.45	0.64
6:T:192:GLN:O	6:T:196:ILE:HG12	1.97	0.64
14:1:55:ILE:HD11	14:1:95:LEU:HD13	1.79	0.64
10:J:136:SER:HA	10:J:139:ASP:HB2	1.79	0.64
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.80	0.64
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.63	0.64
4:R:177:LEU:HA	5:S:58:LEU:HD11	1.79	0.64
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.79	0.64
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.80	0.64
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.33	0.64
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.80	0.64
4:R:185:THR:OG1	4:R:188:GLU:HG3	1.97	0.64
7:U:87:ASN:HD22	7:U:87:ASN:C	2.01	0.63
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.79	0.63
14:1:116:GLY:HA3	16:1:7713:HOH:O	1.98	0.63
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.81	0.63
5:E:227:GLU:CD	5:E:227:GLU:N	2.50	0.63
11:Y:135:TYR:CB	16:Y:7726:HOH:O	2.47	0.63
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.63	0.63
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.34	0.63
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.14	0.63
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.08	0.63
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.80	0.63
7:U:115:ARG:HH12	7:U:119:LEU:HD13	1.64	0.62
13:O:170:SER:HA	16:O:270:HOH:O	1.99	0.62
10:X:136:SER:HA	10:X:139:ASP:HB2	1.80	0.62
11:Y:99:THR:HG22	11:Y:113:VAL:HB	1.80	0.62
1:O:7:ARG:HB2	2:P:5:SER:OG	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:247:HOH:O	11:Y:210:ILE:HB	1.99	0.62
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.00	0.62
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.81	0.62
1:A:85:TYR:O	1:A:89:VAL:HG23	2.00	0.62
14:1:107:LYS:NZ	14:1:145:ASN:HD21	1.97	0.62
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.30	0.62
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.34	0.62
3:Q:55:THR:O	3:Q:56:LEU:HD22	1.99	0.62
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.00	0.62
6:T:237:GLN:O	6:T:240:ILE:HG22	2.00	0.62
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.81	0.62
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.00	0.62
7:G:96:ALA:HA	7:G:107:MET:CE	2.21	0.62
11:Y:104:TYR:CE2	11:Y:108:PRO:HG3	2.35	0.62
4:D:185:THR:OG1	4:D:188:GLU:HG3	1.99	0.62
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.30	0.62
12:L:134:ILE:HD11	12:L:162:ALA:HB2	1.80	0.62
3:C:55:THR:O	3:C:56:LEU:HD22	2.00	0.62
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.15	0.62
7:U:172:ILE:HD12	7:U:197:MET:CE	2.30	0.61
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.35	0.61
5:S:123:ASN:N	5:S:123:ASN:HD22	1.98	0.61
14:1:36:ARG:HG3	14:1:42:TRP:CZ2	2.35	0.61
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.35	0.61
10:X:178:VAL:HG22	10:X:184:ILE:HG12	1.82	0.61
11:K:6:PHE:HA	11:K:123:ASP:O	1.99	0.61
7:G:115:ARG:HH12	7:G:119:LEU:HD13	1.65	0.61
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.92	0.61
16:L:200:HOH:O	9:W:192:ARG:HG3	2.01	0.61
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.00	0.61
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.65	0.61
3:C:175:PHE:O	3:C:179:ASN:HB2	2.00	0.61
13:M:40:ASN:HD22	13:M:40:ASN:N	1.97	0.61
7:G:87:ASN:HD22	7:G:87:ASN:C	2.04	0.61
1:O:121:GLN:O	1:O:124:THR:HB	2.01	0.61
11:K:104:TYR:CE2	11:K:108:PRO:HG3	2.36	0.61
11:Y:6:PHE:HA	11:Y:123:ASP:O	1.99	0.61
1:A:177:GLU:HA	2:B:58:LEU:HD11	1.83	0.61
7:U:236:ILE:HD12	7:U:237:ALA:N	2.15	0.61
7:G:218:ASP:O	7:G:220:LYS:HB2	2.00	0.61
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:179:LEU:HD21	6:T:192:GLN:HG2	1.83	0.60
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.83	0.60
10:X:113:ILE:HA	10:X:118:THR:O	2.01	0.60
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.01	0.60
7:U:218:ASP:O	7:U:220:LYS:HB2	2.00	0.60
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.83	0.60
4:R:207:LEU:C	4:R:207:LEU:HD23	2.21	0.60
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.36	0.60
13:O:40:ASN:HD22	13:O:40:ASN:N	1.98	0.60
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.82	0.60
10:J:178:VAL:HG22	10:J:184:ILE:HG12	1.83	0.60
3:C:15:PHE:N	4:D:23:GLN:HE22	1.95	0.60
4:R:85:ALA:O	4:R:89:ILE:HG12	2.02	0.60
13:M:57:ARG:NE	16:M:246:HOH:O	2.34	0.60
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.30	0.60
13:O:76:PRO:HD2	13:O:105:GLN:OE1	2.02	0.60
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.82	0.60
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.50	0.60
10:J:52:THR:CG2	10:J:53:VAL:N	2.64	0.60
10:J:133:TYR:HE1	16:X:216:HOH:O	1.84	0.60
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.36	0.60
3:C:227:GLU:OE1	3:C:227:GLU:N	2.34	0.60
14:N:18(A):ILE:HD13	14:N:18(B):PHE:N	2.17	0.60
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.37	0.60
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.83	0.60
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.84	0.60
5:E:175:TYR:CD2	5:E:196:ALA:HA	2.37	0.60
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.82	0.60
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.02	0.59
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.67	0.59
13:O:-6:GLN:O	13:O:-6:GLN:HG3	2.01	0.59
8:V:84:LYS:HG3	8:V:85:GLN:N	2.17	0.59
14:N:105:ASP:OD2	14:N:106:ASN:HB2	2.02	0.59
5:E:2(B):THR:H	5:E:2(E):ASN:ND2	1.98	0.59
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.84	0.59
11:K:67:GLU:OE2	11:K:73:ARG:HA	2.02	0.59
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.37	0.59
4:D:207:LEU:HD23	4:D:207:LEU:C	2.23	0.59
11:Y:67:GLU:OE2	11:Y:73:ARG:HA	2.02	0.59
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.84	0.59
6:F:179:LEU:HD11	6:F:192:GLN:CG	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:147:SER:OG	14:N:150:GLU:HG3	2.03	0.59
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.38	0.59
7:G:172:ILE:HD12	7:G:197:MET:CE	2.31	0.59
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.01	0.59
7:G:236:ILE:HD12	7:G:237:ALA:N	2.17	0.59
10:X:48:GLU:HB2	10:X:96:GLN:HB2	1.84	0.59
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.85	0.59
4:D:12(F):GLY:HA3	16:D:271:HOH:O	2.02	0.59
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.85	0.59
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.68	0.59
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.38	0.59
5:S:207:LEU:HA	5:S:2(E):ASN:HD21	1.68	0.59
7:U:59:LEU:O	7:U:61:PRO:HD3	2.03	0.59
4:D:24:VAL:O	4:D:27:SER:HB3	2.03	0.59
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.67	0.59
3:Q:215:VAL:HG23	3:Q:221:ILE:HG12	1.85	0.59
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.84	0.58
6:T:203:GLU:O	6:T:206:LYS:HD2	2.03	0.58
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.84	0.58
4:D:85:ALA:O	4:D:89:ILE:HG12	2.03	0.58
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.02	0.58
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.85	0.58
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.85	0.58
10:X:48:GLU:CB	10:X:96:GLN:HB2	2.33	0.58
7:G:77:VAL:CG1	7:G:137:THR:HB	2.33	0.58
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.85	0.58
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.03	0.58
5:E:123:ASN:HD22	5:E:123:ASN:N	1.98	0.58
14:1:147:SER:OG	14:1:150:GLU:HG3	2.03	0.58
3:Q:15:PHE:H	4:R:23:GLN:NE2	1.94	0.58
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.04	0.58
4:R:40:ILE:CD1	4:R:193:VAL:HG23	2.33	0.58
12:Z:-6:PRO:O	13:0:91:ARG:NH1	2.35	0.58
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.33	0.58
6:F:237:GLN:O	6:F:240:ILE:HG22	2.03	0.58
10:J:113:ILE:HA	10:J:118:THR:O	2.03	0.58
10:X:44:SER:OG	10:X:100:LEU:HB2	2.03	0.58
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.86	0.58
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.84	0.58
4:D:177:LEU:HA	5:E:58:LEU:HD11	1.86	0.58
10:J:143:ARG:HB2	10:J:146:MET:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:VAL:HG11	2:B:216:ARG:HD3	1.85	0.58
10:X:190:PHE:C	10:X:192:ALA:H	2.06	0.58
2:P:224:PHE:N	2:P:224:PHE:CD2	2.72	0.58
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.04	0.58
2:P:186:VAL:HG21	2:P:216:ARG:HG2	1.85	0.58
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.38	0.58
6:F:109:ILE:H	6:F:109:ILE:HD12	1.69	0.58
6:T:69:VAL:HG12	16:T:301:HOH:O	2.02	0.58
3:C:235:GLN:O	3:C:239:GLU:HG2	2.04	0.58
14:1:18(A):ILE:HD13	14:1:18(B):PHE:N	2.19	0.58
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.39	0.58
6:F:203:GLU:O	6:F:206:LYS:HD2	2.04	0.58
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.86	0.58
4:D:205:GLU:HA	4:D:205:GLU:OE2	2.04	0.58
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.86	0.58
5:E:207:LEU:HA	5:E:2(E):ASN:HD21	1.69	0.58
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.03	0.58
2:B:224:PHE:HD2	2:B:224:PHE:N	2.02	0.58
9:I:48:LEU:HG	9:I:50:THR:HG22	1.86	0.58
14:1:163:ILE:HG23	14:1:170:GLY:HA2	1.85	0.58
10:X:52:THR:CG2	10:X:53:VAL:N	2.67	0.57
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.52	0.57
14:1:176:VAL:HG12	14:1:178:LEU:HD13	1.85	0.57
14:1:105:ASP:OD2	14:1:106:ASN:HB2	2.04	0.57
2:P:186:VAL:HG11	2:P:216:ARG:HD3	1.86	0.57
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.16	0.57
7:G:77:VAL:HG12	7:G:137:THR:HB	1.86	0.57
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.86	0.57
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.85	0.57
10:J:19:ALA:HB2	10:J:171:LYS:HG2	1.86	0.57
6:F:20(B):GLU:HG3	6:F:20(C):LYS:H	1.70	0.57
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.86	0.57
11:K:99:THR:CG2	11:K:113:VAL:HB	2.34	0.57
2:P:224:PHE:N	2:P:224:PHE:HD2	2.02	0.57
13:O:110:LEU:HG	13:O:125:LEU:HD12	1.87	0.57
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.85	0.57
13:M:-6:GLN:O	13:M:-6:GLN:HG3	2.03	0.57
2:P:185:LYS:O	2:P:188:ASP:HB2	2.03	0.57
11:Y:135:TYR:HB2	16:Y:7726:HOH:O	2.04	0.57
3:C:227:GLU:CD	3:C:227:GLU:H	2.07	0.57
2:B:224:PHE:CD2	2:B:224:PHE:N	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:17:ASP:HA	13:M:173:PHE:CB	2.34	0.57
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.04	0.57
4:R:121:LEU:HA	4:R:123:PHE:CE1	2.39	0.57
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.68	0.57
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.86	0.57
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.86	0.57
11:K:67:GLU:CD	11:K:73:ARG:HA	2.25	0.57
7:G:136:LEU:O	7:G:150:LYS:HA	2.04	0.57
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.35	0.57
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.04	0.57
5:S:2(B):THR:H	5:S:2(E):ASN:ND2	1.98	0.57
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.35	0.57
10:J:190:PHE:C	10:J:192:ALA:H	2.06	0.57
7:U:136:LEU:O	7:U:150:LYS:HA	2.04	0.57
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.86	0.57
4:R:205:GLU:OE2	4:R:205:GLU:HA	2.04	0.57
7:G:96:ALA:CA	7:G:107:MET:HE2	2.21	0.57
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.87	0.57
13:M:147:THR:HG23	16:M:262:HOH:O	2.04	0.57
14:N:92:ASP:HB2	16:N:7722:HOH:O	2.05	0.57
2:B:185:LYS:O	2:B:188:ASP:HB2	2.04	0.57
6:T:179:LEU:HD21	6:T:192:GLN:CG	2.34	0.57
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.69	0.57
9:I:2:ILE:HD13	9:I:2:ILE:H	1.70	0.57
2:B:41:MET:HE1	3:C:62:ARG:NH2	2.20	0.57
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.86	0.57
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.86	0.57
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.86	0.56
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.05	0.56
9:W:48:LEU:HG	9:W:50:THR:HG22	1.86	0.56
11:K:191:ASP:OD2	11:K:193:GLY:N	2.37	0.56
1:O:60:MET:HE1	16:U:255:HOH:O	2.04	0.56
4:R:140:GLY:HA2	4:R:215:ILE:HG12	1.87	0.56
7:U:77:VAL:CG1	7:U:137:THR:HB	2.35	0.56
10:X:19:ALA:HB2	10:X:171:LYS:HG2	1.86	0.56
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.86	0.56
5:S:175:TYR:CD2	5:S:196:ALA:HA	2.40	0.56
9:I:6:MET:HE1	9:I:155:ILE:HA	1.86	0.56
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.87	0.56
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.88	0.56
2:B:17:PRO:HA	3:C:26:TYR:CE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:135:TYR:HB3	16:Y:7726:HOH:O	2.05	0.56
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.70	0.56
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.05	0.56
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.87	0.56
7:G:59:LEU:O	7:G:61:PRO:HD3	2.05	0.56
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.35	0.56
10:J:48:GLU:CB	10:J:96:GLN:HB2	2.35	0.56
2:B:87:ILE:O	2:B:91:THR:HG23	2.06	0.56
4:D:194:LEU:HD21	4:D:233:ILE:HD12	1.87	0.56
5:E:226:GLY:O	5:E:229:VAL:HG22	2.05	0.56
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.85	0.56
6:F:179:LEU:HD21	6:F:192:GLN:HG2	1.87	0.56
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.05	0.56
6:T:20(B):GLU:HG3	6:T:20(C):LYS:H	1.71	0.56
16:R:831:HOH:O	12:Z:85:HIS:HD2	1.89	0.56
3:C:186:VAL:O	3:C:190:VAL:HG23	2.06	0.56
13:O:39:ASP:HA	13:O:184:LEU:HD12	1.87	0.56
11:Y:78:ALA:O	11:Y:82:ILE:HG12	2.06	0.56
8:V:139:GLU:OE2	8:V:139:GLU:HA	2.06	0.56
6:F:95:GLU:HG3	6:F:115:ARG:NH1	2.14	0.56
1:A:121:GLN:O	1:A:124:THR:HB	2.06	0.56
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.41	0.56
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.41	0.56
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.88	0.56
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.71	0.56
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.21	0.56
10:J:2:ILE:HD12	10:J:162:LEU:HD13	1.88	0.56
2:P:87:ILE:O	2:P:91:THR:HG23	2.06	0.56
9:W:2:ILE:H	9:W:2:ILE:HD13	1.70	0.56
12:Z:21:ILE:C	12:Z:21:ILE:HD12	2.27	0.56
7:U:228:ASN:HB3	16:U:242:HOH:O	2.05	0.56
9:W:101:VAL:O	9:W:110:ILE:HA	2.06	0.56
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.41	0.56
9:W:6:MET:HE3	9:W:155:ILE:CG1	2.32	0.55
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.41	0.55
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.36	0.55
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.71	0.55
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.87	0.55
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.88	0.55
2:P:121:GLN:HG2	3:Q:83:ALA:HB1	1.87	0.55
11:Y:191:ASP:OD2	11:Y:193:GLY:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:179:LEU:HD21	6:F:192:GLN:CG	2.36	0.55
10:J:44:SER:OG	10:J:100:LEU:HB2	2.07	0.55
11:Y:50:ALA:CB	12:Z:116:VAL:HG23	2.35	0.55
10:X:143:ARG:HB2	10:X:146:MET:HG3	1.88	0.55
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.71	0.55
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.07	0.55
14:1:175:MET:HB2	14:1:187:LEU:HB2	1.87	0.55
10:J:-1:MET:CG	10:J:1:ASP:H	2.03	0.55
2:B:186:VAL:HG21	2:B:216:ARG:HG2	1.87	0.55
1:O:69:LEU:HD23	1:O:69:LEU:C	2.27	0.55
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.07	0.55
5:S:15:PHE:H	6:T:23:GLN:NE2	1.95	0.55
11:Y:67:GLU:CD	11:Y:73:ARG:HA	2.26	0.55
4:D:121:LEU:HA	4:D:123:PHE:CE1	2.41	0.55
13:0:17:ASP:HA	13:0:173:PHE:CB	2.36	0.55
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.09	0.55
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.88	0.55
8:H:84:LYS:HG3	8:H:85:GLN:N	2.20	0.55
10:J:2:ILE:O	10:J:3:ILE:HD12	2.07	0.55
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.89	0.55
12:L:21:ILE:HD12	12:L:21:ILE:C	2.27	0.55
13:0:14(C):ARG:HH11	13:0:14(C):ARG:HG3	1.70	0.55
2:B:185:LYS:HD3	2:B:186:VAL:H	1.72	0.55
4:R:24:VAL:O	4:R:27:SER:HB3	2.07	0.55
12:L:79:ALA:O	12:L:83:ILE:HG12	2.07	0.55
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.89	0.55
5:S:15:PHE:N	6:T:23:GLN:HE22	1.96	0.55
7:U:77:VAL:HG12	7:U:137:THR:HB	1.87	0.55
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.36	0.55
13:M:39:ASP:HA	13:M:184:LEU:HD12	1.89	0.55
3:C:224:LEU:N	3:C:224:LEU:HD12	2.21	0.55
10:J:52:THR:HG22	10:J:53:VAL:H	1.70	0.55
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.37	0.54
11:K:195:LEU:O	11:K:199:VAL:HG23	2.07	0.54
4:D:97:VAL:HG11	11:K:65:LEU:HD22	1.89	0.54
1:A:5:THR:O	1:A:7:ARG:HG2	2.07	0.54
5:S:221:PHE:HE1	5:S:223:ILE:HD11	1.72	0.54
5:S:226:GLY:O	5:S:229:VAL:HG22	2.07	0.54
4:D:170:GLU:N	4:D:170:GLU:OE1	2.40	0.54
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.72	0.54
3:C:173:ARG:O	3:C:177:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:184:LEU:CD1	6:T:188:GLU:HB3	2.34	0.54
6:F:109:ILE:CD1	6:F:109:ILE:H	2.19	0.54
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.55	0.54
5:E:4:PHE:CG	5:E:5:ARG:N	2.75	0.54
5:S:4:PHE:CG	5:S:5:ARG:N	2.75	0.54
9:I:2:ILE:HD12	9:I:169:SER:HB3	1.88	0.54
14:N:89:GLU:HG3	16:N:7754:HOH:O	2.08	0.54
16:T:291:HOH:O	7:U:130:ARG:HB2	2.06	0.54
3:Q:224:LEU:N	3:Q:224:LEU:HD12	2.22	0.54
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.06	0.54
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.54	0.54
10:J:48:GLU:HB2	10:J:96:GLN:HB2	1.88	0.54
1:O:85:TYR:O	1:O:89:VAL:HG23	2.06	0.54
10:X:2:ILE:HD12	10:X:162:LEU:HD13	1.89	0.54
6:T:173:LYS:O	6:T:177:GLU:HG3	2.07	0.54
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.36	0.54
12:Z:109:ALA:HA	16:Z:205:HOH:O	2.07	0.54
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.73	0.54
6:T:95:GLU:HG3	6:T:115:ARG:NH1	2.12	0.54
1:A:177:GLU:HG2	2:B:58:LEU:HD13	1.90	0.54
11:K:50:ALA:CB	12:L:116:VAL:HG23	2.37	0.54
8:V:175:VAL:HG12	8:V:176:CYS:N	2.23	0.54
4:R:91:HIS:CG	4:R:119:LEU:HD11	2.43	0.54
1:A:69:LEU:HD23	1:A:69:LEU:C	2.27	0.54
7:U:96:ALA:CA	7:U:107:MET:HE2	2.23	0.54
6:T:109:ILE:CD1	6:T:109:ILE:H	2.20	0.54
14:1:84:LYS:HG3	14:1:119:VAL:HG22	1.89	0.54
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.88	0.54
4:D:91:HIS:CG	4:D:119:LEU:HD11	2.43	0.54
14:1:13:ILE:HD12	14:1:151:THR:CG2	2.38	0.54
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	1.90	0.54
6:F:184:LEU:CD1	6:F:188:GLU:HB3	2.36	0.54
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.23	0.54
2:B:21(C):ASP:OD2	2:B:219:GLU:HB3	2.07	0.54
9:I:101:VAL:O	9:I:110:ILE:HA	2.08	0.54
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.38	0.54
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.90	0.54
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.08	0.54
7:U:115:ARG:NH1	7:U:119:LEU:HD13	2.22	0.54
5:E:221:PHE:HE1	5:E:223:ILE:HD11	1.72	0.54
2:P:21(C):ASP:OD2	2:P:219:GLU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.90	0.54
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.89	0.54
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.90	0.54
1:A:67:VAL:HB	1:A:223:LYS:HZ2	1.73	0.54
4:D:227:GLU:H	4:D:227:GLU:CD	2.11	0.54
5:S:199:GLN:HE21	5:S:199:GLN:N	2.06	0.53
10:X:-1:MET:CG	10:X:1:ASP:H	2.02	0.53
5:E:28:LEU:HD12	5:E:153:PRO:HD2	1.91	0.53
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.37	0.53
10:X:2:ILE:O	10:X:3:ILE:HD12	2.08	0.53
6:F:28:VAL:O	6:F:32:GLU:HG3	2.08	0.53
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.37	0.53
4:R:227:GLU:H	4:R:227:GLU:CD	2.11	0.53
11:K:10(A):ARG:NH1	11:K:10(A):ARG:HG2	2.24	0.53
