



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:46 am BST

PDB ID : 3BDM  
Title : yeast 20S proteasome:glidobactin A-complex  
Authors : Groll, M.; Dudler, R.; Kaiser, M.  
Deposited on : 2007-11-15  
Resolution : 2.70 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  
buster-report : 1.1.7 (2018)  
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

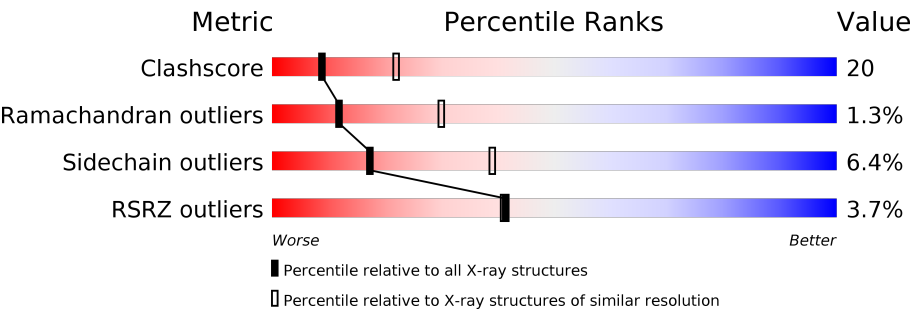
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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><div></div><div>66%</div><div>32%</div><div>.</div></div></div>
1	O	250	<div><div>6%</div><div><div></div><div>66%</div><div>31%</div><div>.</div></div></div>
2	B	258	<div><div>4%</div><div><div></div><div>53%</div><div>37%</div><div>5%</div><div>5%</div></div></div>
2	P	258	<div><div>6%</div><div><div></div><div>53%</div><div>37%</div><div>5%</div><div>5%</div></div></div>
3	C	254	<div><div>6%</div><div><div></div><div>50%</div><div>40%</div><div>5%</div><div>5%</div></div></div>
3	Q	254	<div><div>13%</div><div><div></div><div>50%</div><div>41%</div><div>5%</div><div>5%</div></div></div>
4	D	260	<div><div>3%</div><div><div></div><div>59%</div><div>31%</div><div>.</div><div>7%</div></div></div>

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

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51022 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

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

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

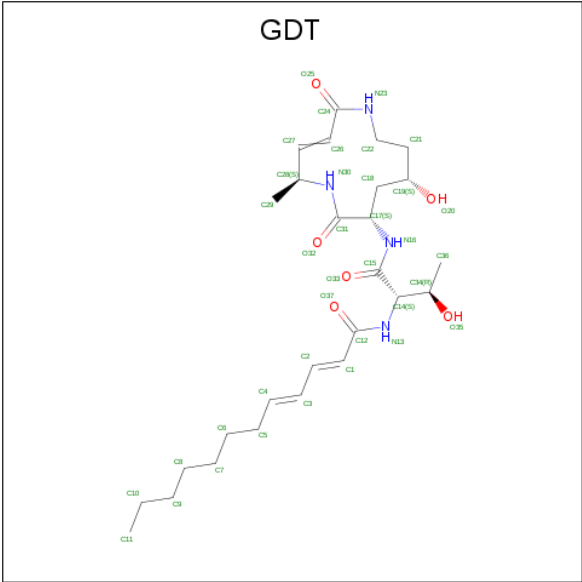
- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is (2E,4E)-N-[(2S,3R)-3-hydroxy-1-[[[(3Z,5S,8S,10S)-10-hydroxy-5-methyl-2,7-dioxo-1,6-diazacyclododec-3-en-8-yl]amino]-1-oxobutan-2-yl]dodeca-2,4-dienamide (three-letter code: GDT) (formula: C<sub>27</sub>H<sub>44</sub>N<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	H	1	Total	C	N	O	0	0
			37	27	4	6		
15	K	1	Total	C	N	O	0	0
			37	27	4	6		
15	V	1	Total	C	N	O	0	0
			37	27	4	6		
15	Y	1	Total	C	N	O	0	0
			37	27	4	6		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	57	Total	O	0	0
			57	57		
16	B	38	Total	O	0	0
			38	38		
16	C	42	Total	O	0	0
			42	42		
16	D	40	Total	O	0	0
			40	40		
16	E	24	Total	O	0	0
			24	24		
16	F	46	Total	O	0	0
			46	46		
16	G	61	Total	O	0	0
			61	61		
16	H	48	Total	O	0	0
			48	48		

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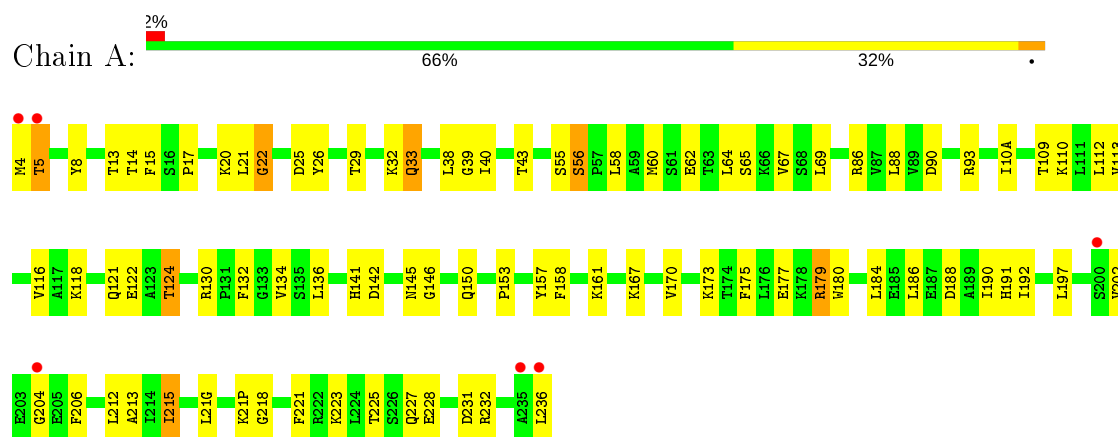
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	I	66	Total 66	O 66	0	0
16	J	52	Total 52	O 52	0	0
16	K	46	Total 46	O 46	0	0
16	L	60	Total 60	O 60	0	0
16	M	69	Total 69	O 69	0	0
16	N	56	Total 56	O 56	0	0
16	O	33	Total 33	O 33	0	0
16	P	32	Total 32	O 32	0	0
16	Q	26	Total 26	O 26	0	0
16	R	34	Total 34	O 34	0	0
16	S	20	Total 20	O 20	0	0
16	T	39	Total 39	O 39	0	0
16	U	58	Total 58	O 58	0	0
16	V	47	Total 47	O 47	0	0
16	W	60	Total 60	O 60	0	0
16	X	42	Total 42	O 42	0	0
16	Y	49	Total 49	O 49	0	0
16	Z	53	Total 53	O 53	0	0
16	0	74	Total 74	O 74	0	0
16	1	64	Total 64	O 64	0	0



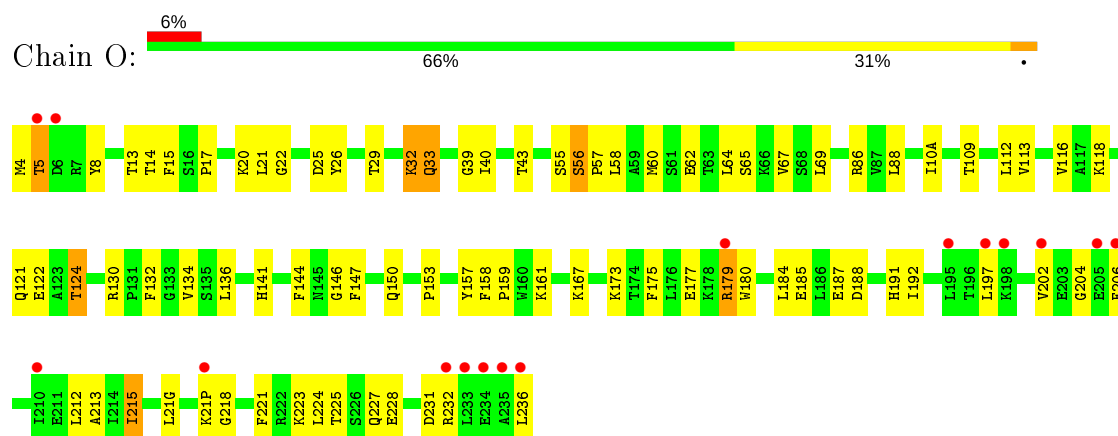
### 3 Residue-property plots [i](#)

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.

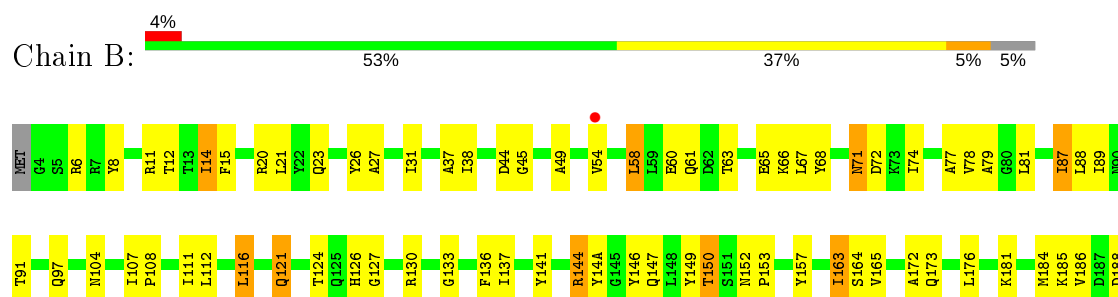
#### • Molecule 1: Proteasome component Y7

