



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 01:51 am BST

PDB ID : 3DY4  
Title : Crystal structure of yeast 20S proteasome in complex with spirolactacystin  
Authors : Groll, M.; Balskus, E.; Jacobsen, E.  
Deposited on : 2008-07-25  
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

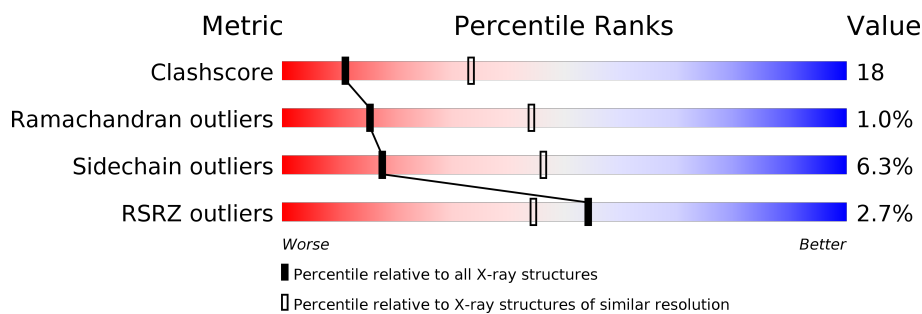
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>2%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>
1	O	250	<div> <div>3%</div> <div>67%</div> <div>32%</div> <div>.</div> </div>
2	B	244	<div> <div>3%</div> <div>59%</div> <div>37%</div> <div>5%</div> </div>
2	P	244	<div> <div>6%</div> <div>57%</div> <div>38%</div> <div>5%</div> </div>
3	C	241	<div> <div>5%</div> <div>57%</div> <div>38%</div> <div>5%</div> </div>
3	Q	241	<div> <div>11%</div> <div>59%</div> <div>37%</div> <div>5%</div> </div>
4	D	242	<div> <div>6%</div> <div>70%</div> <div>26%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50588 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
			1905	1201	321	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	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
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	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
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	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
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	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
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	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			

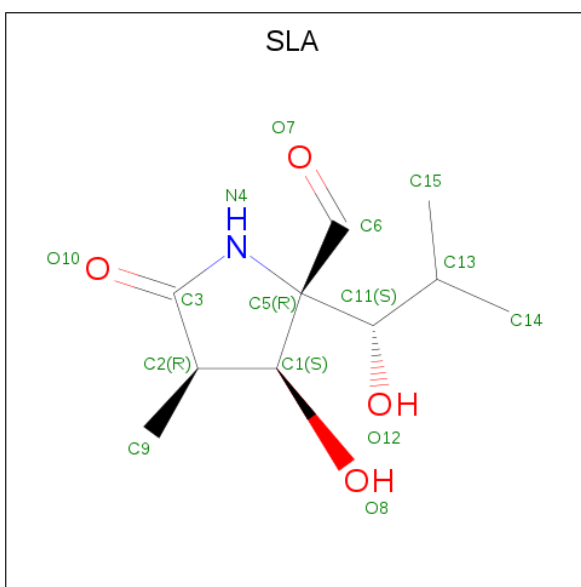
- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	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	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is Omuralide, open form (three-letter code: SLA) (formula: C<sub>10</sub>H<sub>17</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			15	10	1	4		
15	K	1	Total	C	N	O	0	0
			15	10	1	4		
15	V	1	Total	C	N	O	0	0
			15	10	1	4		
15	Y	1	Total	C	N	O	0	0
			15	10	1	4		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	38	Total	O	0	0
			38	38		
16	B	26	Total	O	0	0
			26	26		
16	C	30	Total	O	0	0
			30	30		
16	D	28	Total	O	0	0
			28	28		
16	E	17	Total	O	0	0
			17	17		
16	F	41	Total	O	0	0
			41	41		
16	G	45	Total	O	0	0
			45	45		
16	H	36	Total	O	0	0
			36	36		

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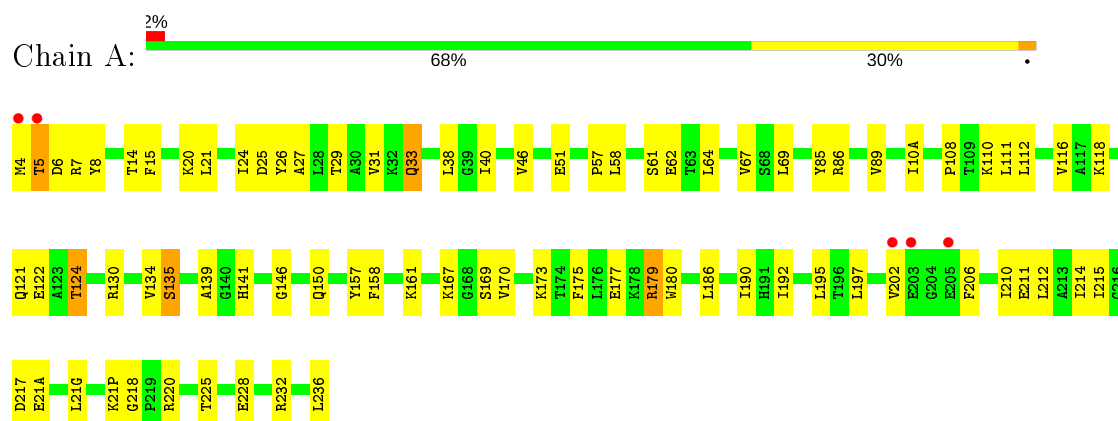
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	I	48	Total 48	O 48	0	0
16	J	33	Total 33	O 33	0	0
16	K	27	Total 27	O 27	0	0
16	L	41	Total 41	O 41	0	0
16	M	54	Total 54	O 54	0	0
16	N	45	Total 45	O 45	0	0
16	O	25	Total 25	O 25	0	0
16	P	19	Total 19	O 19	0	0
16	Q	18	Total 18	O 18	0	0
16	R	21	Total 21	O 21	0	0
16	S	15	Total 15	O 15	0	0
16	T	30	Total 30	O 30	0	0
16	U	50	Total 50	O 50	0	0
16	V	36	Total 36	O 36	0	0
16	W	46	Total 46	O 46	0	0
16	X	36	Total 36	O 36	0	0
16	Y	26	Total 26	O 26	0	0
16	Z	34	Total 34	O 34	0	0
16	1	58	Total 58	O 58	0	0
16	2	57	Total 57	O 57	0	0



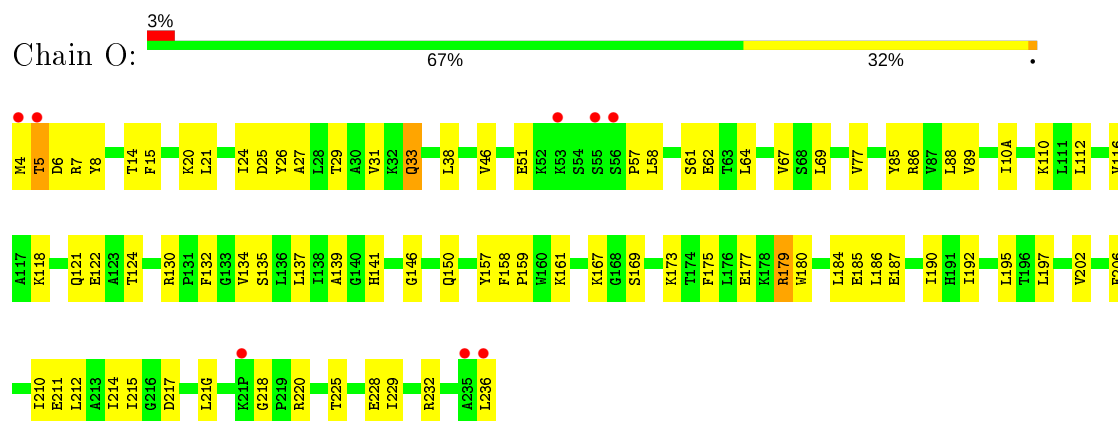
### 3 Residue-property plots [i](#)