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.43	0.53
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.38	0.53
7:U:225:SER:O	7:U:229:ILE:HG12	2.08	0.53
1:O:5:THR:O	1:O:7:ARG:HG2	2.08	0.53
7:G:197:MET:HG2	7:G:205:PHE:CE1	2.43	0.53
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.07	0.53
11:K:207:ASN:ND2	10:X:144:PRO:HD3	2.23	0.53
5:S:123:ASN:ND2	5:S:123:ASN:N	2.56	0.53
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.24	0.53
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.90	0.53
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.56	0.53
1:O:4:MET:O	1:O:5:THR:O	2.27	0.53
3:Q:208:LYS:O	3:Q:208:LYS:HD2	2.08	0.53
4:R:97:VAL:HG11	11:Y:65:LEU:HD22	1.91	0.53
12:L:93:PHE:N	12:L:94:PRO:HD3	2.22	0.53
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.90	0.53
7:G:115:ARG:NH1	7:G:119:LEU:HD13	2.24	0.53
7:G:225:SER:O	7:G:229:ILE:HG12	2.09	0.53
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	2.09	0.53
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.91	0.53
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.90	0.53
1:A:51:GLU:OE1	1:A:202:VAL:HG22	2.09	0.53
5:E:199:GLN:HE21	5:E:199:GLN:N	2.06	0.53
14:N:46:SER:HA	15:N:7710:SRG:H24A	1.91	0.53
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.09	0.53
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.09	0.53
1:A:188:ASP:O	1:A:192:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.91	0.53
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.91	0.53
6:F:173:LYS:O	6:F:177:GLU:HG3	2.09	0.53
2:P:202:THR:CG2	2:P:204:SER:H	2.10	0.53
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.39	0.53
9:W:2:ILE:HD12	9:W:169:SER:HB3	1.90	0.53
10:X:52:THR:HG22	10:X:53:VAL:H	1.73	0.53
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.24	0.53
12:L:-2:ASN:HA	12:L:21:ILE:O	2.08	0.53
12:L:153:LYS:HG2	8:V:201:GLN:HG3	1.90	0.53
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.91	0.53
6:T:172:ALA:O	6:T:176:LEU:HD23	2.09	0.53
11:Y:99:THR:CG2	11:Y:113:VAL:HB	2.39	0.52
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.08	0.52
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.24	0.52
12:Z:79:ALA:O	12:Z:83:ILE:HG12	2.09	0.52
11:K:78:ALA:O	11:K:82:ILE:HG12	2.09	0.52
13:O:179:ASP:HB3	13:O:18(A):THR:OG1	2.09	0.52
11:K:142:TYR:O	11:K:143:LYS:HD2	2.09	0.52
2:P:122:GLY:C	2:P:124:THR:H	2.13	0.52
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.20	0.52
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.90	0.52
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.44	0.52
1:A:13:THR:O	2:B:130:ARG:HD3	2.10	0.52
6:T:136:THR:O	6:T:150:MET:HA	2.09	0.52
5:E:18(C):PHE:HA	5:E:18(F):ILE:CD1	2.40	0.52
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.90	0.52
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.09	0.52
5:S:220:PRO:O	5:S:222:THR:HG23	2.09	0.52
11:K:86:LEU:HD13	11:K:86:LEU:C	2.30	0.52
12:L:5:GLY:O	12:L:124:CYS:HA	2.10	0.52
1:A:212:LEU:HD22	1:A:224:LEU:HD12	1.90	0.52
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.40	0.52
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.40	0.52
12:L:192:LYS:HE3	8:V:195:ASN:HB3	1.92	0.52
13:M:46:SER:OG	13:M:98:ALA:HB3	2.10	0.52
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.92	0.52
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.43	0.52
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.74	0.52
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.23	0.52
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:104:TYR:CD1	11:Y:180:GLU:HG3	2.45	0.52
14:N:67:THR:HA	14:N:72:GLY:O	2.10	0.52
7:U:8:TYR:C	7:U:10:ARG:H	2.13	0.52
11:Y:200:LYS:HG2	16:Y:7731:HOH:O	2.09	0.52
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:N	2.64	0.52
11:K:207:ASN:ND2	10:X:144:PRO:HG3	2.10	0.52
9:W:6:MET:CE	9:W:155:ILE:HA	2.39	0.52
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.40	0.52
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.34	0.52
13:M:139:ARG:NH1	8:V:165:ASN:HD22	2.07	0.52
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.25	0.52
5:S:18(C):PHE:HA	5:S:18(F):ILE:CD1	2.39	0.52
2:B:186:VAL:HG11	2:B:216:ARG:CD	2.39	0.52
2:P:181:LYS:HE2	2:P:183:ASP:OD1	2.10	0.52
4:R:194:LEU:HD21	4:R:233:ILE:HD12	1.90	0.52
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.92	0.52
10:X:77:GLN:C	10:X:77:GLN:NE2	2.63	0.52
8:H:165:ASN:HD22	13:0:139:ARG:NH1	2.07	0.52
6:T:127:ASN:HD22	6:T:127:ASN:C	2.13	0.52
6:T:109:ILE:H	6:T:109:ILE:HD12	1.72	0.52
11:K:200:LYS:HE2	16:K:7731:HOH:O	2.10	0.52
10:X:112:GLN:NE2	16:X:211:HOH:O	2.43	0.52
6:T:186:ALA:O	6:T:190:VAL:HG23	2.10	0.52
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.92	0.52
5:E:123:ASN:ND2	5:E:123:ASN:N	2.58	0.52
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.40	0.52
10:J:189:ASP:O	10:J:193:GLN:HB2	2.09	0.52
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.92	0.52
8:H:175:VAL:HG12	8:H:176:CYS:N	2.24	0.52
7:G:191:GLU:HG3	7:G:232:ARG:HG3	1.90	0.52
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.93	0.52
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.40	0.52
2:P:235:LYS:N	2:P:235:LYS:HD3	2.25	0.52
2:B:202:THR:CG2	2:B:204:SER:H	2.12	0.52
14:1:46:SER:HA	15:1:7710:SRG:H24A	1.93	0.52
6:T:109:ILE:CD1	6:T:109:ILE:N	2.73	0.52
1:O:188:ASP:O	1:O:192:ILE:HG12	2.10	0.52
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.75	0.52
7:U:10:ARG:HG2	7:U:22:TYR:CD2	2.44	0.52
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	1.92	0.52
13:0:14(D):GLU:O	13:0:14(G):ILE:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:227:GLN:OE1	2:P:230:LYS:HD3	2.10	0.52
15:Y:7710:SRG:HN17	15:Y:7710:SRG:H13B	1.75	0.52
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.75	0.52
2:P:186:VAL:HG11	2:P:216:ARG:CD	2.40	0.51
10:X:189:ASP:O	10:X:193:GLN:HB2	2.10	0.51
2:P:41:MET:HE3	16:Q:257:HOH:O	2.09	0.51
1:O:27:ALA:O	1:O:31:VAL:HG23	2.10	0.51
13:O:104:VAL:HG23	13:O:178:ILE:HG22	1.91	0.51
2:B:146:TYR:OH	2:B:21(A):LYS:HB2	2.10	0.51
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.91	0.51
8:H:139:GLU:OE2	8:H:139:GLU:HA	2.09	0.51
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.08	0.51
6:F:127:ASN:HD22	6:F:127:ASN:C	2.13	0.51
7:U:87:ASN:ND2	7:U:87:ASN:C	2.63	0.51
1:A:67:VAL:HB	1:A:223:LYS:NZ	2.26	0.51
11:K:152:LEU:HD11	11:K:187:HIS:CE1	2.45	0.51
13:M:49:ILE:O	13:M:53:GLN:HG3	2.10	0.51
7:G:74:ILE:HD12	7:G:109:CYS:HA	1.92	0.51
13:O:46:SER:OG	13:O:98:ALA:HB3	2.10	0.51
2:P:223:ILE:HD12	2:P:223:ILE:N	2.25	0.51
6:F:95:GLU:CG	6:F:115:ARG:HD2	2.41	0.51
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.10	0.51
4:D:112:LEU:C	4:D:112:LEU:HD13	2.31	0.51
9:I:6:MET:CE	9:I:155:ILE:HA	2.40	0.51
3:Q:57:LYS:HG2	3:Q:208:LYS:NZ	2.25	0.51
12:Z:-8:PHE:HB2	13:O:-8:THR:HG23	1.93	0.51
8:V:46:ALA:HA	15:V:7710:SRG:H24A	1.93	0.51
1:O:51:GLU:OE1	1:O:202:VAL:HG22	2.10	0.51
11:Y:152:LEU:HD11	11:Y:187:HIS:CE1	2.46	0.51
14:N:25:TYR:HD1	13:O:129:PHE:HZ	1.58	0.51
5:S:160:LEU:CD2	6:T:59:LEU:HD12	2.40	0.51
2:P:229:ILE:O	2:P:233:LEU:HB2	2.10	0.51
5:S:198:SER:HA	5:S:201:LEU:HG	1.93	0.51
8:H:53:GLU:O	8:H:57:GLN:HG3	2.11	0.51
9:W:2:ILE:HD13	9:W:2:ILE:N	2.25	0.51
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.46	0.51
4:R:29:GLU:OE2	4:R:32:LYS:HD2	2.10	0.51
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.11	0.51
5:E:220:PRO:O	5:E:222:THR:HG23	2.10	0.51
13:M:129:PHE:HZ	14:1:25:TYR:HD1	1.57	0.51
7:G:172:ILE:HD12	7:G:197:MET:HE1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.40	0.51
10:J:3:ILE:HG22	10:J:3:ILE:O	2.11	0.51
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.92	0.51
7:U:191:GLU:HG3	7:U:232:ARG:HG3	1.92	0.51
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.92	0.51
10:J:88:ALA:O	10:J:90(A):ILE:HG22	2.10	0.51
2:P:146:TYR:OH	2:P:21(A):LYS:HB2	2.11	0.51
8:H:201:GLN:HG3	12:Z:153:LYS:HG2	1.92	0.51
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.93	0.51
4:R:170:GLU:OE1	4:R:170:GLU:N	2.43	0.51
5:E:207:LEU:HD23	5:E:207:LEU:N	2.15	0.51
1:A:4:MET:O	1:A:5:THR:O	2.28	0.51
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.78	0.51
8:V:196:VAL:HG23	16:V:7729:HOH:O	2.11	0.51
14:1:104:TYR:OH	14:1:180:ALA:HB2	2.11	0.51
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.91	0.51
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.92	0.51
4:R:108:ASN:HB3	16:R:828:HOH:O	2.10	0.51
2:B:223:ILE:N	2:B:223:ILE:HD12	2.26	0.51
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.92	0.51
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.93	0.51
1:A:21(A):GLU:OE2	1:A:21(P):LYS:HB2	2.11	0.51
6:T:28:VAL:O	6:T:32:GLU:HG3	2.11	0.51
2:P:150:THR:O	2:P:157:TYR:HA	2.11	0.51
7:U:172:ILE:HD12	7:U:197:MET:HE1	1.92	0.51
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.75	0.51
4:D:97:VAL:HG11	11:K:65:LEU:CD2	2.41	0.51
7:G:74:ILE:HG21	7:G:112:LEU:HD23	1.93	0.51
11:K:156:LYS:HB2	11:K:175:LEU:HD11	1.92	0.51
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.41	0.51
15:K:7710:SRG:H13B	15:K:7710:SRG:HN17	1.75	0.51
14:1:20:THR:HG22	15:1:7710:SRG:C25	2.34	0.50
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.40	0.50
12:L:113:PHE:CD1	12:L:113:PHE:N	2.79	0.50
10:J:112:GLN:NE2	10:J:126:ALA:H	2.09	0.50
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.11	0.50
10:J:77:GLN:NE2	10:J:77:GLN:C	2.64	0.50
7:U:172:ILE:HD11	7:U:201:LEU:HD21	1.93	0.50
2:P:234:VAL:HA	2:P:239:THR:HA	1.92	0.50
13:O:113:VAL:HA	13:O:118:VAL:O	2.11	0.50
2:B:234:VAL:HA	2:B:239:THR:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:67:VAL:HB	1:O:223:LYS:NZ	2.25	0.50
7:U:74:ILE:HG21	7:U:112:LEU:HD23	1.93	0.50
2:B:235:LYS:HD3	2:B:235:LYS:N	2.25	0.50
5:E:198:SER:HA	5:E:201:LEU:HG	1.93	0.50
5:S:207:LEU:N	5:S:207:LEU:HD23	2.16	0.50
11:Y:142:TYR:O	11:Y:143:LYS:HD2	2.12	0.50
12:Z:4:LEU:HD12	12:Z:5:GLY:H	1.75	0.50
6:T:109:ILE:HD13	6:T:142:ASP:HB3	1.93	0.50
10:J:133:TYR:HD1	16:Y:7726:HOH:O	1.87	0.50
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.27	0.50
3:C:208:LYS:HD2	3:C:208:LYS:O	2.11	0.50
7:G:8:TYR:C	7:G:10:ARG:H	2.14	0.50
3:C:232:TYR:O	3:C:236:ILE:HG13	2.12	0.50
9:I:105:ASN:HB3	9:I:10(C):SER:OG	2.10	0.50
10:X:88:ALA:O	10:X:90(A):ILE:HG22	2.11	0.50
2:B:41:MET:HE3	16:B:253:HOH:O	2.11	0.50
2:B:227:GLN:OE1	2:B:230:LYS:HD3	2.12	0.50
14:1:48:SER:HB3	14:1:51:ASP:HB2	1.92	0.50
3:C:35:THR:HB	3:C:51:GLU:HG3	1.93	0.50
12:L:4:LEU:HD12	12:L:5:GLY:H	1.76	0.50
12:L:4:LEU:HD12	12:L:5:GLY:N	2.26	0.50
9:I:2:ILE:N	9:I:2:ILE:HD13	2.26	0.50
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.41	0.50
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.94	0.50
6:F:186:ALA:O	6:F:190:VAL:HG23	2.11	0.50
2:B:150:THR:O	2:B:157:TYR:HA	2.11	0.50
1:A:27:ALA:O	1:A:31:VAL:HG23	2.11	0.50
3:C:57:LYS:HG2	3:C:208:LYS:NZ	2.26	0.50
11:K:44:THR:OG1	11:K:100:MET:HB2	2.11	0.50
2:B:229:ILE:O	2:B:233:LEU:HB2	2.11	0.50
8:V:43:CYS:SG	8:V:99:LEU:HB3	2.51	0.50
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.47	0.50
2:P:185:LYS:HD3	2:P:186:VAL:H	1.73	0.50
12:Z:4:LEU:HD12	12:Z:5:GLY:N	2.26	0.50
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.41	0.50
6:F:109:ILE:CD1	6:F:109:ILE:N	2.74	0.50
11:K:104:TYR:CD1	11:K:180:GLU:HG3	2.47	0.50
5:S:5:ARG:HG3	5:S:22:PHE:CZ	2.46	0.50
4:D:91:HIS:CE1	4:D:119:LEU:HD21	2.47	0.50
7:U:74:ILE:HD12	7:U:109:CYS:HA	1.92	0.50
2:B:160:TRP:HA	3:C:59:GLN:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:236:GLU:O	4:R:240:LYS:HG3	2.11	0.50
1:A:142:ASP:OD1	1:A:145:ASN:HB2	2.11	0.50
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.92	0.50
10:J:144:PRO:HD3	11:Y:207:ASN:ND2	2.27	0.50
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.26	0.50
4:R:233:ILE:HG22	4:R:235:LYS:N	2.27	0.50
14:N:30:VAL:HG11	13:0:199:PHE:CE2	2.46	0.50
4:R:91:HIS:CE1	4:R:119:LEU:HD21	2.47	0.49
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.95	0.49
13:0:1:THR:OG1	13:0:2:SER:N	2.44	0.49
4:R:112:LEU:C	4:R:112:LEU:HD13	2.32	0.49
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.12	0.49
7:U:47:VAL:HG12	7:U:49:ILE:CD1	2.41	0.49
1:A:67:VAL:CG2	1:A:211:GLU:HG2	2.42	0.49
8:V:172:ASN:ND2	8:V:193:THR:HA	2.27	0.49
14:N:20:THR:HG22	15:N:7710:SRG:C25	2.34	0.49
12:Z:-8:PHE:CB	13:0:-8:THR:HG23	2.42	0.49
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.94	0.49
1:A:150:GLN:O	1:A:157:TYR:HA	2.12	0.49
16:T:284:HOH:O	7:U:86:ARG:HD2	2.11	0.49
3:Q:242:GLU:O	3:Q:243:GLN:HB2	2.12	0.49
6:F:136:THR:O	6:F:150:MET:HA	2.12	0.49
6:F:203:GLU:C	6:F:205:ASN:H	2.16	0.49
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.28	0.49
10:J:32:ASP:HA	16:J:204:HOH:O	2.13	0.49
6:T:11:SER:HB3	6:T:14:VAL:HG23	1.95	0.49
5:S:73:HIS:HE1	5:S:107:LEU:O	1.93	0.49
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.09	0.49
7:U:197:MET:HG2	7:U:205:PHE:CE1	2.47	0.49
12:Z:14(E):GLU:HB2	12:Z:14(I):THR:HG21	1.95	0.49
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.12	0.49
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.93	0.49
14:1:156:LYS:HG2	14:1:18(J):LEU:HD11	1.93	0.49
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.11	0.49
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.93	0.49
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.13	0.49
2:P:115:ARG:NH1	2:P:115:ARG:HG3	2.28	0.49
11:K:180:GLU:N	16:K:7728:HOH:O	2.40	0.49
1:O:67:VAL:CG2	1:O:211:GLU:HG2	2.42	0.49
4:R:175:GLU:OE2	4:R:199:GLN:NE2	2.42	0.49
2:B:90:ASN:HB2	16:B:272:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:236:GLU:O	4:D:240:LYS:HG3	2.12	0.49
2:P:163:ILE:HG13	2:P:164:SER:N	2.28	0.49
14:1:161:GLN:NE2	14:1:165:TRP:HE1	2.11	0.49
14:N:13:ILE:HD12	14:N:151:THR:HG22	1.94	0.49
7:U:187:GLU:O	7:U:232:ARG:HD3	2.13	0.49
1:O:142:ASP:OD1	1:O:145:ASN:HB2	2.12	0.49
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.95	0.49
9:W:105:ASN:O	9:W:106:GLY:N	2.43	0.49
7:G:87:ASN:ND2	7:G:87:ASN:C	2.66	0.49
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.47	0.49
2:B:11:ARG:HD2	3:C:10:ARG:NH1	2.27	0.49
10:J:90(A):ILE:CD1	10:J:116:LEU:HD23	2.43	0.49
1:O:67:VAL:HB	1:O:223:LYS:HZ2	1.77	0.49
3:C:197:LEU:O	3:C:201:VAL:HG23	2.13	0.49
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.48	0.49
1:A:190:ILE:O	1:A:193:ALA:HB3	2.13	0.49
13:M:113:VAL:HA	13:M:118:VAL:O	2.12	0.49
7:U:186:TRP:O	7:U:190:VAL:HG23	2.13	0.49
11:K:10(A):ARG:HB3	11:K:10(B):LYS:HE3	1.95	0.49
11:K:7:ARG:HH11	11:K:108:PRO:HB2	1.78	0.49
4:R:123:PHE:HB3	4:R:128:MET:HE2	1.95	0.49
10:J:162:LEU:O	10:J:166:MET:HB2	2.13	0.49
5:E:5:ARG:HG3	5:E:22:PHE:CZ	2.48	0.49
7:G:187:GLU:O	7:G:232:ARG:HD3	2.13	0.49
6:T:77:VAL:HG12	6:T:137:ILE:HB	1.94	0.49
1:O:150:GLN:O	1:O:157:TYR:HA	2.12	0.49
13:O:8:TYR:CE2	13:O:148:VAL:HG22	2.48	0.49
5:E:160:LEU:CD2	6:F:59:LEU:HD12	2.43	0.49
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.43	0.49
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.13	0.49
9:I:29:ASN:HB2	16:I:224:HOH:O	2.12	0.49
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.12	0.48
1:A:225:THR:N	1:A:228:GLU:OE1	2.44	0.48
7:G:47:VAL:HG12	7:G:49:ILE:CD1	2.43	0.48
8:V:172:ASN:HD22	8:V:193:THR:HA	1.78	0.48
9:W:105:ASN:HB3	9:W:10(C):SER:OG	2.12	0.48
4:D:175:GLU:OE2	4:D:199:GLN:NE2	2.44	0.48
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.33	0.48
1:A:224:LEU:HA	1:A:228:GLU:OE1	2.13	0.48
5:S:160:LEU:HD13	5:S:163:THR:HB	1.95	0.48
10:X:90(A):ILE:CD1	10:X:116:LEU:HD23	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:GLN:O	3:C:243:GLN:N	2.43	0.48
8:H:43:CYS:SG	8:H:99:LEU:HB3	2.53	0.48
13:M:133:MET:HG3	8:V:132:LEU:HD23	1.95	0.48
2:P:115:ARG:HH11	2:P:115:ARG:HG3	1.78	0.48
3:C:242:GLU:O	3:C:243:GLN:HB2	2.11	0.48
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.13	0.48
9:W:12:VAL:CG1	9:W:108:PRO:HB3	2.43	0.48
10:J:6:ILE:HD11	10:J:154:LEU:HD23	1.96	0.48
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.28	0.48
14:N:107:LYS:HZ1	14:N:145:ASN:HD21	1.60	0.48
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.74	0.48
6:T:95:GLU:CG	6:T:115:ARG:HD2	2.44	0.48
6:T:203:GLU:C	6:T:205:ASN:H	2.16	0.48
10:X:112:GLN:NE2	10:X:126:ALA:H	2.11	0.48
9:I:105:ASN:O	9:I:106:GLY:N	2.41	0.48
1:O:77:VAL:HG12	1:O:137:LEU:HB2	1.94	0.48
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.42	0.48
13:M:199:PHE:CE2	14:1:30:VAL:HG11	2.48	0.48
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.96	0.48
2:B:181:LYS:HE2	2:B:183:ASP:OD1	2.14	0.48
11:K:97:MET:O	11:K:114:ASP:HA	2.13	0.48
2:P:191:GLU:O	2:P:195:LYS:HG2	2.14	0.48
3:C:122:ARG:NH2	16:C:279:HOH:O	2.46	0.48
11:K:5:ALA:HA	11:K:13:ILE:O	2.14	0.48
4:R:237:LEU:O	4:R:241:GLU:HG3	2.14	0.48
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.97	0.48
9:W:6:MET:HE1	9:W:155:ILE:HA	1.95	0.48
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.49	0.48
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.43	0.48
13:O:205:GLY:HA3	13:O:209:GLN:HB3	1.96	0.48
14:1:66:TYR:CD2	14:1:74:PRO:HB3	2.48	0.48
13:M:11:GLY:HA3	13:M:178:ILE:O	2.12	0.48
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.13	0.48
1:O:21(A):GLU:OE2	1:O:21(P):LYS:HB2	2.13	0.48
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.96	0.48
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.94	0.48
2:P:101:LYS:NZ	10:X:85:GLN:HE22	2.12	0.48
8:V:49:ALA:HB2	15:V:7710:SRG:H25A	1.95	0.48
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.94	0.48
4:D:237:LEU:O	4:D:241:GLU:HG3	2.14	0.48
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.77	0.48
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.79	0.48
13:M:1:THR:OG1	13:M:2:SER:N	2.43	0.48
6:F:77:VAL:HG12	6:F:137:ILE:HB	1.95	0.48
13:0:49:ILE:O	13:0:53:GLN:HG3	2.13	0.48
12:L:14(E):GLU:HB2	12:L:14(I):THR:HG21	1.96	0.48
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.48	0.48
3:Q:93:ARG:HD2	16:Q:258:HOH:O	2.14	0.48
11:Y:97:MET:O	11:Y:114:ASP:HA	2.14	0.48
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.95	0.48
1:O:224:LEU:HA	1:O:228:GLU:OE1	2.14	0.48
9:I:1:GLY:HA2	9:I:17:ASP:OD1	2.14	0.48
6:T:20(B):GLU:OE1	6:T:20(C):LYS:HE3	2.14	0.48
12:L:140:ASN:O	12:L:144:PHE:HA	2.13	0.48
3:C:105:ASP:OD2	3:C:106:PRO:HD2	2.14	0.47
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.79	0.47
1:A:29:THR:O	1:A:33:GLN:HG2	2.13	0.47
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.95	0.47
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.95	0.47
8:H:165:ASN:ND2	13:0:139:ARG:HH11	2.09	0.47
11:K:12:ILE:HG23	11:K:110:ILE:HD11	1.96	0.47
1:O:161:LYS:HD3	1:O:180:TRP:CH2	2.49	0.47
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.45	0.47
4:D:29:GLU:OE2	4:D:32:LYS:HD2	2.14	0.47
10:X:3:ILE:HG22	10:X:3:ILE:O	2.12	0.47
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.96	0.47
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.25	0.47
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.29	0.47
8:V:25:ILE:HB	16:V:7740:HOH:O	2.14	0.47