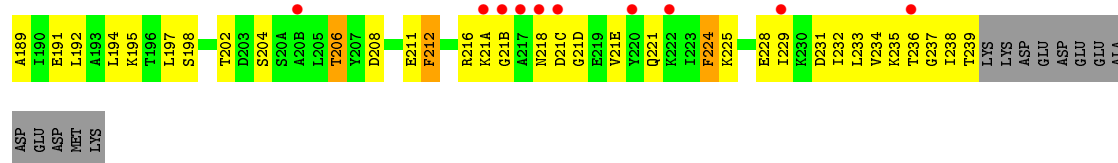


#### • Molecule 1: Proteasome component Y7

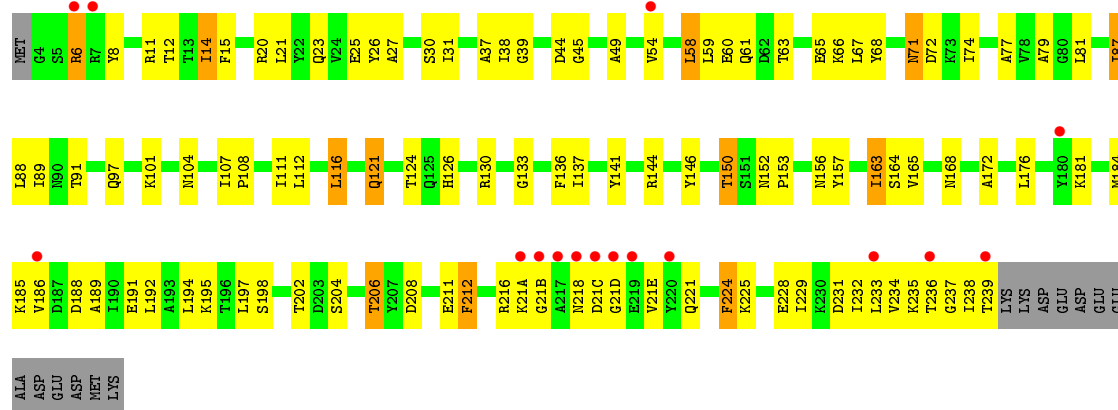


#### • Molecule 2: Proteasome component Y13

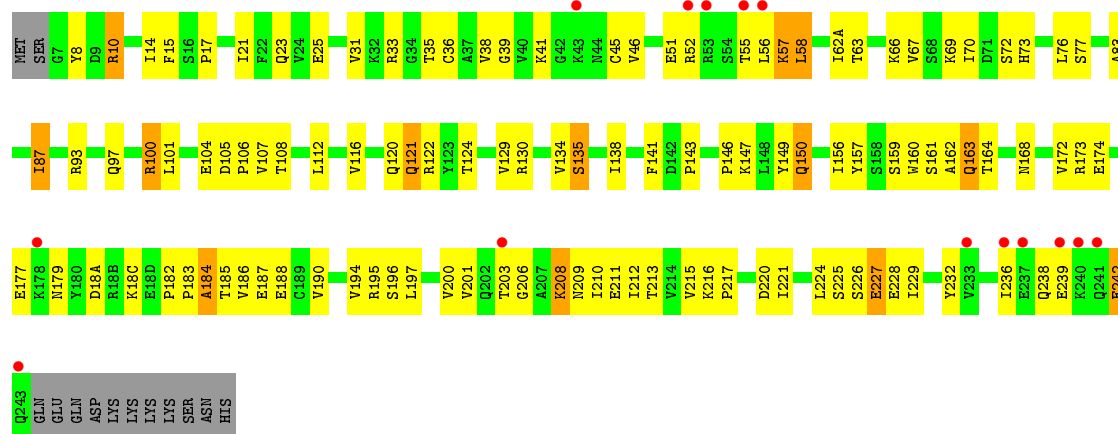




• Molecule 2: Proteasome component Y13

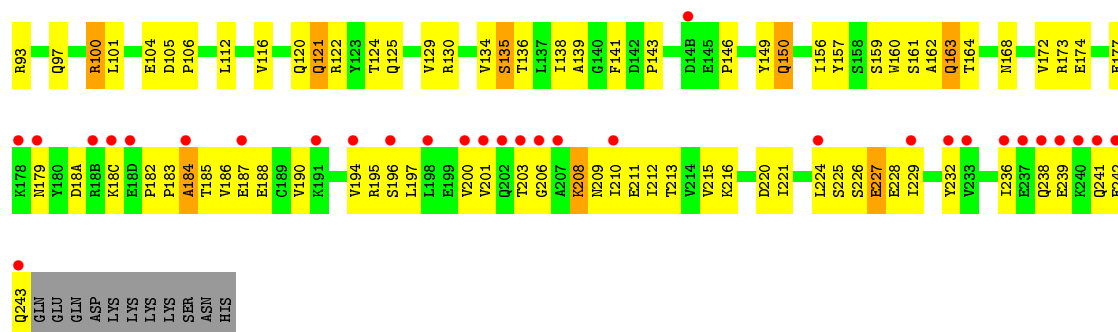


• Molecule 3: Proteasome component PRE6

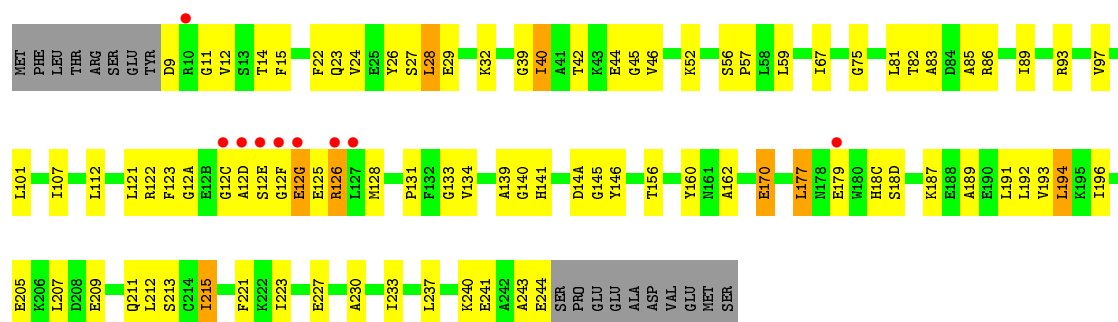


• Molecule 3: Proteasome component PRE6

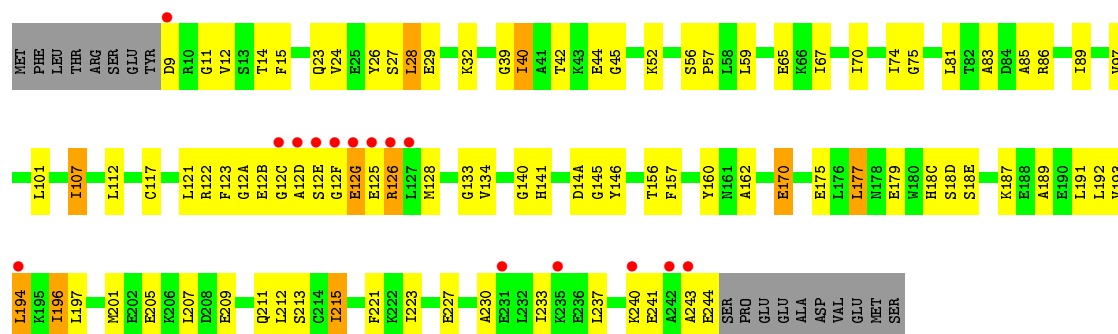




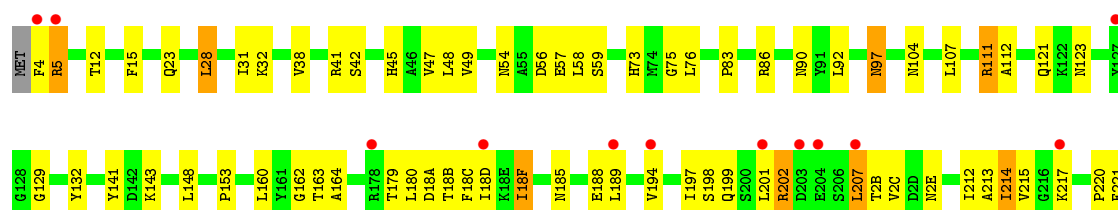
• Molecule 4: Proteasome component PUP2



• Molecule 4: Proteasome component PUP2

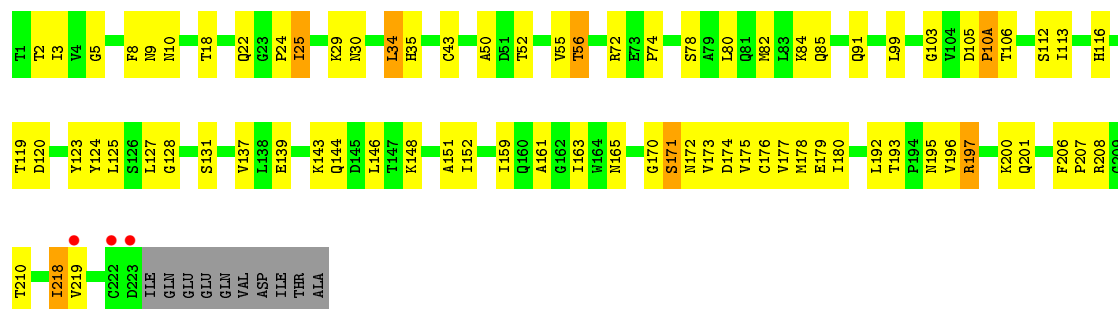


• Molecule 5: Proteasome component PRE5

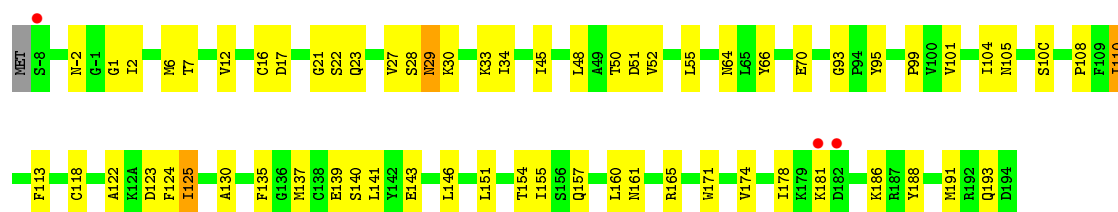




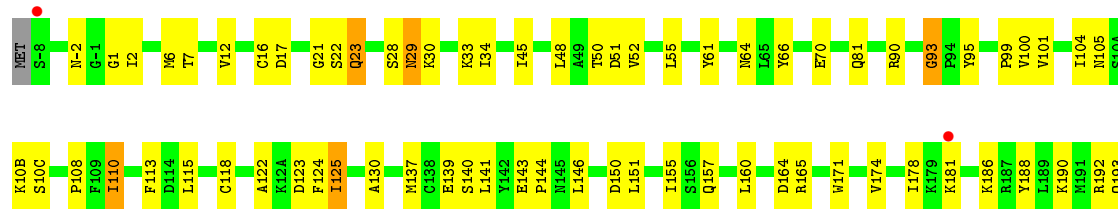




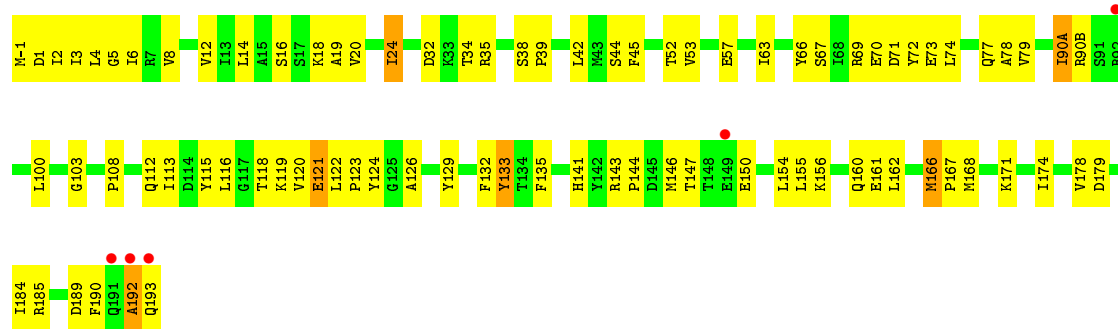
- Molecule 9: Proteasome component PUP3



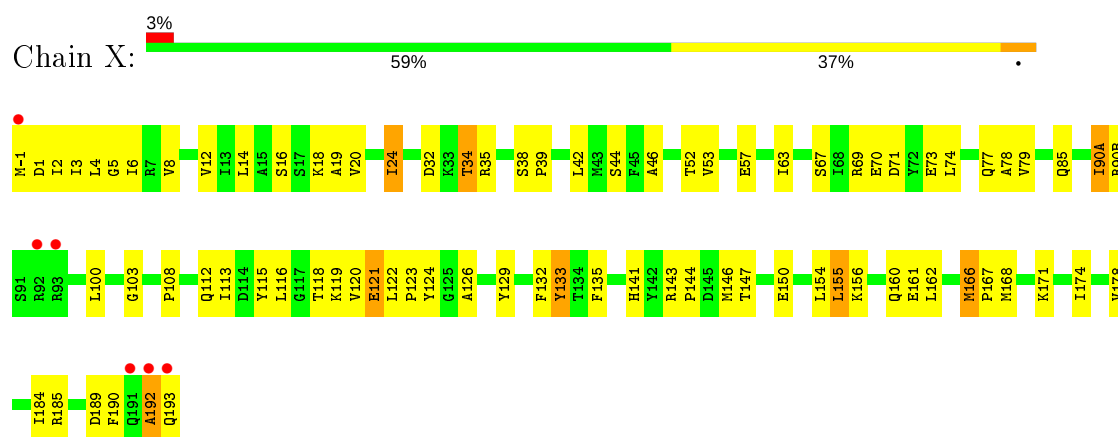
- Molecule 9: Proteasome component PUP3



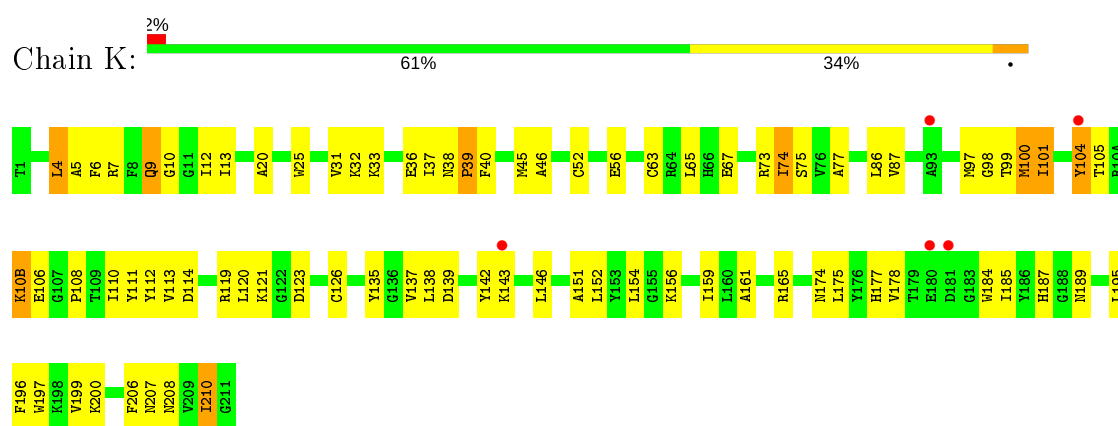
- Molecule 10: Proteasome component C11



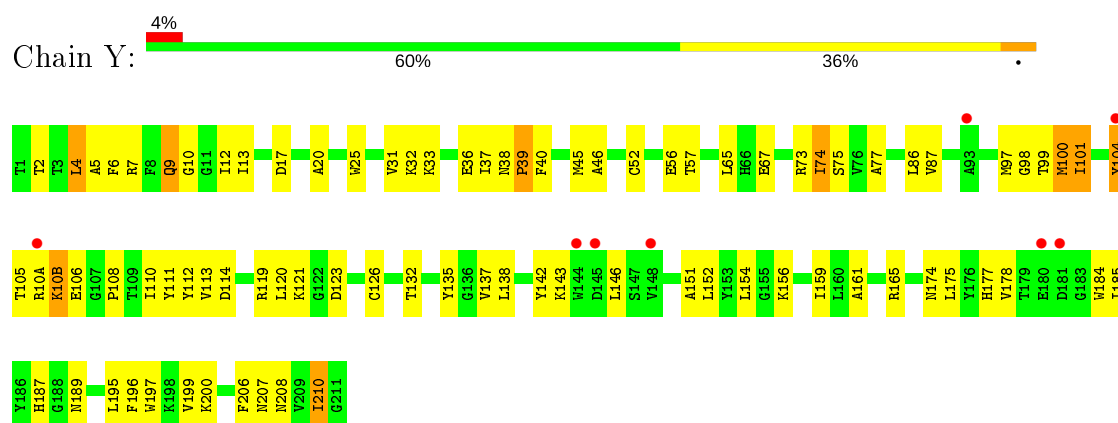
- Molecule 10: Proteasome component C11



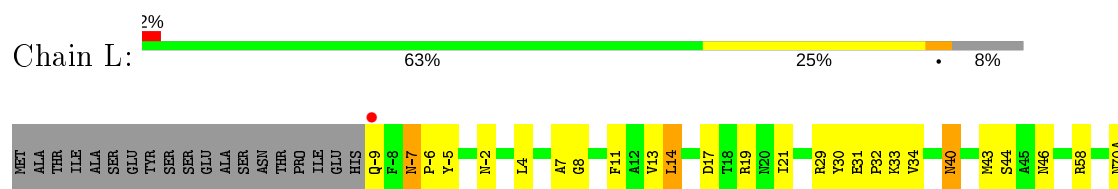
• Molecule 11: Proteasome component PRE2