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

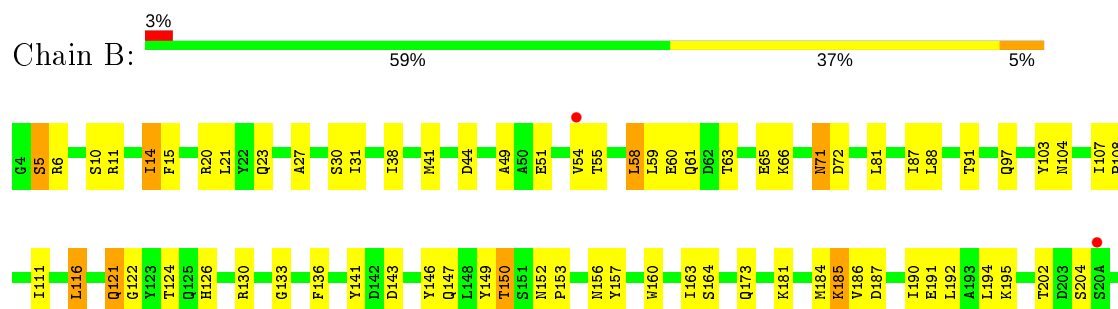
- Molecule 1: Proteasome component Y7



- Molecule 1: Proteasome component Y7

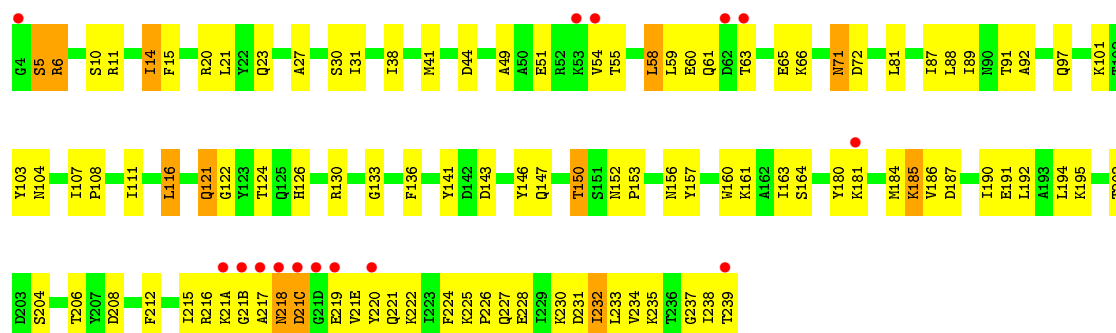


- Molecule 2: Proteasome component Y13

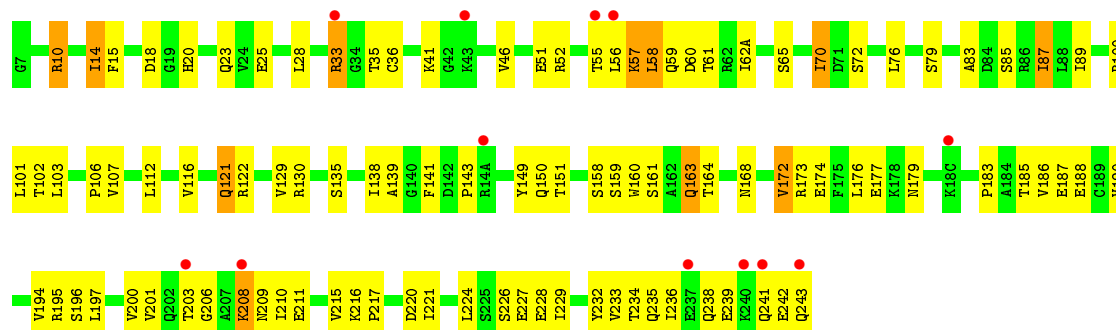




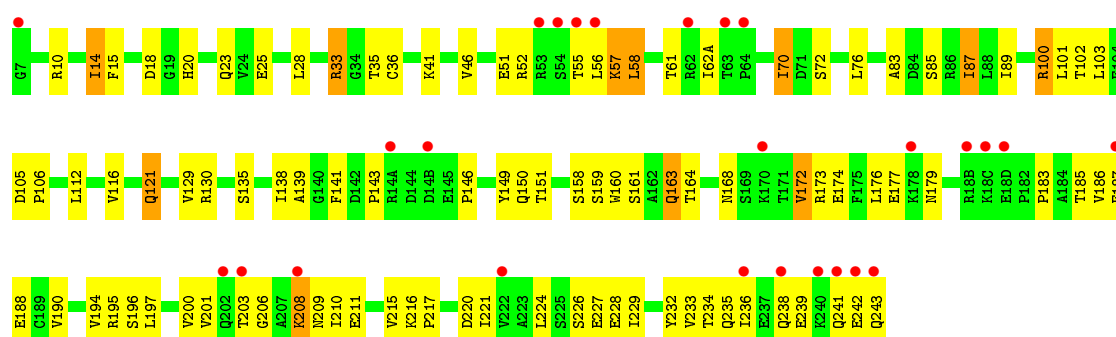
• Molecule 2: Proteasome component Y13



• Molecule 3: Proteasome component PRE6

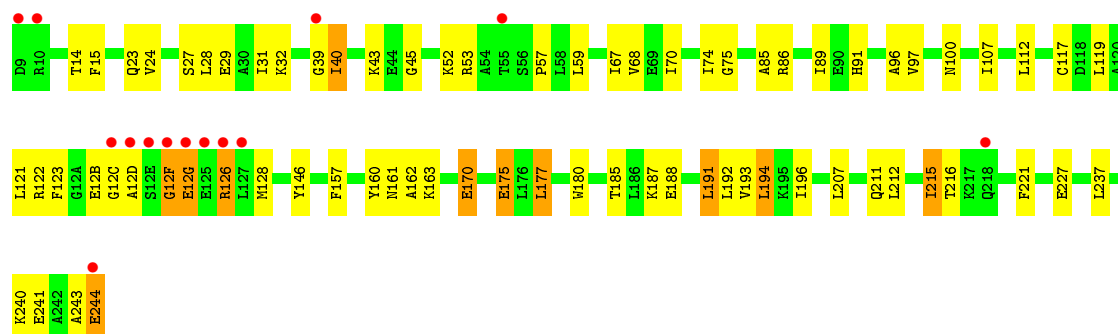


• Molecule 3: Proteasome component PRE6

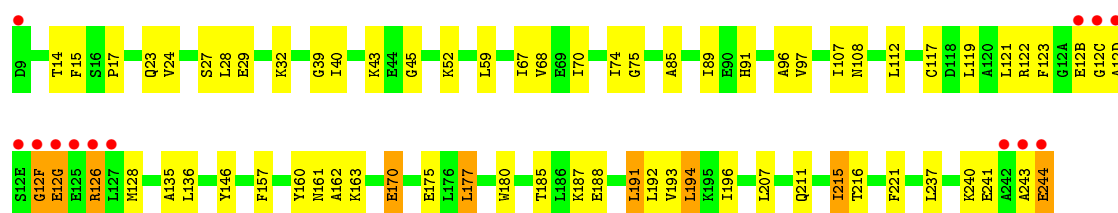


• Molecule 4: Proteasome component PUP2





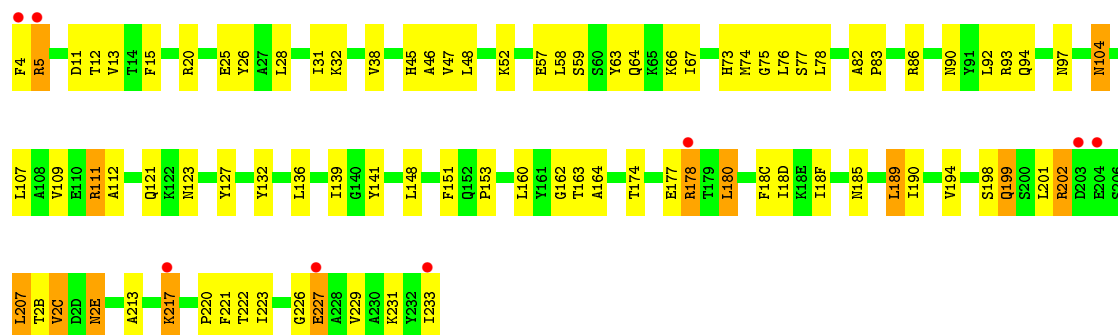
• Molecule 4: Proteasome component PUP2



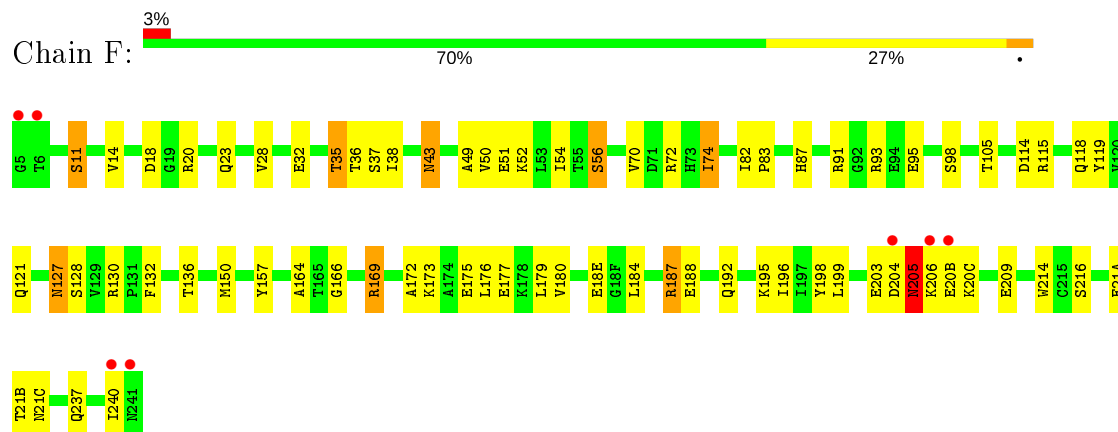
• Molecule 5: Proteasome component PRE5



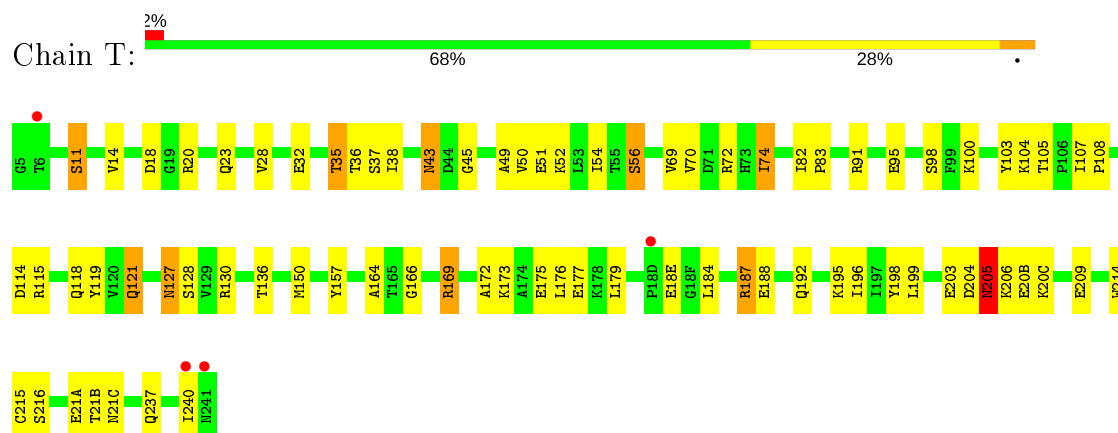
• Molecule 5: Proteasome component PRE5



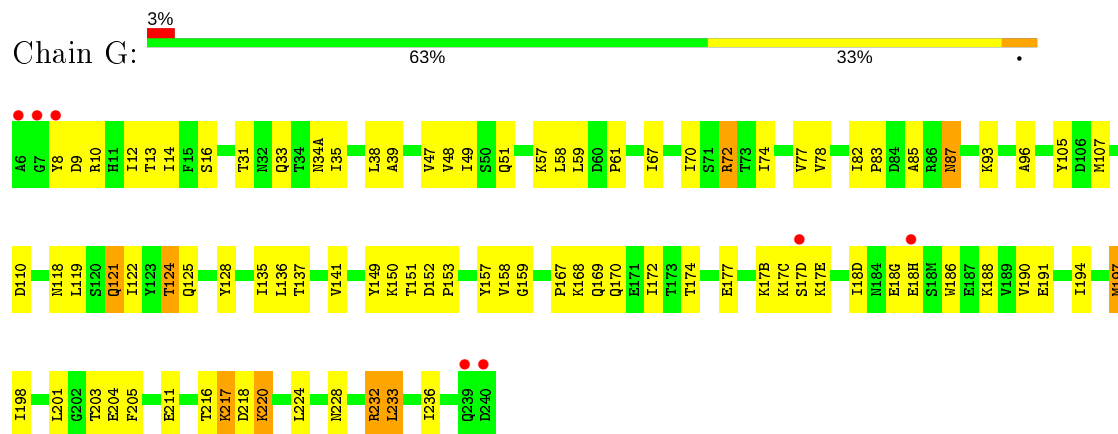
- Molecule 6: Proteasome component C1



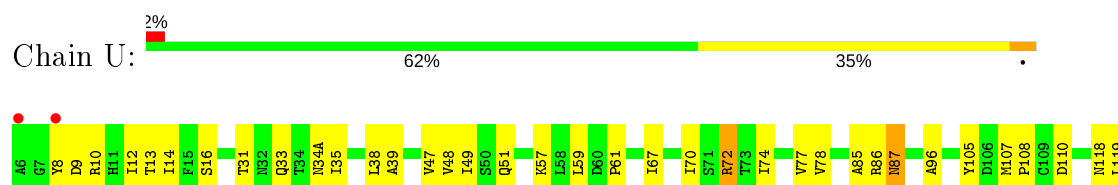
- Molecule 6: Proteasome component C1

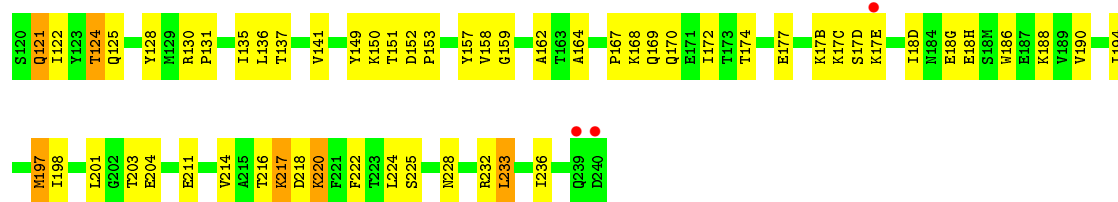


- Molecule 7: Proteasome component C7-alpha

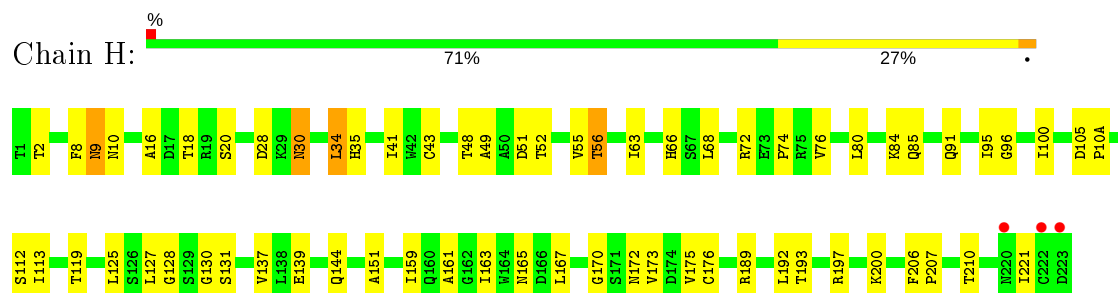


- Molecule 7: Proteasome component C7-alpha

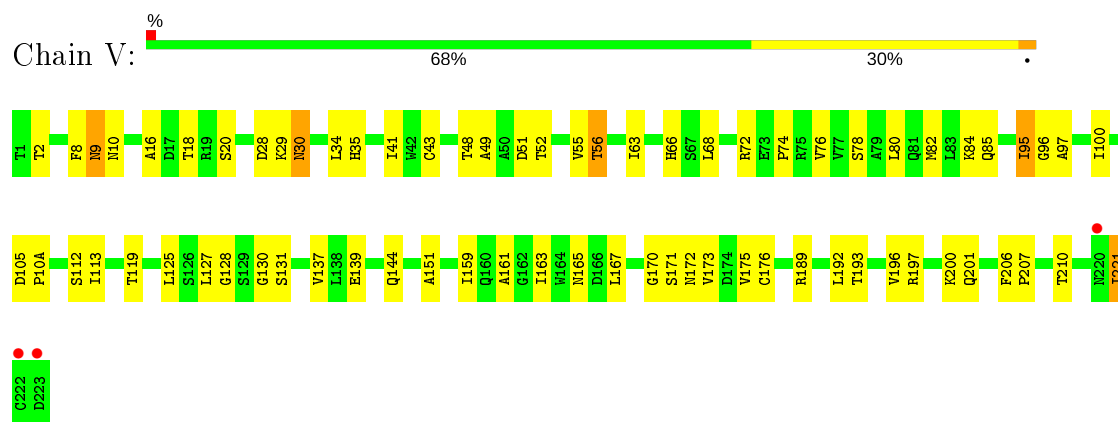




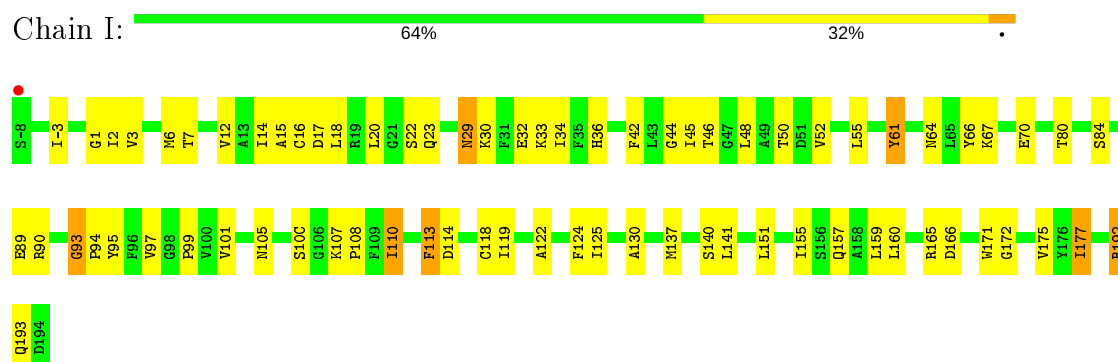
• Molecule 8: Proteasome component PUP1



• Molecule 8: Proteasome component PUP1

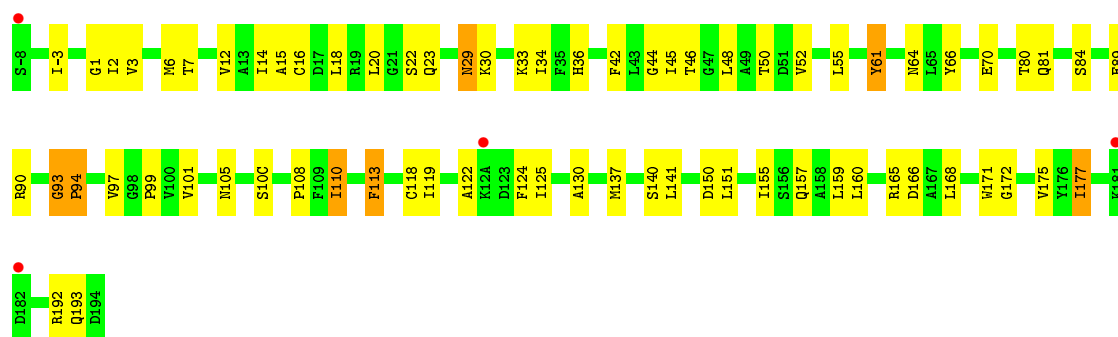


• Molecule 9: Proteasome component PUP3

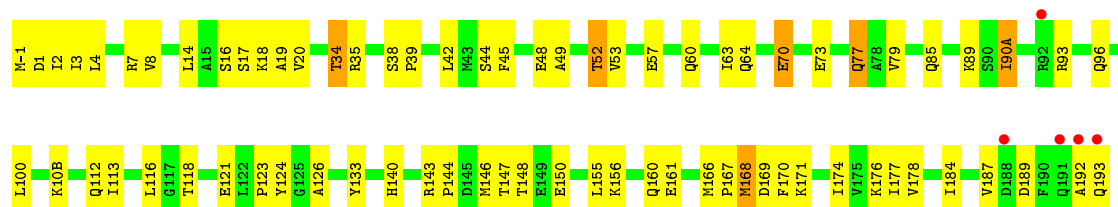


• Molecule 9: Proteasome component PUP3

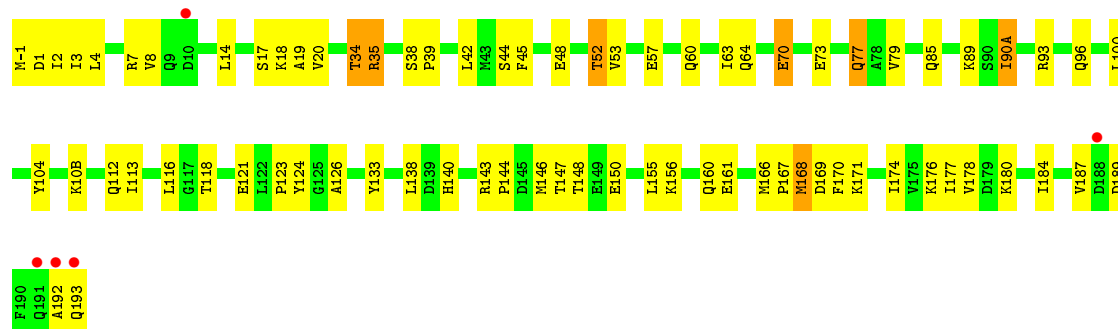




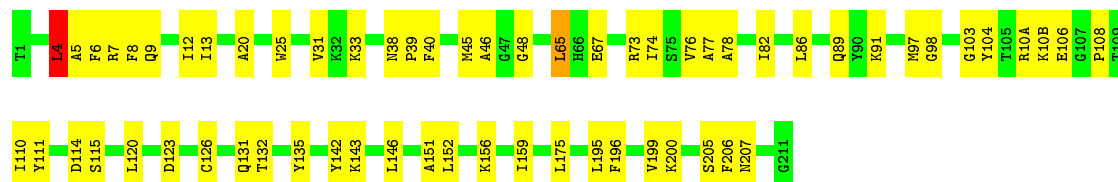
• Molecule 10: Proteasome component C11



• Molecule 10: Proteasome component C11

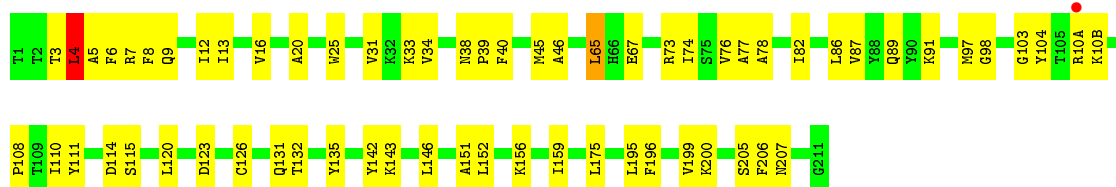


• Molecule 11: Proteasome component PRE2

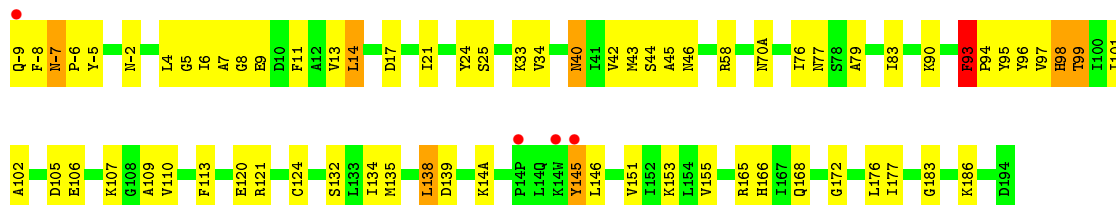


• Molecule 11: Proteasome component PRE2

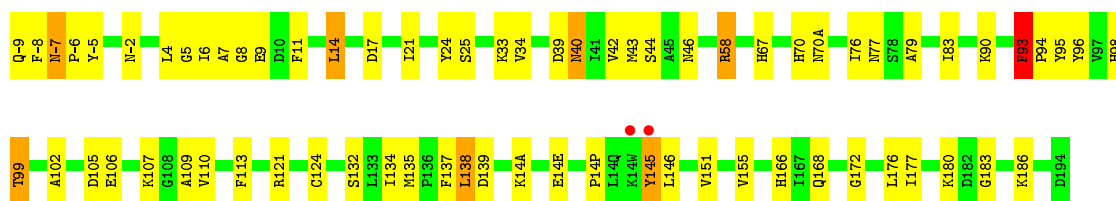




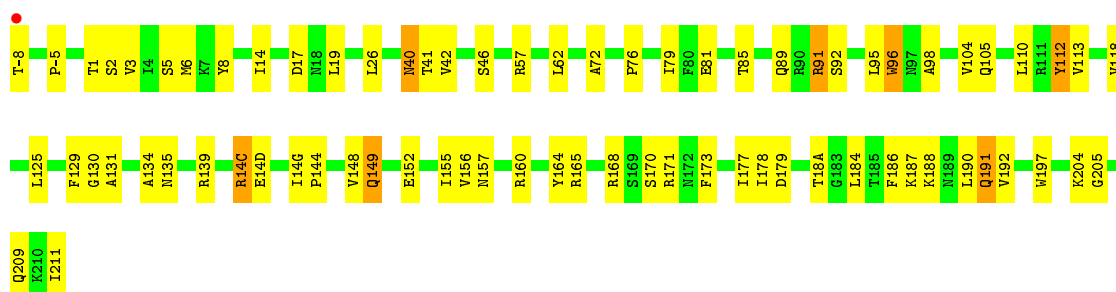
• Molecule 12: Proteasome component C5



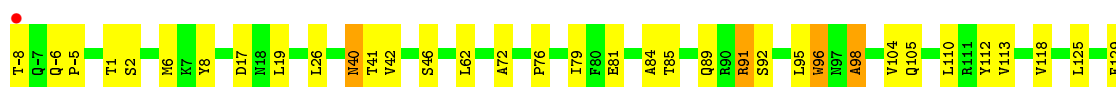
• Molecule 12: Proteasome component C5



• Molecule 13: Proteasome component PRE4

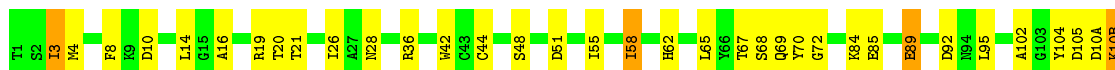


• Molecule 13: Proteasome component PRE4

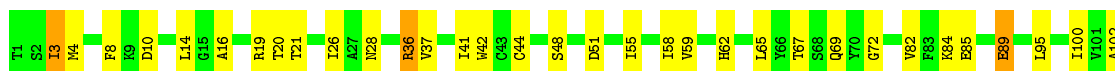




• Molecule 14: Proteasome component PRE3



• 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, $\alpha$ , $\beta$ , $\gamma$	135.16Å 301.97Å 144.05Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 20.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (15.00-2.80) 97.9 (20.01-2.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.227 , 0.256 0.215 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.4	Xtriage
Anisotropy	0.830	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	50588	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.39	0/1952	0.65	0/2642
1	O	0.37	0/1952	0.65	0/2642
2	B	0.38	0/1935	0.64	0/2618
2	P	0.38	0/1935	0.64	0/2618
3	C	0.36	0/1920	0.62	0/2598
3	Q	0.35	0/1920	0.62	0/2598
4	D	0.37	0/1887	0.64	0/2541
4	R	0.36	0/1887	0.63	0/2541
5	E	0.35	0/1823	0.62	0/2463
5	S	0.36	0/1823	0.62	0/2463
6	F	0.38	0/1937	0.62	0/2614
6	T	0.38	0/1937	0.63	0/2614
7	G	0.41	0/1959	0.64	0/2652
7	U	0.40	0/1959	0.64	0/2652
8	H	0.38	0/1716	0.66	0/2326
8	V	0.37	0/1716	0.65	0/2326
9	I	0.38	0/1611	0.65	0/2174
9	W	0.40	0/1611	0.65	0/2174
10	J	0.37	0/1613	0.64	0/2173
10	X	0.39	0/1613	0.65	0/2173
11	K	0.40	0/1681	0.67	1/2274 (0.0%)
11	Y	0.39	0/1681	0.66	1/2274 (0.0%)
12	L	0.40	0/1795	0.66	0/2420
12	Z	0.39	0/1795	0.65	0/2420
13	1	0.40	0/1855	0.67	2/2514 (0.1%)
13	M	0.39	0/1855	0.67	1/2514 (0.0%)
14	2	0.40	0/1541	0.65	0/2087
14	N	0.42	0/1541	0.65	0/2087
All	All	0.38	0/50450	0.64	5/68192 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	4	LEU	CA-CB-CG	5.59	128.16	115.30
11	K	4	LEU	CA-CB-CG	5.48	127.89	115.30
13	1	95	LEU	N-CA-C	-5.31	96.66	111.00
13	M	95	LEU	N-CA-C	-5.15	97.11	111.00
13	1	98	ALA	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	66	0
1	O	1915	0	1926	67	0
2	B	1905	0	1901	102	0
2	P	1905	0	1901	104	0
3	C	1891	0	1900	110	0
3	Q	1891	0	1900	102	0
4	D	1862	0	1836	71	0
4	R	1862	0	1836	66	0
5	E	1795	0	1797	77	0
5	S	1795	0	1797	76	0
6	F	1897	0	1886	66	0
6	T	1897	0	1886	71	0
7	G	1921	0	1910	74	0
7	U	1921	0	1910	77	0
8	H	1685	0	1687	44	0
8	V	1685	0	1687	47	0
9	I	1581	0	1574	60	0
9	W	1581	0	1574	57	0
10	J	1585	0	1590	66	0
10	X	1585	0	1590	69	0
11	K	1644	0	1594	50	0
11	Y	1644	0	1594	51	0
12	L	1757	0	1711	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Z	1757	0	1711	68	0
13	1	1824	0	1832	60	0
13	M	1824	0	1832	64	0
14	2	1512	0	1481	60	0
14	N	1512	0	1481	60	0
15	H	15	0	16	1	0
15	K	15	0	16	1	0
15	V	15	0	16	1	0
15	Y	15	0	16	1	0
16	1	58	0	0	4	0
16	2	57	0	0	2	0
16	A	38	0	0	2	0
16	B	26	0	0	1	0
16	C	30	0	0	5	0
16	D	28	0	0	2	0
16	E	17	0	0	0	0
16	F	41	0	0	3	0
16	G	45	0	0	2	0
16	H	36	0	0	1	0
16	I	48	0	0	3	0
16	J	33	0	0	2	0
16	K	27	0	0	2	0
16	L	41	0	0	2	0
16	M	54	0	0	5	0
16	N	45	0	0	3	0
16	O	25	0	0	2	0
16	P	19	0	0	0	0
16	Q	18	0	0	2	0
16	R	21	0	0	3	0
16	S	15	0	0	3	0
16	T	30	0	0	2	0
16	U	50	0	0	5	0
16	V	36	0	0	2	0
16	W	46	0	0	1	0
16	X	36	0	0	0	0
16	Y	26	0	0	3	0
16	Z	34	0	0	6	0
All	All	50588	0	49314	1770	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 (1770) 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)
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.32	1.11
5:S:2(B):THR:H	5:S:2(E):ASN:ND2	1.49	1.11
5:E:2(B):THR:H	5:E:2(E):ASN:ND2	1.48	1.09
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.31	1.08
7:G:96:ALA:HA	7:G:107:MET:HE2	1.34	1.08
4:R:68:VAL:HG21	4:R:89:ILE:HD13	1.35	1.07
7:U:96:ALA:HA	7:U:107:MET:HE2	1.32	1.05
4:D:68:VAL:HG21	4:D:89:ILE:HD13	1.40	1.02
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.23	1.02
1:A:15:PHE:H	2:B:23:GLN:HE22	1.11	0.98
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.27	0.98
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.07	0.98
1:O:15:PHE:H	2:P:23:GLN:HE22	1.07	0.97
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.65	0.97
2:B:71:ASN:ND2	2:B:72:ASP:H	1.63	0.96
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.03	0.95
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.29	0.95
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.67	0.95
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.07	0.93
5:E:207:LEU:HA	5:E:2(E):ASN:HD21	1.33	0.93
2:P:71:ASN:ND2	2:P:72:ASP:H	1.65	0.93
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.17	0.93
5:S:207:LEU:HA	5:S:2(E):ASN:HD21	1.34	0.92
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.35	0.92
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.17	0.91
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.35	0.91
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.52	0.91
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.04	0.91
3:C:100:ARG:NH1	3:C:106:PRO:HB3	1.87	0.90
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.53	0.89
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.55	0.89
3:C:232:TYR:O	3:C:236:ILE:HG13	1.72	0.89
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.54	0.88
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.88	0.88
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.35	0.88
11:K:142:TYR:O	11:K:143:LYS:HD2	1.72	0.88
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.17	0.88
2:B:202:THR:HG22	2:B:204:SER:H	1.39	0.87
13:M:149:GLN:NE2	13:M:149:GLN:H	1.73	0.87
3:Q:232:TYR:O	3:Q:236:ILE:HG13	1.74	0.87
2:P:202:THR:HG22	2:P:204:SER:H	1.37	0.87
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.59	0.85
3:C:163:GLN:NE2	3:C:164:THR:H	1.75	0.85
6:F:38:ILE:HD11	6:F:49:ALA:HB3	1.58	0.84
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.77	0.84
2:B:71:ASN:HD22	2:B:72:ASP:H	1.26	0.84
12:L:33:LYS:HD2	12:L:46:ASN:ND2	1.93	0.84
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.75	0.84
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.78	0.84
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.89	0.83
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.60	0.83
6:T:38:ILE:HD11	6:T:49:ALA:HB3	1.59	0.83
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.59	0.83
11:Y:143:LYS:O	11:Y:146:LEU:HD13	1.79	0.82
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.77	0.82
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	1.94	0.82
10:J:-1:MET:HG2	10:J:1:ASP:H	1.45	0.82
13:1:149:GLN:H	13:1:149:GLN:NE2	1.78	0.81
3:Q:33:ARG:HH11	3:Q:33:ARG:HB2	1.44	0.81
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.62	0.81
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.79	0.81
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.63	0.81
2:B:15:PHE:H	3:C:23:GLN:HE22	1.26	0.80
3:Q:201:VAL:CG2	3:Q:210:ILE:HD11	2.10	0.80
10:X:-1:MET:HG2	10:X:1:ASP:H	1.44	0.80
6:F:192:GLN:O	6:F:196:ILE:HG12	1.81	0.80
2:P:71:ASN:HD22	2:P:72:ASP:H	1.27	0.80
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.17	0.80
3:C:185:THR:HB	3:C:188:GLU:HG2	1.63	0.80
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.46	0.80
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.63	0.80
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.29	0.80
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.46	0.80
2:B:121:GLN:O	2:B:124:THR:HB	1.82	0.79
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.47	0.79
3:C:201:VAL:CG2	3:C:210:ILE:HD11	2.10	0.79
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.81	0.79
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.28	0.79
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.78	0.79
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.62	0.79
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.95	0.79
3:C:163:GLN:HE21	3:C:164:THR:H	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.65	0.79
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.81	0.79
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	1.96	0.78
5:S:15:PHE:H	6:T:23:GLN:HE22	1.32	0.78
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.66	0.78
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.30	0.78
4:D:40:ILE:HG13	4:D:193:VAL:HG23	1.66	0.78
7:U:121:GLN:O	7:U:124:THR:HB	1.83	0.78
3:C:33:ARG:CB	3:C:33:ARG:HH11	1.97	0.78
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.81	0.78
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.47	0.78
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.49	0.78
7:U:86:ARG:HD2	16:U:248:HOH:O	1.84	0.78
10:J:156:LYS:O	10:J:160:GLN:HG3	1.84	0.78
6:T:192:GLN:O	6:T:196:ILE:HG12	1.83	0.77
3:C:15:PHE:H	4:D:23:GLN:HE22	1.29	0.77
2:P:121:GLN:O	2:P:124:THR:HB	1.85	0.77
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	1.98	0.77
7:G:198:ILE:HG23	7:G:203:THR:O	1.84	0.77
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.19	0.77
9:W:7:THR:HG23	9:W:110:ILE:HD13	1.67	0.77
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.00	0.76
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.82	0.76
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.01	0.76
3:Q:197:LEU:O	3:Q:201:VAL:HG23	1.85	0.76
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.50	0.76
11:K:143:LYS:O	11:K:146:LEU:HD13	1.85	0.76
9:I:7:THR:HG23	9:I:110:ILE:HD13	1.67	0.76
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.86	0.76
3:C:185:THR:HG22	3:C:187:GLU:N	2.01	0.76
3:C:185:THR:HG22	3:C:187:GLU:H	1.49	0.76
10:X:156:LYS:O	10:X:160:GLN:HG3	1.84	0.76
5:E:207:LEU:HD23	5:E:207:LEU:H	1.50	0.76
4:R:40:ILE:HG13	4:R:193:VAL:HG23	1.68	0.76
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.67	0.76
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.51	0.76
13:1:42:VAL:HG23	13:1:178:ILE:HD11	1.69	0.75
5:E:2(B):THR:N	5:E:2(E):ASN:ND2	2.31	0.75
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.87	0.75
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.67	0.75
7:G:217:LYS:HE3	7:G:217:LYS:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.87	0.75
7:G:96:ALA:CA	7:G:107:MET:HE2	2.15	0.74
7:G:121:GLN:O	7:G:124:THR:HB	1.86	0.74
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.52	0.74
5:S:207:LEU:HD23	5:S:207:LEU:H	1.50	0.74
3:C:41:LYS:HG2	3:C:161:SER:O	1.88	0.74
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.36	0.73
5:S:111:ARG:HH11	5:S:111:ARG:HG2	1.53	0.73
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.68	0.73
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.69	0.73
1:O:159:PRO:O	2:P:59:LEU:HD12	1.88	0.73
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.71	0.73
3:C:197:LEU:O	3:C:201:VAL:HG23	1.87	0.73
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.71	0.73
5:S:2(B):THR:N	5:S:2(E):ASN:ND2	2.32	0.73
7:U:198:ILE:HG23	7:U:203:THR:O	1.88	0.72
6:T:175:GLU:HB3	6:T:196:ILE:HD12	1.70	0.72
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.71	0.72
4:R:68:VAL:CG2	4:R:89:ILE:HD13	2.18	0.72
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.53	0.72
7:U:87:ASN:HD22	7:U:87:ASN:C	1.93	0.72
1:O:121:GLN:O	1:O:124:THR:HB	1.90	0.72
7:G:87:ASN:HD22	7:G:87:ASN:C	1.92	0.72
3:Q:163:GLN:HA	3:Q:163:GLN:HE21	1.55	0.72
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.70	0.71
13:1:6:MET:HG2	13:1:155:ILE:HD11	1.73	0.71
1:A:7:ARG:HB2	2:B:5:SER:OG	1.90	0.71
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.72	0.71
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.71	0.71
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.55	0.71
12:Z:-8:PHE:HB2	13:1:-8:THR:HG23	1.71	0.71
12:Z:109:ALA:HA	16:Z:202:HOH:O	1.91	0.71
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.72	0.71
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.55	0.71
9:W:6:MET:HE1	9:W:155:ILE:HA	1.73	0.70
10:X:147:THR:HG23	10:X:150:GLU:OE2	1.91	0.70
7:U:96:ALA:CA	7:U:107:MET:HE2	2.14	0.70
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.73	0.70
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.56	0.70
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.74	0.70
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.73	0.70
5:S:47:VAL:HG23	5:S:189:LEU:HD13	1.73	0.70
12:L:-9:GLN:NE2	12:L:-8:PHE:H	1.90	0.70
2:P:71:ASN:ND2	2:P:72:ASP:N	2.40	0.70
6:T:173:LYS:O	6:T:177:GLU:HG3	1.91	0.70
13:1:41:THR:OG1	13:1:76:PRO:HG3	1.91	0.69
2:B:71:ASN:ND2	2:B:72:ASP:N	2.38	0.69
1:A:121:GLN:O	1:A:124:THR:HB	1.92	0.69
2:B:160:TRP:CE2	2:B:163:ILE:HD12	2.27	0.69
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.57	0.69
13:M:57:ARG:NE	16:M:243:HOH:O	2.25	0.69
2:B:71:ASN:HD22	2:B:72:ASP:N	1.89	0.69
2:P:160:TRP:CE2	2:P:163:ILE:HD12	2.28	0.69
5:E:15:PHE:H	6:F:23:GLN:HE22	1.39	0.69
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.73	0.69
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.74	0.69
10:J:90(A):ILE:HG12	10:J:116:LEU:HA	1.74	0.69
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.38	0.69
6:F:173:LYS:O	6:F:177:GLU:HG3	1.93	0.69
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.74	0.69
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.58	0.69
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.07	0.68
5:S:132:TYR:O	5:S:153:PRO:HB3	1.93	0.68
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.73	0.68
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.06	0.68
10:J:168:MET:HG2	10:X:168:MET:HE3	1.75	0.68
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.75	0.68
10:J:147:THR:HG23	10:J:150:GLU:OE2	1.93	0.68
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.76	0.68
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.74	0.68
12:L:-8:PHE:HB2	13:M:-8:THR:HG23	1.76	0.68
2:P:71:ASN:HD22	2:P:72:ASP:N	1.90	0.68
10:X:-1:MET:HG2	10:X:1:ASP:N	2.09	0.68
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.75	0.68
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.07	0.68
14:N:107:LYS:HG2	14:N:108:GLY:H	1.60	0.67
5:S:207:LEU:H	5:S:207:LEU:CD2	2.06	0.67
5:E:132:TYR:O	5:E:153:PRO:HB3	1.93	0.67
3:C:163:GLN:HE21	3:C:164:THR:N	1.92	0.67
1:O:33:GLN:HA	1:O:33:GLN:HE21	1.59	0.67
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	1.76	0.67
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.91	0.67
14:2:107:LYS:HG2	14:2:108:GLY:H	1.58	0.67
5:E:207:LEU:CD2	5:E:207:LEU:H	2.07	0.67
2:P:234:VAL:HA	2:P:239:THR:HA	1.77	0.67
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.10	0.67
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.77	0.67
12:Z:-9:GLN:NE2	12:Z:-8:PHE:H	1.93	0.67
2:P:190:ILE:HG21	2:P:232:ILE:HD11	1.76	0.66
1:O:57:PRO:HG3	7:U:177:GLU:CD	2.14	0.66
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.76	0.66
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG12	1.77	0.66
4:D:162:ALA:HB3	5:E:58:LEU:HD23	1.77	0.66
10:X:90(A):ILE:HG12	10:X:116:LEU:HA	1.76	0.66
14:2:21:THR:HG22	14:2:26:ILE:HA	1.77	0.66
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.58	0.66
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.76	0.66
11:K:7:ARG:HD2	11:K:108:PRO:O	1.96	0.66
3:C:76:LEU:HD12	3:C:138:ILE:HG12	1.76	0.66
2:P:185:LYS:HD3	2:P:186:VAL:N	2.10	0.66
8:H:165:ASN:ND2	13:1:139:ARG:HH11	1.92	0.66
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.77	0.66
2:B:185:LYS:HD3	2:B:186:VAL:N	2.11	0.66
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.77	0.66
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.78	0.66
3:Q:201:VAL:HG21	3:Q:210:ILE:CD1	2.19	0.66
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.78	0.66
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.78	0.66
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.78	0.66
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.78	0.65
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	1.86	0.65
10:J:-1:MET:HG2	10:J:1:ASP:N	2.10	0.65
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.11	0.65
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.27	0.65
1:O:161:LYS:HD2	2:P:58:LEU:HA	1.78	0.65
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.79	0.65
10:J:168:MET:HE3	10:X:168:MET:HG2	1.79	0.65
3:Q:70:ILE:HD12	3:Q:112:LEU:HD11	1.79	0.65
6:F:35:THR:HG21	6:F:51:GLU:O	1.97	0.65
8:H:165:ASN:HD22	13:1:139:ARG:NH1	1.91	0.65
6:T:177:GLU:OE2	7:U:57:LYS:HE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.61	0.65
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.78	0.65
9:W:124:PHE:O	9:W:125:ILE:HD12	1.98	0.64
8:H:128:GLY:O	8:H:131:SER:HB2	1.96	0.64
14:N:21:THR:HG22	14:N:26:ILE:HA	1.80	0.64
4:R:121:LEU:HA	4:R:123:PHE:CE1	2.32	0.64
2:B:190:ILE:HG21	2:B:232:ILE:HD11	1.79	0.64
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.28	0.64
2:B:234:VAL:HA	2:B:239:THR:HA	1.78	0.64
14:N:3:ILE:HD11	14:N:127:ALA:HB3	1.78	0.64
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.78	0.64
1:O:7:ARG:HB2	2:P:5:SER:OG	1.97	0.64