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.13	0.47
14:1:67:THR:HA	14:1:72:GLY:O	2.14	0.47
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	1.95	0.47
2:B:122:GLY:C	2:B:124:THR:H	2.15	0.47
4:D:233:ILE:HG22	4:D:235:LYS:N	2.29	0.47
4:D:123:PHE:HB3	4:D:128:MET:HE2	1.96	0.47
13:0:14(G):ILE:N	13:0:144:PRO:HD2	2.29	0.47
13:0:11:GLY:HA3	13:0:178:ILE:O	2.13	0.47
2:B:163:ILE:HG13	2:B:164:SER:N	2.29	0.47
5:E:38:VAL:HG12	5:E:39:GLY:N	2.29	0.47
14:N:161:GLN:NE2	14:N:165:TRP:HE1	2.12	0.47
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.96	0.47
12:L:135:MET:CE	9:W:165:ARG:NH2	2.78	0.47
4:D:39:GLY:O	4:D:162:ALA:HA	2.15	0.47
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.50	0.47
13:O:133:MET:O	13:O:136:PRO:HD2	2.15	0.47
12:L:109:ALA:HA	16:L:227:HOH:O	2.13	0.47
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.15	0.47
8:H:46:ALA:HA	15:H:7710:SRG:H24A	1.96	0.47
11:K:10(B):LYS:CD	11:K:10(B):LYS:N	2.64	0.47
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.96	0.47
14:N:146:MET:HB3	14:N:150:GLU:HB2	1.96	0.47
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.95	0.47
4:R:97:VAL:HG11	11:Y:65:LEU:CD2	2.45	0.47
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.14	0.47
7:G:10:ARG:HG2	7:G:22:TYR:CD2	2.50	0.47
6:F:11:SER:HB3	6:F:14:VAL:HG23	1.96	0.47
12:L:176:LEU:CD1	12:L:186:LYS:HG2	2.45	0.47
3:Q:43:LYS:O	3:Q:43:LYS:HG2	2.15	0.47
7:G:192:PHE:CD1	7:G:192:PHE:C	2.88	0.47
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.50	0.47
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.50	0.47
1:A:169:SER:O	1:A:173:LYS:HG3	2.15	0.47
5:S:38:VAL:HG12	5:S:39:GLY:N	2.29	0.47
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.49	0.47
5:S:28:LEU:HD12	5:S:153:PRO:HD2	1.96	0.47
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.50	0.47
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.48	0.47
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.96	0.47
5:E:73:HIS:HE1	5:E:107:LEU:O	1.97	0.47
9:I:156:SER:O	9:I:160:LEU:HB2	2.15	0.47
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	1.97	0.47
5:E:5:ARG:HG3	5:E:22:PHE:CE2	2.49	0.47
4:R:17:PRO:HA	5:S:26:TYR:CD1	2.49	0.47
7:U:158:VAL:HG22	7:U:159:GLY:N	2.30	0.47
10:X:6:ILE:HD11	10:X:154:LEU:HD23	1.96	0.47
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.50	0.47
8:H:172:ASN:ND2	8:H:193:THR:HA	2.30	0.47
3:C:163:GLN:HG3	3:C:164:THR:N	2.30	0.47
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.28	0.47
11:Y:12:ILE:HG23	11:Y:110:ILE:HD11	1.96	0.47
11:K:180:GLU:CB	16:K:7728:HOH:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.13	0.47
1:A:77:VAL:HG12	1:A:137:LEU:HB2	1.96	0.47
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.97	0.47
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.97	0.46
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.50	0.46
7:G:158:VAL:HG22	7:G:159:GLY:N	2.30	0.46
2:B:161:LYS:HB3	2:B:180:TYR:CE2	2.50	0.46
5:E:113:GLY:HA3	16:E:245:HOH:O	2.15	0.46
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.79	0.46
13:O:19:LEU:HD12	13:O:28:PHE:O	2.15	0.46
1:O:225:THR:N	1:O:228:GLU:OE1	2.44	0.46
14:1:146:MET:HB3	14:1:150:GLU:HB2	1.95	0.46
13:M:184:LEU:HD23	13:M:184:LEU:C	2.34	0.46
5:S:5:ARG:HG3	5:S:22:PHE:CE2	2.51	0.46
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.45	0.46
3:C:57:LYS:O	3:C:58:LEU:HB2	2.15	0.46
1:A:57:PRO:HG3	7:G:177:GLU:CD	2.35	0.46
10:J:141:HIS:HB2	10:J:154:LEU:HD11	1.97	0.46
8:H:49:ALA:HB2	15:H:7710:SRG:H25A	1.98	0.46
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.50	0.46
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.16	0.46
14:1:112:THR:CG2	14:1:120:HIS:HB2	2.44	0.46
6:T:175:GLU:HB3	6:T:196:ILE:CD1	2.45	0.46
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.13	0.46
11:K:74:ILE:HA	16:K:7729:HOH:O	2.15	0.46
6:F:91:ARG:HG2	6:F:119:TYR:CD2	2.50	0.46
1:O:190:ILE:O	1:O:193:ALA:HB3	2.15	0.46
2:B:144:ARG:HG2	2:B:144:ARG:O	2.15	0.46
2:P:160:TRP:CD2	2:P:163:ILE:HD13	2.50	0.46
12:L:-8:PHE:HB2	13:M:-8:THR:HG23	1.98	0.46
14:N:26:ILE:HB	13:O:165:ARG:HA	1.97	0.46
13:M:165:ARG:HA	14:1:26:ILE:HB	1.96	0.46
6:T:103:TYR:O	6:T:104:LYS:HB3	2.15	0.46
2:B:115:ARG:HG3	2:B:115:ARG:NH1	2.29	0.46
3:Q:87:ILE:N	3:Q:87:ILE:CD1	2.79	0.46
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.98	0.46
10:J:52:THR:HG22	10:J:53:VAL:HG23	1.98	0.46
1:O:32:LYS:HA	1:O:32:LYS:CE	2.44	0.46
3:C:190:VAL:O	3:C:194:VAL:HG23	2.14	0.46
13:M:1:THR:HG22	16:M:214:HOH:O	2.16	0.46
3:Q:159:SER:HB2	16:Q:272:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ARG:HG3	2:B:115:ARG:HH11	1.79	0.46
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.50	0.46
2:B:97:GLN:NE2	16:B:259:HOH:O	2.48	0.46
7:U:110:ASP:HB3	7:U:149:TYR:CZ	2.50	0.46
5:S:13:VAL:O	5:S:13:VAL:HG13	2.14	0.46
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.15	0.46
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.16	0.46
15:K:7710:SRG:H13B	15:K:7710:SRG:N17	2.31	0.46
3:C:57:LYS:HG2	3:C:208:LYS:HZ3	1.80	0.46
13:M:19:LEU:HD12	13:M:28:PHE:O	2.15	0.46
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.50	0.46
6:T:91:ARG:HG2	6:T:119:TYR:CD2	2.50	0.46
14:N:114:PRO:HD2	14:N:118:SER:O	2.16	0.46
2:B:112:LEU:C	2:B:112:LEU:HD23	2.36	0.46
2:P:112:LEU:HD23	2:P:112:LEU:C	2.36	0.46
11:Y:10(A):ARG:HB3	11:Y:10(B):LYS:HE3	1.98	0.46
3:C:106:PRO:HG2	3:C:143:PRO:HG2	1.94	0.46
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.64	0.46
6:T:179:LEU:CD2	6:T:192:GLN:HG2	2.44	0.46
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.15	0.46
2:P:91:THR:HG22	16:P:263:HOH:O	2.14	0.46
13:O:7:LYS:HG3	13:O:14(G):ILE:HD12	1.97	0.46
3:C:79:SER:HA	16:C:272:HOH:O	2.15	0.46
2:P:161:LYS:HB3	2:P:180:TYR:CE2	2.51	0.46
14:I:107:LYS:HZ1	14:I:145:ASN:HD21	1.63	0.46
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.98	0.46
6:F:109:ILE:HD13	6:F:142:ASP:HB3	1.98	0.46
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.51	0.46
4:D:237:LEU:HD22	4:D:241:GLU:HG3	1.97	0.46
5:S:104:ASN:HB2	13:O:81:GLU:HG2	1.98	0.46
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.97	0.46
3:Q:40:VAL:HG22	3:Q:193:THR:OG1	2.15	0.46
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.51	0.46
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.97	0.46
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.95	0.46
1:O:15:PHE:H	2:P:23:GLN:NE2	1.93	0.46
6:F:36:THR:HB	6:F:168:GLY:H	1.81	0.46
11:Y:7:ARG:HH11	11:Y:108:PRO:HB2	1.81	0.46
1:A:98:THR:HA	1:A:102:ARG:HD2	1.97	0.46
13:M:3:VAL:O	13:M:126:ALA:HA	2.16	0.46
6:F:179:LEU:CD2	6:F:192:GLN:HG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PHE:O	1:A:179:ARG:HG2	2.16	0.45
8:H:72:ARG:NH1	8:H:72:ARG:HG3	2.30	0.45
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.97	0.45
7:G:109:CYS:HB2	7:G:140:SER:OG	2.16	0.45
8:H:5:GLY:O	8:H:124:TYR:HA	2.17	0.45
5:E:86:ARG:NH1	5:E:86:ARG:HG3	2.31	0.45
3:C:224:LEU:N	3:C:224:LEU:CD1	2.79	0.45
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.98	0.45
15:Y:7710:SRG:N17	15:Y:7710:SRG:H13B	2.31	0.45
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.98	0.45
8:H:34:LEU:HB2	16:H:7732:HOH:O	2.15	0.45
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.32	0.45
11:Y:145:ASP:O	11:Y:146:LEU:HD12	2.17	0.45
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.31	0.45
13:O:19:LEU:HB2	13:O:170:SER:HB2	1.96	0.45
3:C:75:VAL:HG13	3:C:221:ILE:HD13	1.98	0.45
3:C:40:VAL:HG22	3:C:193:THR:OG1	2.16	0.45
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.97	0.45
10:J:121:GLU:O	10:J:122:LEU:HD23	2.16	0.45
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.30	0.45
3:Q:121:GLN:C	3:Q:121:GLN:NE2	2.70	0.45
10:X:121:GLU:O	10:X:122:LEU:HD23	2.16	0.45
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.46	0.45
1:A:130:ARG:HG2	7:G:125:GLN:HG3	1.99	0.45
3:Q:87:ILE:N	3:Q:87:ILE:HD12	2.31	0.45
2:B:77:ALA:HB3	2:B:137:ILE:HB	1.98	0.45
11:K:76:VAL:N	11:K:106:GLU:OE2	2.48	0.45
2:B:191:GLU:O	2:B:195:LYS:HG2	2.16	0.45
3:C:43:LYS:HG2	3:C:43:LYS:O	2.17	0.45
6:F:175:GLU:HB3	6:F:196:ILE:CD1	2.47	0.45
10:X:113:ILE:CG1	10:X:119:LYS:HG3	2.45	0.45
3:Q:194:VAL:O	3:Q:198:LEU:HG	2.17	0.45
6:F:20(B):GLU:OE1	6:F:20(C):LYS:HE3	2.16	0.45
1:O:29:THR:O	1:O:33:GLN:HG2	2.15	0.45
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.16	0.45
14:I:13:ILE:HD12	14:I:151:THR:HG22	1.97	0.45
4:R:237:LEU:HD22	4:R:241:GLU:HG3	1.98	0.45
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.83	0.45
10:X:148:THR:CG2	10:X:177:ILE:HD13	2.47	0.45
3:C:87:ILE:N	3:C:87:ILE:HD12	2.31	0.45
1:O:38:LEU:HD12	1:O:38:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:161:GLN:HE22	14:1:165:TRP:HE1	1.65	0.45
6:T:36:THR:HB	6:T:168:GLY:H	1.81	0.45
11:K:142:TYR:C	11:K:143:LYS:HD2	2.37	0.45
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.98	0.45
11:K:12:ILE:HB	11:K:178:VAL:HB	1.99	0.45
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.17	0.45
14:1:84:LYS:HG3	14:1:119:VAL:CG2	2.46	0.45
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.98	0.45
5:S:20:ARG:HB3	5:S:25:GLU:OE2	2.16	0.45
1:O:92:SER:O	1:O:95:VAL:HG12	2.17	0.45
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.52	0.45
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.46	0.45
2:P:97:GLN:NE2	16:P:258:HOH:O	2.48	0.45
13:M:9:ASP:OD1	13:M:10:ASN:N	2.50	0.45
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.51	0.45
1:A:110:LYS:HG2	16:A:246:HOH:O	2.16	0.45
4:D:53:ARG:HG2	4:D:53:ARG:O	2.17	0.45
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.99	0.45
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.45	0.45
8:H:132:LEU:HD23	13:O:133:MET:HG3	1.98	0.45
3:Q:182:PRO:O	3:Q:184:ALA:N	2.50	0.45
1:A:170:VAL:N	16:A:252:HOH:O	2.49	0.45
3:C:182:PRO:O	3:C:184:ALA:N	2.50	0.45
7:U:192:PHE:C	7:U:192:PHE:CD1	2.90	0.45
10:J:190:PHE:HA	10:J:193:GLN:HB2	1.98	0.45
10:X:141:HIS:HB2	10:X:154:LEU:HD11	1.99	0.45
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.98	0.45
8:H:128:GLY:O	8:H:131:SER:HB2	2.17	0.45
11:Y:81:LYS:HA	11:Y:84:SER:HB3	1.98	0.45
6:T:54:ILE:HD11	6:T:209:GLU:HB2	1.99	0.45
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.99	0.45
1:O:141:HIS:HA	1:O:146:GLY:O	2.17	0.45
5:S:134:VAL:O	5:S:153:PRO:HG3	2.16	0.45
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.28	0.45
12:L:134:ILE:HD12	12:L:158:SER:HB3	1.99	0.45
3:C:194:VAL:O	3:C:198:LEU:HG	2.16	0.45
10:X:162:LEU:O	10:X:166:MET:HB2	2.16	0.45
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.99	0.45
3:Q:228:GLU:O	3:Q:232:TYR:HD1	2.00	0.45
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.98	0.45
1:O:98:THR:HA	1:O:102:ARG:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:GLN:NE2	16:C:255:HOH:O	2.49	0.45
10:X:60:GLN:O	10:X:64:GLN:HG3	2.17	0.45
1:A:38:LEU:C	1:A:38:LEU:HD12	2.37	0.45
9:I:6:MET:HE3	9:I:155:ILE:CG1	2.33	0.45
7:U:236:ILE:HD12	7:U:236:ILE:C	2.37	0.45
11:Y:210:ILE:HD12	11:Y:210:ILE:HA	1.88	0.45
1:A:212:LEU:HD23	1:A:212:LEU:C	2.36	0.45
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.98	0.45
12:L:13:VAL:HG12	12:L:177:ILE:HG13	1.98	0.45
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.17	0.45
5:S:78:LEU:HD12	5:S:78:LEU:C	2.38	0.45
7:G:197:MET:HG2	7:G:205:PHE:HE1	1.82	0.44
10:J:17:SER:CB	10:J:170:PHE:HB2	2.47	0.44
5:E:111:ARG:NH1	5:E:111:ARG:HG2	2.32	0.44
11:K:33:LYS:HA	11:K:45:MET:HE2	1.99	0.44
8:V:116:HIS:HB2	16:V:7749:HOH:O	2.16	0.44
3:Q:212:ILE:HG22	3:Q:213:THR:N	2.31	0.44
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.97	0.44
3:C:101:LEU:CD1	10:J:57:GLU:HB3	2.39	0.44
3:Q:75:VAL:HG13	3:Q:221:ILE:HD13	1.99	0.44
2:B:138:TYR:HB2	2:B:149:TYR:HB2	1.98	0.44
5:S:111:ARG:HG2	5:S:111:ARG:NH1	2.31	0.44
5:S:148:LEU:HD23	5:S:162:GLY:HA2	1.99	0.44
10:J:168:MET:HE2	10:X:168:MET:HE2	1.99	0.44
4:D:172:ALA:HB1	4:D:196:ILE:HG21	1.99	0.44
14:I:44:CYS:HB2	14:I:100:ILE:HB	1.99	0.44
6:F:103:TYR:O	6:F:104:LYS:HB3	2.18	0.44
2:P:176:LEU:HD23	2:P:192:LEU:HD22	1.99	0.44
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.98	0.44
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.52	0.44
14:N:156:LYS:HG2	14:N:18(J):LEU:CD1	2.47	0.44
3:Q:47:VAL:HG23	3:Q:189:CYS:SG	2.58	0.44
8:V:18:THR:HB	8:V:30:ASN:HD22	1.82	0.44
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.16	0.44
10:J:148:THR:CG2	10:J:177:ILE:HD13	2.48	0.44
11:K:140:SER:OG	10:X:137:LEU:HD21	2.17	0.44
11:K:147:SER:C	11:K:149:GLU:N	2.70	0.44
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.16	0.44
3:C:33:ARG:HH11	3:C:33:ARG:HB3	1.82	0.44
9:W:29:ASN:HB2	16:W:213:HOH:O	2.17	0.44
1:A:32:LYS:HA	1:A:32:LYS:CE	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:12:ILE:HG13	11:Y:108:PRO:HB3	1.99	0.44
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.80	0.44
3:Q:241:GLN:O	3:Q:243:GLN:N	2.44	0.44
8:H:172:ASN:HD22	8:H:193:THR:HA	1.82	0.44
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.47	0.44
3:Q:33:ARG:HH11	3:Q:33:ARG:HB3	1.81	0.44
2:P:190:ILE:HG21	2:P:232:ILE:HD11	2.00	0.44
5:E:18(A):ASP:O	5:E:18(E):LYS:HD3	2.17	0.44
10:X:17:SER:CB	10:X:170:PHE:HB2	2.47	0.44
14:1:156:LYS:HG2	14:1:18(J):LEU:CD1	2.47	0.44
4:D:240:LYS:O	4:D:243:ALA:HB3	2.17	0.44
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.98	0.44
2:P:97:GLN:HA	2:P:97:GLN:NE2	2.33	0.44
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.83	0.44
6:F:172:ALA:O	6:F:176:LEU:HD23	2.17	0.44
14:N:116:GLY:HA3	16:N:7719:HOH:O	2.17	0.44
11:K:81:LYS:HA	11:K:84:SER:HB3	1.99	0.44
12:Z:45:ALA:HA	12:Z:99:THR:HB	2.00	0.44
10:J:9:GLN:HG3	10:J:10:ASP:OD1	2.18	0.44
10:X:7:ARG:HG2	10:X:7:ARG:HH11	1.82	0.44
7:G:38:LEU:C	7:G:38:LEU:HD12	2.38	0.44
2:B:148:LEU:N	16:B:253:HOH:O	2.41	0.44
1:O:175:PHE:O	1:O:179:ARG:HG2	2.17	0.44
8:V:24:PRO:HG2	8:V:25:ILE:CD1	2.48	0.44
3:C:76:LEU:HD12	3:C:138:ILE:HG12	2.00	0.44
8:H:18:THR:HB	8:H:30:ASN:HD22	1.82	0.44
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.33	0.44
12:Z:123:GLN:HG3	12:Z:145:TYR:HH	1.80	0.44
8:V:53:GLU:O	8:V:57:GLN:HG3	2.17	0.44
2:P:77:ALA:HB3	2:P:137:ILE:HB	1.99	0.44
11:Y:4:LEU:CD1	11:Y:15:ALA:HB3	2.48	0.44
10:X:190:PHE:HA	10:X:193:GLN:HB2	1.98	0.44
11:Y:37:ILE:HB	11:Y:41:LEU:CB	2.48	0.44
13:0:113:VAL:HG23	13:0:119:THR:HG22	1.99	0.44
1:A:186:LEU:O	1:A:190:ILE:HG13	2.18	0.44
3:Q:225:SER:OG	3:Q:228:GLU:HG3	2.16	0.44
12:L:42:VAL:HG23	12:L:102:ALA:HB3	2.00	0.44
13:0:3:VAL:O	13:0:126:ALA:HA	2.17	0.44
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.99	0.44
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.65	0.44
5:S:122:LYS:C	5:S:123:ASN:HD22	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:86:ARG:NH1	5:S:86:ARG:HG3	2.33	0.44
11:Y:200:LYS:HE2	16:Y:7731:HOH:O	2.18	0.44
5:E:160:LEU:HD13	5:E:163:THR:HB	1.98	0.44
10:J:120:VAL:HG13	10:J:122:LEU:HG	1.99	0.44
12:L:148:VAL:O	12:L:152:ILE:HG12	2.18	0.44
11:Y:147:SER:C	11:Y:149:GLU:N	2.70	0.44
8:V:37:ILE:HG23	8:V:60:GLY:HA2	2.00	0.44
11:K:165:ARG:NE	10:X:135:PHE:HB3	2.32	0.44
10:X:143:ARG:HA	10:X:144:PRO:HD3	1.84	0.44
2:B:121:GLN:HG2	3:C:83:ALA:HB1	1.98	0.44
10:X:52:THR:HG22	10:X:53:VAL:HG23	1.99	0.44
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.83	0.44
11:K:4:LEU:HD11	11:K:15:ALA:HB3	2.00	0.44
10:J:48:GLU:HB3	10:J:96:GLN:HB2	2.00	0.44
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.98	0.44
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.47	0.44
3:C:87:ILE:N	3:C:87:ILE:CD1	2.80	0.44
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.53	0.44
6:F:95:GLU:HG2	6:F:115:ARG:HD2	2.00	0.43
10:J:136:SER:N	16:J:198:HOH:O	2.46	0.43
5:E:122:LYS:C	5:E:123:ASN:HD22	2.20	0.43
6:F:199:LEU:HD12	6:F:240:ILE:HD13	2.00	0.43
9:W:113:PHE:HA	9:W:118:CYS:O	2.17	0.43
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.53	0.43
2:B:230:LYS:O	2:B:234:VAL:HG23	2.18	0.43
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.81	0.43
2:B:97:GLN:NE2	2:B:97:GLN:HA	2.33	0.43
9:I:113:PHE:HA	9:I:118:CYS:O	2.18	0.43
4:R:172:ALA:HB1	4:R:196:ILE:HG21	1.99	0.43
3:C:134:VAL:HG12	3:C:135:SER:N	2.32	0.43
12:L:45:ALA:HA	12:L:99:THR:HB	1.99	0.43
7:G:30:ALA:O	7:G:33:GLN:HB2	2.18	0.43
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.33	0.43
13:M:12:VAL:HG21	13:M:102:ALA:HB1	2.01	0.43
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.18	0.43
7:G:171:GLU:OE1	7:G:171:GLU:N	2.51	0.43
8:V:113:ILE:HG12	8:V:119:THR:HG22	2.00	0.43
13:M:17:ASP:HA	13:M:173:PHE:HB3	2.00	0.43
7:U:39:ALA:HA	7:U:47:VAL:O	2.18	0.43
3:C:33:ARG:HG2	3:C:33:ARG:O	2.18	0.43
10:J:60:GLN:O	10:J:64:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:LYS:O	5:E:77:SER:HA	2.18	0.43
2:P:138:TYR:HB2	2:P:149:TYR:HB2	2.00	0.43
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.91	0.43
6:F:54:ILE:HD11	6:F:209:GLU:HB2	1.99	0.43
11:Y:185:ILE:N	11:Y:185:ILE:HD12	2.33	0.43
2:P:144:ARG:O	2:P:144:ARG:HG2	2.18	0.43
6:T:35:THR:CG2	6:T:36:THR:N	2.81	0.43
2:P:121:GLN:NE2	16:P:262:HOH:O	2.51	0.43
6:T:127:ASN:ND2	6:T:127:ASN:C	2.71	0.43
6:T:175:GLU:HB3	6:T:196:ILE:HD12	2.01	0.43
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.38	0.43
9:W:143:GLU:CG	9:W:146:LEU:HD21	2.48	0.43
10:X:6:ILE:CD1	10:X:154:LEU:HD23	2.49	0.43
3:Q:33:ARG:HG2	3:Q:33:ARG:O	2.18	0.43
10:X:9:GLN:HG3	10:X:10:ASP:OD1	2.17	0.43
3:C:212:ILE:HG22	3:C:213:THR:N	2.33	0.43
12:L:180:LYS:HG2	16:L:234:HOH:O	2.19	0.43
16:S:241:HOH:O	6:T:12:ASN:HB2	2.16	0.43
3:C:46:VAL:HG22	3:C:146:PRO:HB2	1.98	0.43
5:E:67:ILE:HG21	5:E:213:ALA:HB2	2.00	0.43
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.53	0.43
3:C:24:VAL:O	3:C:27:ALA:HB3	2.18	0.43
9:W:156:SER:O	9:W:160:LEU:HB2	2.18	0.43
8:H:7:LYS:HG3	8:H:123:TYR:HA	2.00	0.43
9:W:-2:ASN:HA	9:W:21:GLY:O	2.19	0.43
7:G:143:GLU:HG2	16:G:263:HOH:O	2.18	0.43
13:M:39:ASP:OD2	13:M:39:ASP:N	2.51	0.43
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.48	0.43
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.52	0.43
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.53	0.43
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.53	0.43
5:E:104:ASN:HB2	13:M:81:GLU:HG2	2.00	0.43
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.49	0.43
2:B:176:LEU:HD23	2:B:192:LEU:HD22	1.99	0.43
9:I:22:SER:O	9:I:23:GLN:HB2	2.18	0.43
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.53	0.43
3:C:121:GLN:NE2	3:C:121:GLN:C	2.71	0.43
3:Q:172:VAL:O	3:Q:176:LEU:HG	2.17	0.43
12:L:123:GLN:HG3	12:L:145:TYR:CZ	2.53	0.43
10:X:48:GLU:HB3	10:X:96:GLN:HB2	2.00	0.43
3:C:225:SER:OG	3:C:228:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:31:ILE:HD13	4:R:135:ALA:HB2	2.00	0.43
12:Z:176:LEU:CD1	12:Z:186:LYS:HG2	2.49	0.43
1:O:169:SER:O	1:O:173:LYS:HG3	2.18	0.43
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.48	0.43
11:Y:76:VAL:N	11:Y:106:GLU:OE2	2.52	0.43
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.33	0.43
6:T:199:LEU:HD12	6:T:240:ILE:HD13	2.00	0.43
2:B:173:GLN:HG2	3:C:56:LEU:CD1	2.49	0.43
14:N:146:MET:HE3	14:N:150:GLU:HB3	2.00	0.43