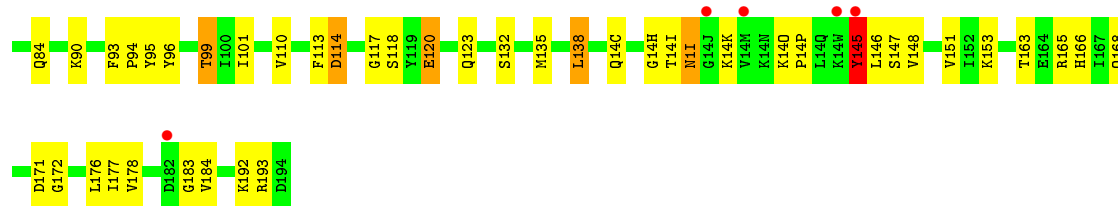


• Molecule 11: Proteasome component PRE2

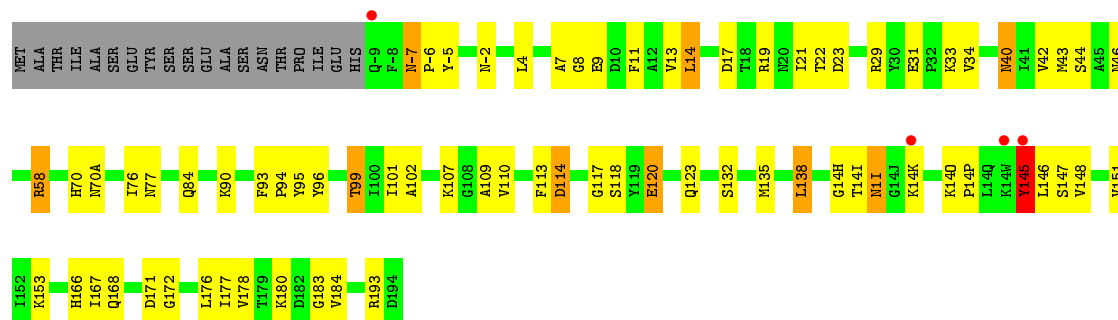


• Molecule 12: Proteasome component C5

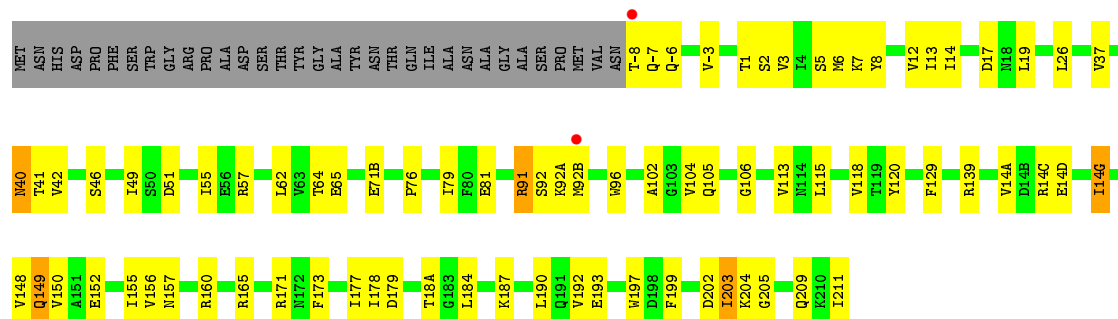




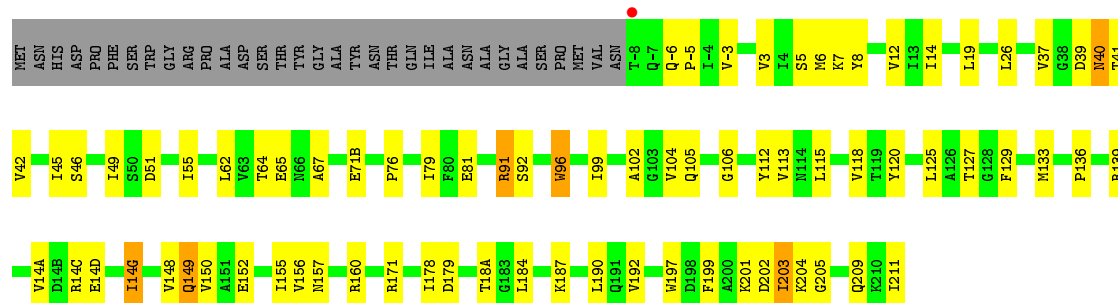
• Molecule 12: Proteasome component C5



• Molecule 13: Proteasome component PRE4

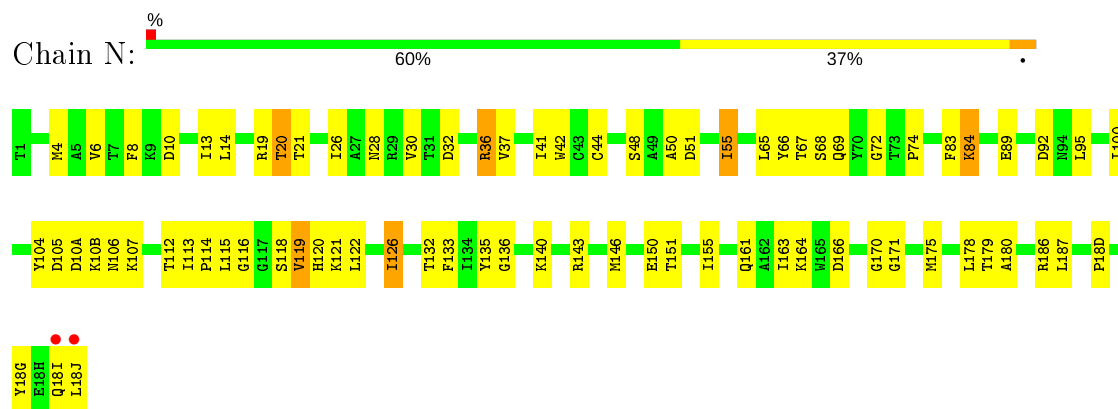


• Molecule 13: Proteasome component PRE4

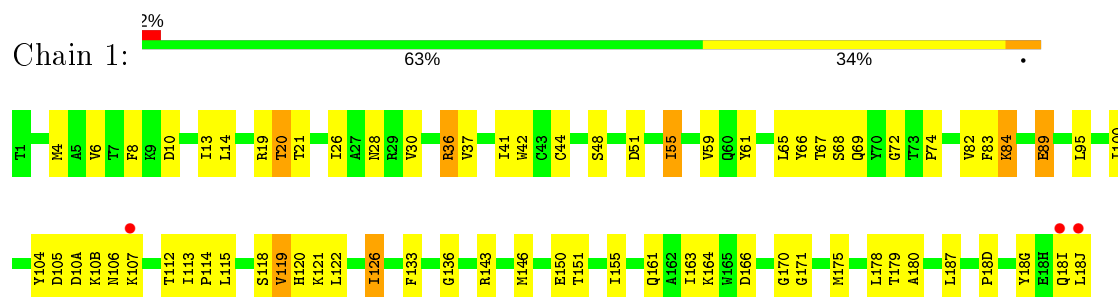


• Molecule 14: Proteasome component PRE3





• 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, $\alpha$ , $\beta$ , $\gamma$	132.77Å 302.79Å 143.21Å 90.00° 112.24° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 49.11 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (15.00-2.70) 97.9 (49.11-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.234 , 0.262 0.217 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 62.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	51022	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: GDT

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	0.40	0/1952	0.64	0/2642
1	O	0.38	0/1952	0.64	0/2642
2	B	0.38	0/1934	0.63	0/2618
2	P	0.38	0/1934	0.63	0/2618
3	C	0.37	0/1919	0.63	0/2598
3	Q	0.36	0/1919	0.63	0/2598
4	D	0.38	0/1886	0.64	0/2541
4	R	0.37	0/1886	0.63	0/2541
5	E	0.36	0/1823	0.62	0/2463
5	S	0.37	0/1823	0.62	0/2463
6	F	0.39	0/1936	0.64	0/2614
6	T	0.39	0/1936	0.64	0/2614
7	G	0.42	0/1959	0.66	0/2652
7	U	0.41	0/1959	0.66	0/2652
8	H	0.39	0/1715	0.67	0/2326
8	V	0.39	0/1715	0.66	0/2326
9	I	0.41	0/1611	0.66	0/2174
9	W	0.42	0/1611	0.67	0/2174
10	J	0.41	0/1613	0.66	0/2173
10	X	0.42	0/1613	0.68	0/2173
11	K	0.40	0/1681	0.66	0/2274
11	Y	0.40	0/1681	0.65	0/2274
12	L	0.42	0/1795	0.66	0/2420
12	Z	0.41	0/1795	0.66	0/2420
13	O	0.41	0/1855	0.69	0/2514
13	M	0.40	0/1855	0.68	0/2514
14	1	0.44	0/1541	0.67	0/2087
14	N	0.44	0/1541	0.68	0/2087
All	All	0.40	0/50440	0.65	0/68192

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	79	0
1	O	1915	0	1926	81	0
2	B	1904	0	1901	110	0
2	P	1904	0	1901	109	0
3	C	1890	0	1900	126	0
3	Q	1890	0	1900	121	0
4	D	1861	0	1836	82	0
4	R	1861	0	1836	83	0
5	E	1795	0	1797	70	0
5	S	1795	0	1797	76	0
6	F	1896	0	1886	83	0
6	T	1896	0	1886	82	0
7	G	1921	0	1910	85	0
7	U	1921	0	1910	95	0
8	H	1684	0	1687	60	0
8	V	1684	0	1687	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1581	0	1574	57	0
9	W	1581	0	1574	66	0
10	J	1585	0	1590	83	0
10	X	1585	0	1590	78	0
11	K	1644	0	1594	76	0
11	Y	1644	0	1594	80	0
12	L	1757	0	1711	61	0
12	Z	1757	0	1711	70	0
13	O	1824	0	1832	63	0
13	M	1824	0	1832	66	0
14	1	1512	0	1481	64	0
14	N	1512	0	1481	68	0
15	H	37	0	43	2	0
15	K	37	0	43	2	0
15	V	37	0	43	3	0
15	Y	37	0	43	4	0
16	O	74	0	0	4	0
16	1	64	0	0	3	0
16	A	57	0	0	5	0
16	B	38	0	0	3	0
16	C	42	0	0	8	0
16	D	40	0	0	4	0
16	E	24	0	0	1	0
16	F	46	0	0	5	0
16	G	61	0	0	5	0
16	H	48	0	0	2	0
16	I	66	0	0	3	0
16	J	52	0	0	4	0
16	K	46	0	0	2	0
16	L	60	0	0	2	0
16	M	69	0	0	4	0
16	N	56	0	0	3	0
16	O	33	0	0	3	0
16	P	32	0	0	4	0
16	Q	26	0	0	3	0
16	R	34	0	0	3	0
16	S	20	0	0	1	0
16	T	39	0	0	6	0
16	U	58	0	0	11	0
16	V	47	0	0	6	0
16	W	60	0	0	4	0
16	X	42	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Y	49	0	0	2	0
16	Z	53	0	0	8	0
All	All	51022	0	49422	2017	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 20.