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.79	0.64
1:A:206:PHE:CE1	1:A:210:ILE:HD11	2.33	0.64
3:C:41:LYS:HD3	3:C:161:SER:HA	1.80	0.64
14:N:107:LYS:HG2	14:N:108:GLY:N	2.13	0.64
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.80	0.64
7:U:59:LEU:O	7:U:61:PRO:HD3	1.97	0.64
13:M:40:ASN:H	13:M:40:ASN:HD22	1.46	0.64
1:O:33:GLN:CA	1:O:33:GLN:HE21	2.11	0.64
3:C:35:THR:HB	3:C:51:GLU:HG3	1.79	0.64
1:O:15:PHE:H	2:P:23:GLN:NE2	1.89	0.63
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.80	0.63
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.80	0.63
10:J:168:MET:HG2	10:X:168:MET:CE	2.28	0.63
6:T:172:ALA:O	6:T:176:LEU:HD23	1.97	0.63
14:2:106:ASN:O	14:2:107:LYS:HB3	1.99	0.63
2:P:228:GLU:O	2:P:232:ILE:HG22	1.99	0.63
8:V:128:GLY:O	8:V:131:SER:HB2	1.99	0.63
10:J:2:ILE:O	10:J:3:ILE:HD13	1.99	0.63
10:J:147:THR:OG1	10:J:150:GLU:HG3	1.98	0.63
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.34	0.63
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.81	0.63
4:D:68:VAL:CG2	4:D:89:ILE:HD13	2.22	0.63
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.32	0.63
12:Z:6:ILE:HG12	12:Z:124:CYS:HB2	1.79	0.63
13:1:40:ASN:HD22	13:1:40:ASN:H	1.46	0.63
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.80	0.63
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.10	0.63
4:D:175:GLU:HG2	4:D:196:ILE:HD13	1.80	0.63
2:B:163:ILE:HG12	2:B:164:SER:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.81	0.62
13:M:139:ARG:HH11	8:V:165:ASN:ND2	1.93	0.62
2:P:239:THR:OXT	2:P:239:THR:HG22	1.99	0.62
3:C:201:VAL:HG21	3:C:210:ILE:CD1	2.19	0.62
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.12	0.62
9:W:113:PHE:CD2	9:W:113:PHE:N	2.66	0.62
11:Y:7:ARG:HD2	11:Y:108:PRO:O	1.99	0.62
14:2:107:LYS:HG2	14:2:108:GLY:N	2.13	0.62
13:M:139:ARG:NH1	8:V:165:ASN:HD22	1.93	0.62
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.80	0.62
10:J:52:THR:HG22	10:J:53:VAL:N	2.14	0.62
2:P:163:ILE:HG12	2:P:164:SER:N	2.13	0.62
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.81	0.62
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.81	0.62
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.15	0.62
4:D:121:LEU:HA	4:D:123:PHE:CE1	2.33	0.62
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.28	0.62
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.35	0.62
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.11	0.62
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.30	0.62
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.79	0.62
2:B:228:GLU:O	2:B:232:ILE:HG22	2.00	0.62
3:C:163:GLN:CA	3:C:163:GLN:HE21	2.13	0.62
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.81	0.62
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.13	0.62
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.30	0.62
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.81	0.62
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.81	0.62
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.00	0.62
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.12	0.62
12:L:6:ILE:HG12	12:L:124:CYS:HB2	1.80	0.62
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.97	0.62
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.82	0.62
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	1.87	0.62
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.35	0.61
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.48	0.61
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.34	0.61
10:X:143:ARG:O	10:X:146:MET:HG3	2.00	0.61
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.65	0.61
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	2.07	0.61
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:172:ASN:ND2	8:V:193:THR:HA	2.14	0.61
3:C:15:PHE:N	4:D:23:GLN:HE22	1.98	0.61
9:I:16:CYS:SG	9:I:34:ILE:HG12	2.39	0.61
10:X:2:ILE:O	10:X:3:ILE:HD13	2.01	0.61
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.66	0.61
7:G:59:LEU:O	7:G:61:PRO:HD3	2.00	0.61
9:I:113:PHE:CD2	9:I:113:PHE:N	2.66	0.61
3:Q:195:ARG:CG	3:Q:236:ILE:HD13	2.31	0.61
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.30	0.61
7:U:218:ASP:O	7:U:220:LYS:HB2	1.99	0.61
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.16	0.61
1:O:206:PHE:CE1	1:O:210:ILE:HD11	2.35	0.61
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.81	0.61
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.29	0.61
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.81	0.61
13:1:149:GLN:H	13:1:149:GLN:HE21	1.49	0.61
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.82	0.61
11:K:156:LYS:HB2	11:K:175:LEU:HD11	1.82	0.61
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.65	0.61
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.31	0.61
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.82	0.60
7:G:77:VAL:HG12	7:G:137:THR:HB	1.82	0.60
6:T:35:THR:HG21	6:T:51:GLU:O	2.01	0.60
6:F:38:ILE:CD1	6:F:49:ALA:HB3	2.31	0.60
14:N:106:ASN:O	14:N:107:LYS:HB3	2.00	0.60
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.96	0.60
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.31	0.60
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.82	0.60
12:Z:151:VAL:O	12:Z:155:VAL:HG23	2.01	0.60
9:W:16:CYS:SG	9:W:34:ILE:HG12	2.41	0.60
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.36	0.60
10:X:52:THR:HG22	10:X:53:VAL:N	2.16	0.60
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.82	0.60
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.01	0.60
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.32	0.60
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.84	0.60
13:1:40:ASN:HD22	13:1:40:ASN:N	2.00	0.60
2:B:181:LYS:O	2:B:184:MET:HG3	2.02	0.60
1:A:20:LYS:HE3	1:A:25:ASP:OD1	2.02	0.60
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.83	0.60
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.16	0.60
10:J:156:LYS:HE2	10:J:160:GLN:NE2	2.17	0.60
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.22	0.60
6:F:177:GLU:OE2	7:G:57:LYS:HE2	2.01	0.60
11:K:142:TYR:C	11:K:143:LYS:HD2	2.21	0.60
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.67	0.60
5:E:227:GLU:CD	5:E:227:GLU:H	2.05	0.59
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.16	0.59
11:K:74:ILE:HA	16:K:322:HOH:O	2.02	0.59
14:N:92:ASP:HB2	16:N:199:HOH:O	2.01	0.59
10:X:156:LYS:HE2	10:X:160:GLN:NE2	2.18	0.59
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.32	0.59
5:S:227:GLU:CD	5:S:227:GLU:H	2.06	0.59
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	1.85	0.59
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.84	0.59
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.48	0.59
2:B:239:THR:OXT	2:B:239:THR:HG22	2.01	0.59
13:M:40:ASN:HD22	13:M:40:ASN:N	2.00	0.59
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.84	0.59
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.84	0.59
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.30	0.59
6:T:187:ARG:HG3	6:T:187:ARG:HH11	1.65	0.59
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.85	0.59
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.37	0.59
3:C:14:ILE:HB	4:D:23:GLN:NE2	2.18	0.59
6:T:130:ARG:HG2	6:T:130:ARG:HH11	1.68	0.59
1:A:173:LYS:O	1:A:177:GLU:HG3	2.03	0.59
10:J:168:MET:CE	10:X:168:MET:HG2	2.33	0.59
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.84	0.59
9:W:110:ILE:HG13	9:W:125:ILE:HD13	1.83	0.59
14:2:3:ILE:O	14:2:3:ILE:HD13	2.03	0.59
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.83	0.59
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.17	0.59
14:N:3:ILE:HD13	14:N:3:ILE:O	2.03	0.59
2:P:190:ILE:CG2	2:P:232:ILE:HD11	2.32	0.59
6:T:127:ASN:HD22	6:T:128:SER:N	2.01	0.59
14:2:3:ILE:HD11	14:2:127:ALA:HB3	1.83	0.59
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.33	0.59
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.85	0.59
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.67	0.59
7:U:12:ILE:HG13	7:U:14:ILE:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:12:ILE:HG13	7:G:14:ILE:HG23	1.83	0.59
9:I:124:PHE:O	9:I:125:ILE:HD12	2.02	0.59
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.67	0.59
13:1:113:VAL:HA	13:1:118:VAL:O	2.03	0.58
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.85	0.58
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.67	0.58
13:1:14(D):GLU:O	13:1:14(G):ILE:HG12	2.03	0.58
14:2:161:GLN:NE2	14:2:165:TRP:HE1	1.99	0.58
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.38	0.58
1:O:20:LYS:HE3	1:O:25:ASP:OD1	2.03	0.58
2:P:181:LYS:O	2:P:184:MET:HG3	2.03	0.58
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.84	0.58
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.68	0.58
7:G:77:VAL:CG1	7:G:137:THR:HB	2.33	0.58
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.33	0.58
6:T:237:GLN:O	6:T:240:ILE:HG22	2.03	0.58
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.85	0.58
7:U:131:PRO:HB3	16:U:258:HOH:O	2.02	0.58
7:U:228:ASN:HB3	16:U:242:HOH:O	2.04	0.58
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.39	0.58
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.51	0.58
6:T:38:ILE:CD1	6:T:49:ALA:HB3	2.31	0.58
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.86	0.58
6:F:172:ALA:O	6:F:176:LEU:HD23	2.03	0.58
6:F:20(B):GLU:HG3	6:F:20(C):LYS:H	1.68	0.58
1:O:173:LYS:O	1:O:177:GLU:HG3	2.03	0.58
3:Q:195:ARG:HG3	3:Q:236:ILE:CD1	2.33	0.58
10:X:113:ILE:HA	10:X:118:THR:O	2.04	0.58
14:2:156:LYS:HG2	14:2:18(J):LEU:CD1	2.33	0.58
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.84	0.58
14:N:156:LYS:HG2	14:N:18(J):LEU:CD1	2.34	0.58
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.68	0.58
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.37	0.58
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.85	0.58
12:L:166:HIS:HD2	12:L:168:GLN:H	1.52	0.58
4:R:107:ILE:HG22	16:R:247:HOH:O	2.03	0.58
7:G:218:ASP:O	7:G:220:LYS:HB2	2.03	0.57
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.86	0.57
4:R:24:VAL:O	4:R:27:SER:HB3	2.04	0.57
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.34	0.57
14:2:172:VAL:HB	14:2:18(A):ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:VAL:O	4:D:27:SER:HB3	2.04	0.57
11:K:33:LYS:HG2	11:K:45:MET:HE1	1.84	0.57
14:N:161:GLN:NE2	14:N:165:TRP:HE1	2.01	0.57
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.87	0.57
3:C:195:ARG:CG	3:C:236:ILE:HD13	2.34	0.57
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.87	0.57
9:I:110:ILE:HG13	9:I:125:ILE:HD13	1.85	0.57
2:P:122:GLY:C	2:P:124:THR:H	2.08	0.57
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.87	0.57
2:P:143:ASP:OD2	10:X:10(B):LYS:HE2	2.04	0.57
2:P:186:VAL:HG21	2:P:216:ARG:HG2	1.85	0.57
7:U:130:ARG:HB2	16:U:262:HOH:O	2.03	0.57
13:M:149:GLN:HE21	13:M:149:GLN:H	1.46	0.57
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.05	0.57
3:C:195:ARG:HG3	3:C:236:ILE:CD1	2.34	0.57
5:E:111:ARG:NH1	5:E:111:ARG:HG2	2.20	0.57
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.87	0.57
12:L:145:TYR:CD1	12:L:146:LEU:N	2.72	0.57
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.40	0.57
5:S:207:LEU:N	5:S:207:LEU:HD23	2.20	0.57
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.86	0.57
5:E:207:LEU:N	5:E:207:LEU:HD23	2.20	0.57
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.39	0.57
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.87	0.57
4:R:207:LEU:C	4:R:207:LEU:HD23	2.26	0.57
2:B:11:ARG:O	2:B:14:ILE:HD13	2.05	0.56
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.40	0.56
7:U:77:VAL:CG1	7:U:137:THR:HB	2.35	0.56
2:B:190:ILE:CG2	2:B:232:ILE:HD11	2.34	0.56
6:F:130:ARG:HG2	6:F:130:ARG:HH11	1.70	0.56
6:F:38:ILE:HG22	6:F:164:ALA:HA	1.87	0.56
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.35	0.56
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.39	0.56
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.38	0.56
2:P:88:LEU:HB3	2:P:116:LEU:HD21	1.87	0.56
9:W:48:LEU:HG	9:W:50:THR:HG22	1.87	0.56
12:Z:-7:ASN:C	12:Z:-7:ASN:HD22	2.06	0.56
12:Z:99:THR:HG22	16:Z:199:HOH:O	2.04	0.56
5:E:86:ARG:O	5:E:90:ASN:HB2	2.05	0.56
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.70	0.56
13:M:14(D):GLU:O	13:M:14(G):ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:14:ILE:HB	4:R:23:GLN:NE2	2.20	0.56
7:U:77:VAL:HG12	7:U:137:THR:HB	1.85	0.56
12:Z:76:ILE:HG22	16:Z:218:HOH:O	2.03	0.56
3:C:242:GLU:O	3:C:243:GLN:HB2	2.06	0.56
4:D:85:ALA:O	4:D:89:ILE:HG13	2.06	0.56
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.06	0.56
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.87	0.56
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.70	0.56
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.70	0.56
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.74	0.56
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.41	0.56
6:F:127:ASN:HD22	6:F:128:SER:N	2.03	0.56
2:P:227:GLN:OE1	2:P:230:LYS:HD3	2.05	0.56
5:S:46:ALA:HB1	5:S:139:ILE:HB	1.87	0.56
5:S:86:ARG:O	5:S:90:ASN:HB2	2.05	0.56
6:T:184:LEU:CD1	6:T:188:GLU:HB3	2.35	0.56
8:H:172:ASN:ND2	8:H:193:THR:HA	2.19	0.56
4:R:192:LEU:O	4:R:196:ILE:HG13	2.06	0.56
6:T:20(B):GLU:HG3	6:T:20(C):LYS:H	1.70	0.56
9:W:122:ALA:HB3	9:W:125:ILE:CD1	2.35	0.56
10:X:7:ARG:HG2	10:X:7:ARG:HH11	1.69	0.56
2:B:227:GLN:OE1	2:B:230:LYS:HD3	2.05	0.56
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.88	0.56
3:C:229:ILE:O	3:C:233:VAL:HG23	2.06	0.56
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.54	0.56
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.88	0.56
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.71	0.56
13:1:41:THR:HG21	13:1:79:ILE:HD12	1.88	0.56
2:B:143:ASP:OD2	10:J:10(B):LYS:HE2	2.06	0.56
2:B:186:VAL:HG21	2:B:216:ARG:HG2	1.88	0.56
2:B:20:ARG:NH2	3:C:33:ARG:HH21	2.03	0.56
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.87	0.56
10:X:44:SER:OG	10:X:100:LEU:HB2	2.05	0.56
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	2.07	0.56
3:C:70:ILE:HD12	3:C:112:LEU:HD11	1.88	0.55
10:J:113:ILE:HA	10:J:118:THR:O	2.06	0.55
13:M:113:VAL:HA	13:M:118:VAL:O	2.06	0.55
1:O:51:GLU:OE1	1:O:202:VAL:HG22	2.06	0.55
8:V:200:LYS:HE3	9:W:140:SER:O	2.06	0.55
14:N:172:VAL:HB	14:N:18(A):ILE:HD11	1.88	0.55
1:O:15:PHE:N	2:P:23:GLN:HE22	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.89	0.55
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.36	0.55
2:B:88:LEU:HB3	2:B:116:LEU:HD21	1.87	0.55
7:G:87:ASN:ND2	7:G:87:ASN:C	2.60	0.55
2:P:87:ILE:O	2:P:91:THR:HG23	2.06	0.55
10:X:-1:MET:CG	10:X:1:ASP:H	2.19	0.55
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.06	0.55
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.89	0.55
3:C:46:VAL:O	3:C:215:VAL:HG12	2.07	0.55
6:F:70:VAL:HB	6:F:74:ILE:HB	1.88	0.55
14:N:67:THR:HA	14:N:72:GLY:O	2.06	0.55
3:Q:242:GLU:O	3:Q:243:GLN:HB2	2.06	0.55
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.04	0.55
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.07	0.55
4:R:85:ALA:O	4:R:89:ILE:HG13	2.06	0.55
1:A:141:HIS:HA	1:A:146:GLY:O	2.06	0.55
11:K:200:LYS:HE3	11:K:206:PHE:O	2.06	0.55
12:L:151:VAL:O	12:L:155:VAL:HG23	2.06	0.55
13:M:41:THR:HG21	13:M:79:ILE:HD12	1.88	0.55
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.07	0.55
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.21	0.55
11:Y:33:LYS:HG2	11:Y:45:MET:HE1	1.89	0.55
7:G:136:LEU:O	7:G:150:LYS:HA	2.07	0.55
12:L:105:ASP:OD2	12:L:107:LYS:HB2	2.07	0.55
3:Q:163:GLN:HA	3:Q:163:GLN:NE2	2.21	0.55
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.88	0.55
8:V:84:LYS:HG3	8:V:85:GLN:N	2.22	0.55
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.37	0.55
5:S:38:VAL:HG22	5:S:164:ALA:HB2	1.88	0.55
8:V:18:THR:HB	8:V:30:ASN:HD22	1.72	0.55
3:C:163:GLN:HA	3:C:163:GLN:NE2	2.21	0.55
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.89	0.55
12:L:177:ILE:HD12	12:L:177:ILE:N	2.22	0.55
1:O:14:THR:O	1:O:21:LEU:HD23	2.06	0.55
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.42	0.55
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.41	0.55
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.07	0.54
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.89	0.54
1:O:8:TYR:HD2	7:U:128:TYR:HB3	1.72	0.54
2:P:11:ARG:O	2:P:14:ILE:HD13	2.07	0.54
6:T:179:LEU:HD21	6:T:192:GLN:CG	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.72	0.54
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.36	0.54
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.23	0.54
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.22	0.54
1:O:141:HIS:HA	1:O:146:GLY:O	2.07	0.54
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.89	0.54
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.07	0.54
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.89	0.54
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.07	0.54
10:J:133:TYR:HD1	16:Y:319:HOH:O	1.89	0.54
13:M:187:LYS:HB3	13:M:190:LEU:HD11	1.89	0.54
3:Q:85:SER:O	3:Q:89:ILE:HD12	2.06	0.54
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.42	0.54
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.90	0.54
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.41	0.54
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.88	0.54
6:F:179:LEU:HD11	6:F:192:GLN:CG	2.37	0.54
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.90	0.54
9:I:48:LEU:HG	9:I:50:THR:HG22	1.88	0.54
11:Y:45:MET:HE3	15:Y:301:SLA:H11	1.88	0.54
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.90	0.54
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.43	0.54
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.89	0.54
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.89	0.54
2:B:27:ALA:O	2:B:31:ILE:HG12	2.08	0.54
6:F:237:GLN:O	6:F:240:ILE:HG22	2.08	0.54
11:K:48:GLY:HA2	16:K:318:HOH:O	2.08	0.54
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.07	0.54
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.23	0.54
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.89	0.54
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.23	0.54
8:H:139:GLU:OE1	13:1:165:ARG:NH1	2.36	0.54
8:H:18:THR:HB	8:H:30:ASN:HD22	1.73	0.54
8:H:41:ILE:HG12	8:H:76:VAL:HG22	1.89	0.54
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.11	0.54
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.38	0.54
6:T:70:VAL:HB	6:T:74:ILE:HB	1.89	0.54
8:V:172:ASN:HD22	8:V:193:THR:HA	1.73	0.54
2:B:87:ILE:O	2:B:91:THR:HG23	2.07	0.54
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.38	0.54
9:I:122:ALA:HB3	9:I:125:ILE:CD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:172:ILE:HD12	7:U:197:MET:CE	2.37	0.54
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.90	0.54
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.72	0.54