2:P:21(A):LYS:O	2:P:217:ALA:N	2.52	0.43
8:H:24:PRO:HG2	8:H:25:ILE:CD1	2.47	0.43
3:Q:170:LYS:HB2	16:Q:267:HOH:O	2.18	0.43
7:G:186:TRP:O	7:G:190:VAL:HG23	2.19	0.43
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.48	0.43
12:Z:43:MET:CB	12:Z:101:ILE:HG22	2.35	0.43
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.49	0.43
12:L:90:LYS:HE3	12:L:93:PHE:O	2.18	0.43
1:O:33:GLN:CA	1:O:33:GLN:HE21	2.28	0.43
4:D:194:LEU:HD12	4:D:194:LEU:HA	1.88	0.43
12:Z:83:ILE:HB	12:Z:113:PHE:CE2	2.53	0.43
1:O:186:LEU:O	1:O:190:ILE:HG13	2.19	0.43
10:J:168:MET:HG2	10:X:168:MET:CE	2.49	0.43
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.49	0.43
4:D:31:ILE:HD13	4:D:135:ALA:HB2	2.00	0.43
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.53	0.43
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.39	0.43
2:B:206:THR:HB	2:B:208:ASP:OD1	2.19	0.43
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.86	0.43
8:H:147:THR:HG23	8:H:150:GLU:OE1	2.18	0.43
8:V:128:GLY:O	8:V:131:SER:HB2	2.18	0.43
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.18	0.43
13:O:9:ASP:OD1	13:O:10:ASN:N	2.51	0.43
5:S:67:ILE:HG21	5:S:213:ALA:HB2	2.00	0.43
6:T:18:ASP:N	6:T:18:ASP:OD2	2.45	0.43
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.19	0.43
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.34	0.43
14:1:113:ILE:HG12	14:1:119:VAL:HG13	2.00	0.43
5:S:18(F):ILE:O	5:S:18(F):ILE:HG22	2.19	0.43
3:C:228:GLU:O	3:C:232:TYR:HD1	2.02	0.43
14:1:114:PRO:HD2	14:1:118:SER:O	2.19	0.43
10:J:51:ASP:HB3	10:J:95:TYR:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:22:SER:O	9:W:23:GLN:HB2	2.19	0.43
8:H:113:ILE:HG12	8:H:119:THR:HG22	2.01	0.43
6:F:179:LEU:HD11	6:F:192:GLN:HG2	2.01	0.43
10:J:133:TYR:CE1	16:Y:7726:HOH:O	2.68	0.43
1:O:212:LEU:HD23	1:O:212:LEU:C	2.39	0.43
5:E:148:LEU:HD23	5:E:162:GLY:HA2	2.00	0.43
2:B:21(A):LYS:O	2:B:217:ALA:N	2.52	0.43
13:M:113:VAL:HG23	13:M:119:THR:HG22	2.00	0.43
13:O:112:TYR:HE1	13:O:127:THR:HG22	1.83	0.43
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.84	0.43
8:H:174:ASP:OD2	8:H:189:ARG:NH1	2.49	0.43
9:W:80:THR:HG22	9:W:119:ILE:HD13	2.01	0.43
6:T:157:TYR:CD1	6:T:157:TYR:C	2.92	0.43
2:B:20:ARG:HG2	2:B:20:ARG:NH1	2.34	0.43
7:G:107:MET:HA	7:G:108:PRO:HD3	1.87	0.42
2:P:44:ASP:OD2	2:P:186:VAL:HG23	2.19	0.42
13:O:149:GLN:NE2	13:O:149:GLN:N	2.58	0.42
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.19	0.42
5:S:86:ARG:O	5:S:90:ASN:HB2	2.19	0.42
11:K:4:LEU:C	11:K:4:LEU:HD22	2.40	0.42
11:K:37:ILE:HB	11:K:41:LEU:CB	2.48	0.42
1:A:136:LEU:O	1:A:150:GLN:HA	2.19	0.42
2:B:190:ILE:HG21	2:B:232:ILE:HD11	2.01	0.42
2:B:156:ASN:HB2	16:C:285:HOH:O	2.18	0.42
16:F:286:HOH:O	7:G:86:ARG:HD2	2.18	0.42
5:E:78:LEU:HD12	5:E:78:LEU:C	2.39	0.42
10:J:157:LEU:HA	10:J:157:LEU:HD12	1.87	0.42
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.99	0.42
7:G:236:ILE:HD12	7:G:236:ILE:C	2.39	0.42
14:1:14:LEU:O	14:1:175:MET:HA	2.18	0.42
13:M:-3:VAL:HA	13:M:21:SER:O	2.20	0.42
10:J:7:ARG:HG2	10:J:7:ARG:HH11	1.84	0.42
2:B:107:ILE:HD11	2:B:111:ILE:HG22	2.00	0.42
3:C:15:PHE:H	4:D:23:GLN:NE2	1.97	0.42
11:K:145:ASP:O	11:K:146:LEU:HD12	2.20	0.42
12:Z:134:ILE:HD12	12:Z:158:SER:HB3	2.01	0.42
7:U:38:LEU:C	7:U:38:LEU:HD12	2.39	0.42
3:C:57:LYS:HD2	3:C:57:LYS:C	2.40	0.42
10:J:105:ASP:O	10:J:106:ASN:N	2.47	0.42
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.20	0.42
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:202:THR:CG2	2:P:204:SER:HB2	2.49	0.42
13:O:40:ASN:ND2	13:O:40:ASN:N	2.67	0.42
4:D:122:ARG:NH1	4:D:122:ARG:HG2	2.34	0.42
3:C:39:GLY:O	3:C:162:ALA:HA	2.19	0.42
7:U:109:CYS:HB2	7:U:140:SER:OG	2.19	0.42
6:T:119:TYR:O	6:T:122:ALA:HB3	2.20	0.42
10:X:120:VAL:HG13	10:X:122:LEU:HG	2.01	0.42
10:X:9:GLN:HG3	10:X:10:ASP:CG	2.40	0.42
5:S:18(A):ASP:O	5:S:18(E):LYS:HD3	2.19	0.42
4:R:78:MET:HG3	4:R:82:THR:HG22	2.01	0.42
11:K:207:ASN:ND2	10:X:144:PRO:CD	2.82	0.42
11:Y:145:ASP:C	11:Y:146:LEU:HD12	2.40	0.42
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.35	0.42
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.01	0.42
6:T:109:ILE:CD1	6:T:142:ASP:HB3	2.48	0.42
10:J:113:ILE:CG1	10:J:119:LYS:HG3	2.48	0.42
14:N:14:LEU:O	14:N:175:MET:HA	2.18	0.42
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.49	0.42
7:G:74:ILE:CD1	7:G:109:CYS:HA	2.50	0.42
1:A:141:HIS:HA	1:A:146:GLY:O	2.19	0.42
6:F:210:LEU:HD21	6:F:212:ILE:HD11	2.02	0.42
10:J:35:ARG:HA	10:J:35:ARG:HD3	1.84	0.42
6:T:95:GLU:HG2	6:T:115:ARG:CG	2.49	0.42
5:E:18(F):ILE:HG22	5:E:18(F):ILE:O	2.19	0.42
6:F:119:TYR:O	6:F:122:ALA:HB3	2.19	0.42
8:V:7:LYS:HG3	8:V:123:TYR:HA	2.00	0.42
9:W:137:MET:HE3	9:W:141:LEU:HD11	2.02	0.42
9:I:-2:ASN:HA	9:I:21:GLY:O	2.19	0.42
4:R:238:LYS:HE2	4:R:238:LYS:HB3	1.88	0.42
7:U:107:MET:HA	7:U:108:PRO:HD3	1.87	0.42
6:F:109:ILE:CD1	6:F:142:ASP:HB3	2.50	0.42
11:K:12:ILE:HG13	11:K:108:PRO:HB3	2.00	0.42
10:X:19:ALA:HB2	10:X:171:LYS:CG	2.49	0.42
4:D:194:LEU:HD22	4:D:212:LEU:HD11	2.01	0.42
2:P:230:LYS:O	2:P:234:VAL:HG23	2.20	0.42
10:J:168:MET:CE	10:X:168:MET:CE	2.98	0.42
2:P:149:TYR:OH	3:Q:62(A):ILE:HB	2.20	0.42
7:G:228:ASN:HB3	16:G:253:HOH:O	2.19	0.42
6:T:45:GLY:HA3	6:T:215:CYS:O	2.20	0.42
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.34	0.42
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:0:12:VAL:HG21	13:0:102:ALA:HB1	2.02	0.42
5:S:66:LYS:O	5:S:77:SER:HA	2.19	0.42
7:U:30:ALA:O	7:U:33:GLN:HB2	2.19	0.42
6:T:95:GLU:CG	6:T:115:ARG:HH11	2.17	0.42
2:P:206:THR:HB	2:P:208:ASP:OD1	2.19	0.42
6:F:175:GLU:HB3	6:F:196:ILE:HD12	2.01	0.42
12:Z:42:VAL:HG23	12:Z:102:ALA:HB3	2.02	0.42
9:I:137:MET:CE	9:I:141:LEU:HD11	2.49	0.42
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.33	0.42
9:W:178:ILE:HG23	9:W:184:VAL:HG22	2.02	0.42
10:J:135:PHE:HB3	11:Y:165:ARG:NE	2.35	0.42
4:D:100:ASN:HB3	16:D:257:HOH:O	2.19	0.42
8:H:148:LYS:O	8:H:152:ILE:HG13	2.20	0.42
11:K:137:VAL:HG21	11:K:161:ALA:HB2	2.02	0.42
7:G:72:ARG:HB2	7:G:72:ARG:NH1	2.35	0.42
2:P:122:GLY:C	2:P:124:THR:N	2.73	0.42
13:M:91:ARG:HG3	13:M:92:SER:N	2.34	0.42
10:J:45:PHE:CE1	10:J:52:THR:HG23	2.55	0.42
6:T:179:LEU:HD11	6:T:192:GLN:HG2	2.02	0.42
13:0:184:LEU:HD23	13:0:184:LEU:C	2.39	0.42
6:T:176:LEU:O	6:T:180:VAL:HG23	2.20	0.42
1:O:31:VAL:HG13	1:O:79:SER:O	2.20	0.42
1:O:21(G):LEU:HA	1:O:21(G):LEU:HD12	1.88	0.42
10:J:6:ILE:CD1	10:J:154:LEU:HD23	2.49	0.42
10:J:168:MET:HE1	10:X:167:PRO:CB	2.50	0.42
1:A:92:SER:O	1:A:95:VAL:HG12	2.20	0.42
11:Y:137:VAL:HG21	11:Y:161:ALA:HB2	2.02	0.42
10:X:76:PRO:HD2	16:X:202:HOH:O	2.20	0.42
6:F:157:TYR:C	6:F:157:TYR:CD1	2.92	0.42
10:X:185:ARG:HG2	10:X:185:ARG:HH11	1.85	0.42
2:B:186:VAL:CB	2:B:216:ARG:HD3	2.50	0.42
1:O:232:ARG:CG	1:O:232:ARG:NH1	2.83	0.42
6:F:127:ASN:ND2	6:F:127:ASN:C	2.72	0.42
1:A:4:MET:HG3	6:F:126:TYR:CE2	2.54	0.42
1:O:179:ARG:HB3	1:O:192:ILE:HD12	2.02	0.42
1:A:67:VAL:HG23	1:A:211:GLU:HG2	2.02	0.42
14:N:113:ILE:HG12	14:N:119:VAL:HG13	2.01	0.42
6:F:176:LEU:O	6:F:180:VAL:HG23	2.19	0.42
6:F:52:LYS:HB2	6:F:209:GLU:O	2.20	0.42
11:K:9:GLN:HB3	11:K:144:TRP:O	2.20	0.42
3:Q:120:GLN:O	3:Q:124:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.35	0.42
5:E:233:ILE:OXT	5:E:233:ILE:HG22	2.20	0.42
11:K:205:SER:C	11:K:207:ASN:N	2.72	0.41
11:K:7:ARG:HG2	11:K:108:PRO:HB2	2.02	0.41
10:X:190:PHE:C	10:X:192:ALA:N	2.73	0.41
8:V:175:VAL:CG1	8:V:176:CYS:N	2.83	0.41
10:J:112:GLN:HE22	10:J:126:ALA:H	1.67	0.41
11:Y:147:SER:O	11:Y:150:ASP:N	2.53	0.41
9:I:80:THR:HG22	9:I:119:ILE:HD13	2.00	0.41
10:X:157:LEU:HD12	10:X:157:LEU:HA	1.87	0.41
10:X:146:MET:HB3	10:X:146:MET:HE2	1.92	0.41
2:B:202:THR:CG2	2:B:204:SER:HB2	2.50	0.41
3:C:172:VAL:O	3:C:176:LEU:HG	2.20	0.41
2:P:186:VAL:CB	2:P:216:ARG:HD3	2.50	0.41
2:P:134:VAL:O	2:P:153:PRO:HD3	2.20	0.41
1:O:232:ARG:HH11	1:O:232:ARG:CG	2.30	0.41
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.55	0.41
3:Q:57:LYS:HG2	3:Q:208:LYS:HZ3	1.86	0.41
13:O:14(G):ILE:HB	13:O:144:PRO:CD	2.50	0.41
9:I:113:PHE:CD2	9:I:113:PHE:N	2.88	0.41
13:O:3:VAL:HA	13:O:21:SER:O	2.20	0.41
4:D:78:MET:HG3	4:D:82:THR:HG22	2.03	0.41
10:J:140:HIS:CE1	11:Y:203:GLU:OE2	2.73	0.41
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.86	0.41
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.90	0.41
13:O:14(A):VAL:O	13:O:14(A):VAL:HG23	2.20	0.41
2:B:186:VAL:CG1	2:B:216:ARG:HD3	2.50	0.41
13:O:125:LEU:HA	16:O:217:HOH:O	2.19	0.41
7:U:18(G):GLU:CG	7:U:188:LYS:HB2	2.50	0.41
1:A:12:LEU:HD11	7:G:127:ALA:HB2	2.02	0.41
12:L:39:ASP:OD2	12:L:67:HIS:HE1	2.03	0.41
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.88	0.41
4:R:53:ARG:O	4:R:53:ARG:HG2	2.20	0.41
11:K:210:ILE:HA	11:K:210:ILE:HD12	1.87	0.41
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.35	0.41
6:F:50:VAL:HG22	6:F:51:GLU:N	2.35	0.41
5:E:141:TYR:HA	5:E:145:GLY:O	2.20	0.41
7:U:38:LEU:HD23	7:U:197:MET:HE3	2.02	0.41
10:J:18:LYS:HD3	10:J:174:ILE:CG1	2.50	0.41
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.50	0.41
10:J:191:GLN:O	10:J:192:ALA:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1:GLY:HA2	9:W:17:ASP:OD1	2.20	0.41
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.56	0.41
13:0:42:VAL:CG2	13:0:178:ILE:HD11	2.50	0.41
8:H:201:GLN:HG2	12:Z:153:LYS:HA	2.02	0.41
1:O:214:ILE:HD13	1:O:222:ARG:O	2.21	0.41
3:C:93:ARG:HD2	16:C:260:HOH:O	2.19	0.41
8:H:19:ARG:NH1	8:H:167:LEU:O	2.54	0.41
8:H:26:VAL:HG11	8:H:29:LYS:HG2	2.01	0.41
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	2.19	0.41
4:R:39:GLY:O	4:R:162:ALA:HA	2.20	0.41
3:Q:185:THR:CB	3:Q:188:GLU:HG2	2.39	0.41
5:S:141:TYR:HA	5:S:145:GLY:O	2.20	0.41
2:B:126:HIS:HA	16:C:276:HOH:O	2.20	0.41
10:J:124:TYR:CE2	10:J:138:LEU:HB2	2.55	0.41
4:D:185:THR:HG23	4:D:188:GLU:OE1	2.21	0.41
8:H:201:GLN:CG	12:Z:153:LYS:HG2	2.51	0.41
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.55	0.41
12:L:9:GLU:O	12:L:107:LYS:HA	2.20	0.41
7:G:75:GLY:HA3	7:G:221:PHE:CE2	2.55	0.41
10:J:143:ARG:HA	10:J:144:PRO:HD3	1.83	0.41
10:J:146:MET:HB3	10:J:146:MET:HE2	1.90	0.41
11:Y:9:GLN:HB3	11:Y:144:TRP:O	2.20	0.41
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.24	0.41
7:G:18(G):GLU:CG	7:G:188:LYS:HB2	2.50	0.41
4:R:240:LYS:O	4:R:243:ALA:HB3	2.19	0.41
3:Q:212:ILE:CG2	3:Q:213:THR:N	2.83	0.41
3:Q:24:VAL:O	3:Q:27:ALA:HB3	2.20	0.41
12:Z:2:THR:HG21	12:Z:130:ALA:HB3	2.03	0.41
4:D:101:LEU:CD1	11:K:57:THR:HG22	2.50	0.41
7:U:171:GLU:N	7:U:171:GLU:OE1	2.52	0.41
6:T:95:GLU:HG2	6:T:115:ARG:HD2	2.03	0.41
13:M:157:ASN:ND2	16:M:273:HOH:O	2.54	0.41
2:P:186:VAL:HG21	2:P:216:ARG:CG	2.49	0.41
10:X:34:THR:HG21	10:X:176:LYS:HZ2	1.84	0.41
7:U:172:ILE:HG12	7:U:172:ILE:H	1.61	0.41
9:I:143:GLU:CG	9:I:146:LEU:HD21	2.49	0.41
9:I:55:LEU:HD12	9:I:97:VAL:HG21	2.02	0.41
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.55	0.41
3:C:59:GLN:HG3	3:C:59:GLN:H	1.51	0.41
7:U:116:MET:HE3	16:U:257:HOH:O	2.20	0.41
5:S:233:ILE:OXT	5:S:233:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:185:THR:CB	3:C:188:GLU:HG2	2.40	0.41
11:Y:9:GLN:NE2	11:Y:146:LEU:O	2.52	0.41
1:A:179:ARG:HB3	1:A:192:ILE:HD12	2.02	0.41
4:R:122:ARG:HG2	4:R:122:ARG:NH1	2.36	0.41
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.84	0.41
10:J:167:PRO:CB	10:X:168:MET:HE1	2.50	0.41
10:J:9:GLN:HG3	10:J:10:ASP:CG	2.40	0.41
9:W:160:LEU:HA	9:W:160:LEU:HD12	1.93	0.41
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.84	0.41
3:C:136:THR:O	3:C:150:GLN:HA	2.21	0.41
4:D:219:ASP:O	4:D:222:LYS:HE2	2.20	0.41
2:P:39:GLY:O	2:P:148:LEU:HD21	2.21	0.41
3:Q:136:THR:O	3:Q:150:GLN:HA	2.20	0.41
6:F:70:VAL:HG11	6:F:112:PHE:CE1	2.54	0.41
1:O:122:GLU:C	1:O:124:THR:H	2.24	0.41
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.21	0.41
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	2.02	0.41
13:M:149:GLN:NE2	13:M:149:GLN:N	2.56	0.41
2:B:122:GLY:C	2:B:124:THR:N	2.74	0.41
7:U:203:THR:HG22	7:U:204:GLU:O	2.21	0.41
10:X:36:GLN:OE1	10:X:39:PRO:HA	2.21	0.41
14:1:146:MET:HE3	14:1:150:GLU:HB3	2.03	0.41
10:X:18:LYS:HD3	10:X:174:ILE:CG1	2.50	0.41
6:F:205:ASN:C	6:F:20(B):GLU:H	2.24	0.41
7:U:188:LYS:HA	7:U:188:LYS:HD3	1.90	0.41
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	2.02	0.41
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.51	0.41
7:G:39:ALA:HA	7:G:47:VAL:O	2.20	0.41
3:Q:201:VAL:HG12	3:Q:201:VAL:O	2.21	0.41
7:U:74:ILE:CD1	7:U:109:CYS:HA	2.50	0.41
13:O:133:MET:C	13:O:136:PRO:HD2	2.41	0.41
2:P:99:TYR:CD2	2:P:107:ILE:HA	2.56	0.41
2:P:107:ILE:HA	2:P:108:PRO:HD3	1.99	0.41
2:B:20:ARG:HH11	2:B:20:ARG:HG2	1.86	0.41
7:G:224:LEU:HB3	7:G:228:ASN:HB2	2.03	0.41
2:B:211:GLU:HA	16:B:265:HOH:O	2.21	0.41
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.56	0.41
8:H:2:THR:OG1	8:H:130:GLY:HA3	2.20	0.41
6:T:147:HIS:HD2	16:T:282:HOH:O	2.04	0.41
4:D:117:CYS:O	4:D:120:ALA:HB3	2.20	0.41
12:Z:9:GLU:O	12:Z:107:LYS:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:24:ILE:HG13	10:J:24:ILE:O	2.21	0.41
7:G:17(C):LYS:HB2	7:G:17(C):LYS:HE3	1.87	0.41
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.51	0.41
12:L:17:ASP:HA	12:L:172:GLY:O	2.21	0.41
11:K:173:VAL:O	11:K:189:ASN:HA	2.21	0.41
1:O:162:ALA:O	2:P:58:LEU:HD23	2.21	0.41
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.34	0.41
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.21	0.41
7:G:203:THR:HG22	7:G:204:GLU:O	2.21	0.41
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.51	0.41
12:L:166:HIS:CD2	12:L:168:GLN:H	2.29	0.41
2:P:5:SER:O	2:P:7:ARG:N	2.54	0.41
10:X:191:GLN:O	10:X:192:ALA:HB2	2.20	0.41
13:O:39:ASP:N	13:O:39:ASP:OD2	2.53	0.41
4:D:97:VAL:HG21	11:K:65:LEU:HD13	2.02	0.41
8:H:175:VAL:CG1	8:H:176:CYS:N	2.84	0.41
8:H:25:ILE:N	8:H:25:ILE:HD12	2.36	0.41
1:O:136:LEU:O	1:O:150:GLN:HA	2.21	0.41
9:W:14:ILE:HG12	9:W:34:ILE:CD1	2.51	0.41
1:A:46:VAL:HG11	1:A:139:ALA:HB1	2.03	0.41
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.56	0.41
10:J:46:ALA:HA	16:J:212:HOH:O	2.21	0.41
6:T:187:ARG:NH1	6:T:228:LEU:HD13	2.36	0.41
4:R:107:ILE:HG22	16:R:338:HOH:O	2.20	0.41
12:Z:39:ASP:OD2	12:Z:67:HIS:HE1	2.04	0.41
2:B:28:LEU:HA	2:B:31:ILE:HG13	2.03	0.41
5:E:13:VAL:HG13	5:E:13:VAL:O	2.21	0.41
14:1:107:LYS:CG	14:1:108:GLY:N	2.54	0.40
3:C:100:ARG:HH12	3:C:106:PRO:HB3	1.74	0.40
6:F:95:GLU:HG2	6:F:115:ARG:CB	2.49	0.40
6:T:196:ILE:HG12	6:T:196:ILE:H	1.72	0.40
10:X:103:GLY:HA2	10:X:178:VAL:HG11	2.03	0.40
6:T:205:ASN:C	6:T:20(B):GLU:H	2.24	0.40
1:O:26:TYR:O	1:O:29:THR:HB	2.20	0.40
9:W:7:THR:HG23	9:W:110:ILE:HD13	2.03	0.40
5:S:4:PHE:CD2	5:S:5:ARG:N	2.89	0.40
15:V:7710:SRG:N17	15:V:7710:SRG:H13B	2.36	0.40
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	2.02	0.40
7:G:8:TYR:C	7:G:10:ARG:N	2.75	0.40
13:M:133:MET:O	13:M:136:PRO:HD2	2.21	0.40
10:J:168:MET:CE	10:X:168:MET:HG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:82:ILE:HG22	7:U:83:PRO:HD3	2.03	0.40
10:X:14:LEU:HD12	10:X:42:LEU:HD23	2.03	0.40
8:H:200:LYS:HE3	9:I:140:SER:O	2.21	0.40
9:I:34:ILE:HB	16:I:243:HOH:O	2.21	0.40
8:H:3:ILE:HG22	8:H:16:ALA:HB2	2.03	0.40
1:O:13:THR:O	2:P:130:ARG:HD3	2.21	0.40
8:V:34:LEU:HD22	8:V:174:ASP:HB3	2.02	0.40
5:E:86:ARG:O	5:E:90:ASN:HB2	2.21	0.40
8:V:72:ARG:NH1	8:V:72:ARG:HG3	2.32	0.40
7:U:224:LEU:HB3	7:U:228:ASN:HB2	2.02	0.40
12:L:153:LYS:HA	8:V:201:GLN:HG2	2.02	0.40
6:T:172:ALA:O	6:T:176:LEU:CD2	2.69	0.40
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.36	0.40
14:1:3:ILE:HB	14:1:44:CYS:HB3	2.03	0.40
11:K:147:SER:O	11:K:150:ASP:N	2.54	0.40
12:Z:99:THR:CG2	16:Z:201:HOH:O	2.69	0.40
11:Y:147:SER:O	11:Y:149:GLU:N	2.54	0.40
4:D:135:ALA:O	4:D:136:LEU:HD23	2.22	0.40
8:H:137:VAL:HG21	8:H:161:ALA:HB2	2.03	0.40
7:G:151:THR:HG22	7:G:157:TYR:HB2	2.03	0.40
12:Z:151:VAL:O	12:Z:155:VAL:HG23	2.21	0.40
9:I:93:GLY:N	9:I:94:PRO:CD	2.85	0.40
1:O:46:VAL:HG11	1:O:139:ALA:HB1	2.03	0.40
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.56	0.40
1:O:121:GLN:CG	2:P:83:ALA:HB1	2.52	0.40
2:B:184:MET:HE3	2:B:188:ASP:HB3	2.04	0.40
6:F:35:THR:CG2	6:F:36:THR:N	2.84	0.40
12:L:4:LEU:HD13	12:L:138:LEU:HD21	2.01	0.40
4:R:121:LEU:HA	4:R:123:PHE:HE1	1.86	0.40
9:I:7:THR:HG23	9:I:110:ILE:HD13	2.03	0.40
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	2.03	0.40
14:1:18(G):TYR:HA	14:1:18(J):LEU:HG	2.03	0.40
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.56	0.40
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.55	0.40
8:V:5:GLY:O	8:V:124:TYR:HA	2.21	0.40
12:L:22:THR:O	12:L:23:ASP:HB2	2.21	0.40
3:C:120:GLN:O	3:C:124:THR:HG23	2.22	0.40
14:N:32:ASP:OD1	14:N:186:ARG:NH2	2.52	0.40
4:R:219:ASP:O	4:R:222:LYS:HE2	2.21	0.40
5:E:189:LEU:HA	5:E:189:LEU:HD23	1.86	0.40
3:Q:97:GLN:NE2	3:Q:97:GLN:HA	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:205:SER:C	11:Y:207:ASN:N	2.72	0.40
2:P:66:LYS:O	2:P:77:ALA:HA	2.21	0.40
15:H:7710:SRG:H13B	15:H:7710:SRG:N17	2.37	0.40
12:Z:148:VAL:HG13	12:Z:149:GLU:N	2.36	0.40
14:I:65:LEU:HG	14:I:69:GLN:HE21	1.86	0.40
11:K:145:ASP:C	11:K:146:LEU:HD12	2.41	0.40
13:O:91:ARG:HG3	13:O:92:SER:N	2.36	0.40
2:B:173:GLN:HG2	3:C:56:LEU:HD12	2.04	0.40
7:G:119:LEU:HD12	7:G:119:LEU:HA	1.88	0.40
12:L:83:ILE:HB	12:L:113:PHE:CE2	2.57	0.40
10:X:112:GLN:HE22	10:X:126:ALA:H	1.69	0.40
1:O:31:VAL:HG11	1:O:135:SER:HB2	2.03	0.40
3:C:58:LEU:HD12	3:C:58:LEU:HA	1.88	0.40
2:B:107:ILE:HA	2:B:108:PRO:HD3	1.98	0.40
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.85	0.40
4:R:117:CYS:O	4:R:120:ALA:HB3	2.21	0.40
5:E:97:ASN:HA	5:E:97:ASN:HD22	1.70	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	248/250 (99%)	232 (94%)	15 (6%)	1 (0%)	39	74
1	O	248/250 (99%)	233 (94%)	14 (6%)	1 (0%)	39	74
2	B	242/258 (94%)	219 (90%)	19 (8%)	4 (2%)	11	38
2	P	242/258 (94%)	218 (90%)	20 (8%)	4 (2%)	11	38
3	C	239/254 (94%)	218 (91%)	17 (7%)	4 (2%)	11	38
3	Q	239/254 (94%)	219 (92%)	17 (7%)	3 (1%)	15	46
4	D	240/260 (92%)	215 (90%)	19 (8%)	6 (2%)	7	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	240/260 (92%)	215 (90%)	19 (8%)	6 (2%)	7	27
5	E	231/234 (99%)	210 (91%)	16 (7%)	5 (2%)	8	31
5	S	231/234 (99%)	211 (91%)	15 (6%)	5 (2%)	8	31
6	F	242/287 (84%)	230 (95%)	10 (4%)	2 (1%)	24	60
6	T	242/287 (84%)	230 (95%)	10 (4%)	2 (1%)	24	60
7	G	241/252 (96%)	226 (94%)	14 (6%)	1 (0%)	39	74
7	U	241/252 (96%)	227 (94%)	13 (5%)	1 (0%)	39	74
8	H	220/232 (95%)	204 (93%)	14 (6%)	2 (1%)	21	57
8	V	220/232 (95%)	207 (94%)	12 (6%)	1 (0%)	34	71
9	I	202/205 (98%)	188 (93%)	13 (6%)	1 (0%)	34	71
9	W	202/205 (98%)	187 (93%)	14 (7%)	1 (0%)	34	71
10	J	196/198 (99%)	181 (92%)	11 (6%)	4 (2%)	9	33
10	X	196/198 (99%)	182 (93%)	10 (5%)	4 (2%)	9	33
11	K	210/212 (99%)	196 (93%)	11 (5%)	3 (1%)	14	44
11	Y	210/212 (99%)	196 (93%)	11 (5%)	3 (1%)	14	44
12	L	220/241 (91%)	208 (94%)	11 (5%)	1 (0%)	34	71
12	Z	220/241 (91%)	209 (95%)	11 (5%)	0	100	100
13	O	231/266 (87%)	215 (93%)	15 (6%)	1 (0%)	39	74
13	M	231/266 (87%)	216 (94%)	14 (6%)	1 (0%)	39	74
14	1	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6312/6690 (94%)	5867 (93%)	378 (6%)	67 (1%)	17	51