All (2017) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.14	1.10
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.15	1.09
14:N:136:GLY:HA2	14:1:161:GLN:HE21	1.12	1.07
14:N:161:GLN:HE21	14:1:136:GLY:HA2	1.15	1.06
2:P:71:ASN:ND2	2:P:72:ASP:H	1.56	1.04
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.24	1.01
2:B:71:ASN:ND2	2:B:72:ASP:H	1.58	1.01
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.06	1.00
3:Q:52:ARG:HH21	3:Q:211:GLU:HB3	1.29	0.98
2:P:202:THR:HG22	2:P:204:SER:H	1.29	0.97
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.28	0.96
3:C:52:ARG:HH21	3:C:211:GLU:HB3	1.31	0.95
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.31	0.94
1:O:86:ARG:HE	7:U:118:ASN:HD21	0.97	0.94
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	1.47	0.94
7:G:96:ALA:HA	7:G:107:MET:HE2	1.49	0.94
3:C:76:LEU:HD12	3:C:138:ILE:HG12	1.50	0.94
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.67	0.93
7:U:96:ALA:HA	7:U:107:MET:HE2	1.51	0.93
1:O:15:PHE:H	2:P:23:GLN:HE22	1.14	0.92
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.31	0.92
2:B:202:THR:HG22	2:B:204:SER:H	1.32	0.92
14:N:136:GLY:HA2	14:1:161:GLN:NE2	1.83	0.92
10:J:-1:MET:HG2	10:J:1:ASP:H	1.34	0.91
13:M:149:GLN:NE2	13:M:149:GLN:H	1.69	0.91
10:J:133:TYR:HD1	16:Y:524:HOH:O	1.53	0.90
14:N:161:GLN:NE2	14:1:136:GLY:HA2	1.85	0.90
1:A:15:PHE:H	2:B:23:GLN:HE22	1.18	0.90
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.54	0.90
10:X:-1:MET:HG2	10:X:1:ASP:H	1.34	0.90
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.17	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:12:ILE:HB	11:K:178:VAL:HB	1.55	0.89
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.54	0.88
10:J:156:LYS:O	10:J:160:GLN:HG3	1.74	0.88
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.89	0.88
7:G:77:VAL:HG12	7:G:137:THR:HB	1.56	0.88
3:C:163:GLN:HE21	3:C:164:THR:H	1.15	0.88
11:Y:143:LYS:O	11:Y:146:LEU:HD13	1.73	0.87
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.56	0.87
3:C:163:GLN:NE2	3:C:164:THR:H	1.72	0.87
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	1.89	0.87
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	1.88	0.87
13:O:149:GLN:H	13:O:149:GLN:NE2	1.73	0.87
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.40	0.86
3:C:100:ARG:NH1	3:C:106:PRO:HB3	1.88	0.86
10:X:156:LYS:O	10:X:160:GLN:HG3	1.74	0.86
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.19	0.86
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.88	0.86
14:1:84:LYS:HG3	14:1:119:VAL:HG22	1.56	0.86
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.58	0.85
7:U:77:VAL:HG12	7:U:137:THR:HB	1.58	0.85
2:B:163:ILE:HD13	2:B:164:SER:H	1.39	0.85
11:K:143:LYS:O	11:K:146:LEU:HD13	1.76	0.85
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.20	0.85
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.57	0.85
3:Q:52:ARG:NH2	3:Q:211:GLU:HB3	1.91	0.85
5:S:214:ILE:HD12	5:S:215:VAL:N	1.92	0.85
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.58	0.85
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.21	0.85
3:C:52:ARG:NH2	3:C:211:GLU:HB3	1.92	0.84
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.21	0.84
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.75	0.84
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.42	0.83
2:B:15:PHE:H	3:C:23:GLN:HE22	1.26	0.83
1:O:33:GLN:HA	1:O:33:GLN:HE21	1.43	0.83
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.61	0.83
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.92	0.82
13:M:149:GLN:HE21	13:M:149:GLN:H	1.27	0.82
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.43	0.82
3:C:185:THR:HG22	3:C:187:GLU:H	1.44	0.82
6:F:192:GLN:O	6:F:196:ILE:HG12	1.80	0.82
11:Y:10(B):LYS:N	11:Y:10(B):LYS:HD2	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	1.94	0.81
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.44	0.81
14:N:126:ILE:HD13	14:N:126:ILE:H	1.46	0.81
6:T:69:VAL:HG12	16:T:306:HOH:O	1.78	0.81
2:B:185:LYS:HD3	2:B:186:VAL:N	1.97	0.80
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.81	0.80
13:O:149:GLN:H	13:O:149:GLN:HE21	1.30	0.80
6:T:192:GLN:O	6:T:196:ILE:HG12	1.82	0.80
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.79	0.80
7:G:217:LYS:HE3	7:G:217:LYS:HA	1.63	0.80
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	1.97	0.80
13:O:157:ASN:HD22	13:O:160:ARG:HH11	1.29	0.79
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.31	0.79
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.62	0.79
2:P:185:LYS:HD3	2:P:186:VAL:N	1.97	0.79
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.45	0.79
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.65	0.78
11:Y:210:ILE:HB	16:Y:539:HOH:O	1.83	0.78
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.96	0.78
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.66	0.78
14:1:126:ILE:H	14:1:126:ILE:HD13	1.49	0.78
3:Q:33:ARG:HH11	3:Q:33:ARG:HB2	1.48	0.78
5:E:214:ILE:HD12	5:E:215:VAL:N	1.99	0.77
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.47	0.77
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.83	0.77
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.66	0.77
6:T:175:GLU:HB3	6:T:196:ILE:HD12	1.66	0.77
3:C:33:ARG:HB2	3:C:33:ARG:NH1	1.98	0.77
2:P:163:ILE:CD1	2:P:164:SER:H	1.98	0.77
13:O:76:PRO:HD2	13:O:105:GLN:OE1	1.85	0.77
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.67	0.77
11:K:142:TYR:O	11:K:143:LYS:HD2	1.85	0.77
2:P:71:ASN:ND2	2:P:72:ASP:N	2.33	0.77
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.32	0.76
6:T:179:LEU:HD21	6:T:192:GLN:HG2	1.67	0.76
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.67	0.76
12:L:123:GLN:HG3	12:L:145:TYR:OH	1.86	0.76
2:B:71:ASN:ND2	2:B:72:ASP:N	2.34	0.75
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.69	0.75
3:C:163:GLN:HE21	3:C:164:THR:N	1.84	0.75
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	1.86	0.75
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.67	0.75
2:B:163:ILE:CD1	2:B:164:SER:H	1.99	0.75
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.87	0.75
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.69	0.75
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.50	0.75
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.50	0.74
7:U:87:ASN:HD22	7:U:87:ASN:C	1.90	0.74
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.87	0.74
6:F:35:THR:HG21	6:F:51:GLU:O	1.87	0.74
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.50	0.74
14:N:51:ASP:O	14:N:55:ILE:HD12	1.86	0.74
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.01	0.74
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.88	0.74
14:1:51:ASP:O	14:1:55:ILE:HD12	1.86	0.73
9:I:6:MET:HE1	9:I:155:ILE:HA	1.70	0.73
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.88	0.73
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.34	0.73
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.68	0.73
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.01	0.73
7:G:87:ASN:HD22	7:G:87:ASN:C	1.91	0.73
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.88	0.73
6:F:179:LEU:HD21	6:F:192:GLN:HG2	1.69	0.73
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.52	0.73
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.01	0.73
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.69	0.73
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.89	0.73
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.02	0.72
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.71	0.72
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.54	0.72
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.71	0.72
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.87	0.72
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.38	0.72
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.36	0.71
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.72	0.71
3:C:35:THR:HB	3:C:51:GLU:HG3	1.72	0.71
6:T:35:THR:HG21	6:T:51:GLU:O	1.91	0.71
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.72	0.71
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.37	0.71
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.03	0.71
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:96:ALA:HA	7:G:107:MET:CE	2.20	0.71
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.25	0.71
6:F:122:ALA:HA	6:F:125:LEU:HD12	1.71	0.71
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.74	0.70
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.73	0.70
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.55	0.70
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.73	0.70
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.72	0.70
7:U:96:ALA:HA	7:U:107:MET:CE	2.20	0.70
14:1:36:ARG:HG3	14:1:42:TRP:CE2	2.26	0.70
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.74	0.70
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.07	0.70
13:O:37:VAL:HG11	13:O:79:ILE:HD13	1.74	0.70
4:D:40:ILE:HG13	4:D:193:VAL:CG2	2.22	0.70
4:D:162:ALA:HB3	5:E:58:LEU:HD23	1.73	0.70
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.73	0.69
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.72	0.69
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.74	0.69
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.72	0.69
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.36	0.69
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.74	0.69
14:N:161:GLN:HE21	14:1:136:GLY:CA	1.99	0.69
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.75	0.69
11:K:184:TRP:C	11:K:185:ILE:HD13	2.11	0.69
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.75	0.69
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.74	0.69
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.73	0.69
6:T:68:GLN:HA	16:T:312:HOH:O	1.91	0.69
10:J:133:TYR:HE1	16:X:222:HOH:O	1.75	0.69
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.90	0.69
11:Y:184:TRP:C	11:Y:185:ILE:HD13	2.14	0.68
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.74	0.68
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.04	0.68
13:O:6:MET:HG2	13:O:155:ILE:HD11	1.74	0.68
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.27	0.68
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.76	0.68
3:C:232:TYR:O	3:C:236:ILE:HG13	1.94	0.68
3:C:15:PHE:H	4:D:23:GLN:HE22	1.39	0.68
2:B:27:ALA:O	2:B:31:ILE:HG12	1.94	0.68
13:M:37:VAL:HG11	13:M:79:ILE:HD13	1.75	0.68
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:232:TYR:O	3:Q:236:ILE:HG13	1.93	0.68
13:M:211:ILE:HG12	16:M:243:HOH:O	1.93	0.68
14:1:36:ARG:HG3	14:1:42:TRP:CZ2	2.29	0.67
1:O:121:GLN:O	1:O:124:THR:HB	1.94	0.67
4:R:40:ILE:HG13	4:R:193:VAL:CG2	2.24	0.67
6:T:122:ALA:HA	6:T:125:LEU:HD12	1.75	0.67
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.76	0.67
4:R:140:GLY:HA2	4:R:215:ILE:HG12	1.74	0.67
5:S:38:VAL:HG22	5:S:164:ALA:HB2	1.75	0.67
12:L:1(I):ASN:O	12:L:14(K):LYS:HG2	1.94	0.67
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.76	0.67
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.10	0.67
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.76	0.67
11:K:104:TYR:CE2	11:K:108:PRO:HG3	2.30	0.67
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.76	0.67
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.77	0.67
13:M:40:ASN:H	13:M:40:ASN:HD22	1.43	0.67
2:P:87:ILE:O	2:P:91:THR:HG23	1.95	0.67
7:U:218:ASP:O	7:U:220:LYS:HB2	1.95	0.67
14:1:112:THR:HG22	14:1:120:HIS:HB2	1.77	0.66
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.77	0.66
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.77	0.66
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.77	0.66
1:A:121:GLN:O	1:A:124:THR:HB	1.94	0.66