13:M:1:THR:HG22	16:M:214:HOH:O	2.07	0.54
5:S:73:HIS:HE1	5:S:107:LEU:O	1.90	0.54
8:V:196:VAL:HG23	16:V:319:HOH:O	2.07	0.54
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.08	0.54
12:L:134:ILE:HG22	12:L:138:LEU:HD22	1.90	0.54
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.42	0.54
12:Z:-5:TYR:CE2	12:Z:96:TYR:HB2	2.43	0.54
2:B:163:ILE:HG12	2:B:164:SER:H	1.72	0.53
2:P:44:ASP:OD2	2:P:186:VAL:HG23	2.08	0.53
2:P:224:PHE:N	2:P:224:PHE:CD2	2.76	0.53
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.08	0.53
5:S:111:ARG:NH1	5:S:111:ARG:HG2	2.17	0.53
7:U:136:LEU:O	7:U:150:LYS:HA	2.08	0.53
10:X:48:GLU:HB2	10:X:96:GLN:HB2	1.89	0.53
3:C:150:GLN:HG2	3:C:151:THR:N	2.22	0.53
8:H:200:LYS:HE3	9:I:140:SER:O	2.08	0.53
11:K:25:TRP:CH2	12:L:132:SER:HA	2.42	0.53
3:Q:229:ILE:O	3:Q:233:VAL:HG23	2.08	0.53
10:X:19:ALA:HB2	10:X:171:LYS:HG2	1.90	0.53
5:E:46:ALA:HB1	5:E:139:ILE:HB	1.90	0.53
5:E:18(C):PHE:O	5:E:18(F):ILE:HG12	2.09	0.53
8:H:2:THR:HG22	8:H:159:ILE:HD13	1.90	0.53
10:J:143:ARG:O	10:J:146:MET:HG3	2.08	0.53
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.38	0.53
7:U:87:ASN:ND2	7:U:87:ASN:C	2.60	0.53
1:A:51:GLU:OE1	1:A:202:VAL:HG22	2.07	0.53
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.91	0.53
10:J:44:SER:OG	10:J:100:LEU:HB2	2.09	0.53
13:M:125:LEU:HA	16:M:225:HOH:O	2.09	0.53
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.38	0.53
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.44	0.53
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.91	0.53
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.91	0.53
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.89	0.53
13:M:17:ASP:HA	13:M:173:PHE:CB	2.38	0.53
2:P:181:LYS:HG3	2:P:184:MET:HG3	1.90	0.53
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.89	0.53
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:163:ILE:HG12	2:P:164:SER:H	1.73	0.53
6:T:11:SER:HB3	6:T:14:VAL:HG23	1.90	0.53
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.90	0.53
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.44	0.53
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.73	0.53
2:B:224:PHE:N	2:B:224:PHE:CD2	2.76	0.53
5:E:73:HIS:HE1	5:E:107:LEU:O	1.90	0.53
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.91	0.53
7:G:172:ILE:HD12	7:G:197:MET:CE	2.39	0.53
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.91	0.53
3:C:57:LYS:O	3:C:58:LEU:HB2	2.09	0.53
4:D:185:THR:HG23	4:D:188:GLU:OE1	2.09	0.53
4:D:207:LEU:HD23	4:D:207:LEU:C	2.29	0.53
4:D:215:ILE:HD13	4:D:215:ILE:C	2.29	0.53
3:Q:172:VAL:O	3:Q:176:LEU:HG	2.09	0.53
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.24	0.53
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	1.90	0.53
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.62	0.53
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.89	0.53
2:B:122:GLY:C	2:B:124:THR:H	2.11	0.53
2:B:224:PHE:HD2	2:B:224:PHE:N	2.07	0.53
3:C:190:VAL:O	3:C:194:VAL:HG23	2.08	0.53
3:C:224:LEU:N	3:C:224:LEU:HD12	2.24	0.53
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.09	0.53
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.74	0.53
9:I:16:CYS:HB3	9:I:34:ILE:HD11	1.91	0.53
12:L:5:GLY:O	12:L:124:CYS:HA	2.08	0.53
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.44	0.53
4:D:40:ILE:HG13	4:D:193:VAL:CG2	2.38	0.53
12:L:90:LYS:HE3	12:L:93:PHE:O	2.07	0.53
14:N:159:LEU:O	14:N:163:ILE:HD12	2.09	0.53
3:Q:224:LEU:N	3:Q:224:LEU:HD12	2.24	0.53
6:T:38:ILE:HG22	6:T:164:ALA:HA	1.91	0.53
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.90	0.52
6:F:179:LEU:HD21	6:F:192:GLN:CG	2.38	0.52
7:G:233:LEU:O	7:G:236:ILE:HG12	2.09	0.52
9:I:67:LYS:HB3	16:I:216:HOH:O	2.09	0.52
10:J:19:ALA:HB2	10:J:171:LYS:HG2	1.89	0.52
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.90	0.52
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.92	0.52
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:224:PHE:N	2:P:224:PHE:HD2	2.07	0.52
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.39	0.52
6:T:179:LEU:HD21	6:T:192:GLN:HG2	1.91	0.52
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.91	0.52
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.39	0.52
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.08	0.52
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	1.90	0.52
7:G:96:ALA:HA	7:G:107:MET:CE	2.24	0.52
9:I:29:ASN:H	9:I:29:ASN:ND2	2.07	0.52
2:P:150:THR:O	2:P:157:TYR:HA	2.09	0.52
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.55	0.52
5:S:201:LEU:O	5:S:202:ARG:HB2	2.09	0.52
14:2:48:SER:HB3	14:2:51:ASP:HB2	1.90	0.52
1:A:69:LEU:HD23	1:A:69:LEU:C	2.29	0.52
13:1:187:LYS:HB3	13:1:190:LEU:HD11	1.91	0.52
4:D:192:LEU:O	4:D:196:ILE:HG13	2.10	0.52
10:J:52:THR:CG2	10:J:53:VAL:N	2.73	0.52
12:L:-9:GLN:CD	12:L:-8:PHE:N	2.63	0.52
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.73	0.52
7:U:233:LEU:O	7:U:236:ILE:HG12	2.09	0.52
9:W:29:ASN:H	9:W:29:ASN:ND2	2.08	0.52
13:1:17:ASP:HA	13:1:173:PHE:CB	2.39	0.52
1:A:170:VAL:N	16:A:250:HOH:O	2.43	0.52
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.90	0.52
6:F:11:SER:HB3	6:F:14:VAL:HG23	1.91	0.52
10:J:63:ILE:HD12	10:J:79:VAL:HG22	1.91	0.52
14:N:3:ILE:HB	14:N:44:CYS:HB3	1.91	0.52
2:P:186:VAL:HG11	2:P:216:ARG:HD3	1.92	0.52
3:Q:150:GLN:HG2	3:Q:151:THR:N	2.24	0.52
3:Q:15:PHE:H	4:R:23:GLN:NE2	2.04	0.52
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.90	0.52
10:J:168:MET:HE2	10:X:168:MET:HE2	1.91	0.52
2:B:126:HIS:HA	16:C:264:HOH:O	2.10	0.52
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.92	0.52
8:H:84:LYS:HE2	8:H:119:THR:HG23	1.90	0.52
11:K:86:LEU:HD13	11:K:86:LEU:C	2.30	0.52
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.92	0.52
1:O:69:LEU:HD23	1:O:69:LEU:C	2.30	0.52
4:R:52:LYS:HE3	4:R:211:GLN:HB2	1.91	0.52
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.09	0.52
1:A:112:LEU:O	1:A:116:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:GLU:OE1	3:C:227:GLU:N	2.30	0.52
2:P:27:ALA:O	2:P:31:ILE:HG12	2.09	0.52
1:A:150:GLN:O	1:A:157:TYR:HA	2.10	0.52
7:G:72:ARG:HH11	7:G:72:ARG:HB2	1.73	0.52
8:H:34:LEU:HB2	16:H:323:HOH:O	2.10	0.52
12:L:-9:GLN:CD	12:L:-8:PHE:H	2.13	0.52
2:P:108:PRO:HB2	2:P:111:ILE:HD12	1.92	0.52
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.45	0.52
5:S:18(C):PHE:O	5:S:18(F):ILE:HG12	2.09	0.52
2:B:108:PRO:HB2	2:B:111:ILE:HD12	1.92	0.52
10:X:193:GLN:HG2	10:X:193:GLN:OXT	2.08	0.52
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.92	0.52
7:U:172:ILE:HD11	7:U:201:LEU:HD21	1.91	0.52
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.45	0.52
12:Z:105:ASP:OD2	12:Z:107:LYS:HB2	2.10	0.52
2:B:160:TRP:HA	3:C:59:GLN:HA	1.92	0.51
8:H:52:THR:O	8:H:56:THR:HB	2.10	0.51
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.59	0.51
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.10	0.51
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.93	0.51
2:B:150:THR:O	2:B:157:TYR:HA	2.10	0.51
2:B:220:TYR:CE1	2:B:222:LYS:HB2	2.45	0.51
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.32	0.51
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.10	0.51
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.11	0.51
2:B:44:ASP:OD2	2:B:186:VAL:HG23	2.10	0.51
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.92	0.51
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.90	0.51
2:P:190:ILE:HG21	2:P:232:ILE:CD1	2.40	0.51
3:Q:228:GLU:O	3:Q:232:TYR:HD1	1.93	0.51
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.10	0.51
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.92	0.51
10:X:148:THR:CG2	10:X:177:ILE:HD13	2.41	0.51
10:J:48:GLU:HB2	10:J:96:GLN:HB2	1.91	0.51
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.39	0.51
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.41	0.51
13:1:1:THR:OG1	13:1:2:SER:N	2.43	0.51
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.74	0.51
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.46	0.51
1:O:150:GLN:O	1:O:157:TYR:HA	2.10	0.51
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:184:LEU:CD1	6:F:188:GLU:HB3	2.37	0.51
6:F:28:VAL:O	6:F:32:GLU:HG3	2.10	0.51
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.93	0.51
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.10	0.51
9:W:122:ALA:HB3	9:W:125:ILE:HD11	1.93	0.51
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.31	0.51
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.46	0.51
14:2:67:THR:HA	14:2:72:GLY:O	2.11	0.51
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.46	0.51
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.09	0.51
10:J:16:SER:HB2	16:J:202:HOH:O	2.10	0.51
10:J:148:THR:CG2	10:J:177:ILE:HD13	2.41	0.51
4:R:117:CYS:HG	4:R:157:PHE:HD2	1.57	0.51
5:S:123:ASN:N	5:S:123:ASN:HD22	2.07	0.51
4:R:177:LEU:HA	5:S:58:LEU:HD11	1.93	0.51
11:Y:33:LYS:HG2	11:Y:45:MET:CE	2.40	0.51
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.92	0.51
10:J:7:ARG:HG2	10:J:7:ARG:HH11	1.74	0.51
9:W:16:CYS:HB3	9:W:34:ILE:HD11	1.92	0.51
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.92	0.51
4:D:240:LYS:O	4:D:243:ALA:HB3	2.11	0.51
9:I:105:ASN:HB3	9:I:10(C):SER:OG	2.11	0.51
10:J:148:THR:HG21	10:J:177:ILE:HD13	1.93	0.51
2:P:160:TRP:CD2	2:P:163:ILE:HD12	2.46	0.51
4:R:237:LEU:O	4:R:241:GLU:HG3	2.11	0.51
7:U:168:LYS:O	7:U:172:ILE:HG12	2.11	0.51
2:B:20:ARG:HH11	2:B:20:ARG:HG2	1.76	0.51
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.92	0.51
9:W:101:VAL:O	9:W:110:ILE:HA	2.11	0.51
1:A:27:ALA:O	1:A:31:VAL:HG23	2.11	0.50
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.10	0.50
1:A:7:ARG:NH1	5:E:127:TYR:HD2	2.08	0.50
4:D:177:LEU:HA	5:E:58:LEU:HD11	1.93	0.50
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.45	0.50
12:L:79:ALA:O	12:L:83:ILE:HG13	2.11	0.50
1:A:29:THR:O	1:A:33:GLN:HG2	2.11	0.50
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.93	0.50
8:H:84:LYS:HG3	8:H:85:GLN:N	2.26	0.50
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.45	0.50
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.47	0.50
10:X:14:LEU:HD12	10:X:42:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:42:VAL:HG23	12:Z:102:ALA:HB3	1.94	0.50
3:C:52:ARG:HD2	3:C:208:LYS:O	2.11	0.50
4:D:237:LEU:O	4:D:241:GLU:HG3	2.12	0.50
13:M:184:LEU:HD23	13:M:184:LEU:C	2.31	0.50
3:Q:159:SER:HB2	16:Q:257:HOH:O	2.11	0.50
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	1.92	0.50
3:C:235:GLN:O	3:C:239:GLU:HG2	2.11	0.50
1:O:27:ALA:O	1:O:31:VAL:HG23	2.12	0.50
8:V:2:THR:HG22	8:V:159:ILE:HD13	1.92	0.50
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.46	0.50
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.47	0.50
2:B:111:ILE:HD11	10:J:70:GLU:HG2	1.92	0.50
3:C:224:LEU:N	3:C:224:LEU:CD1	2.75	0.50
4:D:185:THR:OG1	4:D:188:GLU:HG3	2.12	0.50
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.76	0.50
5:S:199:GLN:HE21	5:S:199:GLN:N	2.09	0.50
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.47	0.50
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.12	0.50
3:C:173:ARG:O	3:C:177:GLU:HG3	2.12	0.50
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.41	0.50
8:H:175:VAL:HG12	8:H:176:CYS:N	2.25	0.50
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.12	0.50
5:S:177:GLU:OE1	6:T:56:SER:HB2	2.11	0.50
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.92	0.50
12:Z:180:LYS:HG2	16:Z:228:HOH:O	2.10	0.50
3:C:172:VAL:O	3:C:176:LEU:HG	2.11	0.50
3:C:228:GLU:O	3:C:232:TYR:HD1	1.94	0.50
4:D:70:ILE:HG13	4:D:74:ILE:HG22	1.93	0.50
6:F:199:LEU:HD12	6:F:240:ILE:HD12	1.94	0.50
14:N:147:SER:OG	14:N:150:GLU:HG3	2.11	0.50
1:O:10(A):ILE:HD12	1:O:10(A):ILE:N	2.27	0.50
10:X:52:THR:CG2	10:X:53:VAL:N	2.74	0.50
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.94	0.50
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.93	0.50
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.47	0.50
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.93	0.50
10:J:45:PHE:CE1	10:J:52:THR:HG23	2.46	0.50
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.94	0.50
11:K:46:ALA:HB3	11:K:98:GLY:O	2.12	0.50
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.27	0.50
4:R:185:THR:HG23	4:R:188:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.42	0.49
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.40	0.49
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.46	0.49
6:F:179:LEU:HD21	6:F:192:GLN:HG2	1.93	0.49
7:G:18(D):ILE:HD12	7:G:18(D):ILE:N	2.27	0.49
8:H:16:ALA:HA	8:H:159:ILE:HD12	1.94	0.49
9:I:29:ASN:HD22	9:I:30:LYS:HG3	1.76	0.49
2:P:202:THR:CG2	2:P:204:SER:HB2	2.42	0.49
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.11	0.49
6:T:130:ARG:NH1	6:T:130:ARG:HG2	2.27	0.49
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.77	0.49
1:O:29:THR:O	1:O:33:GLN:HG2	2.11	0.49
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.75	0.49
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.11	0.49
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.43	0.49
13:1:125:LEU:HA	16:1:217:HOH:O	2.12	0.49
5:E:233:ILE:OXT	5:E:233:ILE:HG22	2.12	0.49
12:L:-5:TYR:CE2	12:L:96:TYR:HB2	2.47	0.49
14:N:3:ILE:H	14:N:3:ILE:HD12	1.77	0.49
2:P:202:THR:HG21	2:P:204:SER:HB2	1.92	0.49
7:U:70:ILE:HG13	7:U:74:ILE:HG22	1.94	0.49
2:P:111:ILE:HD11	10:X:70:GLU:HG2	1.93	0.49
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.42	0.49
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.12	0.49
7:G:70:ILE:HG13	7:G:74:ILE:HG22	1.94	0.49
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.47	0.49
2:P:235:LYS:C	2:P:237:GLY:H	2.16	0.49
4:R:121:LEU:HA	4:R:123:PHE:HE1	1.78	0.49
5:S:220:PRO:O	5:S:222:THR:HG23	2.12	0.49
8:V:52:THR:O	8:V:56:THR:HB	2.11	0.49
10:J:168:MET:HE1	10:X:167:PRO:CB	2.43	0.49
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.47	0.49
2:B:20:ARG:CZ	3:C:33:ARG:HH21	2.26	0.49
5:E:123:ASN:HD22	5:E:123:ASN:N	2.10	0.49
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.12	0.49
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.66	0.49
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.95	0.49
5:S:104:ASN:HB2	13:1:81:GLU:HG2	1.94	0.49
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.94	0.49
1:A:14:THR:O	1:A:21:LEU:HD23	2.13	0.49
2:B:61:GLN:NE2	2:B:226:PRO:HG3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:201:LEU:O	5:E:202:ARG:HB2	2.11	0.49
3:Q:87:ILE:N	3:Q:87:ILE:CD1	2.76	0.49
4:R:240:LYS:O	4:R:243:ALA:HB3	2.13	0.49
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.92	0.49
9:W:105:ASN:HB3	9:W:10(C):SER:OG	2.11	0.49
11:Y:131:GLN:HG3	11:Y:132:THR:N	2.27	0.49
1:A:10(A):ILE:HD12	1:A:10(A):ILE:N	2.28	0.49
3:C:159:SER:O	4:D:59:LEU:HD22	2.13	0.49
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.43	0.49
4:D:52:LYS:HE3	4:D:211:GLN:HB2	1.93	0.49
6:F:38:ILE:HG22	6:F:164:ALA:CA	2.41	0.49
1:O:112:LEU:O	1:O:116:VAL:HG23	2.12	0.49
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.93	0.49
10:J:-1:MET:CG	10:J:1:ASP:H	2.19	0.49
11:K:33:LYS:HG2	11:K:45:MET:CE	2.43	0.49
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.47	0.49
3:Q:159:SER:O	4:R:59:LEU:HD22	2.13	0.49
3:Q:241:GLN:O	3:Q:243:GLN:N	2.41	0.49
2:B:191:GLU:O	2:B:195:LYS:HG2	2.13	0.49
2:B:51:GLU:OE1	2:B:202:THR:HG23	2.12	0.49
7:G:151:THR:HG22	7:G:157:TYR:CB	2.42	0.49
12:L:43:MET:HG2	12:L:44:SER:N	2.28	0.49
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.94	0.49
11:K:131:GLN:HG3	11:K:132:THR:N	2.28	0.49
11:K:45:MET:HE3	15:K:301:SLA:H11	1.95	0.49
3:Q:55:THR:HG22	3:Q:56:LEU:CD2	2.41	0.49
5:S:148:LEU:HD23	5:S:162:GLY:HA2	1.95	0.49
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.48	0.49
12:Z:-9:GLN:CD	12:Z:-8:PHE:N	2.65	0.49
1:A:130:ARG:HG2	7:G:125:GLN:HG3	1.94	0.48
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.48	0.48
9:I:101:VAL:O	9:I:110:ILE:HA	2.14	0.48
4:R:40:ILE:HG13	4:R:193:VAL:CG2	2.42	0.48
10:X:166:MET:CE	10:X:168:MET:HB2	2.43	0.48
11:K:97:MET:O	11:K:114:ASP:HA	2.13	0.48
12:L:109:ALA:HA	16:L:225:HOH:O	2.13	0.48
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.29	0.48
6:T:18:ASP:OD1	6:T:20:ARG:HD3	2.14	0.48
8:V:49:ALA:HB2	15:V:301:SLA:H16	1.95	0.48
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.48	0.48
12:L:76:ILE:HG23	12:L:77:ASN:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.42	0.48
7:U:18(D):ILE:HD12	7:U:18(D):ILE:N	2.29	0.48
12:L:135:MET:HE2	9:W:165:ARG:NH2	2.29	0.48
10:X:148:THR:HG21	10:X:177:ILE:HD13	1.96	0.48
10:X:4:LEU:HD23	10:X:126:ALA:HB2	1.95	0.48
11:Y:86:LEU:O	11:Y:89:GLN:HB2	2.13	0.48
13:1:150:VAL:HG21	16:1:232:HOH:O	2.13	0.48
14:2:105:ASP:OD2	14:2:106:ASN:N	2.44	0.48
2:B:160:TRP:CD2	2:B:163:ILE:HD12	2.48	0.48
4:D:112:LEU:C	4:D:112:LEU:HD13	2.34	0.48
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.15	0.48
11:K:207:ASN:HD21	10:X:144:PRO:HG2	1.78	0.48
12:L:42:VAL:HG23	12:L:102:ALA:HB3	1.95	0.48
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.48	0.48
9:W:113:PHE:HA	9:W:118:CYS:O	2.14	0.48
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.28	0.48
3:C:102:THR:OG1	3:C:103:LEU:HD22	2.13	0.48
3:C:65:SER:HB2	16:C:252:HOH:O	2.14	0.48
5:E:227:GLU:N	5:E:227:GLU:CD	2.66	0.48
5:E:226:GLY:O	5:E:229:VAL:HG22	2.14	0.48
7:G:9:ASP:OD2	7:G:16:SER:HA	2.13	0.48
13:M:1:THR:OG1	13:M:2:SER:N	2.46	0.48
2:P:220:TYR:CE1	2:P:222:LYS:HB2	2.48	0.48
13:1:91:ARG:HG3	13:1:92:SER:N	2.28	0.48
2:B:186:VAL:HG11	2:B:216:ARG:HD3	1.95	0.48
2:B:235:LYS:C	2:B:237:GLY:H	2.17	0.48
5:E:190:ILE:O	5:E:194:VAL:HG23	2.13	0.48
5:E:199:GLN:N	5:E:199:GLN:HE21	2.10	0.48
11:K:40:PHE:CD1	11:K:73:ARG:NH1	2.82	0.48
1:O:169:SER:O	1:O:173:LYS:HG3	2.14	0.48
5:S:233:ILE:OXT	5:S:233:ILE:HG22	2.14	0.48
6:T:127:ASN:HD22	6:T:127:ASN:C	2.17	0.48
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.44	0.48
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.44	0.48
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.49	0.48
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.14	0.48
5:E:220:PRO:O	5:E:222:THR:HG23	2.13	0.48
7:G:47:VAL:HG12	7:G:49:ILE:CD1	2.44	0.48
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.49	0.48
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.96	0.48
2:P:191:GLU:O	2:P:195:LYS:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:9:ASP:OD2	7:U:16:SER:HA	2.14	0.48
7:U:203:THR:HG22	7:U:204:GLU:O	2.13	0.48
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.13	0.48
8:V:175:VAL:HG12	8:V:176:CYS:N	2.29	0.48
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.95	0.48
8:H:172:ASN:HD22	8:H:193:THR:HA	1.79	0.48
12:Z:43:MET:HG2	12:Z:44:SER:N	2.28	0.48
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.49	0.48
2:P:215:ILE:HG12	2:P:221:GLN:HG2	1.96	0.48
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.13	0.48
9:W:29:ASN:HD22	9:W:30:LYS:HG3	1.77	0.48
1:A:169:SER:O	1:A:173:LYS:HG3	2.14	0.48