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
3	C	58	LEU
3	C	203	THR
4	D	12(G)	GLU
10	J	192	ALA
1	O	5	THR
3	Q	58	LEU
3	Q	203	THR
4	R	12(G)	GLU

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Mol	Chain	Res	Type
10	X	192	ALA
2	B	21(B)	GLY
2	B	21(C)	ASP
4	D	12(E)	SER
4	D	128	MET
4	D	18(D)	SER
5	E	180	LEU
8	H	9	ASN
10	J	8	VAL
2	P	6	ARG
2	P	21(B)	GLY
2	P	21(C)	ASP
4	R	12(E)	SER
4	R	18(D)	SER
5	S	180	LEU
8	V	9	ASN
10	X	8	VAL
2	B	6	ARG
3	C	183	PRO
4	D	12(F)	GLY
5	E	202	ARG
6	F	205	ASN
6	F	206	LYS
7	G	220	LYS
10	J	132	PHE
13	M	2	SER
3	Q	183	PRO
4	R	128	MET
5	S	202	ARG
5	S	217	LYS
6	T	205	ASN
6	T	206	LYS
7	U	220	LYS
10	X	132	PHE
2	B	54	VAL
5	E	5	ARG
5	E	203	ASP
5	E	217	LYS
12	L	71	ASP
2	P	54	VAL
4	R	12(F)	GLY
5	S	5	ARG