2:B:87:ILE:O	2:B:91:THR:HG23	1.95	0.66
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.93	0.66
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.08	0.66
3:Q:101:LEU:HD11	10:X:57:GLU:HB3	1.77	0.66
3:C:41:LYS:HG2	3:C:161:SER:O	1.94	0.66
3:C:177:GLU:OE2	4:D:57:PRO:HD2	1.95	0.66
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.44	0.66
7:G:77:VAL:CG1	7:G:137:THR:HB	2.25	0.66
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.61	0.66
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.78	0.66
12:Z:-6:PRO:O	13:O:91:ARG:NH1	2.29	0.66
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.10	0.66
7:G:198:ILE:HG23	7:G:203:THR:O	1.95	0.66
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.76	0.66
13:M:57:ARG:NE	16:M:245:HOH:O	2.29	0.66
1:O:177:GLU:HG2	2:P:58:LEU:HD22	1.78	0.66
11:Y:104:TYR:CE2	11:Y:108:PRO:HG3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.78	0.66
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.78	0.66
10:X:63:ILE:HD11	10:X:79:VAL:HG13	1.77	0.66
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	1.94	0.66
10:J:63:ILE:HD11	10:J:79:VAL:HG13	1.77	0.66
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.09	0.66
2:P:163:ILE:HD13	2:P:164:SER:H	1.61	0.66
2:P:163:ILE:HD12	2:P:164:SER:N	2.11	0.66
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.78	0.66
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.77	0.65
1:A:188:ASP:O	1:A:192:ILE:HG12	1.96	0.65
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.77	0.65
7:U:130:ARG:HB2	16:U:293:HOH:O	1.96	0.65
16:X:222:HOH:O	11:Y:132:THR:HG22	1.95	0.65
16:B:254:HOH:O	3:C:62(A):ILE:HD11	1.95	0.65
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.78	0.65
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.32	0.65
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.78	0.65
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	1.94	0.65
7:U:77:VAL:CG1	7:U:137:THR:HB	2.26	0.65
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.26	0.65
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.77	0.65
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.32	0.65
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.78	0.65
1:A:67:VAL:HB	1:A:223:LYS:NZ	2.12	0.65
2:B:108:PRO:HB2	2:B:111:ILE:HD12	1.79	0.65
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.78	0.65
13:O:40:ASN:H	13:O:40:ASN:HD22	1.41	0.65
2:P:234:VAL:HA	2:P:239:THR:HA	1.79	0.65
6:T:79:SER:HA	16:T:316:HOH:O	1.96	0.65
1:O:86:ARG:NE	7:U:118:ASN:HD21	1.82	0.65
1:A:170:VAL:HB	16:A:253:HOH:O	1.96	0.65
2:P:27:ALA:O	2:P:31:ILE:HG12	1.97	0.65
5:S:73:HIS:HE1	5:S:107:LEU:O	1.79	0.65
12:Z:1(I):ASN:O	12:Z:14(K):LYS:HG2	1.97	0.65
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.77	0.65
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.32	0.65
4:R:24:VAL:O	4:R:28:LEU:HD22	1.96	0.65
7:U:121:GLN:O	7:U:124:THR:HB	1.96	0.65
5:E:73:HIS:HE1	5:E:107:LEU:O	1.80	0.65
7:U:59:LEU:O	7:U:61:PRO:HD3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.77	0.64
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.79	0.64
14:N:105:ASP:OD2	14:N:106:ASN:N	2.30	0.64
7:G:218:ASP:O	7:G:220:LYS:HB2	1.96	0.64
11:K:73:ARG:NH2	11:K:104:TYR:O	2.30	0.64
1:O:188:ASP:O	1:O:192:ILE:HG12	1.97	0.64
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.33	0.64
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.28	0.64
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.80	0.64
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.63	0.64
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.80	0.64
2:P:163:ILE:CD1	2:P:164:SER:N	2.61	0.64
8:V:18:THR:HB	8:V:30:ASN:HD22	1.63	0.64
10:X:44:SER:OG	10:X:100:LEU:HB2	1.98	0.64
12:Z:109:ALA:HA	16:Z:207:HOH:O	1.98	0.64
5:E:231:LYS:HD2	5:E:231:LYS:H	1.63	0.64
16:L:201:HOH:O	9:W:192:ARG:HG3	1.96	0.64
10:X:52:THR:HG23	10:X:53:VAL:N	2.13	0.64
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.28	0.64
14:N:136:GLY:CA	14:1:161:GLN:HE21	1.99	0.63
1:A:86:ARG:NE	7:G:118:ASN:HD21	1.89	0.63
7:G:177:GLU:O	7:G:17(B):LYS:HG3	1.99	0.63
5:S:231:LYS:HD2	5:S:231:LYS:H	1.63	0.63
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.80	0.63
6:F:33:ASN:HB2	16:F:326:HOH:O	1.98	0.63
10:J:52:THR:HG23	10:J:53:VAL:N	2.13	0.63
3:C:101:LEU:HD11	10:J:57:GLU:HB3	1.78	0.63
6:T:173:LYS:O	6:T:177:GLU:HG3	1.98	0.63
9:W:101:VAL:O	9:W:110:ILE:HA	1.98	0.63
2:P:163:ILE:HD12	2:P:164:SER:H	1.64	0.63
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.33	0.63
7:G:121:GLN:O	7:G:124:THR:HB	1.97	0.63
2:P:71:ASN:HD22	2:P:72:ASP:H	1.42	0.63
6:T:127:ASN:HD22	6:T:127:ASN:N	1.96	0.63
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.79	0.63
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.79	0.63
2:B:234:VAL:HA	2:B:239:THR:HA	1.80	0.63
5:S:198:SER:HA	5:S:201:LEU:HG	1.81	0.63
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.81	0.63
5:E:198:SER:HA	5:E:201:LEU:HG	1.80	0.63
11:K:142:TYR:C	11:K:143:LYS:HD2	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:208:ASN:HD21	9:W:29:ASN:HD21	1.45	0.63
2:P:202:THR:HG22	2:P:204:SER:N	2.09	0.63
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.81	0.63
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.80	0.62
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.99	0.62
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.62	0.62
3:Q:211:GLU:C	3:Q:212:ILE:HD13	2.19	0.62
8:V:128:GLY:O	8:V:131:SER:HB2	1.98	0.62
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.81	0.62
6:F:127:ASN:N	6:F:127:ASN:HD22	1.97	0.62
10:J:141:HIS:HB2	10:J:154:LEU:HD11	1.82	0.62
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.80	0.62
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.64	0.62
13:O:157:ASN:ND2	13:O:160:ARG:HH11	1.96	0.62
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.79	0.62
5:E:132:TYR:O	5:E:153:PRO:HB3	1.99	0.62
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.80	0.62
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.81	0.62
2:B:163:ILE:CD1	2:B:164:SER:N	2.62	0.62
12:L:13:VAL:HG12	12:L:177:ILE:HG13	1.82	0.62
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.80	0.62
7:U:12:ILE:HG13	7:U:14:ILE:HG23	1.82	0.62
7:U:16:SER:HA	16:U:316:HOH:O	2.00	0.62
11:Y:12:ILE:HG13	11:Y:108:PRO:HB3	1.81	0.62
11:Y:74:ILE:HG13	11:Y:75:SER:N	2.13	0.62
7:G:93:LYS:HD3	14:N:68:SER:HB3	1.82	0.62
11:K:12:ILE:HG13	11:K:108:PRO:HB3	1.82	0.62
5:S:15:PHE:H	6:T:23:GLN:HE22	1.46	0.62
8:H:18:THR:HB	8:H:30:ASN:HD22	1.65	0.62
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.15	0.62
4:R:121:LEU:HA	4:R:123:PHE:CE1	2.35	0.62
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.64	0.61
8:V:34:LEU:HD22	8:V:174:ASP:HB3	1.81	0.61
4:D:24:VAL:O	4:D:28:LEU:HD22	2.00	0.61
6:F:173:LYS:O	6:F:177:GLU:HG3	2.00	0.61
7:G:172:ILE:HD11	7:G:201:LEU:CD2	2.30	0.61
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.82	0.61
1:O:67:VAL:HB	1:O:223:LYS:NZ	2.15	0.61
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.35	0.61
9:W:6:MET:HE1	9:W:155:ILE:HA	1.80	0.61
12:Z:178:VAL:HG22	12:Z:184:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:63:ILE:CD1	10:J:79:VAL:HG13	2.31	0.61
11:K:111:TYR:CE1	11:K:121:LYS:HB2	2.34	0.61
3:Q:14:ILE:HB	4:R:23:GLN:NE2	2.15	0.61
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.65	0.61
10:X:141:HIS:HB2	10:X:154:LEU:HD11	1.81	0.61
14:1:146:MET:HE3	14:1:150:GLU:HB3	1.82	0.61
14:1:175:MET:HB2	14:1:187:LEU:HB2	1.82	0.61
4:D:121:LEU:HA	4:D:123:PHE:CE1	2.36	0.61
1:O:197:LEU:O	1:O:202:VAL:HG23	2.01	0.61
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.01	0.61
14:1:105:ASP:OD2	14:1:106:ASN:N	2.32	0.61
14:1:44:CYS:HB2	14:1:100:ILE:HB	1.83	0.61
1:A:197:LEU:O	1:A:202:VAL:HG23	2.01	0.61
8:H:5:GLY:O	8:H:124:TYR:HA	2.01	0.61
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.00	0.61
10:X:-1:MET:CG	10:X:1:ASP:H	2.12	0.61
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.63	0.61
12:L:166:HIS:HD2	12:L:168:GLN:H	1.46	0.61
10:X:63:ILE:CD1	10:X:79:VAL:HG13	2.29	0.61
3:C:14:ILE:HB	4:D:23:GLN:NE2	2.16	0.61
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.66	0.61
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.83	0.61
9:I:104:ILE:HD12	9:I:178:ILE:HG22	1.83	0.61
12:L:178:VAL:HG22	12:L:184:VAL:HG22	1.82	0.61
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.82	0.61
5:S:207:LEU:HA	5:S:2(E):ASN:HD21	1.64	0.61
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.31	0.60
11:K:74:ILE:HG13	11:K:75:SER:N	2.15	0.60
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.83	0.60
10:J:133:TYR:CE1	16:X:222:HOH:O	2.50	0.60
5:S:220:PRO:O	5:S:222:THR:HG23	2.00	0.60
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.83	0.60
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.97	0.60
7:U:198:ILE:HG23	7:U:203:THR:O	2.01	0.60
8:V:196:VAL:HG23	16:V:520:HOH:O	2.00	0.60
2:B:202:THR:HG22	2:B:204:SER:N	2.11	0.60
3:C:182:PRO:O	3:C:184:ALA:N	2.35	0.60
13:M:40:ASN:HD22	13:M:40:ASN:N	1.98	0.60
3:C:211:GLU:C	3:C:212:ILE:HD13	2.21	0.60
11:K:99:THR:HG22	11:K:113:VAL:O	2.01	0.60
10:X:42:LEU:HB2	10:X:184:ILE:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:48:SER:HB3	14:1:51:ASP:HB2	1.84	0.60
7:G:59:LEU:O	7:G:61:PRO:HD3	2.02	0.60
1:O:60:MET:HB3	1:O:62:GLU:OE1	2.02	0.60
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.83	0.60
14:1:84:LYS:HG3	14:1:119:VAL:CG2	2.30	0.60
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.84	0.60
8:H:34:LEU:HD22	8:H:174:ASP:HB3	1.82	0.60
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.65	0.60
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.84	0.60
2:P:71:ASN:HD22	2:P:72:ASP:N	1.96	0.60
2:P:79:ALA:HA	16:P:281:HOH:O	2.02	0.60
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.21	0.60
6:F:63:LYS:O	6:F:65:VAL:N	2.34	0.60
4:R:15:PHE:HB2	5:S:23:GLN:OE1	2.02	0.60
11:K:208:ASN:ND2	9:W:29:ASN:HD21	1.99	0.59
14:N:21:THR:HG22	14:N:26:ILE:HA	1.84	0.59
7:U:17:PRO:HD3	16:U:316:HOH:O	2.01	0.59
6:F:179:LEU:HD11	6:F:192:GLN:CG	2.31	0.59
9:W:104:ILE:HD12	9:W:178:ILE:HG22	1.83	0.59
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.03	0.59
2:B:181:LYS:O	2:B:184:MET:HG3	2.03	0.59
5:E:220:PRO:O	5:E:222:THR:HG23	2.02	0.59
7:G:12:ILE:HG13	7:G:14:ILE:HG23	1.85	0.59
10:J:44:SER:OG	10:J:100:LEU:HB2	2.02	0.59
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.38	0.59
2:P:108:PRO:HB2	2:P:111:ILE:HD12	1.85	0.59
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	1.84	0.59
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.14	0.59
7:U:225:SER:O	7:U:229:ILE:HD12	2.03	0.59
1:O:33:GLN:CA	1:O:33:GLN:HE21	2.12	0.59
3:Q:228:GLU:O	3:Q:232:TYR:HD1	1.86	0.59
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	2.01	0.59
14:1:21:THR:HG22	14:1:26:ILE:HA	1.83	0.59
3:C:107:VAL:HA	16:C:260:HOH:O	2.02	0.59
5:E:226:GLY:O	5:E:229:VAL:HG22	2.02	0.59
5:S:132:TYR:O	5:S:153:PRO:HB3	2.02	0.59
6:T:109:ILE:HD13	6:T:142:ASP:HB3	1.82	0.59
6:T:109:ILE:CD1	6:T:109:ILE:N	2.65	0.59
6:T:63:LYS:O	6:T:65:VAL:N	2.34	0.59
7:U:53:LYS:O	7:U:55:PRO:HD3	2.02	0.59
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:101:VAL:O	9:I:110:ILE:HA	2.02	0.59
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.83	0.59
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.66	0.59
14:N:44:CYS:HB2	14:N:100:ILE:HB	1.85	0.59
4:R:86:ARG:HB2	16:R:1021:HOH:O	2.02	0.59
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.32	0.59
8:V:208:ARG:HG3	16:V:537:HOH:O	2.00	0.59
9:W:29:ASN:H	9:W:29:ASN:ND2	2.01	0.59
6:F:109:ILE:CD1	6:F:109:ILE:N	2.65	0.59
7:G:122:ILE:HA	16:G:273:HOH:O	2.02	0.59
3:Q:224:LEU:H	3:Q:224:LEU:CD1	2.15	0.59
7:U:172:ILE:HD11	7:U:201:LEU:CD2	2.32	0.59
8:V:5:GLY:O	8:V:124:TYR:HA	2.03	0.59