4:D:86:ARG:HD3	4:D:86:ARG:HA	1.77	0.48
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.13	0.48
9:W:80:THR:HG22	9:W:119:ILE:HD13	1.96	0.48
10:X:93:ARG:NH2	11:Y:91:LYS:HD3	2.28	0.48
14:2:58:ILE:HG22	14:2:62:HIS:HD2	1.79	0.47
2:B:202:THR:HG21	2:B:204:SER:HB2	1.95	0.47
2:B:51:GLU:CD	2:B:202:THR:HG23	2.34	0.47
2:B:55:THR:HG22	2:B:59:LEU:HD23	1.96	0.47
6:F:52:LYS:HB2	6:F:209:GLU:O	2.14	0.47
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.43	0.47
2:P:41:MET:HE3	16:Q:247:HOH:O	2.14	0.47
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.17	0.47
7:U:47:VAL:HG12	7:U:49:ILE:CD1	2.44	0.47
16:F:252:HOH:O	14:N:70:TYR:HE2	1.97	0.47
6:T:28:VAL:O	6:T:32:GLU:HG3	2.14	0.47
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.68	0.47
8:H:2:THR:OG1	8:H:130:GLY:HA3	2.14	0.47
9:I:29:ASN:HD22	9:I:29:ASN:C	2.18	0.47
10:J:189:ASP:O	10:J:193:GLN:HB2	2.15	0.47
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.80	0.47
11:K:38:ASN:HB2	11:K:39:PRO:CD	2.44	0.47
9:W:45:ILE:HB	9:W:52:VAL:HG13	1.96	0.47
10:X:63:ILE:HD12	10:X:79:VAL:HG22	1.95	0.47
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	1.95	0.47
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.30	0.47
1:A:186:LEU:O	1:A:190:ILE:HG13	2.14	0.47
3:C:87:ILE:CD1	3:C:87:ILE:N	2.76	0.47
10:J:166:MET:CE	10:J:168:MET:HB2	2.43	0.47
14:N:18(A):ILE:HD13	14:N:18(B):PHE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.15	0.47
2:P:21(A):LYS:O	2:P:217:ALA:N	2.47	0.47
5:S:67:ILE:HG21	5:S:213:ALA:HB2	1.96	0.47
7:U:35:ILE:HD11	16:U:285:HOH:O	2.14	0.47
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	1.95	0.47
16:R:258:HOH:O	12:Z:70:HIS:HE1	1.95	0.47
14:2:116:GLY:HA3	16:2:190:HOH:O	2.14	0.47
14:2:3:ILE:HB	14:2:44:CYS:HB3	1.95	0.47
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.93	0.47
4:D:170:GLU:N	4:D:170:GLU:OE1	2.46	0.47
7:G:93:LYS:HD3	14:N:68:SER:HB3	1.96	0.47
4:R:70:ILE:HG13	4:R:74:ILE:HG22	1.95	0.47
6:T:136:THR:O	6:T:150:MET:HA	2.14	0.47
12:L:135:MET:CE	9:W:165:ARG:NH2	2.78	0.47
14:2:18(A):ILE:HD13	14:2:18(B):PHE:N	2.29	0.47
4:D:121:LEU:HA	4:D:123:PHE:HE1	1.79	0.47
4:D:91:HIS:CE1	4:D:119:LEU:HD21	2.49	0.47
13:M:168:ARG:HB2	16:M:240:HOH:O	2.14	0.47
1:O:8:TYR:CD2	7:U:128:TYR:HB3	2.49	0.47
3:Q:102:THR:OG1	3:Q:103:LEU:HD22	2.13	0.47
3:Q:121:GLN:C	3:Q:121:GLN:NE2	2.68	0.47
9:W:124:PHE:C	9:W:125:ILE:HD12	2.34	0.47
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.29	0.47
1:A:8:TYR:CD2	7:G:128:TYR:HB3	2.48	0.47
2:B:11:ARG:HD2	3:C:10:ARG:CZ	2.44	0.47
2:B:190:ILE:HG21	2:B:232:ILE:CD1	2.42	0.47
4:D:59:LEU:C	4:D:59:LEU:HD13	2.34	0.47
7:G:168:LYS:O	7:G:172:ILE:HG12	2.14	0.47
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.96	0.47
2:P:60:GLU:OE1	2:P:60:GLU:HA	2.14	0.47
4:R:112:LEU:C	4:R:112:LEU:HD13	2.35	0.47
5:S:227:GLU:CD	5:S:227:GLU:N	2.67	0.47
9:W:12:VAL:CG1	9:W:108:PRO:HB3	2.45	0.47
9:W:89:GLU:HG2	9:W:90:ARG:NH1	2.30	0.47
4:D:122:ARG:NH1	4:D:122:ARG:HG2	2.29	0.47
6:F:130:ARG:NH1	6:F:130:ARG:HG2	2.29	0.47
7:G:203:THR:HG22	7:G:204:GLU:O	2.15	0.47
9:I:6:MET:HE1	9:I:155:ILE:HA	1.97	0.47
10:J:133:TYR:HE1	16:Y:219:HOH:O	1.97	0.47
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.29	0.47
3:Q:163:GLN:NE2	3:Q:163:GLN:CA	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.96	0.47
10:X:45:PHE:CE1	10:X:52:THR:HG23	2.50	0.47
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.15	0.47
3:C:85:SER:O	3:C:89:ILE:HD12	2.14	0.47
9:I:192:ARG:HD3	16:I:242:HOH:O	2.14	0.47
11:K:38:ASN:HB2	11:K:39:PRO:HD2	1.96	0.47
13:M:149:GLN:NE2	13:M:149:GLN:N	2.54	0.47
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.97	0.47
2:P:38:ILE:HG12	2:P:164:SER:HB3	1.97	0.47
2:P:20:ARG:HH11	2:P:20:ARG:HG2	1.78	0.47
2:P:27:ALA:O	2:P:30:SER:HB3	2.15	0.47
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.15	0.47
5:S:18(D):ILE:O	5:S:18(D):ILE:HG12	2.14	0.47
6:T:52:LYS:HB2	6:T:209:GLU:O	2.14	0.47
7:U:18(H):GLU:CD	7:U:18(H):GLU:H	2.18	0.47
8:V:16:ALA:HA	8:V:159:ILE:HD12	1.95	0.47
10:X:189:ASP:O	10:X:193:GLN:HB2	2.14	0.47
13:1:157:ASN:HB3	16:1:248:HOH:O	2.13	0.47
2:B:21(A):LYS:O	2:B:217:ALA:N	2.47	0.47
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.49	0.47
10:J:112:GLN:NE2	10:J:126:ALA:H	2.12	0.47
2:P:122:GLY:C	2:P:124:THR:N	2.68	0.47
2:P:55:THR:HG22	2:P:59:LEU:HD23	1.96	0.47
4:R:170:GLU:N	4:R:170:GLU:OE1	2.48	0.47
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.29	0.47
9:W:29:ASN:C	9:W:29:ASN:HD22	2.18	0.47
11:K:205:SER:HB2	10:X:140:HIS:HA	1.96	0.47
5:E:67:ILE:HG21	5:E:213:ALA:HB2	1.97	0.47
12:L:176:LEU:CD1	12:L:186:LYS:HG2	2.45	0.47
1:O:5:THR:O	1:O:7:ARG:HG2	2.15	0.47
4:R:59:LEU:HD13	4:R:59:LEU:C	2.35	0.47
5:S:15:PHE:H	6:T:23:GLN:NE2	2.06	0.47
8:V:41:ILE:HG12	8:V:76:VAL:HG22	1.97	0.47
8:V:206:PHE:CE2	9:W:157:GLN:HG3	2.50	0.47
9:W:177:ILE:N	9:W:177:ILE:HD13	2.30	0.47
9:W:61:TYR:C	9:W:61:TYR:CD1	2.89	0.47
10:X:7:ARG:NH1	10:X:7:ARG:HG2	2.29	0.47
13:1:184:LEU:C	13:1:184:LEU:HD23	2.35	0.46
2:B:202:THR:CG2	2:B:204:SER:HB2	2.45	0.46
2:B:60:GLU:HA	2:B:60:GLU:OE1	2.15	0.46
2:P:232:ILE:HG13	2:P:232:ILE:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:33:ARG:HG2	3:Q:33:ARG:O	2.15	0.46
4:R:215:ILE:HD13	4:R:215:ILE:C	2.36	0.46
11:Y:97:MET:O	11:Y:114:ASP:HA	2.14	0.46
12:Z:-9:GLN:CD	12:Z:-8:PHE:H	2.17	0.46
1:A:5:THR:O	1:A:7:ARG:HG2	2.15	0.46
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.45	0.46
3:C:234:THR:HG22	3:C:238:GLN:HE21	1.80	0.46
5:E:18(D):ILE:O	5:E:18(D):ILE:HG12	2.14	0.46
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.62	0.46
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.97	0.46
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.97	0.46
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.30	0.46
8:V:63:ILE:CG2	8:V:74:PRO:HB3	2.45	0.46
9:W:89:GLU:O	9:W:90:ARG:NH1	2.48	0.46
10:X:90(A):ILE:HA	10:X:90(A):ILE:HD13	1.79	0.46
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.16	0.46
13:1:171:ARG:O	13:1:192:VAL:HG23	2.16	0.46
2:B:122:GLY:C	2:B:124:THR:N	2.69	0.46
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.97	0.46
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.43	0.46
14:N:26:ILE:HB	13:1:165:ARG:HA	1.98	0.46
11:Y:132:THR:HG22	16:Y:219:HOH:O	2.15	0.46
13:1:133:MET:O	13:1:136:PRO:HD2	2.16	0.46
3:C:122:ARG:NH2	16:C:267:HOH:O	2.49	0.46
5:E:47:VAL:CG2	5:E:189:LEU:HD13	2.42	0.46
9:I:124:PHE:C	9:I:125:ILE:HD12	2.36	0.46
9:I:122:ALA:HB3	9:I:125:ILE:HD11	1.96	0.46
11:K:12:ILE:HG23	11:K:110:ILE:HD11	1.97	0.46
2:P:51:GLU:OE1	2:P:202:THR:HG23	2.16	0.46
5:S:90:ASN:ND2	16:S:245:HOH:O	2.47	0.46
6:T:38:ILE:HG22	6:T:164:ALA:CA	2.44	0.46
12:Z:79:ALA:O	12:Z:83:ILE:HG13	2.15	0.46
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.15	0.46
1:A:110:LYS:HG2	16:A:245:HOH:O	2.14	0.46
3:C:15:PHE:H	4:D:23:GLN:NE2	2.03	0.46
5:E:198:SER:HA	5:E:201:LEU:HG	1.98	0.46
6:F:166:GLY:O	6:F:169:ARG:HB3	2.15	0.46
12:L:9:GLU:O	12:L:107:LYS:HD3	2.16	0.46
14:N:116:GLY:HA3	16:N:195:HOH:O	2.15	0.46
1:O:130:ARG:HG2	7:U:125:GLN:HG3	1.98	0.46
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:146:TYR:OH	2:P:21(A):LYS:HB2	2.15	0.46
4:R:29:GLU:OE2	4:R:32:LYS:HD2	2.16	0.46
9:W:33:LYS:O	9:W:44:GLY:HA2	2.16	0.46
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.16	0.46
7:G:141:VAL:HG21	7:G:216:THR:HA	1.97	0.46
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	1.98	0.46
3:Q:185:THR:CB	3:Q:188:GLU:HG2	2.41	0.46
3:Q:234:THR:HG22	3:Q:238:GLN:HE21	1.80	0.46
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.97	0.46
7:U:158:VAL:HG22	7:U:159:GLY:N	2.31	0.46
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.16	0.46
9:W:22:SER:O	9:W:23:GLN:HB2	2.15	0.46
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.80	0.46
11:Y:12:ILE:HG23	11:Y:110:ILE:HD11	1.98	0.46
14:2:147:SER:OG	14:2:150:GLU:HG3	2.16	0.46
14:2:3:ILE:HG22	14:2:16:ALA:HB1	1.97	0.46
14:2:19:ARG:HG3	14:2:26:ILE:HG23	1.98	0.46
10:J:85:GLN:O	10:J:89:LYS:HG3	2.16	0.46
13:M:40:ASN:ND2	13:M:40:ASN:N	2.64	0.46
4:R:122:ARG:HG2	4:R:122:ARG:NH1	2.31	0.46
8:V:100:ILE:HD11	8:V:127:LEU:HG	1.98	0.46
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.50	0.46
2:B:20:ARG:HG2	2:B:20:ARG:NH1	2.28	0.46
2:B:232:ILE:O	2:B:232:ILE:HG13	2.14	0.46
2:B:6:ARG:HH12	4:D:12(B):GLU:CD	2.18	0.46
5:E:148:LEU:HD23	5:E:162:GLY:HA2	1.97	0.46
8:H:9:ASN:OD1	8:H:10:ASN:N	2.49	0.46
1:O:212:LEU:C	1:O:212:LEU:HD23	2.36	0.46
1:A:217:ASP:O	1:A:220:ARG:HA	2.16	0.46
9:I:33:LYS:O	9:I:44:GLY:HA2	2.16	0.46
10:J:140:HIS:HA	11:Y:205:SER:HB2	1.97	0.46
11:K:13:ILE:HD12	11:K:152:LEU:HD23	1.98	0.46
12:L:-2:ASN:HA	12:L:21:ILE:O	2.15	0.46
5:S:190:ILE:O	5:S:194:VAL:HG23	2.15	0.46
6:T:91:ARG:HG2	6:T:119:TYR:CD2	2.51	0.46
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.16	0.46
7:G:158:VAL:HG22	7:G:159:GLY:N	2.31	0.46
11:K:4:LEU:C	11:K:4:LEU:CD2	2.84	0.46
13:M:171:ARG:O	13:M:192:VAL:HG23	2.16	0.46
4:R:29:GLU:HA	4:R:29:GLU:OE2	2.15	0.46
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.16	0.46
13:1:148:VAL:HG23	16:1:227:HOH:O	2.16	0.45
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.98	0.45
2:B:146:TYR:OH	2:B:21(A):LYS:HB2	2.16	0.45
9:I:22:SER:O	9:I:23:GLN:HB2	2.16	0.45
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.16	0.45
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.51	0.45
7:U:190:VAL:O	7:U:194:ILE:HD12	2.16	0.45
9:W:130:ALA:HB2	9:W:166:ASP:HB2	1.97	0.45
11:Y:4:LEU:C	11:Y:4:LEU:CD2	2.85	0.45
12:Z:9:GLU:O	12:Z:107:LYS:HD3	2.15	0.45
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.97	0.45
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.99	0.45
3:C:79:SER:HA	16:C:261:HOH:O	2.15	0.45
4:D:187:LYS:O	4:D:191:LEU:HD22	2.16	0.45
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.97	0.45
2:P:136:PHE:O	2:P:150:THR:HA	2.17	0.45
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.51	0.45
4:R:91:HIS:CE1	4:R:119:LEU:HD21	2.51	0.45
10:X:166:MET:HA	10:X:167:PRO:HD3	1.80	0.45
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.98	0.45
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.17	0.45
14:2:10(B):LYS:HD3	14:2:10(B):LYS:O	2.17	0.45
3:C:121:GLN:C	3:C:121:GLN:NE2	2.69	0.45
13:M:17:ASP:HA	13:M:173:PHE:HA	1.98	0.45
2:P:121:GLN:HG2	3:Q:83:ALA:HB1	1.97	0.45
8:V:9:ASN:OD1	8:V:10:ASN:N	2.48	0.45
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	1.99	0.45
1:A:4:MET:O	1:A:5:THR:O	2.34	0.45
4:D:91:HIS:CG	4:D:119:LEU:HD11	2.52	0.45
6:F:199:LEU:HD12	6:F:240:ILE:CD1	2.46	0.45
8:H:48:THR:HB	8:H:51:ASP:HB2	1.97	0.45
9:I:113:PHE:HA	9:I:118:CYS:O	2.16	0.45
10:J:14:LEU:HD12	10:J:42:LEU:HD23	1.98	0.45
11:K:146:LEU:HD23	11:K:151:ALA:HA	1.98	0.45
2:P:194:LEU:HD13	2:P:233:LEU:HD12	1.98	0.45
5:S:226:GLY:O	5:S:229:VAL:HG22	2.16	0.45
7:U:13:THR:HB	7:U:124:THR:O	2.16	0.45
10:X:60:GLN:O	10:X:64:GLN:HG3	2.16	0.45
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.80	0.45
13:1:149:GLN:N	13:1:149:GLN:NE2	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:35:SER:HB3	5:E:66:LYS:NZ	2.32	0.45
7:G:190:VAL:O	7:G:194:ILE:HD12	2.15	0.45
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.14	0.45
10:J:167:PRO:CB	10:X:168:MET:HE1	2.46	0.45
12:L:139:ASP:O	12:L:14(A):LYS:HG2	2.17	0.45
12:L:17:ASP:HA	12:L:172:GLY:O	2.17	0.45
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.98	0.45
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.15	0.45
3:Q:112:LEU:O	3:Q:116:VAL:HG23	2.16	0.45
5:S:52:LYS:HB3	5:S:63:TYR:HB3	1.99	0.45
6:T:11:SER:HB3	6:T:14:VAL:CG2	2.46	0.45
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.97	0.45
3:Q:101:LEU:HD11	10:X:57:GLU:HB3	1.99	0.45
11:Y:40:PHE:CD1	11:Y:73:ARG:NH1	2.85	0.45
12:Z:139:ASP:O	12:Z:14(A):LYS:HG2	2.16	0.45
14:2:172:VAL:HB	14:2:18(A):ILE:CD1	2.46	0.45
1:A:206:PHE:CD1	1:A:210:ILE:HD11	2.51	0.45
1:A:67:VAL:CG2	1:A:211:GLU:HG2	2.47	0.45
3:C:186:VAL:O	3:C:190:VAL:HG23	2.17	0.45
9:I:89:GLU:O	9:I:90:ARG:NH1	2.50	0.45
13:M:46:SER:OG	13:M:98:ALA:HB3	2.16	0.45
14:N:105:ASP:OD2	14:N:106:ASN:N	2.45	0.45
6:T:166:GLY:O	6:T:169:ARG:HB3	2.17	0.45
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.52	0.45
6:F:136:THR:O	6:F:150:MET:HA	2.17	0.45
6:F:18:ASP:OD1	6:F:20:ARG:HD3	2.16	0.45
8:H:49:ALA:HB2	15:H:301:SLA:H16	1.97	0.45
12:L:-9:GLN:NE2	12:L:-8:PHE:N	2.64	0.45
11:Y:146:LEU:HD23	11:Y:151:ALA:HA	1.98	0.45
14:2:14:LEU:O	14:2:175:MET:HA	2.16	0.45
1:A:212:LEU:HD23	1:A:212:LEU:C	2.36	0.45
1:A:7:ARG:NH1	5:E:127:TYR:CD2	2.85	0.45
14:N:58:ILE:HG22	14:N:62:HIS:HD2	1.82	0.45
1:O:122:GLU:C	1:O:124:THR:H	2.21	0.45
1:O:4:MET:O	1:O:5:THR:O	2.35	0.45
2:P:51:GLU:CD	2:P:202:THR:HG23	2.36	0.45
2:P:61:GLN:NE2	2:P:226:PRO:HG3	2.31	0.45
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.52	0.45
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.51	0.45
3:Q:158:SER:CB	4:R:59:LEU:HD21	2.46	0.45
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:96:ALA:HA	7:U:107:MET:CE	2.23	0.45
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.99	0.45
10:X:112:GLN:NE2	10:X:126:ALA:H	2.14	0.45
12:Z:99:THR:CG2	16:Z:199:HOH:O	2.64	0.45
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.81	0.45
13:M:164:TYR:O	14:2:26:ILE:HD12	2.17	0.45
2:B:38:ILE:HG12	2:B:164:SER:HB3	1.98	0.45
2:B:235:LYS:C	2:B:237:GLY:N	2.70	0.45
9:I:137:MET:CE	9:I:141:LEU:HD11	2.47	0.45
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.47	0.45
11:K:6:PHE:HA	11:K:123:ASP:O	2.16	0.45
14:N:3:ILE:HG22	14:N:16:ALA:HB1	1.98	0.45
12:Z:58:ARG:NH2	16:Z:227:HOH:O	2.50	0.45
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.98	0.45
3:C:112:LEU:O	3:C:116:VAL:HG23	2.17	0.45
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.17	0.45
6:F:127:ASN:ND2	6:F:127:ASN:H	2.15	0.45
7:G:203:THR:HG22	7:G:204:GLU:N	2.32	0.45
9:I:3:VAL:HG23	9:I:46:THR:HG22	1.98	0.45
11:K:67:GLU:OE1	11:K:74:ILE:HG22	2.17	0.45
1:O:217:ASP:O	1:O:220:ARG:HA	2.17	0.45
5:S:2(C):VAL:O	5:S:226:GLY:HA2	2.17	0.45
6:T:157:TYR:CD1	6:T:157:TYR:C	2.90	0.45
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.80	0.45
13:1:40:ASN:ND2	13:1:40:ASN:N	2.64	0.44
14:2:4:MET:CB	14:2:126:ILE:HG22	2.47	0.44
1:A:197:LEU:HD23	1:A:210:ILE:HD13	1.98	0.44
6:F:127:ASN:N	6:F:127:ASN:HD22	2.15	0.44
13:M:165:ARG:HA	14:2:26:ILE:HB	1.98	0.44
1:A:85:TYR:O	1:A:89:VAL:HG23	2.17	0.44
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.17	0.44
2:B:21(C):ASP:OD2	2:B:219:GLU:HB3	2.16	0.44
5:E:2(C):VAL:O	5:E:226:GLY:HA2	2.18	0.44
6:F:127:ASN:C	6:F:127:ASN:HD22	2.20	0.44
1:A:57:PRO:HG3	7:G:177:GLU:CD	2.38	0.44
7:G:211:GLU:HA	16:G:256:HOH:O	2.18	0.44
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.53	0.44
13:M:91:ARG:HG3	13:M:92:SER:N	2.31	0.44
14:N:19:ARG:HG3	14:N:26:ILE:HG23	1.99	0.44
3:Q:18:ASP:OD2	3:Q:20:HIS:ND1	2.50	0.44
3:Q:52:ARG:NH2	3:Q:211:GLU:HB3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:123:ASN:ND2	5:S:123:ASN:N	2.65	0.44
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.16	0.44
5:S:93:ARG:HD2	16:S:245:HOH:O	2.16	0.44
3:C:52:ARG:NH2	3:C:211:GLU:HB3	2.32	0.44
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.99	0.44
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.98	0.44
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.99	0.44
14:N:18(A):ILE:HD13	14:N:18(B):PHE:H	1.82	0.44
14:N:85:GLU:O	14:N:89:GLU:HB2	2.18	0.44
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.98	0.44
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.67	0.44
5:S:90:ASN:O	5:S:94:GLN:HG3	2.17	0.44
7:U:8:TYR:C	7:U:10:ARG:H	2.21	0.44
8:V:84:LYS:HE2	8:V:119:THR:CG2	2.47	0.44
11:Y:76:VAL:HG22	11:Y:103:GLY:HA3	1.98	0.44
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.99	0.44
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.98	0.44
3:C:241:GLN:O	3:C:243:GLN:N	2.41	0.44
3:C:55:THR:HG22	3:C:56:LEU:CD2	2.44	0.44
4:D:12(F):GLY:HA3	16:D:262:HOH:O	2.17	0.44
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.51	0.44
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.99	0.44
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.98	0.44
1:O:184:LEU:HB2	16:O:246:HOH:O	2.17	0.44
2:P:21(C):ASP:OD2	2:P:219:GLU:HB3	2.17	0.44
4:R:91:HIS:CG	4:R:119:LEU:HD11	2.52	0.44
7:U:224:LEU:HB3	7:U:228:ASN:HB2	1.99	0.44
14:2:18(A):ILE:HD13	14:2:18(B):PHE:H	1.83	0.44
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.82	0.44
3:C:107:VAL:HA	16:C:250:HOH:O	2.17	0.44
13:M:130:GLY:O	13:M:134:ALA:HB3	2.17	0.44
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.53	0.44
7:U:203:THR:HG22	7:U:204:GLU:N	2.33	0.44
10:X:178:VAL:HG22	10:X:184:ILE:HG12	2.00	0.44
3:C:72:SER:O	3:C:221:ILE:HD12	2.17	0.44
5:E:66:LYS:O	5:E:77:SER:HA	2.18	0.44
6:F:43:ASN:N	6:F:43:ASN:ND2	2.66	0.44
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.48	0.44
3:C:101:LEU:HD11	10:J:57:GLU:HB3	1.99	0.44
11:K:31:VAL:HG11	11:K:45:MET:HE3	2.00	0.44
1:O:186:LEU:O	1:O:190:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:198:SER:HA	5:S:201:LEU:HG	1.99	0.44
6:T:187:ARG:CG	6:T:187:ARG:HH11	2.30	0.44
7:U:141:VAL:HG21	7:U:216:THR:HA	2.00	0.44
8:V:78:SER:O	8:V:82:MET:HG3	2.18	0.44
9:W:15:ALA:HB2	9:W:175:VAL:HG22	2.00	0.44
2:B:97:GLN:NE2	16:B:246:HOH:O	2.50	0.44
3:C:18:ASP:OD2	3:C:20:HIS:ND1	2.51	0.44
9:I:15:ALA:HB1	9:I:159:LEU:HD22	2.00	0.44
9:I:80:THR:HG22	9:I:119:ILE:HD13	1.98	0.44
9:I:84:SER:HB2	9:I:119:ILE:HD11	2.00	0.44
12:L:93:PHE:N	12:L:94:PRO:HD3	2.33	0.44
13:M:85:THR:O	13:M:89:GLN:HG3	2.18	0.44
10:X:52:THR:HG22	10:X:53:VAL:H	1.83	0.44
13:1:177:ILE:HD12	13:1:177:ILE:N	2.33	0.44
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.53	0.44
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.17	0.44
4:D:29:GLU:HA	4:D:29:GLU:OE2	2.18	0.44
5:E:4:PHE:CG	5:E:5:ARG:N	2.86	0.44
9:I:15:ALA:HB2	9:I:175:VAL:HG22	1.98	0.44
11:K:195:LEU:O	11:K:199:VAL:HG23	2.18	0.44
11:K:200:LYS:HG3	11:K:206:PHE:HB2	2.00	0.44
13:M:112:TYR:C	13:M:112:TYR:CD2	2.91	0.44
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.53	0.44
3:Q:215:VAL:HG23	3:Q:221:ILE:HG13	1.99	0.44
5:S:20:ARG:HB3	5:S:25:GLU:OE2	2.17	0.44
7:U:38:LEU:C	7:U:38:LEU:HD12	2.38	0.44
9:W:3:VAL:HG23	9:W:46:THR:HG22	1.99	0.44
10:X:85:GLN:O	10:X:89:LYS:HG3	2.17	0.44
14:2:146:MET:HB3	14:2:150:GLU:HB2	2.00	0.44
5:E:104:ASN:HB2	13:M:81:GLU:HG2	2.00	0.44
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.18	0.44
9:I:61:TYR:C	9:I:61:TYR:CD1	2.92	0.44
11:K:86:LEU:O	11:K:89:GLN:HB2	2.17	0.44
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.53	0.44
1:O:67:VAL:CG2	1:O:211:GLU:HG2	2.48	0.44
7:U:152:ASP:HB2	7:U:153:PRO:HD2	2.00	0.44
13:1:131:ALA:HA	13:1:135:ASN:ND2	2.33	0.43
1:A:62:GLU:H	1:A:62:GLU:CD	2.21	0.43
7:G:8:TYR:C	7:G:10:ARG:H	2.21	0.43
10:J:4:LEU:HD23	10:J:126:ALA:HB2	2.00	0.43
13:M:177:ILE:HD12	13:M:177:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:186:PHE:CE1	13:M:188:LYS:HG3	2.53	0.43