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Mol	Chain	Res	Type
5	S	203	ASP
11	K	39	PRO
11	K	208	ASN
11	K	209	VAL
11	Y	208	ASN
11	Y	209	VAL
13	O	2	SER
8	H	91	GLN
10	J	191	GLN
10	X	191	GLN
11	Y	39	PRO
4	D	12(C)	GLY
9	I	93	GLY
4	R	12(C)	GLY
9	W	93	GLY
3	C	206	GLY

### 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	209/209 (100%)	203 (97%)	6 (3%)	50	83
1	O	209/209 (100%)	203 (97%)	6 (3%)	50	83
2	B	203/216 (94%)	191 (94%)	12 (6%)	24	58
2	P	203/216 (94%)	190 (94%)	13 (6%)	22	53
3	C	213/226 (94%)	204 (96%)	9 (4%)	36	73
3	Q	213/226 (94%)	203 (95%)	10 (5%)	32	68
4	D	198/215 (92%)	189 (96%)	9 (4%)	34	70
4	R	198/215 (92%)	190 (96%)	8 (4%)	38	74
5	E	192/193 (100%)	172 (90%)	20 (10%)	9	26
5	S	192/193 (100%)	172 (90%)	20 (10%)	9	26
6	F	201/238 (84%)	186 (92%)	15 (8%)	17	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	201/238 (84%)	187 (93%)	14 (7%)	19	47
7	G	207/210 (99%)	194 (94%)	13 (6%)	22	54
7	U	207/210 (99%)	195 (94%)	12 (6%)	25	58
8	H	181/190 (95%)	174 (96%)	7 (4%)	39	75
8	V	181/190 (95%)	174 (96%)	7 (4%)	39	75
9	I	172/173 (99%)	165 (96%)	7 (4%)	37	73
9	W	172/173 (99%)	165 (96%)	7 (4%)	37	73
10	J	175/175 (100%)	169 (97%)	6 (3%)	44	79
10	X	175/175 (100%)	168 (96%)	7 (4%)	38	74
11	K	169/169 (100%)	158 (94%)	11 (6%)	21	52
11	Y	169/169 (100%)	157 (93%)	12 (7%)	18	47
12	L	185/201 (92%)	171 (92%)	14 (8%)	16	43
12	Z	185/201 (92%)	170 (92%)	15 (8%)	15	39
13	O	199/224 (89%)	190 (96%)	9 (4%)	34	70
13	M	199/224 (89%)	190 (96%)	9 (4%)	34	70
14	I	162/162 (100%)	152 (94%)	10 (6%)	23	55
14	N	162/162 (100%)	153 (94%)	9 (6%)	26	60
All	All	5332/5602 (95%)	5035 (94%)	297 (6%)	26	60