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.03	0.59
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.35	0.59
3:C:185:THR:HB	3:C:188:GLU:HG2	1.84	0.59
6:F:109:ILE:HD13	6:F:109:ILE:H	1.68	0.59
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.33	0.59
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.66	0.59
2:P:137:ILE:HD11	2:P:165:VAL:HG22	1.85	0.59
6:F:40:ILE:HD12	6:F:193:ALA:HB2	1.85	0.58
9:I:29:ASN:H	9:I:29:ASN:ND2	2.01	0.58
2:P:181:LYS:O	2:P:184:MET:HG3	2.03	0.58
4:R:177:LEU:HD13	5:S:58:LEU:HD11	1.84	0.58
8:V:84:LYS:HG3	8:V:85:GLN:N	2.18	0.58
13:O:179:ASP:HB3	13:O:18(A):THR:OG1	2.04	0.58
6:F:90:ASN:O	6:F:94:GLU:HG3	2.03	0.58
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.03	0.58
10:J:135:PHE:HB3	11:Y:165:ARG:HE	1.67	0.58
13:M:197:TRP:CH2	14:1:171:GLY:HA2	2.38	0.58
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.68	0.58
3:C:185:THR:HG22	3:C:187:GLU:N	2.14	0.58
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.03	0.58
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.86	0.58
5:S:226:GLY:O	5:S:229:VAL:HG22	2.04	0.58
2:B:163:ILE:HD13	2:B:164:SER:N	2.13	0.58
5:E:207:LEU:HA	5:E:2(E):ASN:HD21	1.66	0.58
12:L:135:MET:CE	9:W:165:ARG:NH2	2.66	0.58
1:A:60:MET:HB3	1:A:62:GLU:OE1	2.02	0.58
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.86	0.58
2:P:181:LYS:HG3	2:P:184:MET:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:45:ILE:HB	9:W:52:VAL:HG13	1.86	0.58
14:1:133:PHE:HE2	14:1:166:ASP:HB2	1.67	0.58
5:E:207:LEU:HD23	5:E:207:LEU:H	1.68	0.58
3:Q:182:PRO:O	3:Q:184:ALA:N	2.37	0.58
8:H:128:GLY:O	8:H:131:SER:HB2	2.04	0.58
7:U:72:ARG:HG2	16:U:321:HOH:O	2.03	0.58
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.39	0.58
2:B:71:ASN:HD22	2:B:72:ASP:N	1.99	0.58
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.04	0.58
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.86	0.58
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.86	0.58
4:D:192:LEU:O	4:D:196:ILE:HG13	2.04	0.58
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.69	0.58
11:Y:111:TYR:CE1	11:Y:121:LYS:HB2	2.39	0.58
3:C:224:LEU:H	3:C:224:LEU:CD1	2.17	0.57
5:E:15:PHE:H	6:F:23:GLN:HE22	1.50	0.57
7:G:151:THR:HG22	7:G:157:TYR:CB	2.34	0.57
8:H:24:PRO:HG2	8:H:25:ILE:HD13	1.86	0.57
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.86	0.57
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.86	0.57
5:S:49:VAL:HG13	5:S:212:ILE:CD1	2.34	0.57
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.19	0.57
7:U:172:ILE:HD11	7:U:201:LEU:HD21	1.85	0.57
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.85	0.57
6:F:69:VAL:HG12	16:F:289:HOH:O	2.04	0.57
14:N:133:PHE:HE2	14:N:166:ASP:HB2	1.69	0.57
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.39	0.57
8:V:106:THR:HG21	16:V:511:HOH:O	2.03	0.57
10:J:-1:MET:CG	10:J:1:ASP:H	2.12	0.57
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.70	0.57
7:U:87:ASN:ND2	7:U:87:ASN:C	2.56	0.57
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.18	0.57
3:C:190:VAL:O	3:C:194:VAL:HG23	2.05	0.57
3:C:36:CYS:H	3:C:51:GLU:HG2	1.69	0.57
7:G:53:LYS:O	7:G:55:PRO:HD3	2.04	0.57
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.34	0.57
1:O:69:LEU:HD23	1:O:69:LEU:C	2.24	0.57
11:K:13:ILE:HD12	11:K:152:LEU:HD23	1.85	0.57
11:K:25:TRP:CH2	12:L:132:SER:HA	2.39	0.57
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.69	0.57
2:P:112:LEU:HD23	2:P:112:LEU:C	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.04	0.57
10:X:156:LYS:HE2	10:X:160:GLN:NE2	2.19	0.57
10:X:52:THR:CG2	10:X:53:VAL:N	2.67	0.57
2:B:112:LEU:C	2:B:112:LEU:HD23	2.25	0.57
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.35	0.57
11:K:184:TRP:O	11:K:185:ILE:HD13	2.04	0.57
13:M:91:ARG:HG3	13:M:92:SER:N	2.18	0.57
1:O:159:PRO:O	2:P:59:LEU:HD12	2.04	0.57
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.85	0.57
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	1.85	0.57
13:O:152:GLU:O	13:O:156:VAL:HG23	2.04	0.57
11:K:7:ARG:HD2	11:K:108:PRO:O	2.04	0.57
6:T:109:ILE:HD12	6:T:109:ILE:N	2.18	0.57
6:T:136:THR:O	6:T:150:MET:HA	2.05	0.57
10:J:-1:MET:HG2	10:J:1:ASP:N	2.14	0.57
10:X:90(A):ILE:HG12	10:X:116:LEU:HA	1.86	0.57
13:O:12:VAL:HG21	13:O:102:ALA:HB1	1.87	0.57
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.87	0.57
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.87	0.57
4:D:205:GLU:HA	4:D:205:GLU:OE2	2.05	0.57
6:F:63:LYS:O	6:F:65:VAL:HG23	2.05	0.57
6:F:91:ARG:O	6:F:95:GLU:HB2	2.05	0.57
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.02	0.56
2:B:121:GLN:O	2:B:124:THR:HB	2.05	0.56
6:F:136:THR:O	6:F:150:MET:HA	2.05	0.56
14:N:30:VAL:HG11	13:O:199:PHE:CE2	2.40	0.56
6:T:91:ARG:O	6:T:95:GLU:HB2	2.05	0.56
3:C:228:GLU:O	3:C:232:TYR:HD1	1.89	0.56
3:Q:224:LEU:N	3:Q:224:LEU:HD12	2.20	0.56
6:T:90:ASN:O	6:T:94:GLU:HG3	2.05	0.56
8:V:200:LYS:HE3	9:W:140:SER:O	2.05	0.56
11:K:165:ARG:HE	10:X:135:PHE:HB3	1.70	0.56
5:E:45:HIS:HB3	5:E:214:ILE:HD11	1.88	0.56
10:J:52:THR:CG2	10:J:53:VAL:N	2.68	0.56
10:J:74:LEU:HD23	16:J:205:HOH:O	2.05	0.56
2:B:71:ASN:HD22	2:B:72:ASP:H	1.45	0.56
5:S:207:LEU:HD23	5:S:207:LEU:H	1.69	0.56
6:T:63:LYS:O	6:T:65:VAL:HG23	2.05	0.56
9:I:154:THR:HG23	16:I:224:HOH:O	2.04	0.56
4:R:177:LEU:HA	5:S:58:LEU:HD11	1.87	0.56
8:V:25:ILE:N	8:V:25:ILE:HD13	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.86	0.56
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.41	0.56
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.40	0.56
13:O:51:ASP:O	13:O:55:ILE:HD12	2.05	0.56
14:1:61:TYR:HA	16:1:214:HOH:O	2.05	0.56
7:U:228:ASN:HB3	16:U:295:HOH:O	2.04	0.56
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.06	0.56
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.09	0.56
1:A:69:LEU:HD23	1:A:69:LEU:C	2.25	0.56
11:K:40:PHE:HB3	11:K:73:ARG:HH21	1.71	0.56
3:Q:227:GLU:OE1	3:Q:227:GLU:N	2.38	0.56
4:R:85:ALA:O	4:R:89:ILE:HG12	2.05	0.56
5:S:45:HIS:HB3	5:S:214:ILE:HD11	1.88	0.56
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.05	0.56
13:O:19:LEU:HD21	13:O:26:LEU:HD22	1.87	0.56
8:H:84:LYS:HG3	8:H:85:GLN:N	2.20	0.56
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.87	0.56
7:U:18(A):ILE:CD1	7:U:18(C):HIS:O	2.53	0.56
7:U:172:ILE:HD12	7:U:197:MET:CE	2.36	0.56
12:Z:21:ILE:HD12	12:Z:21:ILE:C	2.26	0.56
3:C:55:THR:O	3:C:56:LEU:HD22	2.05	0.56
7:G:87:ASN:ND2	7:G:87:ASN:C	2.59	0.56
8:H:105:ASP:O	8:H:106:THR:N	2.38	0.56
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.53	0.56
3:Q:224:LEU:H	3:Q:224:LEU:HD12	1.70	0.56
14:1:19:ARG:HG3	14:1:26:ILE:HG23	1.88	0.56
14:1:8:PHE:CE1	14:1:10:ASP:HB2	2.41	0.56
4:D:177:LEU:HD13	5:E:58:LEU:CD1	2.36	0.56
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.41	0.56
13:M:13:ILE:HB	13:M:155:ILE:HD12	1.88	0.56
2:P:38:ILE:HG13	2:P:164:SER:HB3	1.88	0.56
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.41	0.56
13:O:157:ASN:HD22	13:O:160:ARG:NH1	2.03	0.55
5:E:207:LEU:CD2	5:E:207:LEU:H	2.19	0.55
5:E:227:GLU:CD	5:E:227:GLU:N	2.59	0.55
11:K:45:MET:HG3	11:K:52:CYS:HB2	1.88	0.55
8:V:148:LYS:O	8:V:152:ILE:HG13	2.05	0.55
13:O:14(D):GLU:O	13:O:14(G):ILE:HG13	2.05	0.55
7:G:172:ILE:HD12	7:G:197:MET:CE	2.37	0.55
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.06	0.55
10:X:113:ILE:HA	10:X:118:THR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.06	0.55
13:O:41:THR:OG1	13:O:76:PRO:HG3	2.06	0.55
2:B:38:ILE:HG13	2:B:164:SER:HB3	1.88	0.55
3:C:173:ARG:O	3:C:177:GLU:HG3	2.07	0.55
3:C:224:LEU:N	3:C:224:LEU:HD12	2.22	0.55
4:D:227:GLU:OE2	4:D:227:GLU:N	2.34	0.55
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.71	0.55
9:I:6:MET:CE	9:I:155:ILE:HA	2.36	0.55
10:J:156:LYS:HE2	10:J:160:GLN:NE2	2.21	0.55
11:K:4:LEU:HD11	11:K:159:ILE:HG12	1.89	0.55
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.42	0.55
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.33	0.55
2:B:194:LEU:HD12	2:B:236:THR:HG21	1.88	0.55
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.35	0.55
8:H:165:ASN:ND2	13:O:139:ARG:HH11	2.04	0.55
13:M:152:GLU:O	13:M:156:VAL:HG23	2.06	0.55
6:T:179:LEU:HD21	6:T:192:GLN:CG	2.34	0.55
3:C:186:VAL:O	3:C:190:VAL:HG23	2.07	0.55
7:G:18(A):ILE:CD1	7:G:18(C):HIS:O	2.53	0.55
8:H:196:VAL:HG23	16:H:521:HOH:O	2.06	0.55
11:K:32:LYS:N	11:K:32:LYS:HD2	2.22	0.55
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.42	0.55
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.06	0.55
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.87	0.55
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.07	0.55
4:R:205:GLU:OE2	4:R:205:GLU:HA	2.06	0.55
11:Y:4:LEU:HD11	11:Y:159:ILE:HG12	1.89	0.55
11:Y:45:MET:HG3	11:Y:52:CYS:HB2	1.89	0.55
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.07	0.55
2:B:224:PHE:N	2:B:224:PHE:CD2	2.75	0.55
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.36	0.55
5:S:207:LEU:H	5:S:207:LEU:CD2	2.20	0.55
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.88	0.55
10:X:190:PHE:C	10:X:192:ALA:H	2.10	0.55
14:1:133:PHE:CE2	14:1:166:ASP:HB2	2.41	0.55
3:C:227:GLU:OE1	3:C:227:GLU:N	2.37	0.55
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.37	0.55
5:S:227:GLU:N	5:S:227:GLU:CD	2.60	0.55
13:O:178:ILE:CD1	13:O:184:LEU:HG	2.36	0.55
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.42	0.55
3:C:122:ARG:NH2	16:C:280:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:PHE:N	3:C:23:GLN:HE22	2.02	0.55
4:D:85:ALA:O	4:D:89:ILE:HG12	2.07	0.55
10:J:190:PHE:HA	10:J:193:GLN:HB2	1.89	0.55
13:M:12:VAL:HG21	13:M:102:ALA:HB1	1.89	0.55
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.42	0.55
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.89	0.55
14:1:146:MET:CE	14:1:150:GLU:HB3	2.37	0.55
13:M:199:PHE:CE2	14:1:30:VAL:HG11	2.41	0.55
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.21	0.55
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.02	0.55
8:H:200:LYS:HE3	9:I:140:SER:O	2.06	0.54
10:J:113:ILE:HA	10:J:118:THR:O	2.07	0.54
11:K:207:ASN:HD21	10:X:144:PRO:HG2	1.73	0.54
12:L:163:THR:HG21	16:L:247:HOH:O	2.06	0.54
3:Q:57:LYS:HG2	3:Q:208:LYS:NZ	2.23	0.54
3:Q:87:ILE:HD13	3:Q:87:ILE:N	2.21	0.54
6:T:187:ARG:HG3	6:T:187:ARG:HH11	1.71	0.54
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.22	0.54
2:B:224:PHE:HD2	2:B:224:PHE:N	2.04	0.54
8:H:148:LYS:O	8:H:152:ILE:HG13	2.07	0.54
8:H:218:ILE:N	8:H:218:ILE:HD13	2.23	0.54
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.88	0.54
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.07	0.54
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.06	0.54
6:T:127:ASN:H	6:T:127:ASN:HD22	1.53	0.54
14:1:18(G):TYR:HA	14:1:18(J):LEU:HG	1.88	0.54
10:J:190:PHE:C	10:J:192:ALA:H	2.10	0.54
10:J:2:ILE:O	10:J:3:ILE:HD13	2.07	0.54
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.23	0.54
13:M:51:ASP:O	13:M:55:ILE:HD12	2.07	0.54
14:N:6:VAL:HG23	14:N:155:ILE:HD11	1.89	0.54
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.07	0.54
2:P:121:GLN:O	2:P:124:THR:HB	2.06	0.54
2:P:185:LYS:HD3	2:P:186:VAL:H	1.72	0.54
7:U:151:THR:HG22	7:U:157:TYR:CB	2.37	0.54
7:U:158:VAL:HG22	7:U:159:GLY:N	2.22	0.54
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.38	0.54
3:C:57:LYS:HG2	3:C:208:LYS:NZ	2.23	0.54
3:C:224:LEU:H	3:C:224:LEU:HD12	1.72	0.54
6:F:179:LEU:HD21	6:F:192:GLN:CG	2.36	0.54
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:200:LYS:HE3	11:K:206:PHE:O	2.07	0.54
11:K:33:LYS:HE2	15:K:500:GDT:H29	1.88	0.54
3:Q:65:SER:HB2	16:Q:257:HOH:O	2.07	0.54
5:S:143:LYS:HD2	13:O:71(B):GLU:O	2.07	0.54
5:E:194:VAL:O	5:E:197:ILE:HG22	2.07	0.54
11:K:63:CYS:HB2	16:K:540:HOH:O	2.07	0.54
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.42	0.54