14:N:14:LEU:O	14:N:175:MET:HA	2.17	0.43
4:R:187:LYS:O	4:R:191:LEU:HD22	2.18	0.43
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.18	0.43
3:C:215:VAL:HG23	3:C:221:ILE:HG13	1.99	0.43
5:E:90:ASN:O	5:E:94:GLN:HG3	2.17	0.43
6:F:180:VAL:HG21	7:G:58:LEU:HD23	2.00	0.43
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.33	0.43
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.33	0.43
10:J:178:VAL:HG22	10:J:184:ILE:HG12	2.00	0.43
10:J:45:PHE:CD1	10:J:52:THR:HG23	2.53	0.43
13:M:3:VAL:HG23	13:M:46:SER:HB3	2.00	0.43
1:O:197:LEU:HD23	1:O:210:ILE:HD13	1.99	0.43
3:Q:215:VAL:HG23	3:Q:221:ILE:CG1	2.48	0.43
5:S:180:LEU:O	5:S:18(D):ILE:HG22	2.19	0.43
7:U:151:THR:HG22	7:U:157:TYR:CB	2.46	0.43
8:V:221:ILE:HD13	8:V:221:ILE:N	2.33	0.43
10:J:144:PRO:HG2	11:Y:207:ASN:HD21	1.83	0.43
8:H:30:ASN:O	8:H:189:ARG:NH2	2.51	0.43
9:I:114:ASP:HB2	16:I:231:HOH:O	2.17	0.43
10:J:39:PRO:HG2	10:J:73:GLU:CD	2.38	0.43
12:L:13:VAL:HG12	12:L:177:ILE:HG13	2.00	0.43
13:M:211:ILE:HD11	16:2:196:HOH:O	2.18	0.43
2:P:235:LYS:C	2:P:237:GLY:N	2.70	0.43
5:S:4:PHE:CG	5:S:5:ARG:N	2.86	0.43
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.89	0.43
8:V:48:THR:HB	8:V:51:ASP:HB2	1.99	0.43
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.16	0.43
13:1:186:PHE:CE1	13:1:188:LYS:HG3	2.53	0.43
14:2:44:CYS:HB2	14:2:100:ILE:HB	2.00	0.43
2:B:15:PHE:N	3:C:23:GLN:HE22	2.05	0.43
3:C:55:THR:O	3:C:56:LEU:HD22	2.17	0.43
2:P:235:LYS:N	2:P:235:LYS:HD3	2.33	0.43
2:P:6:ARG:HH12	4:R:12(B):GLU:CD	2.22	0.43
4:R:68:VAL:HG21	4:R:89:ILE:CD1	2.27	0.43
6:T:100:LYS:NZ	16:T:267:HOH:O	2.47	0.43
7:U:188:LYS:HA	7:U:188:LYS:HD3	1.78	0.43
7:U:186:TRP:O	7:U:190:VAL:HG23	2.18	0.43
10:X:39:PRO:HG2	10:X:73:GLU:CD	2.39	0.43
12:Z:113:PHE:N	12:Z:113:PHE:CD1	2.87	0.43
13:1:17:ASP:HA	13:1:173:PHE:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:146:TYR:HE1	4:D:216:THR:HA	1.83	0.43
5:E:177:GLU:OE1	6:F:56:SER:HB2	2.19	0.43
8:H:84:LYS:HE2	8:H:119:THR:CG2	2.48	0.43
8:H:167:LEU:HD12	12:Z:24:TYR:HA	2.00	0.43
9:I:45:ILE:HB	9:I:52:VAL:HG13	2.00	0.43
12:L:113:PHE:CD1	12:L:113:PHE:N	2.86	0.43
14:N:10(B):LYS:O	14:N:10(B):LYS:HD3	2.18	0.43
4:R:241:GLU:C	4:R:243:ALA:H	2.21	0.43
6:T:199:LEU:HD12	6:T:240:ILE:CD1	2.49	0.43
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	2.01	0.43
13:1:-6:GLN:HG3	13:1:-6:GLN:O	2.18	0.43
2:B:41:MET:HE3	3:C:60:ASP:OD1	2.19	0.43
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.53	0.43
12:L:43:MET:HG3	12:L:101:ILE:HG22	2.01	0.43
14:N:105:ASP:HB2	16:N:218:HOH:O	2.18	0.43
1:O:186:LEU:HD21	1:O:214:ILE:HD12	2.01	0.43
5:S:66:LYS:O	5:S:77:SER:HA	2.18	0.43
4:D:161:ASN:HB3	4:D:180:TRP:CZ2	2.53	0.43
14:N:172:VAL:HB	14:N:18(A):ILE:CD1	2.48	0.43
2:P:103:TYR:O	2:P:104:ASN:HB2	2.18	0.43
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.18	0.43
5:E:54:ASN:ND2	5:E:56:ASP:O	2.52	0.43
7:G:18(H):GLU:H	7:G:18(H):GLU:CD	2.21	0.43
7:G:186:TRP:O	7:G:190:VAL:HG23	2.19	0.43
9:I:15:ALA:CB	9:I:175:VAL:HG22	2.49	0.43
12:L:17:ASP:OD2	12:L:33:LYS:NZ	2.45	0.43
12:L:98:HIS:HD2	16:L:198:HOH:O	2.01	0.43
14:N:114:PRO:HD2	14:N:118:SER:O	2.19	0.43
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.82	0.43
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.83	0.43
3:C:215:VAL:HG23	3:C:221:ILE:CG1	2.49	0.43
3:C:33:ARG:O	3:C:33:ARG:HG2	2.19	0.43
4:D:241:GLU:C	4:D:243:ALA:H	2.21	0.43
4:D:243:ALA:O	4:D:244:GLU:HB2	2.18	0.43
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.99	0.43
8:H:100:ILE:HD11	8:H:127:LEU:HG	2.01	0.43
10:J:60:GLN:O	10:J:64:GLN:HG3	2.18	0.43
10:J:85:GLN:HG2	10:J:89:LYS:HE3	2.00	0.43
11:K:97:MET:HG2	11:K:115:SER:HB3	2.01	0.43
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.18	0.43
3:Q:72:SER:O	3:Q:221:ILE:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.48	0.43
14:N:140:LYS:NZ	14:2:157:HIS:HD2	2.17	0.43
4:D:14:THR:HG22	4:D:15:PHE:N	2.33	0.43
3:C:158:SER:CB	4:D:59:LEU:HD21	2.49	0.43
6:F:11:SER:HB3	6:F:14:VAL:CG2	2.49	0.43
7:G:38:LEU:C	7:G:38:LEU:HD12	2.39	0.43
8:H:63:ILE:CG2	8:H:74:PRO:HB3	2.49	0.43
10:J:166:MET:HA	10:J:167:PRO:HD3	1.82	0.43
12:L:24:TYR:HA	8:V:167:LEU:HD12	2.00	0.43
16:V:334:HOH:O	9:W:150:ASP:HA	2.19	0.43
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.54	0.42
14:N:14:LEU:HD11	14:N:102:ALA:CB	2.49	0.42
14:N:146:MET:HB3	14:N:150:GLU:HB2	1.99	0.42
14:N:4:MET:CB	14:N:126:ILE:HG22	2.49	0.42
1:O:77:VAL:CG1	1:O:137:LEU:HB2	2.49	0.42
4:R:243:ALA:O	4:R:244:GLU:HB2	2.19	0.42
5:S:174:THR:O	5:S:178:ARG:HB2	2.19	0.42
4:R:17:PRO:HA	5:S:26:TYR:CD1	2.54	0.42
6:T:199:LEU:HD12	6:T:240:ILE:HD12	2.00	0.42
7:U:110:ASP:HB3	7:U:149:TYR:CZ	2.54	0.42
12:Z:-5:TYR:CD2	12:Z:96:TYR:HB2	2.54	0.42
3:C:52:ARG:HB2	3:C:209:ASN:HA	2.01	0.42
3:C:215:VAL:O	3:C:215:VAL:HG13	2.19	0.42
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.83	0.42
6:F:91:ARG:HG2	6:F:119:TYR:CD2	2.53	0.42
9:I:89:GLU:HG2	9:I:90:ARG:NH1	2.33	0.42
2:P:21(E):VAL:HG12	2:P:220:TYR:N	2.34	0.42
5:S:2(C):VAL:HG22	5:S:226:GLY:C	2.40	0.42
1:O:58:LEU:HB3	7:U:162:ALA:O	2.19	0.42
9:W:84:SER:HB2	9:W:119:ILE:HD11	2.01	0.42
13:1:130:GLY:O	13:1:134:ALA:HB3	2.20	0.42
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.19	0.42
1:O:62:GLU:CD	1:O:62:GLU:H	2.22	0.42
4:R:14:THR:HG22	4:R:15:PHE:N	2.33	0.42
10:X:169:ASP:OD1	10:X:171:LYS:HD3	2.19	0.42
2:B:136:PHE:O	2:B:150:THR:HA	2.19	0.42
3:C:106:PRO:HG2	3:C:143:PRO:HG2	2.00	0.42
7:G:170:GLN:HB3	16:G:265:HOH:O	2.18	0.42
9:I:14:ILE:HG23	9:I:14:ILE:O	2.20	0.42
8:H:206:PHE:CE2	9:I:157:GLN:HG3	2.55	0.42
11:K:5:ALA:HA	11:K:13:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:145:TYR:HD1	12:L:146:LEU:N	2.15	0.42
12:L:14:LEU:HD13	12:L:34:VAL:HG13	2.00	0.42
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.35	0.42
1:O:33:GLN:CA	1:O:33:GLN:NE2	2.80	0.42
1:O:85:TYR:O	1:O:89:VAL:HG23	2.19	0.42
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	2.01	0.42
3:Q:215:VAL:O	3:Q:215:VAL:HG13	2.19	0.42
2:P:147:GLN:HG2	3:Q:62(A):ILE:HG21	2.01	0.42
10:X:124:TYR:CD2	10:X:138:LEU:HD13	2.54	0.42
14:2:159:LEU:O	14:2:163:ILE:HD12	2.20	0.42
1:A:108:PRO:HG2	1:A:111:LEU:HG	2.01	0.42
2:B:194:LEU:HD13	2:B:233:LEU:HD12	2.00	0.42
9:I:1:GLY:HA2	9:I:17:ASP:OD1	2.19	0.42
11:K:33:LYS:O	11:K:45:MET:N	2.52	0.42
14:N:65:LEU:HG	14:N:69:GLN:HE21	1.84	0.42
6:T:127:ASN:ND2	6:T:127:ASN:H	2.17	0.42
7:U:31:THR:HG21	7:U:135:ILE:HG13	2.02	0.42
8:V:207:PRO:O	8:V:210:THR:OG1	2.30	0.42
10:X:85:GLN:HG2	10:X:89:LYS:HE3	2.00	0.42
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.54	0.42
14:2:36:ARG:HG3	14:2:42:TRP:NE1	2.34	0.42
4:D:194:LEU:HD22	4:D:212:LEU:HD11	2.02	0.42
4:D:39:GLY:O	4:D:162:ALA:HA	2.20	0.42
9:I:6:MET:HB3	9:I:151:LEU:HD11	2.01	0.42
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.83	0.42
2:P:185:LYS:HD3	2:P:186:VAL:H	1.85	0.42
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.85	0.42
6:T:43:ASN:ND2	6:T:43:ASN:N	2.67	0.42
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.02	0.42
9:I:165:ARG:NH2	12:Z:135:MET:HE2	2.34	0.42
1:A:33:GLN:CA	1:A:33:GLN:NE2	2.80	0.42
3:C:36:CYS:H	3:C:51:GLU:HG2	1.85	0.42
3:C:160:TRP:NE1	4:D:59:LEU:HD23	2.35	0.42
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.50	0.42
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.54	0.42
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.84	0.42
9:W:15:ALA:HB1	9:W:159:LEU:HD22	2.01	0.42
9:W:20:LEU:C	9:W:20:LEU:HD13	2.39	0.42
11:Y:67:GLU:OE1	11:Y:74:ILE:HG22	2.19	0.42
11:Y:78:ALA:O	11:Y:82:ILE:HG12	2.20	0.42
13:1:46:SER:OG	13:1:98:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197:LEU:HD13	3:C:210:ILE:HD12	2.02	0.42
4:D:117:CYS:HG	4:D:157:PHE:HD2	1.66	0.42
5:E:45:HIS:HB2	5:E:189:LEU:HD12	2.02	0.42
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.55	0.42
6:F:157:TYR:C	6:F:157:TYR:CD1	2.92	0.42
6:F:205:ASN:O	6:F:20(B):GLU:N	2.53	0.42
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.20	0.42
3:Q:197:LEU:HD13	3:Q:210:ILE:HD12	2.02	0.42
4:R:12(D):ALA:HB3	4:R:126:ARG:CG	2.50	0.42
9:W:15:ALA:CB	9:W:175:VAL:HG22	2.49	0.42
12:Z:134:ILE:O	12:Z:137:PHE:HB3	2.20	0.42
12:Z:-6:PRO:HG2	12:Z:-5:TYR:CD1	2.55	0.42
2:B:186:VAL:HG21	2:B:216:ARG:CG	2.50	0.42
3:C:209:ASN:O	3:C:210:ILE:HD13	2.19	0.42
5:E:180:LEU:O	5:E:18(D):ILE:HG22	2.18	0.42
7:G:48:VAL:C	7:G:49:ILE:HD12	2.41	0.42
14:N:3:ILE:HG22	14:N:16:ALA:HB2	2.01	0.42
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.85	0.42
8:V:30:ASN:O	8:V:189:ARG:NH2	2.50	0.42
7:G:17(C):LYS:HB2	7:G:17(C):LYS:HE3	1.80	0.42
9:I:93:GLY:N	9:I:94:PRO:CD	2.83	0.42
13:M:5:SER:HB3	13:M:14:ILE:HG13	2.01	0.42
14:N:4:MET:HB3	14:N:126:ILE:HG22	2.02	0.42
1:O:195:LEU:HD23	1:O:236:LEU:HD11	2.02	0.42
2:P:186:VAL:HG11	2:P:216:ARG:CD	2.50	0.42
4:R:96:ALA:HA	4:R:107:ILE:HG21	2.02	0.42
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.49	0.42
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.84	0.42
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.83	0.42
2:B:235:LYS:HD3	2:B:235:LYS:N	2.34	0.41
4:D:29:GLU:OE2	4:D:32:LYS:HD2	2.20	0.41
6:F:87:HIS:HD2	6:F:132:PHE:CE2	2.38	0.41
7:G:31:THR:HG21	7:G:135:ILE:HG13	2.01	0.41
12:L:45:ALA:HB1	12:L:97:VAL:HG21	2.02	0.41
13:M:131:ALA:HA	13:M:135:ASN:ND2	2.35	0.41
13:M:40:ASN:HD22	13:M:41:THR:N	2.18	0.41
1:O:7:ARG:HD3	5:S:127:TYR:CD2	2.55	0.41
6:T:127:ASN:HD22	6:T:127:ASN:N	2.16	0.41
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.81	0.41
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.55	0.41
2:B:27:ALA:O	2:B:30:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.45	0.41
6:F:93:ARG:HD3	16:F:268:HOH:O	2.20	0.41
8:H:72:ARG:NH1	8:H:72:ARG:HG3	2.34	0.41
9:I:20:LEU:HD13	9:I:20:LEU:C	2.41	0.41
9:I:18:LEU:CD2	9:I:32:GLU:HG2	2.49	0.41
1:O:88:LEU:HG	1:O:132:PHE:CE2	2.55	0.41
2:P:161:LYS:HB3	2:P:180:TYR:CE2	2.55	0.41
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.40	0.41
4:R:108:ASN:HB3	16:R:255:HOH:O	2.21	0.41
5:S:45:HIS:HB2	5:S:189:LEU:HD12	2.01	0.41
5:S:93:ARG:NH1	16:S:245:HOH:O	2.53	0.41
6:T:114:ASP:O	6:T:118:GLN:HG2	2.19	0.41
6:T:69:VAL:HG23	6:T:74:ILE:O	2.20	0.41
12:Z:14(E):GLU:OE2	12:Z:14(P):PRO:HD2	2.21	0.41
4:D:100:ASN:HB3	16:D:248:HOH:O	2.19	0.41
5:E:123:ASN:ND2	5:E:123:ASN:N	2.68	0.41
5:E:174:THR:O	5:E:178:ARG:HB2	2.21	0.41
6:F:21(B):THR:O	6:F:21(C):ASN:CB	2.68	0.41
8:H:172:ASN:HB3	8:H:192:LEU:O	2.20	0.41
9:I:177:ILE:HD13	9:I:177:ILE:N	2.35	0.41
12:L:107:LYS:HA	12:L:107:LYS:HD3	1.93	0.41
5:S:46:ALA:CB	5:S:139:ILE:HB	2.50	0.41
5:S:160:LEU:HD13	5:S:163:THR:HB	2.02	0.41
5:S:28:LEU:HA	5:S:31:ILE:HD12	2.02	0.41
6:T:169:ARG:O	6:T:173:LYS:HG3	2.20	0.41
9:W:14:ILE:HG23	9:W:14:ILE:O	2.20	0.41
9:W:168:LEU:HD22	16:W:205:HOH:O	2.19	0.41
10:X:104:TYR:CD1	10:X:180:LYS:HA	2.55	0.41
10:X:48:GLU:CB	10:X:96:GLN:HB2	2.49	0.41
11:Y:87:VAL:CG1	11:Y:115:SER:HA	2.50	0.41
11:Y:97:MET:HG2	11:Y:115:SER:HB3	2.02	0.41
1:A:195:LEU:HD23	1:A:236:LEU:HD11	2.03	0.41
6:F:127:ASN:ND2	6:F:127:ASN:N	2.68	0.41
7:G:191:GLU:HG3	7:G:232:ARG:HG3	2.03	0.41
9:I:18:LEU:HD12	9:I:172:GLY:HA3	2.03	0.41
11:K:76:VAL:HG22	11:K:103:GLY:HA3	2.01	0.41
12:L:120:GLU:HA	12:L:120:GLU:OE1	2.20	0.41
3:Q:76:LEU:HD22	3:Q:89:ILE:HG13	2.01	0.41
4:R:194:LEU:HA	4:R:194:LEU:HD12	1.92	0.41
5:S:74:MET:HE2	5:S:109:VAL:HA	2.01	0.41
6:T:103:TYR:O	6:T:104:LYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:172:ALA:C	6:T:176:LEU:HD23	2.41	0.41
6:T:45:GLY:HA3	6:T:215:CYS:O	2.20	0.41
9:W:6:MET:HB3	9:W:151:LEU:HD11	2.03	0.41
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.56	0.41
9:W:93:GLY:N	9:W:94:PRO:CD	2.83	0.41
14:2:85:GLU:O	14:2:89:GLU:HB2	2.20	0.41
1:A:26:TYR:O	1:A:29:THR:HB	2.20	0.41
3:C:185:THR:CB	3:C:188:GLU:HG2	2.43	0.41
5:E:185:ASN:OD1	5:E:188:GLU:HG2	2.21	0.41
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.51	0.41
2:P:233:LEU:HA	2:P:233:LEU:HD12	1.92	0.41
3:Q:209:ASN:O	3:Q:210:ILE:HD13	2.20	0.41
7:U:107:MET:HA	7:U:108:PRO:HD3	1.90	0.41
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.86	0.41
7:U:225:SER:H	7:U:228:ASN:HB2	1.85	0.41
8:V:95:ILE:O	8:V:97:ALA:N	2.53	0.41
11:Y:3:THR:HG22	11:Y:16:VAL:HG12	2.02	0.41
14:2:107:LYS:CG	14:2:108:GLY:H	2.26	0.41
14:2:37:VAL:HG22	14:2:41:ILE:O	2.21	0.41
4:D:227:GLU:OE2	4:D:227:GLU:N	2.39	0.41
4:D:96:ALA:HA	4:D:107:ILE:HG21	2.02	0.41
6:F:43:ASN:N	6:F:43:ASN:HD22	2.18	0.41
7:G:39:ALA:CB	7:G:48:VAL:HG12	2.48	0.41
10:J:90(A):ILE:HA	10:J:90(A):ILE:HD13	1.79	0.41
2:P:89:ILE:O	2:P:92:ALA:HB3	2.21	0.41
6:T:21(B):THR:O	6:T:21(C):ASN:CB	2.68	0.41
7:U:164:ALA:CB	7:U:172:ILE:HB	2.51	0.41
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.33	0.41
2:B:15:PHE:H	3:C:23:GLN:NE2	2.06	0.41
3:C:46:VAL:HG11	3:C:139:ALA:HB1	2.02	0.41
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.88	0.41
10:J:77:GLN:HB2	16:J:206:HOH:O	2.21	0.41
2:P:215:ILE:HG22	2:P:215:ILE:O	2.20	0.41
14:2:59:VAL:HG22	14:2:82:VAL:HG12	2.03	0.41
6:F:91:ARG:O	6:F:95:GLU:HB2	2.20	0.41
7:G:152:ASP:HB2	7:G:153:PRO:HD2	2.01	0.41
7:G:82:ILE:HG22	7:G:83:PRO:HD3	2.02	0.41
10:J:7:ARG:NH1	10:J:7:ARG:HG2	2.34	0.41
11:K:78:ALA:O	11:K:82:ILE:HG12	2.20	0.41
14:N:172:VAL:CB	14:N:18(A):ILE:HD11	2.50	0.41
4:R:161:ASN:HB3	4:R:180:TRP:CZ2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:18:LEU:HD12	9:W:172:GLY:HA3	2.02	0.41
10:X:77:GLN:C	10:X:77:GLN:NE2	2.74	0.41
14:2:172:VAL:CB	14:2:18(A):ILE:HD11	2.49	0.41
1:A:186:LEU:HD21	1:A:214:ILE:HD12	2.01	0.41
1:A:21(A):GLU:OE2	1:A:21(P):LYS:HB2	2.21	0.41
2:B:103:TYR:O	2:B:104:ASN:HB2	2.20	0.41
5:E:160:LEU:HD13	5:E:163:THR:HB	2.03	0.41
13:M:191:GLN:HE21	13:M:191:GLN:HB3	1.61	0.41
1:O:175:PHE:O	1:O:179:ARG:HG2	2.21	0.41
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.51	0.41
12:Z:107:LYS:HD3	12:Z:107:LYS:HA	1.94	0.41
12:Z:17:ASP:OD2	12:Z:33:LYS:NZ	2.45	0.41
12:Z:176:LEU:CD1	12:Z:186:LYS:HG2	2.51	0.41
1:A:46:VAL:HG11	1:A:139:ALA:HB1	2.03	0.41
1:A:232:ARG:NH1	1:A:232:ARG:HG3	2.36	0.41
4:D:12(D):ALA:HB3	4:D:126:ARG:CG	2.51	0.41
5:E:2(C):VAL:HG22	5:E:226:GLY:C	2.41	0.41
6:F:114:ASP:O	6:F:118:GLN:HG2	2.20	0.41
7:G:13:THR:HB	7:G:124:THR:O	2.20	0.41
13:M:152:GLU:O	13:M:156:VAL:HG23	2.20	0.41
13:M:-5:PRO:HD3	13:M:96:TRP:CE2	2.56	0.41
1:O:58:LEU:HD23	1:O:58:LEU:HA	1.83	0.41
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.20	0.41
4:R:135:ALA:O	4:R:136:LEU:HD23	2.20	0.41
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.50	0.41
6:T:127:ASN:ND2	6:T:127:ASN:N	2.69	0.41
1:A:38:LEU:HD12	1:A:38:LEU:C	2.40	0.41
1:A:58:LEU:HD23	1:A:58:LEU:HA	1.86	0.41
5:E:38:VAL:HG12	5:E:39:GLY:N	2.35	0.41
10:J:169:ASP:OD1	10:J:171:LYS:HD3	2.21	0.41
10:J:93:ARG:NH2	11:K:91:LYS:HD3	2.36	0.41
2:P:231:ASP:O	2:P:235:LYS:HG2	2.21	0.41
2:P:63:THR:HG22	2:P:63:THR:O	2.20	0.41
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	2.01	0.41
4:R:146:TYR:HE1	4:R:216:THR:HA	1.85	0.41
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.64	0.41
12:Z:145:TYR:HD1	12:Z:146:LEU:N	2.17	0.41
12:Z:39:ASP:OD2	12:Z:67:HIS:HE1	2.04	0.41
5:E:20:ARG:HB3	5:E:25:GLU:OE2	2.21	0.40
7:G:197:MET:HG2	7:G:205:PHE:CE1	2.56	0.40
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:76:VAL:N	11:K:106:GLU:OE2	2.50	0.40
2:P:235:LYS:O	2:P:237:GLY:N	2.54	0.40
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.56	0.40
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.36	0.40
14:2:14:LEU:HD11	14:2:102:ALA:CB	2.51	0.40
14:2:51:ASP:O	14:2:55:ILE:HG13	2.21	0.40
1:A:31:VAL:HG11	1:A:135:SER:HB2	2.04	0.40
1:A:175:PHE:O	1:A:179:ARG:HG2	2.21	0.40
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.19	0.40
1:O:110:LYS:HG2	16:O:243:HOH:O	2.20	0.40
1:O:26:TYR:O	1:O:29:THR:HB	2.20	0.40
1:O:46:VAL:HG11	1:O:139:ALA:HB1	2.02	0.40
6:T:205:ASN:O	6:T:20(B):GLU:N	2.53	0.40
9:W:177:ILE:N	9:W:177:ILE:CD1	2.85	0.40
9:W:81:GLN:HA	9:W:81:GLN:NE2	2.35	0.40
3:C:36:CYS:N	3:C:51:GLU:HG2	2.36	0.40
3:C:58:LEU:HA	3:C:58:LEU:HD12	1.79	0.40
4:D:52:LYS:O	4:D:53:ARG:HB3	2.21	0.40
10:J:48:GLU:CB	10:J:96:GLN:HB2	2.51	0.40
13:M:157:ASN:ND2	16:M:265:HOH:O	2.54	0.40
4:R:39:GLY:O	4:R:162:ALA:HA	2.20	0.40
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	2.04	0.40
12:Z:-9:GLN:NE2	12:Z:-8:PHE:N	2.65	0.40
13:1:84:ALA:HA	13:1:113:VAL:HG21	2.04	0.40
13:1:133:MET:C	13:1:136:PRO:HD2	2.42	0.40
13:1:85:THR:O	13:1:89:GLN:HG3	2.22	0.40
2:B:63:THR:HG22	2:B:63:THR:O	2.20	0.40
5:E:38:VAL:CG1	5:E:39:GLY:N	2.84	0.40
8:H:175:VAL:CG1	8:H:176:CYS:N	2.84	0.40
9:I:55:LEU:HD21	9:I:95:TYR:CD1	2.57	0.40
1:O:185:GLU:OE1	1:O:187:GLU:HB2	2.21	0.40
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.37	0.40
12:L:153:LYS:HG2	8:V:201:GLN:CG	2.52	0.40
13:1:175:LEU:HD23	13:1:175:LEU:C	2.42	0.40
1:A:122:GLU:C	1:A:124:THR:H	2.23	0.40
2:B:231:ASP:O	2:B:235:LYS:HG2	2.21	0.40
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.84	0.40
6:F:195:LYS:NZ	16:F:282:HOH:O	2.55	0.40
1:O:38:LEU:HD12	1:O:38:LEU:C	2.42	0.40
6:T:121:GLN:NE2	16:T:248:HOH:O	2.54	0.40
7:U:214:VAL:HB	7:U:222:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:48:VAL:C	7:U:49:ILE:HD12	2.42	0.40
9:W:137:MET:CE	9:W:141:LEU:HD11	2.52	0.40
10:X:143:ARG:HA	10:X:144:PRO:HD3	1.95	0.40
10:X:45:PHE:CD1	10:X:52:THR:HG23	2.57	0.40
11:Y:33:LYS:O	11:Y:45:MET:N	2.52	0.40
12:Z:42:VAL:HG12	12:Z:176:LEU:HD23	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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%)	230 (93%)	15 (6%)	3 (1%)	13	39
1	O	248/250 (99%)	230 (93%)	15 (6%)	3 (1%)	13	39
2	B	242/244 (99%)	220 (91%)	19 (8%)	3 (1%)	13	39
2	P	242/244 (99%)	220 (91%)	18 (7%)	4 (2%)	9	29
3	C	239/241 (99%)	218 (91%)	17 (7%)	4 (2%)	9	29
3	Q	239/241 (99%)	218 (91%)	17 (7%)	4 (2%)	9	29
4	D	240/242 (99%)	219 (91%)	16 (7%)	5 (2%)	7	23
4	R	240/242 (99%)	217 (90%)	18 (8%)	5 (2%)	7	23
5	E	231/233 (99%)	212 (92%)	15 (6%)	4 (2%)	9	29
5	S	231/233 (99%)	211 (91%)	16 (7%)	4 (2%)	9	29
6	F	242/244 (99%)	229 (95%)	11 (4%)	2 (1%)	19	49
6	T	242/244 (99%)	228 (94%)	12 (5%)	2 (1%)	19	49
7	G	241/243 (99%)	228 (95%)	12 (5%)	1 (0%)	34	66
7	U	241/243 (99%)	228 (95%)	12 (5%)	1 (0%)	34	66
8	H	220/222 (99%)	207 (94%)	10 (4%)	3 (1%)	11	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	220/222 (99%)	209 (95%)	8 (4%)	3 (1%)	11	34
9	I	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	29	61
9	W	202/204 (99%)	193 (96%)	8 (4%)	1 (0%)	29	61
10	J	196/198 (99%)	188 (96%)	4 (2%)	4 (2%)	7	24
10	X	196/198 (99%)	187 (95%)	6 (3%)	3 (2%)	10	33
11	K	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
11	Y	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
12	L	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	29	61
12	Z	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	29	61
13	1	231/233 (99%)	214 (93%)	15 (6%)	2 (1%)	17	46
13	M	231/233 (99%)	214 (93%)	15 (6%)	2 (1%)	17	46
14	2	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6312/6368 (99%)	5892 (93%)	354 (6%)	66 (1%)	15	44