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	124	THR
1	A	158	PHE
1	A	179	ARG
1	A	214	ILE
2	B	31	ILE
2	B	58	LEU
2	B	71	ASN
2	B	91	THR
2	B	121	GLN
2	B	150	THR
2	B	185	LYS
2	B	192	LEU

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Mol	Chain	Res	Type
2	B	206	THR
2	B	218	ASN
2	B	221	GLN
2	B	224	PHE
3	C	10	ARG
3	C	57	LYS
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	172	VAL
3	C	174	GLU
3	C	208	LYS
3	C	227	GLU
4	D	12	VAL
4	D	28	LEU
4	D	76	CYS
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	194	LEU
4	D	237	LEU
4	D	244	GLU
5	E	12	THR
5	E	13	VAL
5	E	32	LYS
5	E	56	ASP
5	E	57	GLU
5	E	64	GLN
5	E	76	LEU
5	E	90	ASN
5	E	97	ASN
5	E	104	ASN
5	E	111	ARG
5	E	121	GLN
5	E	18(D)	ILE
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	2(C)	VAL
5	E	227	GLU
5	E	231	LYS

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Mol	Chain	Res	Type
6	F	11	SER
6	F	35	THR
6	F	43	ASN
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
6	F	135	SER
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
6	F	225	LYS
7	G	33	GLN
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	169	GLN
7	G	172	ILE
7	G	184	ASN
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	240	ASP
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	144	GLN
8	H	197	ARG
8	H	223	ASP
9	I	2	ILE
9	I	29	ASN
9	I	90	ARG
9	I	113	PHE
9	I	115	LEU
9	I	160	LEU
9	I	171	TRP

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Mol	Chain	Res	Type
10	J	3	ILE
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	121	GLU
10	J	168	MET
11	K	4	LEU
11	K	8	PHE
11	K	9	GLN
11	K	65	LEU
11	K	69	ARG
11	K	99	THR
11	K	100	MET
11	K	104	TYR
11	K	10(B)	LYS
11	K	129	SER
11	K	181	ASP
12	L	-7	ASN
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	43	MET
12	L	58	ARG
12	L	70(A)	ASN
12	L	99	THR
12	L	106	GLU
12	L	114	ASP
12	L	120	GLU
12	L	123	GLN
12	L	138	LEU
12	L	145	TYR
13	M	40	ASN
13	M	62	LEU
13	M	71(A)	ASP
13	M	91	ARG
13	M	115	LEU
13	M	14(C)	ARG
13	M	149	GLN
13	M	191	GLN
13	M	204	LYS
14	N	70	TYR
14	N	84	LYS

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Mol	Chain	Res	Type
14	N	89	GLU
14	N	105	ASP
14	N	10(A)	ASP
14	N	115	LEU
14	N	119	VAL
14	N	18(A)	ILE
14	N	18(I)	GLN
1	O	33	GLN
1	O	64	LEU
1	O	124	THR
1	O	158	PHE
1	O	179	ARG
1	O	214	ILE
2	P	31	ILE
2	P	41	MET
2	P	58	LEU
2	P	71	ASN
2	P	91	THR
2	P	121	GLN
2	P	150	THR
2	P	185	LYS
2	P	192	LEU
2	P	206	THR
2	P	218	ASN
2	P	221	GLN
2	P	224	PHE
3	Q	10	ARG
3	Q	57	LYS
3	Q	59	GLN
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	172	VAL
3	Q	174	GLU
3	Q	208	LYS
3	Q	227	GLU
4	R	12	VAL
4	R	28	LEU
4	R	76	CYS
4	R	126	ARG
4	R	170	GLU
4	R	177	LEU

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Mol	Chain	Res	Type
4	R	237	LEU
4	R	244	GLU
5	S	12	THR
5	S	13	VAL
5	S	32	LYS
5	S	56	ASP
5	S	57	GLU
5	S	64	GLN
5	S	76	LEU
5	S	90	ASN
5	S	97	ASN
5	S	104	ASN
5	S	111	ARG
5	S	121	GLN
5	S	18(D)	ILE
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	2(C)	VAL
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	35	THR
6	T	43	ASN
6	T	98	SER
6	T	105	THR
6	T	121	GLN
6	T	127	ASN
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
6	T	225	LYS
7	U	33	GLN
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR

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Mol	Chain	Res	Type
7	U	128	TYR
7	U	169	GLN
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	240	ASP
8	V	30	ASN
8	V	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	144	GLN
8	V	197	ARG
8	V	223	ASP
9	W	2	ILE
9	W	29	ASN
9	W	90	ARG
9	W	113	PHE
9	W	115	LEU
9	W	160	LEU
9	W	171	TRP
10	X	3	ILE
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	121	GLU
10	X	140	HIS
10	X	168	MET
11	Y	4	LEU
11	Y	8	PHE
11	Y	9	GLN
11	Y	65	LEU
11	Y	69	ARG
11	Y	99	THR
11	Y	100	MET
11	Y	104	TYR
11	Y	10(B)	LYS
11	Y	129	SER
11	Y	181	ASP
11	Y	208	ASN
12	Z	-7	ASN
12	Z	14	LEU
12	Z	25	SER

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Mol	Chain	Res	Type
12	Z	40	ASN
12	Z	43	MET
12	Z	58	ARG
12	Z	70(A)	ASN
12	Z	99	THR
12	Z	106	GLU
12	Z	114	ASP
12	Z	120	GLU
12	Z	123	GLN
12	Z	138	LEU
12	Z	1(I)	ASN
12	Z	145	TYR
13	0	40	ASN
13	0	62	LEU
13	0	71(A)	ASP
13	0	91	ARG
13	0	115	LEU
13	0	14(C)	ARG
13	0	149	GLN
13	0	191	GLN
13	0	204	LYS
14	1	36	ARG
14	1	70	TYR
14	1	84	LYS
14	1	89	GLU
14	1	105	ASP
14	1	10(A)	ASP
14	1	115	LEU
14	1	119	VAL
14	1	18(A)	ILE
14	1	18(I)	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (200) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN

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Mol	Chain	Res	Type
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	238	GLN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	73	HIS
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	156	ASN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	87	HIS
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
6	F	237	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN

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Mol	Chain	Res	Type
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	18(C)	HIS
7	G	184	ASN
7	G	228	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
9	I	81	GLN
10	J	54	GLN
10	J	64	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	186	GLN
11	K	85	ASN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	85	HIS
12	L	1(I)	ASN
12	L	166	HIS
13	M	-7	GLN
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	132	HIS
13	M	149	GLN

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Mol	Chain	Res	Type
13	M	157	ASN
13	M	191	GLN
14	N	69	GLN
14	N	141	ASN
14	N	145	ASN
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	238	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	211	GLN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	73	HIS
5	S	97	ASN
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	156	ASN
5	S	199	GLN

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Mol	Chain	Res	Type
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	87	HIS
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	192	GLN
6	T	237	GLN
7	U	11	HIS
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	18(C)	HIS
7	U	184	ASN
7	U	228	ASN
8	V	30	ASN
8	V	66	HIS
8	V	91	GLN
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	64	ASN
9	W	81	GLN
10	X	54	GLN
10	X	64	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	186	GLN
10	X	193	GLN
11	Y	85	ASN
11	Y	174	ASN
11	Y	207	ASN
11	Y	208	ASN