1:O:191:HIS:HE1	1:O:236:LEU:HA	1.72	0.54
2:P:6:ARG:HD2	4:R:9:ASP:N	2.22	0.54
12:Z:29:ARG:NH1	12:Z:193:ARG:HB3	2.22	0.54
14:N:171:GLY:HA2	13:O:197:TRP:CH2	2.42	0.54
1:O:86:ARG:NE	7:U:118:ASN:ND2	2.46	0.54
11:Y:33:LYS:HE2	15:Y:500:GDT:H29	1.88	0.54
4:D:40:ILE:HG13	4:D:193:VAL:HG23	1.89	0.54
7:G:8:TYR:C	7:G:10:ARG:H	2.10	0.54
1:O:212:LEU:HD23	1:O:212:LEU:C	2.28	0.54
2:P:126:HIS:CB	3:Q:129:VAL:HG12	2.36	0.54
7:U:8:TYR:C	7:U:10:ARG:H	2.11	0.54
11:Y:32:LYS:HD2	11:Y:32:LYS:N	2.22	0.54
2:B:15:PHE:H	3:C:23:GLN:NE2	2.02	0.54
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.89	0.54
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.71	0.54
13:O:113:VAL:HA	13:O:118:VAL:O	2.08	0.54
1:A:17:PRO:HA	2:B:26:TYR:CD1	2.43	0.54
8:H:159:ILE:O	8:H:163:ILE:HD12	2.08	0.54
14:N:146:MET:CE	14:N:150:GLU:HB3	2.37	0.54
8:H:165:ASN:HD22	13:O:139:ARG:HH11	1.56	0.54
13:O:40:ASN:N	13:O:40:ASN:HD22	1.97	0.54
1:A:191:HIS:HE1	1:A:236:LEU:HA	1.72	0.54
12:L:177:ILE:HD12	12:L:177:ILE:N	2.22	0.54
3:Q:122:ARG:NH2	16:Q:261:HOH:O	2.40	0.54
4:R:177:LEU:HD13	5:S:58:LEU:CD1	2.36	0.54
7:U:79:ASN:HA	16:U:302:HOH:O	2.07	0.54
10:X:52:THR:CG2	10:X:53:VAL:H	2.21	0.54
11:Y:184:TRP:O	11:Y:185:ILE:HD13	2.08	0.54
6:F:121:GLN:NE2	16:F:300:HOH:O	2.41	0.53
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.89	0.53
8:V:172:ASN:ND2	8:V:193:THR:HA	2.23	0.53
7:G:225:SER:O	7:G:229:ILE:HD12	2.08	0.53
8:H:143:LYS:HG2	8:H:146:LEU:HD21	1.90	0.53
8:H:34:LEU:HB2	16:H:522:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:135:PHE:HB3	11:Y:165:ARG:NE	2.23	0.53
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.39	0.53
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.10	0.53
13:M:184:LEU:C	13:M:184:LEU:HD23	2.28	0.53
2:P:224:PHE:N	2:P:224:PHE:HD2	2.06	0.53
7:U:87:ASN:HD22	7:U:88:ALA:N	2.07	0.53
2:B:141:TYR:C	2:B:141:TYR:CD1	2.82	0.53
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.23	0.53
8:V:22:GLN:HG2	15:V:500:GDT:H36B	1.90	0.53
3:C:227:GLU:CD	3:C:227:GLU:H	2.11	0.53
5:E:49:VAL:HG13	5:E:212:ILE:CD1	2.39	0.53
8:H:25:ILE:HD13	8:H:25:ILE:N	2.23	0.53
9:I:29:ASN:HD21	11:Y:208:ASN:HD21	1.55	0.53
13:M:149:GLN:NE2	13:M:149:GLN:N	2.49	0.53
14:N:133:PHE:CE2	14:N:166:ASP:HB2	2.43	0.53
1:O:150:GLN:O	1:O:157:TYR:HA	2.08	0.53
1:O:62:GLU:CD	1:O:62:GLU:H	2.12	0.53
7:U:131:PRO:HB3	16:U:312:HOH:O	2.08	0.53
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.90	0.53
9:W:6:MET:CE	9:W:155:ILE:HA	2.38	0.53
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.23	0.53
13:O:8:TYR:CE2	13:O:148:VAL:HG22	2.43	0.53
4:D:29:GLU:OE2	4:D:32:LYS:HD2	2.08	0.53
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.56	0.53
7:G:30:ALA:O	7:G:33:GLN:HB2	2.08	0.53
12:L:93:PHE:N	12:L:94:PRO:HD3	2.22	0.53
4:R:192:LEU:O	4:R:196:ILE:HG13	2.09	0.53
9:W:48:LEU:HG	9:W:50:THR:HG22	1.91	0.53
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.38	0.53
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	1.90	0.53
13:O:149:GLN:NE2	13:O:149:GLN:N	2.52	0.53
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.44	0.53
4:D:81:LEU:O	4:D:134:VAL:HB	2.09	0.53
7:G:172:ILE:HD12	7:G:197:MET:HE2	1.91	0.53
10:J:162:LEU:O	10:J:166:MET:HB2	2.08	0.53
11:K:37:ILE:O	11:K:38:ASN:HB3	2.09	0.53
8:V:18:THR:CB	8:V:30:ASN:HD22	2.22	0.53
11:Y:38:ASN:O	11:Y:40:PHE:N	2.41	0.53
15:Y:500:GDT:H8	12:Z:96:TYR:CE2	2.44	0.53
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.90	0.53
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:14(H):GLY:C	12:L:1(I):ASN:H	2.12	0.53
8:V:74:PRO:HA	16:V:516:HOH:O	2.09	0.53
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	1.99	0.53
13:O:205:GLY:HA3	13:O:209:GLN:HB3	1.91	0.53
13:O:91:ARG:HG3	13:O:92:SER:N	2.24	0.53
9:I:104:ILE:HG21	9:I:181:LYS:HG2	1.91	0.53
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.44	0.53
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.89	0.53
3:Q:15:PHE:N	4:R:23:GLN:HE22	2.06	0.53
4:R:29:GLU:OE2	4:R:32:LYS:HD2	2.09	0.53
1:A:212:LEU:HD23	1:A:212:LEU:C	2.29	0.53
9:I:48:LEU:HG	9:I:50:THR:HG22	1.90	0.53
10:J:189:ASP:O	10:J:193:GLN:HB2	2.08	0.53
10:J:90(A):ILE:HG12	10:J:116:LEU:HA	1.91	0.53
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.09	0.53
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.90	0.53
11:Y:40:PHE:HB3	11:Y:73:ARG:HH21	1.73	0.53
14:I:114:PRO:HD2	14:I:118:SER:O	2.09	0.52
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.43	0.52
1:A:62:GLU:H	1:A:62:GLU:CD	2.12	0.52
2:B:137:ILE:HD11	2:B:165:VAL:HG22	1.90	0.52
14:N:19:ARG:HG3	14:N:26:ILE:HG23	1.91	0.52
2:P:224:PHE:N	2:P:224:PHE:CD2	2.77	0.52
5:S:214:ILE:HD12	5:S:215:VAL:H	1.70	0.52
6:T:109:ILE:CD1	6:T:109:ILE:H	2.21	0.52
7:U:30:ALA:O	7:U:33:GLN:HB2	2.09	0.52
8:V:143:LYS:HG2	8:V:146:LEU:HD21	1.90	0.52
1:A:227:GLN:NE2	1:A:231:ASP:OD1	2.42	0.52
7:G:136:LEU:O	7:G:150:LYS:HA	2.09	0.52
8:H:172:ASN:ND2	8:H:193:THR:HA	2.24	0.52
5:S:194:VAL:O	5:S:197:ILE:HG22	2.08	0.52
8:V:105:ASP:O	8:V:106:THR:N	2.43	0.52
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.43	0.52
13:O:7:LYS:HG3	13:O:14(G):ILE:HD13	1.91	0.52
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.90	0.52
5:E:214:ILE:CD1	5:E:215:VAL:N	2.71	0.52
6:F:186:ALA:O	6:F:190:VAL:HG23	2.10	0.52
9:I:45:ILE:HB	9:I:52:VAL:HG13	1.90	0.52
10:J:19:ALA:HB2	10:J:171:LYS:HG2	1.91	0.52
10:X:190:PHE:HA	10:X:193:GLN:HB2	1.89	0.52
1:A:150:GLN:O	1:A:157:TYR:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:158:VAL:HG22	7:G:159:GLY:N	2.24	0.52
12:L:21:ILE:HD12	12:L:21:ILE:C	2.30	0.52
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.12	0.52
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.45	0.52
6:T:70:VAL:HB	6:T:74:ILE:HB	1.90	0.52
8:V:78:SER:O	8:V:82:MET:HG3	2.09	0.52
4:D:22:PHE:HB2	16:D:280:HOH:O	2.09	0.52
4:D:24:VAL:O	4:D:27:SER:HB3	2.10	0.52
13:M:14(D):GLU:O	13:M:14(G):ILE:HG13	2.08	0.52
3:Q:112:LEU:O	3:Q:116:VAL:HG23	2.09	0.52
8:V:218:ILE:N	8:V:218:ILE:HD13	2.24	0.52
13:O:171:ARG:O	13:O:192:VAL:HG23	2.10	0.52
13:M:113:VAL:HA	13:M:118:VAL:O	2.08	0.52
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.91	0.52
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.91	0.52
7:U:18(A):ILE:HD12	7:U:18(C):HIS:O	2.10	0.52
14:1:163:ILE:HG23	14:1:170:GLY:HA2	1.92	0.52
3:C:15:PHE:N	4:D:23:GLN:HE22	2.08	0.52
5:E:54:ASN:ND2	5:E:56:ASP:O	2.43	0.52
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.92	0.52
10:J:42:LEU:HB2	10:J:184:ILE:HD13	1.90	0.52
1:O:161:LYS:HD3	1:O:180:TRP:CH2	2.45	0.52
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.91	0.52
3:C:212:ILE:HG22	3:C:213:THR:N	2.25	0.52
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.44	0.52
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.45	0.52
14:N:67:THR:HA	14:N:72:GLY:O	2.10	0.52
4:R:175:GLU:HG2	4:R:196:ILE:HD13	1.91	0.52
9:W:29:ASN:HB2	16:W:218:HOH:O	2.10	0.52
10:X:103:GLY:HA2	10:X:178:VAL:HG11	1.92	0.52
9:I:29:ASN:HD21	11:Y:208:ASN:ND2	2.07	0.52
14:N:106:ASN:O	14:N:107:LYS:HB3	2.09	0.52
9:W:12:VAL:CG1	9:W:108:PRO:HB3	2.40	0.52
7:U:93:LYS:HD3	14:1:68:SER:HB3	1.91	0.52
2:B:185:LYS:HD3	2:B:186:VAL:H	1.72	0.52
16:P:258:HOH:O	3:Q:62(A):ILE:HD11	2.10	0.52
10:X:189:ASP:O	10:X:193:GLN:HB2	2.10	0.52
12:Z:180:LYS:HG2	16:Z:247:HOH:O	2.10	0.52
13:O:105:GLN:HG3	16:O:260:HOH:O	2.09	0.51
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.74	0.51
4:D:121:LEU:HA	4:D:123:PHE:HE1	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:124:PHE:O	9:I:125:ILE:HD13	2.10	0.51
11:K:38:ASN:O	11:K:40:PHE:N	2.43	0.51
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.91	0.51
6:T:72:ARG:HD2	13:O:64:THR:OG1	2.10	0.51
11:Y:101:ILE:HD13	11:Y:101:ILE:N	2.25	0.51
3:C:39:GLY:O	3:C:162:ALA:HA	2.11	0.51
2:P:206:THR:HB	2:P:208:ASP:OD1	2.11	0.51
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.46	0.51
12:Z:14(H):GLY:C	12:Z:1(I):ASN:H	2.13	0.51
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.93	0.51
6:F:109:ILE:HD13	6:F:142:ASP:HB3	1.91	0.51
6:F:70:VAL:HB	6:F:74:ILE:HB	1.92	0.51
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.92	0.51
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.25	0.51
15:K:500:GDT:H8	12:L:96:TYR:CE2	2.45	0.51
13:M:7:LYS:HG3	13:M:14(G):ILE:HD13	1.92	0.51
13:M:157:ASN:HD22	13:M:160:ARG:NH1	2.05	0.51
13:M:40:ASN:ND2	13:M:40:ASN:N	2.58	0.51
2:P:141:TYR:C	2:P:141:TYR:CD1	2.83	0.51
3:Q:212:ILE:HG22	3:Q:213:THR:N	2.26	0.51
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.91	0.51
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.93	0.51
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.45	0.51
3:C:197:LEU:O	3:C:201:VAL:HG23	2.11	0.51
3:C:160:TRP:NE1	4:D:59:LEU:HD23	2.25	0.51
13:M:203:ILE:O	13:M:203:ILE:HG22	2.09	0.51
14:1:106:ASN:O	14:1:107:LYS:HB3	2.10	0.51
4:D:112:LEU:C	4:D:112:LEU:HD13	2.30	0.51
7:G:87:ASN:HD22	7:G:88:ALA:N	2.08	0.51
3:Q:163:GLN:HA	3:Q:163:GLN:HE21	1.75	0.51
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.45	0.51
10:J:24:ILE:HD11	10:X:129:TYR:HB3	1.92	0.51
11:Y:9:GLN:CD	11:Y:10:GLY:N	2.64	0.51
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.92	0.51
2:P:194:LEU:HD12	2:P:236:THR:HG21	1.92	0.51
5:S:41:ARG:NH1	5:S:42:SER:O	2.43	0.51
11:Y:37:ILE:O	11:Y:38:ASN:HB3	2.09	0.51
1:A:202:VAL:HG21	1:A:206:PHE:CD1	2.45	0.51
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.93	0.51
4:D:12(E):SER:HB2	5:E:123:ASN:OD1	2.11	0.51
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.93	0.51
6:T:45:GLY:HA3	6:T:215:CYS:O	2.11	0.51
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.46	0.51
6:F:127:ASN:HD22	6:F:127:ASN:H	1.56	0.51
7:G:18(D):ILE:O	7:G:18(G):GLU:N	2.44	0.51
13:M:205:GLY:HA2	16:1:193:HOH:O	2.11	0.51
13:M:-3:VAL:HG12	13:M:49:ILE:HG13	1.92	0.51
7:U:172:ILE:HD12	7:U:197:MET:HE2	1.92	0.51
10:X:121:GLU:O	10:X:122:LEU:HD23	2.10	0.51
13:O:-3:VAL:HG12	13:O:49:ILE:HG13	1.91	0.51
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.92	0.51
9:I:30:LYS:NZ	11:Y:210:ILE:HD13	2.26	0.51
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.91	0.51
1:O:227:GLN:NE2	1:O:231:ASP:OD1	2.43	0.51
2:P:67:LEU:HD22	2:P:211:GLU:HB3	1.93	0.51
4:R:121:LEU:HA	4:R:123:PHE:HE1	1.73	0.51
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.92	0.51
14:1:10(B):LYS:O	14:1:10(B):LYS:HD3	2.11	0.51
9:I:101:VAL:HG23	9:I:113:PHE:HE2	1.76	0.51
9:I:1:GLY:HA2	9:I:17:ASP:OD1	2.11	0.51
13:M:3:VAL:HG23	13:M:46:SER:HB3	1.93	0.51
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.40	0.51
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.10	0.51
11:Y:146:LEU:HD23	11:Y:151:ALA:HA	1.93	0.51
12:Z:70:HIS:HE1	16:Z:226:HOH:O	1.94	0.51
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.92	0.50
2:B:136:PHE:O	2:B:150:THR:HA	2.10	0.50
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.11	0.50
10:J:69:ARG:HD2	16:J:216:HOH:O	2.10	0.50
12:L:19:ARG:NE	12:L:171:ASP:OD2	2.37	0.50
13:M:178:ILE:CD1	13:M:184:LEU:HG	2.40	0.50
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.92	0.50
14:N:13:ILE:HD12	14:N:151:THR:HG22	1.92	0.50
10:X:16:SER:HB2	16:X:229:HOH:O	2.11	0.50
10:X:2:ILE:O	10:X:3:ILE:HD13	2.11	0.50
11:Y:31:VAL:HA	12:Z:120:GLU:OE2	2.11	0.50
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.41	0.50
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.06	0.50
6:T:237:GLN:O	6:T:240:ILE:HG22	2.11	0.50
9:W:45:ILE:HG22	9:W:52:VAL:HG22	1.93	0.50
3:C:112:LEU:O	3:C:116:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.92	0.50
8:H:18:THR:CB	8:H:30:ASN:HD22	2.24	0.50
10:J:103:GLY:HA2	10:J:178:VAL:HG11	1.93	0.50
5:E:143:LYS:HD2	13:M:71(B):GLU:O	2.11	0.50
7:U:81:PRO:HD2	7:U:133:GLY:O	2.11	0.50
2:B:127:GLY:N	16:B:275:HOH:O	2.44	0.50
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.93	0.50