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
3	C	58	LEU
4	D	12(G)	GLU
6	F	205	ASN
10	J	192	ALA
1	O	5	THR
3	Q	58	LEU
4	R	12(G)	GLU
6	T	205	ASN
10	X	192	ALA
1	A	61	SER
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	203	THR
5	E	202	ARG
6	F	206	LYS
2	P	54	VAL
2	P	21(B)	GLY

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Mol	Chain	Res	Type
2	P	21(C)	ASP
3	Q	203	THR
5	S	202	ARG
6	T	206	LYS
3	C	179	ASN
3	C	183	PRO
4	D	128	MET
5	E	180	LEU
7	G	220	LYS
9	I	93	GLY
1	O	61	SER
3	Q	179	ASN
3	Q	183	PRO
4	R	128	MET
5	S	180	LEU
7	U	220	LYS
9	W	93	GLY
5	E	217	LYS
10	J	49	ALA
13	M	96	TRP
2	P	6	ARG
5	S	217	LYS
8	V	96	GLY
4	D	43	LYS
4	D	12(C)	GLY
5	E	5	ARG
8	H	91	GLN
1	O	167	LYS
4	R	12(C)	GLY
8	V	171	SER
1	A	167	LYS
8	H	9	ASN
10	J	8	VAL
13	M	72	ALA
4	R	43	LYS
5	S	5	ARG
8	V	9	ASN
10	X	8	VAL
13	1	72	ALA
13	1	96	TRP
10	X	187	VAL
12	Z	93	PHE