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Mol	Chain	Res	Type
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	85	HIS
12	Z	1(I)	ASN
12	Z	166	HIS
13	0	-7	GLN
13	0	10	ASN
13	0	40	ASN
13	0	89	GLN
13	0	93	ASN
13	0	132	HIS
13	0	149	GLN
13	0	157	ASN
13	0	191	GLN
14	1	60	GLN
14	1	69	GLN
14	1	141	ASN
14	1	145	ASN
14	1	157	HIS
14	1	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	SRG	1	7710	14	31,35,35	2.19	4 (12%)	31,47,47	1.84	6 (19%)
15	SRG	H	7710	8	31,35,35	2.38	6 (19%)	31,47,47	2.00	6 (19%)
15	SRG	K	7710	11	31,35,35	2.50	6 (19%)	31,47,47	1.96	7 (22%)
15	SRG	N	7710	14	31,35,35	2.15	5 (16%)	31,47,47	1.91	6 (19%)
15	SRG	V	7710	8	31,35,35	2.31	5 (16%)	31,47,47	2.03	6 (19%)
15	SRG	Y	7710	11	31,35,35	2.46	7 (22%)	31,47,47	1.99	6 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SRG	1	7710	14	-	2/49/53/53	0/0/1/1
15	SRG	H	7710	8	-	2/49/53/53	0/0/1/1
15	SRG	K	7710	11	-	2/49/53/53	0/0/1/1
15	SRG	N	7710	14	-	2/49/53/53	0/0/1/1
15	SRG	V	7710	8	-	2/49/53/53	0/0/1/1
15	SRG	Y	7710	11	-	2/49/53/53	0/0/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	7710	SRG	C22-N21	-2.45	1.43	1.46
15	Y	7710	SRG	C22-C26	2.04	1.55	1.49
15	Y	7710	SRG	C18-C34	2.19	1.56	1.50
15	K	7710	SRG	C18-C34	2.35	1.56	1.50
15	N	7710	SRG	C27-C28	2.56	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	1	7710	SRG	C27-C28	2.56	1.53	1.48
15	Y	7710	SRG	C27-C28	2.66	1.53	1.48
15	N	7710	SRG	C23-C22	2.76	1.57	1.54
15	K	7710	SRG	C27-C28	2.96	1.54	1.48
15	V	7710	SRG	C27-C28	3.02	1.54	1.48
15	N	7710	SRG	C31-C32	3.02	1.56	1.53
15	1	7710	SRG	C31-C32	3.03	1.56	1.53
15	H	7710	SRG	C23-C22	3.36	1.58	1.54
15	N	7710	SRG	C28-N30	3.41	1.39	1.34
15	V	7710	SRG	C28-N30	3.55	1.39	1.34
15	H	7710	SRG	C28-N30	3.55	1.39	1.34
15	V	7710	SRG	C23-C22	3.72	1.58	1.54
15	H	7710	SRG	C27-C28	3.75	1.55	1.48
15	1	7710	SRG	C28-N30	3.81	1.39	1.34
15	V	7710	SRG	C31-C32	3.83	1.57	1.53
15	Y	7710	SRG	C23-C22	3.83	1.58	1.54
15	Y	7710	SRG	C28-N30	3.96	1.39	1.34
15	K	7710	SRG	C28-N30	4.10	1.40	1.34
15	H	7710	SRG	C31-C32	4.17	1.57	1.53
15	K	7710	SRG	C23-C22	4.20	1.59	1.54
15	K	7710	SRG	C31-C32	4.75	1.58	1.53
15	Y	7710	SRG	C31-C32	4.95	1.58	1.53
15	N	7710	SRG	C27-C26	9.60	1.57	1.32
15	V	7710	SRG	C27-C26	9.89	1.58	1.32
15	1	7710	SRG	C27-C26	9.90	1.58	1.32
15	H	7710	SRG	C27-C26	10.06	1.59	1.32
15	K	7710	SRG	C27-C26	10.08	1.59	1.32
15	Y	7710	SRG	C27-C26	10.17	1.59	1.32

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	7710	SRG	C1-C3-N7	-4.70	104.09	113.51
15	H	7710	SRG	O29-C28-N30	-4.26	117.05	122.53
15	K	7710	SRG	C1-C3-N7	-4.25	104.98	113.51
15	1	7710	SRG	C1-C3-N7	-4.22	105.06	113.51
15	Y	7710	SRG	C1-C3-N7	-4.14	105.21	113.51
15	V	7710	SRG	O29-C28-N30	-3.93	117.47	122.53
15	1	7710	SRG	O29-C28-C27	-3.79	115.72	123.01
15	Y	7710	SRG	O29-C28-C27	-3.78	115.73	123.01
15	N	7710	SRG	O29-C28-N30	-3.74	117.71	122.53
15	V	7710	SRG	O29-C28-C27	-3.73	115.83	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	7710	SRG	C1-C3-N7	-3.72	106.05	113.51
15	K	7710	SRG	O29-C28-C27	-3.65	115.98	123.01
15	V	7710	SRG	C1-C3-N7	-3.63	106.23	113.51
15	N	7710	SRG	O29-C28-C27	-3.59	116.09	123.01
15	K	7710	SRG	O29-C28-N30	-3.50	118.02	122.53
15	Y	7710	SRG	O29-C28-N30	-3.50	118.03	122.53
15	1	7710	SRG	O29-C28-N30	-3.45	118.09	122.53
15	H	7710	SRG	O29-C28-C27	-3.31	116.64	123.01
15	N	7710	SRG	C5-C4-C3	-2.88	108.67	111.30
15	V	7710	SRG	C5-C4-C3	-2.78	108.76	111.30
15	Y	7710	SRG	C5-C4-C3	-2.64	108.89	111.30
15	H	7710	SRG	C5-C4-C3	-2.62	108.91	111.30
15	K	7710	SRG	C5-C4-C3	-2.18	109.31	111.30
15	1	7710	SRG	C5-C4-C3	-2.13	109.35	111.30
15	K	7710	SRG	C32-C31-N30	2.08	113.47	110.16
15	N	7710	SRG	C31-N30-C28	4.29	128.83	122.41
15	1	7710	SRG	C31-N30-C28	4.37	128.96	122.41
15	K	7710	SRG	C31-N30-C28	4.38	128.97	122.41
15	H	7710	SRG	C31-N30-C28	4.62	129.33	122.41
15	Y	7710	SRG	C31-N30-C28	4.65	129.38	122.41
15	V	7710	SRG	C31-N30-C28	4.67	129.40	122.41
15	K	7710	SRG	C27-C28-N30	4.83	125.99	114.87
15	1	7710	SRG	C27-C28-N30	4.91	126.19	114.87
15	N	7710	SRG	C27-C28-N30	4.92	126.20	114.87
15	Y	7710	SRG	C27-C28-N30	4.94	126.25	114.87
15	H	7710	SRG	C27-C28-N30	4.97	126.32	114.87
15	V	7710	SRG	C27-C28-N30	5.13	126.70	114.87

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	Y	7710	SRG	O29-C28-N30-C31
15	H	7710	SRG	O29-C28-N30-C31
15	H	7710	SRG	C27-C28-N30-C31
15	Y	7710	SRG	C27-C28-N30-C31
15	N	7710	SRG	C27-C28-N30-C31
15	1	7710	SRG	C27-C28-N30-C31
15	K	7710	SRG	O29-C28-N30-C31
15	V	7710	SRG	C27-C28-N30-C31
15	1	7710	SRG	O29-C28-N30-C31
15	K	7710	SRG	C27-C28-N30-C31

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Mol	Chain	Res	Type	Atoms
15	N	7710	SRG	O29-C28-N30-C31
15	V	7710	SRG	O29-C28-N30-C31

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	1	7710	SRG	3	0
15	H	7710	SRG	3	0
15	K	7710	SRG	2	0
15	N	7710	SRG	3	0
15	V	7710	SRG	3	0
15	Y	7710	SRG	2	0

## 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	250/250 (100%)	-0.27	2 (0%)	87 86	32, 46, 76, 99	0
1	O	250/250 (100%)	-0.21	8 (3%)	51 43	31, 48, 77, 99	0
2	B	244/258 (94%)	-0.05	11 (4%)	37 31	32, 49, 83, 112	0
2	P	244/258 (94%)	0.00	16 (6%)	22 16	33, 50, 84, 111	0
3	C	241/254 (94%)	0.11	16 (6%)	22 16	34, 54, 103, 116	0
3	Q	241/254 (94%)	0.26	26 (10%)	8 4	35, 55, 104, 116	0
4	D	242/260 (93%)	0.05	12 (4%)	32 26	35, 52, 85, 115	0
4	R	242/260 (93%)	0.05	12 (4%)	32 26	34, 53, 85, 115	0
5	E	233/234 (99%)	-0.15	4 (1%)	73 70	35, 53, 79, 104	0
5	S	233/234 (99%)	-0.22	8 (3%)	49 41	36, 52, 79, 104	0
6	F	244/287 (85%)	-0.32	8 (3%)	50 42	30, 45, 84, 99	0
6	T	244/287 (85%)	-0.35	5 (2%)	68 64	29, 45, 83, 99	0
7	G	243/252 (96%)	-0.31	6 (2%)	61 55	26, 41, 68, 107	0
7	U	243/252 (96%)	-0.30	6 (2%)	61 55	25, 41, 69, 107	0
8	H	222/232 (95%)	-0.48	3 (1%)	78 76	26, 38, 59, 87	0
8	V	222/232 (95%)	-0.57	3 (1%)	78 76	27, 39, 58, 87	0
9	I	204/205 (99%)	-0.58	2 (0%)	84 82	29, 41, 57, 75	0
9	W	204/205 (99%)	-0.52	3 (1%)	76 74	29, 41, 58, 74	0
10	J	198/198 (100%)	-0.27	5 (2%)	61 55	31, 45, 62, 115	0
10	X	198/198 (100%)	-0.27	5 (2%)	61 55	30, 45, 62, 116	0
11	K	212/212 (100%)	-0.34	4 (1%)	70 66	28, 43, 65, 72	0
11	Y	212/212 (100%)	-0.37	6 (2%)	56 50	31, 44, 64, 72	0
12	L	222/241 (92%)	-0.43	4 (1%)	71 68	27, 41, 62, 84	0
12	Z	222/241 (92%)	-0.43	5 (2%)	64 59	28, 41, 62, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	0	233/266 (87%)	-0.53	1 (0%)	93	92	27, 38, 51, 57	0
13	M	233/266 (87%)	-0.54	1 (0%)	93	92	28, 39, 52, 59	0
14	1	196/196 (100%)	-0.53	1 (0%)	91	90	25, 36, 54, 73	0
14	N	196/196 (100%)	-0.54	2 (1%)	84	82	26, 35, 55, 72	0
All	All	6368/6690 (95%)	-0.28	185 (2%)	55	49	25, 44, 76, 116	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	55	THR	10.9
4	D	12(D)	ALA	10.6
4	D	12(C)	GLY	9.7
4	R	12(E)	SER	9.2
7	U	240	ASP	8.8
4	D	12(E)	SER	8.6
4	R	12(D)	ALA	8.2
4	R	12(F)	GLY	7.6
10	X	192	ALA	7.5
10	J	191	GLN	7.2
2	B	218	ASN	7.1
7	G	240	ASP	7.1
10	J	192	ALA	7.0
10	X	193	GLN	6.8
3	Q	55	THR	6.8
6	F	5	GLY	6.7
4	R	12(C)	GLY	6.6
2	P	217	ALA	6.4
2	P	218	ASN	6.3
2	B	54	VAL	6.0
10	X	191	GLN	6.0
4	D	12(F)	GLY	5.9
3	C	56	LEU	5.6
7	U	6	ALA	5.6
2	B	217	ALA	5.5
2	P	54	VAL	5.2
1	O	5	THR	5.0
2	P	219	GLU	4.9
10	J	193	GLN	4.9
9	I	-8	SER	4.9
7	G	6	ALA	4.8
5	E	203	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	5	THR	4.6
12	L	145	TYR	4.6
3	Q	56	LEU	4.5
3	Q	243	GLN	4.4
9	W	-8	SER	4.3
1	A	4	MET	4.3
1	O	4	MET	4.2
3	Q	54	SER	4.1
4	D	12(G)	GLU	4.1
6	F	204	ASP	4.1
3	Q	63	THR	4.0
14	1	18(I)	GLN	4.0
1	O	21(P)	LYS	4.0
12	Z	145	TYR	4.0
3	Q	203	THR	4.0
4	R	125	GLU	3.9
4	D	125	GLU	3.9
3	Q	240	LYS	3.9
8	H	222	CYS	3.9
13	M	-8	THR	3.8
4	R	242	ALA	3.8
4	R	12(G)	GLU	3.8
3	Q	242	GLU	3.8
2	P	21(B)	GLY	3.8
3	Q	241	GLN	3.7
8	V	222	CYS	3.7
11	K	181	ASP	3.7
11	Y	181	ASP	3.6
3	Q	223	ALA	3.6
2	P	21(C)	ASP	3.6
3	C	241	GLN	3.6
2	P	21(A)	LYS	3.6
5	S	5	ARG	3.6
13	0	-8	THR	3.6
5	S	4	PHE	3.5
3	Q	64	PRO	3.5
6	F	20(B)	GLU	3.5
3	Q	238	GLN	3.4
2	B	219	GLU	3.4
1	O	53	LYS	3.4
2	B	20(A)	SER	3.3
1	O	235	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
3	Q	202	GLN	3.3
7	G	239	GLN	3.3
4	R	12(B)	GLU	3.2
6	F	206	LYS	3.2
6	F	6	THR	3.2
3	Q	187	GLU	3.1
4	R	126	ARG	3.1
8	V	223	ASP	3.0
4	R	127	LEU	3.0
4	D	126	ARG	3.0
5	E	5	ARG	3.0
4	R	243	ALA	3.0
2	B	21(B)	GLY	3.0
3	Q	14(B)	ASP	2.9
2	P	20(A)	SER	2.9
5	S	203	ASP	2.9
5	E	4	PHE	2.9
7	G	7	GLY	2.9
8	V	220	ASN	2.8
2	B	21(A)	LYS	2.8
7	U	17(E)	LYS	2.8
7	G	8	TYR	2.7
4	D	218	GLN	2.7
2	P	63(A)	SER	2.7
8	H	223	ASP	2.7
11	Y	180	GLU	2.7
9	W	182	ASP	2.7
3	Q	57	LYS	2.7
3	C	234	THR	2.7
2	B	21(C)	ASP	2.7
7	U	239	GLN	2.7
6	T	18(E)	GLU	2.6
5	S	178	ARG	2.6
11	K	180	GLU	2.6
6	T	6	THR	2.6
1	O	55	SER	2.6
3	C	243	GLN	2.6
3	C	240	LYS	2.6
2	P	181	LYS	2.5
4	D	244	GLU	2.5
2	P	53	LYS	2.5
3	C	203	THR	2.5

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Mol	Chain	Res	Type	RSRZ
7	U	8	TYR	2.5
12	L	14(W)	LYS	2.5
9	I	182	ASP	2.5
11	Y	10(A)	ARG	2.5
10	X	189	ASP	2.5
5	S	204	GLU	2.5
5	S	233	ILE	2.5
6	T	240	ILE	2.5
3	Q	225	SER	2.4
3	Q	18(C)	LYS	2.4
2	P	62	ASP	2.4
4	R	244	GLU	2.4
11	K	10(A)	ARG	2.4
6	F	18(E)	GLU	2.4
2	P	183	ASP	2.4
2	P	63	THR	2.4
3	C	18(C)	LYS	2.4
3	C	14(A)	ARG	2.4
4	D	55	THR	2.4
6	F	205	ASN	2.3
8	H	220	ASN	2.3
7	U	7	GLY	2.3
3	C	43	LYS	2.3
12	L	14(P)	PRO	2.3
4	D	12(A)	GLY	2.3
3	Q	222	VAL	2.3
5	S	217	LYS	2.3
11	Y	207	ASN	2.3
6	T	241	ASN	2.3
3	Q	14(A)	ARG	2.3
5	S	127	TYR	2.3
1	O	234	GLU	2.3
6	T	18(D)	PRO	2.3
12	L	70(A)	ASN	2.2
2	B	21(D)	GLY	2.2
2	P	239	THR	2.2
3	C	14(B)	ASP	2.2
4	D	127	LEU	2.2
3	C	57	LYS	2.2
10	J	-1	MET	2.2
3	C	237	GLU	2.2
12	Z	14(W)	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
10	J	92	ARG	2.2
1	O	203	GLU	2.2
12	Z	-9	GLN	2.1
7	G	218	ASP	2.1
3	C	178	LYS	2.1
9	W	181	LYS	2.1
11	Y	145	ASP	2.1
12	Z	70(A)	ASN	2.1
3	Q	18(B)	ARG	2.1
3	Q	65	SER	2.1
3	Q	208	LYS	2.1
14	N	18(I)	GLN	2.1
3	C	227	GLU	2.1
12	Z	96	TYR	2.1
2	B	183	ASP	2.0
3	C	218	ASP	2.0
10	X	145	ASP	2.0
3	Q	170	LYS	2.0
11	K	145	ASP	2.0
5	E	233	ILE	2.0
11	Y	104	TYR	2.0
2	B	20(B)	ALA	2.0
3	Q	178	LYS	2.0
2	P	20(B)	ALA	2.0
3	Q	227	GLU	2.0
14	N	18(J)	LEU	2.0
6	F	241	ASN	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
15	SRG	N	7710	35/35	0.90	0.24	4.19	25,40,59,61	0
15	SRG	1	7710	35/35	0.86	0.25	3.80	25,40,58,61	0
15	SRG	Y	7710	35/35	0.91	0.20	3.66	36,42,47,48	0
15	SRG	H	7710	35/35	0.91	0.22	3.11	34,38,45,47	0
15	SRG	V	7710	35/35	0.92	0.21	2.36	33,39,46,47	0
15	SRG	K	7710	35/35	0.94	0.17	1.57	34,41,47,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.