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Mol	Chain	Res	Type
8	H	96	GLY
10	J	187	VAL
4	D	12(F)	GLY
12	L	93	PHE
4	R	12(F)	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%)	198 (95%)	11 (5%)	22	54
1	O	209/209 (100%)	199 (95%)	10 (5%)	25	58
2	B	203/203 (100%)	188 (93%)	15 (7%)	13	37
2	P	203/203 (100%)	188 (93%)	15 (7%)	13	37
3	C	213/213 (100%)	198 (93%)	15 (7%)	15	40
3	Q	213/213 (100%)	197 (92%)	16 (8%)	13	37
4	D	198/198 (100%)	187 (94%)	11 (6%)	21	51
4	R	198/198 (100%)	189 (96%)	9 (4%)	27	60
5	E	192/192 (100%)	170 (88%)	22 (12%)	5	17
5	S	192/192 (100%)	170 (88%)	22 (12%)	5	17
6	F	201/201 (100%)	183 (91%)	18 (9%)	9	28
6	T	201/201 (100%)	183 (91%)	18 (9%)	9	28
7	G	207/207 (100%)	195 (94%)	12 (6%)	20	50
7	U	207/207 (100%)	195 (94%)	12 (6%)	20	50
8	H	181/181 (100%)	171 (94%)	10 (6%)	21	52
8	V	181/181 (100%)	171 (94%)	10 (6%)	21	52
9	I	172/172 (100%)	163 (95%)	9 (5%)	23	55
9	W	172/172 (100%)	162 (94%)	10 (6%)	20	50
10	J	175/175 (100%)	166 (95%)	9 (5%)	24	55
10	X	175/175 (100%)	166 (95%)	9 (5%)	24	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	169/169 (100%)	164 (97%)	5 (3%)	41	75
11	Y	169/169 (100%)	164 (97%)	5 (3%)	41	75
12	L	185/185 (100%)	173 (94%)	12 (6%)	17	44
12	Z	185/185 (100%)	173 (94%)	12 (6%)	17	44
13	1	199/199 (100%)	191 (96%)	8 (4%)	31	65
13	M	199/199 (100%)	190 (96%)	9 (4%)	27	60
14	2	162/162 (100%)	150 (93%)	12 (7%)	13	37
14	N	162/162 (100%)	151 (93%)	11 (7%)	16	42
All	All	5332/5332 (100%)	4995 (94%)	337 (6%)	18	46

All (337) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	33	GLN
1	A	40	ILE
1	A	64	LEU
1	A	124	THR
1	A	134	VAL
1	A	135	SER
1	A	158	PHE
1	A	179	ARG
1	A	192	ILE
1	A	215	ILE
2	B	5	SER
2	B	10	SER
2	B	14	ILE
2	B	58	LEU
2	B	71	ASN
2	B	116	LEU
2	B	121	GLN
2	B	150	THR
2	B	156	ASN
2	B	185	LYS
2	B	192	LEU
2	B	206	THR
2	B	218	ASN
2	B	232	ILE
2	B	238	ILE

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Mol	Chain	Res	Type
3	C	10	ARG
3	C	14	ILE
3	C	25	GLU
3	C	28	LEU
3	C	33	ARG
3	C	57	LYS
3	C	61	THR
3	C	70	ILE
3	C	87	ILE
3	C	121	GLN
3	C	135	SER
3	C	163	GLN
3	C	172	VAL
3	C	174	GLU
3	C	208	LYS
4	D	28	LEU
4	D	31	ILE
4	D	40	ILE
4	D	126	ARG
4	D	170	GLU
4	D	175	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	244	GLU
5	E	11	ASP
5	E	12	THR
5	E	13	VAL
5	E	32	LYS
5	E	57	GLU
5	E	64	GLN
5	E	76	LEU
5	E	78	LEU
5	E	97	ASN
5	E	104	ASN
5	E	111	ARG
5	E	121	GLN
5	E	178	ARG
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN

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Mol	Chain	Res	Type
5	E	207	LEU
5	E	2(C)	VAL
5	E	2(E)	ASN
5	E	223	ILE
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	35	THR
6	F	43	ASN
6	F	54	ILE
6	F	56	SER
6	F	72	ARG
6	F	74	ILE
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
6	F	169	ARG
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
7	G	33	GLN
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	122	ILE
7	G	124	THR
7	G	169	GLN
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	30	ASN
8	H	34	LEU
8	H	43	CYS
8	H	55	VAL
8	H	56	THR
8	H	68	LEU

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Mol	Chain	Res	Type
8	H	95	ILE
8	H	144	GLN
8	H	197	ARG
8	H	221	ILE
9	I	-3	ILE
9	I	29	ASN
9	I	61	TYR
9	I	110	ILE
9	I	113	PHE
9	I	160	LEU
9	I	171	TRP
9	I	177	ILE
9	I	192	ARG
10	J	34	THR
10	J	35	ARG
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	90(A)	ILE
10	J	121	GLU
10	J	155	LEU
10	J	168	MET
11	K	4	LEU
11	K	8	PHE
11	K	9	GLN
11	K	65	LEU
11	K	104	TYR
12	L	-7	ASN
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	58	ARG
12	L	70(A)	ASN
12	L	93	PHE
12	L	98	HIS
12	L	99	THR
12	L	106	GLU
12	L	138	LEU
12	L	145	TYR
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG

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Mol	Chain	Res	Type
13	M	112	TYR
13	M	129	PHE
13	M	14(C)	ARG
13	M	149	GLN
13	M	191	GLN
13	M	204	LYS
14	N	3	ILE
14	N	58	ILE
14	N	84	LYS
14	N	89	GLU
14	N	10(A)	ASP
14	N	10(B)	LYS
14	N	119	VAL
14	N	149	GLU
14	N	163	ILE
14	N	18(A)	ILE
14	N	18(I)	GLN
1	O	24	ILE
1	O	33	GLN
1	O	64	LEU
1	O	134	VAL
1	O	135	SER
1	O	158	PHE
1	O	179	ARG
1	O	192	ILE
1	O	215	ILE
1	O	229	ILE
2	P	5	SER
2	P	10	SER
2	P	14	ILE
2	P	58	LEU
2	P	71	ASN
2	P	116	LEU
2	P	121	GLN
2	P	150	THR
2	P	156	ASN
2	P	185	LYS
2	P	192	LEU
2	P	206	THR
2	P	218	ASN
2	P	232	ILE
2	P	238	ILE

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Mol	Chain	Res	Type
3	Q	10	ARG
3	Q	14	ILE
3	Q	25	GLU
3	Q	28	LEU
3	Q	33	ARG
3	Q	57	LYS
3	Q	61	THR
3	Q	70	ILE
3	Q	87	ILE
3	Q	100	ARG
3	Q	121	GLN
3	Q	135	SER
3	Q	163	GLN
3	Q	172	VAL
3	Q	174	GLU
3	Q	208	LYS
4	R	28	LEU
4	R	126	ARG
4	R	170	GLU
4	R	175	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	244	GLU
5	S	11	ASP
5	S	12	THR
5	S	13	VAL
5	S	32	LYS
5	S	57	GLU
5	S	64	GLN
5	S	76	LEU
5	S	78	LEU
5	S	97	ASN
5	S	104	ASN
5	S	111	ARG
5	S	121	GLN
5	S	178	ARG
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU

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Mol	Chain	Res	Type
5	S	2(C)	VAL
5	S	2(E)	ASN
5	S	223	ILE
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	35	THR
6	T	43	ASN
6	T	54	ILE
6	T	56	SER
6	T	72	ARG
6	T	74	ILE
6	T	98	SER
6	T	105	THR
6	T	121	GLN
6	T	127	ASN
6	T	169	ARG
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
7	U	33	GLN
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	122	ILE
7	U	124	THR
7	U	169	GLN
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	30	ASN
8	V	34	LEU
8	V	43	CYS
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	95	ILE

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Mol	Chain	Res	Type
8	V	144	GLN
8	V	197	ARG
8	V	221	ILE
9	W	-3	ILE
9	W	29	ASN
9	W	61	TYR
9	W	94	PRO
9	W	110	ILE
9	W	113	PHE
9	W	160	LEU
9	W	171	TRP
9	W	177	ILE
9	W	192	ARG
10	X	34	THR
10	X	35	ARG
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	90(A)	ILE
10	X	121	GLU
10	X	155	LEU
10	X	168	MET
11	Y	4	LEU
11	Y	8	PHE
11	Y	9	GLN
11	Y	65	LEU
11	Y	104	TYR
12	Z	-7	ASN
12	Z	14	LEU
12	Z	25	SER
12	Z	40	ASN
12	Z	58	ARG
12	Z	70(A)	ASN
12	Z	93	PHE
12	Z	98	HIS
12	Z	99	THR
12	Z	106	GLU
12	Z	138	LEU
12	Z	145	TYR
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG

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Mol	Chain	Res	Type
13	1	112	TYR
13	1	129	PHE
13	1	14(C)	ARG
13	1	149	GLN
13	1	204	LYS
14	2	3	ILE
14	2	36	ARG
14	2	84	LYS
14	2	89	GLU
14	2	10(A)	ASP
14	2	10(B)	LYS
14	2	119	VAL
14	2	149	GLU
14	2	163	ILE
14	2	178	LEU
14	2	18(A)	ILE
14	2	18(I)	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (207) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
1	A	145	ASN
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
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	209	ASN
3	C	238	GLN
3	C	243	GLN

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Mol	Chain	Res	Type
4	D	23	GLN
4	D	108	ASN
4	D	161	ASN
4	D	211	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	170	GLN
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
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
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	91	GLN
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN

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Mol	Chain	Res	Type
9	I	29	ASN
9	I	81	GLN
10	J	36	GLN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	160	GLN
10	J	186	GLN
11	K	9	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
11	K	208	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	98	HIS
12	L	1(I)	ASN
12	L	166	HIS
12	L	168	GLN
13	M	-7	GLN
13	M	10	ASN
13	M	18	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	191	GLN
14	N	62	HIS
14	N	69	GLN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN

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Mol	Chain	Res	Type
1	O	97	HIS
1	O	145	ASN
1	O	191	HIS
2	P	23	GLN
2	P	71	ASN
2	P	97	GLN
2	P	104	ASN
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	209	ASN
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	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	156	ASN
5	S	170	GLN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	87	HIS

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Mol	Chain	Res	Type
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	192	GLN
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	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	81	GLN
10	X	36	GLN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	160	GLN
10	X	186	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	67	HIS
12	Z	70(A)	ASN

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Mol	Chain	Res	Type
12	Z	85	HIS
12	Z	1(I)	ASN
12	Z	166	HIS
12	Z	168	GLN
13	1	-7	GLN
13	1	10	ASN
13	1	18	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	191	GLN
14	2	62	HIS
14	2	69	GLN
14	2	141	ASN
14	2	157	HIS
14	2	161	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	SLA	V	301	8	10,15,15	3.14	2 (20%)	12,23,23	1.24	2 (16%)
15	SLA	K	301	11	10,15,15	2.71	1 (10%)	12,23,23	1.47	2 (16%)
15	SLA	Y	301	11	10,15,15	2.79	1 (10%)	12,23,23	1.44	2 (16%)
15	SLA	H	301	8	10,15,15	2.86	2 (20%)	12,23,23	1.26	2 (16%)

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	SLA	V	301	8	-	0/6/32/32	0/1/1/1
15	SLA	K	301	11	-	0/6/32/32	0/1/1/1
15	SLA	Y	301	11	-	0/6/32/32	0/1/1/1
15	SLA	H	301	8	-	0/6/32/32	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	301	SLA	C13-C11	9.16	1.61	1.53
15	H	301	SLA	C13-C11	8.24	1.60	1.53
15	Y	301	SLA	C13-C11	8.11	1.60	1.53
15	K	301	SLA	C13-C11	7.88	1.60	1.53
15	H	301	SLA	O8-C1	2.29	1.47	1.42
15	V	301	SLA	C9-C2	2.02	1.57	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	301	SLA	C5-N4-C3	3.47	117.00	114.58
15	K	301	SLA	C5-N4-C3	3.45	116.98	114.58
15	K	301	SLA	O10-C3-C2	-2.98	123.80	126.17
15	Y	301	SLA	O10-C3-C2	-2.88	123.89	126.17
15	H	301	SLA	C5-N4-C3	2.61	116.40	114.58
15	V	301	SLA	O10-C3-C2	-2.53	124.16	126.17
15	H	301	SLA	O10-C3-C2	-2.35	124.30	126.17
15	V	301	SLA	C5-N4-C3	2.35	116.22	114.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	V	301	SLA	1	0
15	K	301	SLA	1	0
15	Y	301	SLA	1	0
15	H	301	SLA	1	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%)	-0.24	5 (2%) 65 56	32, 46, 77, 100	0
1	O	250/250 (100%)	-0.14	8 (3%) 47 37	35, 54, 79, 99	0
2	B	244/244 (100%)	-0.08	8 (3%) 46 36	31, 51, 84, 113	0
2	P	244/244 (100%)	0.05	15 (6%) 21 13	34, 53, 88, 114	0
3	C	241/241 (100%)	0.02	12 (4%) 28 19	35, 55, 105, 122	0
3	Q	241/241 (100%)	0.18	26 (10%) 5 3	38, 58, 106, 122	0
4	D	242/242 (100%)	0.02	14 (5%) 23 15	38, 54, 87, 119	0
4	R	242/242 (100%)	0.11	13 (5%) 25 17	41, 56, 89, 119	0
5	E	233/233 (100%)	-0.20	4 (1%) 70 63	37, 54, 80, 105	0
5	S	233/233 (100%)	-0.19	8 (3%) 45 35	37, 55, 80, 106	0
6	F	244/244 (100%)	-0.27	7 (2%) 51 41	31, 48, 85, 103	0
6	T	244/244 (100%)	-0.37	4 (1%) 72 66	30, 45, 85, 99	0
7	G	243/243 (100%)	-0.32	7 (2%) 51 41	28, 43, 71, 108	0
7	U	243/243 (100%)	-0.29	5 (2%) 63 54	29, 44, 70, 106	0
8	H	222/222 (100%)	-0.48	3 (1%) 75 70	28, 42, 59, 91	0
8	V	222/222 (100%)	-0.49	3 (1%) 75 70	33, 45, 62, 93	0
9	I	204/204 (100%)	-0.55	1 (0%) 91 88	26, 44, 62, 78	0
9	W	204/204 (100%)	-0.51	4 (1%) 65 56	32, 43, 64, 77	0
10	J	198/198 (100%)	-0.32	5 (2%) 57 47	32, 46, 62, 118	0
10	X	198/198 (100%)	-0.24	5 (2%) 57 47	32, 46, 64, 120	0
11	K	212/212 (100%)	-0.40	0 100 100	30, 45, 61, 73	0
11	Y	212/212 (100%)	-0.44	1 (0%) 91 88	30, 46, 63, 74	0
12	L	222/222 (100%)	-0.33	4 (1%) 68 61	28, 46, 69, 89	0
12	Z	222/222 (100%)	-0.39	2 (0%) 84 80	31, 45, 70, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
13	1	233/233 (100%)	-0.52	1 (0%)	92 91	29, 40, 54, 62	0
13	M	233/233 (100%)	-0.50	1 (0%)	92 91	27, 42, 56, 63	0
14	2	196/196 (100%)	-0.48	2 (1%)	82 77	23, 39, 58, 78	0
14	N	196/196 (100%)	-0.52	1 (0%)	91 88	29, 38, 58, 76	0
All	All	6368/6368 (100%)	-0.27	169 (2%)	54 44	23, 47, 79, 122	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(D)	ALA	15.0
7	U	240	ASP	11.0
4	D	12(E)	SER	10.2
4	R	12(E)	SER	10.1
4	R	12(D)	ALA	10.1
4	R	12(C)	GLY	10.0
3	C	55	THR	9.0
4	D	12(C)	GLY	8.5
6	F	5	GLY	8.4
7	U	6	ALA	7.0
10	X	193	GLN	7.0
2	P	218	ASN	6.9
10	X	192	ALA	6.7
3	Q	55	THR	6.6
10	J	192	ALA	6.3
4	D	12(F)	GLY	6.3
2	B	218	ASN	6.1
7	G	240	ASP	6.1
2	B	217	ALA	6.0
4	R	12(F)	GLY	6.0
10	X	191	GLN	5.9
2	P	21(C)	ASP	5.7
2	P	54	VAL	5.5
3	C	56	LEU	5.5
1	O	5	THR	5.4
13	1	-8	THR	5.4
4	R	127	LEU	5.4
10	J	191	GLN	5.2
7	G	6	ALA	5.2
2	P	217	ALA	5.1
6	F	204	ASP	5.0
1	A	5	THR	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	54	VAL	5.0
1	A	4	MET	4.9
4	R	126	ARG	4.6
3	Q	203	THR	4.5
1	O	4	MET	4.4
8	H	222	CYS	4.3
2	P	219	GLU	4.0
5	S	4	PHE	4.0
12	L	145	TYR	3.9
8	H	223	ASP	3.8
4	D	12(G)	GLU	3.8
1	O	235	ALA	3.8
5	E	203	ASP	3.8
9	W	-8	SER	3.7
4	R	125	GLU	3.7
3	Q	242	GLU	3.7
13	M	-8	THR	3.7
8	V	223	ASP	3.6
3	Q	63	THR	3.6
10	J	193	GLN	3.5
3	Q	56	LEU	3.5
3	Q	243	GLN	3.5
3	Q	238	GLN	3.4
4	D	244	GLU	3.4
4	D	126	ARG	3.4
2	P	63	THR	3.4
8	V	222	CYS	3.4
5	S	5	ARG	3.3
2	B	219	GLU	3.3
6	F	6	THR	3.3
3	Q	54	SER	3.3
4	R	243	ALA	3.2
12	L	14(P)	PRO	3.2
5	E	5	ARG	3.2
3	Q	241	GLN	3.2
3	C	240	LYS	3.2
14	2	18(I)	GLN	3.2
1	O	21(P)	LYS	3.2
9	I	-8	SER	3.2
2	P	21(A)	LYS	3.2
2	B	21(C)	ASP	3.2
8	V	220	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
4	R	12(B)	GLU	3.1
14	N	18(I)	GLN	3.1
3	Q	170	LYS	3.1
7	G	239	GLN	3.0
2	B	21(B)	GLY	3.0
1	O	53	LYS	2.9
4	D	127	LEU	2.9
1	A	203	GLU	2.9
4	R	12(G)	GLU	2.9
12	L	14(W)	LYS	2.9
3	C	243	GLN	2.9
5	S	233	ILE	2.9
3	Q	18(D)	GLU	2.8
6	F	241	ASN	2.8
3	C	241	GLN	2.8
6	F	20(B)	GLU	2.8
1	O	56	SER	2.8
3	Q	240	LYS	2.8
12	Z	145	TYR	2.8
5	S	178	ARG	2.7
12	Z	14(W)	LYS	2.7
5	S	203	ASP	2.7
5	E	4	PHE	2.7
6	T	241	ASN	2.7
4	D	125	GLU	2.7
7	G	8	TYR	2.7
2	P	62	ASP	2.7
10	J	188	ASP	2.7
2	P	21(B)	GLY	2.7
3	C	33	ARG	2.7
5	E	204	GLU	2.6
3	C	208	LYS	2.6
4	R	242	ALA	2.6
6	F	240	ILE	2.6
3	Q	64	PRO	2.6
7	U	239	GLN	2.6
5	S	217	LYS	2.6
1	A	202	VAL	2.6
3	Q	18(C)	LYS	2.6
6	T	240	ILE	2.5
1	O	236	LEU	2.5
11	Y	10(A)	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	O	55	SER	2.5
3	Q	187	GLU	2.5
4	R	244	GLU	2.5
14	2	107	LYS	2.5
6	F	206	LYS	2.5
7	G	17(D)	SER	2.4
3	C	14(A)	ARG	2.4
12	L	-9	GLN	2.4
9	W	182	ASP	2.4
2	P	53	LYS	2.4
3	C	18(C)	LYS	2.4
4	D	218	GLN	2.4
3	Q	178	LYS	2.4
3	Q	62	ARG	2.3
3	Q	18(B)	ARG	2.3
5	S	204	GLU	2.3
1	A	205	GLU	2.3
2	B	21(A)	LYS	2.3
2	P	181	LYS	2.3
4	D	39	GLY	2.3
3	Q	14(B)	ASP	2.3
3	Q	236	ILE	2.3
7	G	7	GLY	2.3
4	D	10	ARG	2.3
3	Q	202	GLN	2.2
3	Q	14(A)	ARG	2.2
3	Q	53	ARG	2.2
2	P	239	THR	2.2
9	W	12(A)	LYS	2.2
10	X	10	ASP	2.2
6	T	6	THR	2.2
7	U	8	TYR	2.2
5	S	227	GLU	2.2
2	P	4	GLY	2.2
3	Q	7	GLY	2.2
6	T	18(D)	PRO	2.2
2	P	220	TYR	2.1
3	Q	208	LYS	2.1
3	C	203	THR	2.1
4	D	55	THR	2.1
3	C	237	GLU	2.1
10	J	92	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
4	R	9	ASP	2.1
8	H	220	ASN	2.1
2	P	21(D)	GLY	2.1
7	G	18(H)	GLU	2.1
2	B	20(A)	SER	2.0
10	X	188	ASP	2.0
3	C	43	LYS	2.0
9	W	181	LYS	2.0
4	D	9	ASP	2.0
7	U	17(E)	LYS	2.0
3	Q	222	VAL	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
15	SLA	V	301	15/15	0.93	0.21	47,49,53,53	0
15	SLA	Y	301	15/15	0.95	0.19	36,40,43,44	0
15	SLA	H	301	15/15	0.95	0.19	47,49,50,53	0
15	SLA	K	301	15/15	0.96	0.18	41,43,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.