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.93	0.50
13:O:104:VAL:HG13	13:O:106:GLY:O	2.11	0.50
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.12	0.50
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.77	0.50
3:Q:120:GLN:O	3:Q:124:THR:HG23	2.12	0.50
5:S:226:GLY:O	5:S:228:ALA:N	2.44	0.50
14:1:10:ASP:O	14:1:179:THR:HG22	2.12	0.50
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.94	0.50
8:H:10:ASN:HD22	8:H:179:GLU:CG	2.24	0.50
10:J:179:ASP:HB2	16:J:217:HOH:O	2.10	0.50
11:K:101:ILE:N	11:K:101:ILE:HD13	2.27	0.50
10:X:74:LEU:HD22	10:X:78:ALA:CB	2.42	0.50
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.27	0.50
3:C:163:GLN:CA	3:C:163:GLN:HE21	2.25	0.50
11:K:6:PHE:HA	11:K:123:ASP:O	2.12	0.50
11:K:32:LYS:HB2	16:K:542:HOH:O	2.11	0.50
10:J:129:TYR:HB3	10:X:24:ILE:HD11	1.92	0.50
2:B:206:THR:HB	2:B:208:ASP:OD1	2.11	0.50
3:C:87:ILE:N	3:C:87:ILE:HD13	2.26	0.50
4:D:177:LEU:HA	5:E:58:LEU:HD11	1.93	0.50
7:G:228:ASN:HB3	16:G:255:HOH:O	2.12	0.50
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.47	0.50
11:K:9:GLN:CD	11:K:10:GLY:N	2.65	0.50
3:Q:45:CYS:HA	3:Q:141:PHE:HZ	1.77	0.50
1:O:58:LEU:HD12	7:U:173:THR:HG23	1.93	0.50
9:W:104:ILE:HG21	9:W:181:LYS:HG2	1.93	0.50
10:X:39:PRO:HG2	10:X:73:GLU:OE2	2.12	0.50
10:J:52:THR:CG2	10:J:53:VAL:H	2.24	0.50
11:K:67:GLU:HG2	11:K:73:ARG:HA	1.94	0.50
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.12	0.50
4:D:81:LEU:HD12	4:D:133:GLY:HA3	1.94	0.49
7:G:38:LEU:HD23	7:G:197:MET:CE	2.42	0.49
8:H:22:GLN:HG2	15:H:500:GDT:H36B	1.94	0.49
14:N:114:PRO:HD2	14:N:118:SER:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.12	0.49
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.94	0.49
5:S:86:ARG:O	5:S:90:ASN:HB2	2.11	0.49
6:T:186:ALA:O	6:T:190:VAL:HG23	2.12	0.49
7:U:49:ILE:HD12	7:U:212:VAL:HG22	1.93	0.49
10:X:19:ALA:HB2	10:X:171:LYS:HG2	1.92	0.49
13:O:184:LEU:HD23	13:O:184:LEU:C	2.32	0.49
14:1:6:VAL:HG23	14:1:155:ILE:HD11	1.93	0.49
3:C:69:LYS:HG3	16:C:277:HOH:O	2.12	0.49
4:D:29:GLU:HA	4:D:29:GLU:OE2	2.12	0.49
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.47	0.49
10:J:112:GLN:NE2	10:J:126:ALA:H	2.10	0.49
11:K:67:GLU:CD	11:K:73:ARG:HA	2.33	0.49
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.12	0.49
2:P:136:PHE:O	2:P:150:THR:HA	2.12	0.49
2:P:168:ASN:HA	16:P:275:HOH:O	2.12	0.49
3:Q:201:VAL:HG21	3:Q:210:ILE:CD1	2.41	0.49
4:R:42:THR:C	4:R:44:GLU:H	2.16	0.49
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.74	0.49
10:X:162:LEU:O	10:X:166:MET:HB2	2.11	0.49
12:Z:147:SER:O	12:Z:151:VAL:HG23	2.12	0.49
1:A:109:THR:O	1:A:113:VAL:HG23	2.12	0.49
1:A:67:VAL:HB	1:A:223:LYS:HZ2	1.77	0.49
3:C:121:GLN:C	3:C:121:GLN:NE2	2.65	0.49
11:K:46:ALA:HB3	11:K:98:GLY:O	2.12	0.49
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.27	0.49
3:Q:39:GLY:O	3:Q:162:ALA:HA	2.11	0.49
3:Q:62(A):ILE:HG13	3:Q:63:THR:N	2.28	0.49
7:U:136:LEU:O	7:U:150:LYS:HA	2.12	0.49
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.94	0.49
9:W:186:LYS:HE2	9:W:188:TYR:CE1	2.47	0.49
5:E:226:GLY:O	5:E:228:ALA:N	2.44	0.49
6:F:45:GLY:HA3	6:F:215:CYS:O	2.12	0.49
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.41	0.49
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.93	0.49
8:V:10:ASN:HD22	8:V:179:GLU:CG	2.26	0.49
8:V:52:THR:O	8:V:56:THR:HB	2.13	0.49
12:Z:11:PHE:CZ	12:Z:148:VAL:HA	2.47	0.49
13:O:40:ASN:ND2	13:O:40:ASN:N	2.58	0.49
13:O:-6:GLN:O	13:O:-6:GLN:HG3	2.13	0.49
1:A:86:ARG:NE	7:G:118:ASN:ND2	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.93	0.49
11:K:146:LEU:HD23	11:K:151:ALA:HA	1.93	0.49
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	1.94	0.49
4:R:112:LEU:C	4:R:112:LEU:HD13	2.32	0.49
4:R:194:LEU:HD12	4:R:207:LEU:HD11	1.94	0.49
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.48	0.49
2:P:97:GLN:OE1	9:W:64:ASN:HB3	2.13	0.49
11:K:165:ARG:NE	10:X:135:PHE:HB3	2.27	0.49
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.13	0.49
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.12	0.49
14:1:104:TYR:OH	14:1:180:ALA:HB2	2.12	0.49
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.26	0.49
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.77	0.49
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.93	0.49
4:D:194:LEU:HD12	4:D:207:LEU:HD11	1.95	0.49
4:D:14:THR:HG23	5:E:23:GLN:NE2	2.28	0.49
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.27	0.49
2:P:225:LYS:HB2	2:P:228:GLU:HG3	1.95	0.49
2:P:12:THR:HB	2:P:23:GLN:HG3	1.93	0.49
4:R:81:LEU:O	4:R:134:VAL:HB	2.13	0.49
10:X:4:LEU:HD23	10:X:126:ALA:HB2	1.94	0.49
2:B:235:LYS:HD3	2:B:235:LYS:N	2.28	0.49
7:G:81:PRO:HD2	7:G:133:GLY:O	2.13	0.49
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.95	0.49
11:K:126:CYS:HB2	11:K:135:TYR:CZ	2.48	0.49
3:Q:125:GLN:NE2	16:Q:270:HOH:O	2.46	0.49
7:U:18(D):ILE:O	7:U:18(G):GLU:N	2.45	0.49
10:X:100:LEU:CD2	10:X:112:GLN:HG3	2.42	0.49
3:C:120:GLN:O	3:C:124:THR:HG23	2.13	0.49
2:B:126:HIS:CB	3:C:129:VAL:HG12	2.35	0.49
4:D:101:LEU:N	16:D:257:HOH:O	2.45	0.49
4:D:56:SER:OG	4:D:57:PRO:HD2	2.12	0.49
6:F:70:VAL:HG11	6:F:112:PHE:CE1	2.48	0.49
7:G:192:PHE:CD1	7:G:192:PHE:C	2.85	0.49
8:H:159:ILE:HG22	8:H:163:ILE:CD1	2.43	0.49
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.95	0.49
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.48	0.49
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.12	0.49
8:H:52:THR:O	8:H:56:THR:HB	2.12	0.49
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.93	0.49
4:D:240:LYS:O	4:D:243:ALA:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:165:ARG:HG2	16:Z:218:HOH:O	2.13	0.49
12:L:11:PHE:CZ	12:L:148:VAL:HA	2.48	0.49
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.11	0.49
4:R:40:ILE:HG13	4:R:193:VAL:HG23	1.93	0.49
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.39	0.49
6:T:127:ASN:ND2	6:T:127:ASN:H	2.11	0.49
8:V:24:PRO:HG2	8:V:25:ILE:HD13	1.94	0.49
3:C:225:SER:O	3:C:229:ILE:HG13	2.12	0.48
6:F:109:ILE:CD1	6:F:109:ILE:H	2.24	0.48
7:G:79:ASN:HA	16:G:284:HOH:O	2.13	0.48
12:L:145:TYR:CD1	12:L:146:LEU:N	2.81	0.48
2:P:72:ASP:O	2:P:221:GLN:HG3	2.12	0.48
4:R:29:GLU:HA	4:R:29:GLU:OE2	2.12	0.48
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.43	0.48
5:S:49:VAL:HG13	5:S:212:ILE:HD11	1.95	0.48
9:W:104:ILE:CD1	9:W:178:ILE:HG22	2.43	0.48
10:X:-1:MET:HG2	10:X:1:ASP:N	2.15	0.48
10:X:39:PRO:HG2	10:X:73:GLU:CD	2.34	0.48
12:Z:123:GLN:CG	12:Z:145:TYR:OH	2.61	0.48
13:O:42:VAL:HG23	13:O:178:ILE:HD11	1.94	0.48
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.94	0.48
9:I:12:VAL:CG1	9:I:108:PRO:HB3	2.43	0.48
13:M:171:ARG:O	13:M:192:VAL:HG23	2.13	0.48
14:N:10:ASP:O	14:N:179:THR:HG22	2.13	0.48
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.28	0.48
4:R:240:LYS:O	4:R:243:ALA:HB3	2.13	0.48
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.48	0.48
7:G:233:LEU:O	7:G:236:ILE:HG12	2.13	0.48
5:S:207:LEU:HD23	5:S:207:LEU:N	2.29	0.48
5:S:48:LEU:HB2	5:S:213:ALA:HB3	1.95	0.48
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.82	0.48
13:O:42:VAL:CG2	13:O:178:ILE:HD11	2.44	0.48
5:E:207:LEU:HD23	5:E:207:LEU:N	2.28	0.48
4:R:24:VAL:O	4:R:27:SER:HB3	2.13	0.48
5:S:54:ASN:ND2	5:S:56:ASP:O	2.45	0.48
7:U:192:PHE:C	7:U:192:PHE:CD1	2.86	0.48
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.95	0.48
11:Y:67:GLU:HG2	11:Y:73:ARG:HA	1.96	0.48
14:1:67:THR:HA	14:1:72:GLY:O	2.13	0.48
2:B:21(A):LYS:HE2	2:B:21(D):GLY:O	2.14	0.48
3:C:45:CYS:HA	3:C:141:PHE:HZ	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:227:GLU:CD	5:E:227:GLU:H	2.17	0.48
14:N:83:PHE:HB3	14:N:113:ILE:HD13	1.95	0.48
1:O:14:THR:O	1:O:21:LEU:HD23	2.12	0.48
3:Q:225:SER:O	3:Q:229:ILE:HG13	2.12	0.48
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.48	0.48
7:U:226:ALA:HB3	16:U:344:HOH:O	2.14	0.48
9:W:100:VAL:HG13	9:W:125:ILE:HG21	1.95	0.48
11:Y:67:GLU:CD	11:Y:73:ARG:HA	2.33	0.48
5:S:104:ASN:HB2	13:O:81:GLU:HG2	1.96	0.48
14:1:121:LYS:O	14:1:122:LEU:HD23	2.13	0.48
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.37	0.48
2:B:12:THR:HB	2:B:23:GLN:HG3	1.94	0.48
2:B:74:ILE:C	2:B:221:GLN:HE22	2.17	0.48
10:J:100:LEU:CD2	10:J:112:GLN:HG3	2.43	0.48
11:K:210:ILE:HG22	11:K:210:ILE:O	2.14	0.48
1:O:22:GLY:O	1:O:25:ASP:HB2	2.14	0.48
6:T:240:ILE:O	6:T:240:ILE:HD12	2.14	0.48
7:U:197:MET:HA	7:U:197:MET:HE3	1.96	0.48
9:W:1:GLY:HA2	9:W:17:ASP:OD1	2.13	0.48
10:X:14:LEU:HD12	10:X:42:LEU:HD23	1.96	0.48
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.95	0.48
11:Y:112:TYR:O	11:Y:119:ARG:HA	2.13	0.48
2:B:225:LYS:HB2	2:B:228:GLU:HG3	1.95	0.48
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.13	0.48
9:I:104:ILE:CD1	9:I:178:ILE:HG22	2.43	0.48
10:J:121:GLU:O	10:J:122:LEU:HD23	2.13	0.48
8:V:197:ARG:NH2	9:W:139:GLU:O	2.47	0.48
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.14	0.48
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.33	0.48
1:A:14:THR:O	1:A:21:LEU:HD23	2.13	0.48
3:Q:70:ILE:HG21	3:Q:112:LEU:HD21	1.96	0.48
13:O:203:ILE:HG22	13:O:203:ILE:O	2.13	0.48
14:1:146:MET:HE2	14:1:150:GLU:O	2.14	0.48
1:A:90:ASP:OD1	16:A:245:HOH:O	2.20	0.48
3:C:70:ILE:HG21	3:C:112:LEU:HD21	1.95	0.48
4:D:52:LYS:HE3	4:D:211:GLN:HB2	1.95	0.48
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.49	0.48
5:E:4:PHE:CG	5:E:5:ARG:N	2.81	0.48
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.14	0.48
10:J:67:SER:O	10:J:71:ASP:N	2.46	0.48
11:K:67:GLU:OE1	11:K:73:ARG:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.67	0.48
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.14	0.48
2:P:11:ARG:O	2:P:14:ILE:HD13	2.14	0.48
4:R:52:LYS:HE3	4:R:211:GLN:HB2	1.94	0.48
5:S:49:VAL:HG22	5:S:212:ILE:HD12	1.96	0.48
7:U:233:LEU:O	7:U:236:ILE:HG12	2.13	0.48
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.62	0.48
9:W:22:SER:O	9:W:23:GLN:HB2	2.14	0.48
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.79	0.48
14:1:66:TYR:CD2	14:1:74:PRO:HB3	2.49	0.47
11:K:195:LEU:O	11:K:199:VAL:HG23	2.14	0.47
1:O:202:VAL:HG21	1:O:206:PHE:CD1	2.48	0.47
3:Q:121:GLN:C	3:Q:121:GLN:NE2	2.68	0.47
10:X:129:TYR:O	10:X:132:PHE:HB2	2.14	0.47
5:E:41:ARG:NH1	5:E:42:SER:O	2.47	0.47
10:J:168:MET:HE3	10:X:168:MET:HE3	1.96	0.47
11:K:112:TYR:O	11:K:119:ARG:HA	2.14	0.47
12:L:84:GLN:HG3	12:L:117:GLY:O	2.13	0.47
1:O:109:THR:O	1:O:113:VAL:HG23	2.13	0.47
7:U:38:LEU:HD23	7:U:197:MET:CE	2.44	0.47
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.97	0.47
12:Z:84:GLN:HG3	12:Z:117:GLY:O	2.14	0.47
13:O:14(A):VAL:O	13:O:14(A):VAL:HG23	2.14	0.47
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.49	0.47
7:G:55:PRO:HG2	7:G:56:ASP:H	1.78	0.47
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.95	0.47
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.96	0.47
8:H:78:SER:O	8:H:82:MET:HG3	2.15	0.47
10:J:74:LEU:HD22	10:J:78:ALA:CB	2.44	0.47
2:P:235:LYS:N	2:P:235:LYS:HD3	2.28	0.47
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.44	0.47
3:Q:57:LYS:HG2	3:Q:208:LYS:HZ3	1.79	0.47
9:W:7:THR:CG2	9:W:110:ILE:HG13	2.45	0.47
1:A:215:ILE:HD11	1:A:221:PHE:HD1	1.79	0.47
2:B:38:ILE:HD13	2:B:197:LEU:HG	1.96	0.47
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.43	0.47
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.77	0.47
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.29	0.47
7:U:120:SER:HA	7:U:123:TYR:CD2	2.50	0.47
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.95	0.47
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:31:GLU:OE1	13:O:120:TYR:HA	2.15	0.47
13:O:37:VAL:HG11	13:O:79:ILE:CD1	2.43	0.47
3:Q:15:PHE:H	4:R:23:GLN:NE2	2.10	0.47
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.96	0.47
6:T:114:ASP:O	6:T:118:GLN:HG2	2.14	0.47
14:1:65:LEU:HG	14:1:69:GLN:NE2	2.29	0.47
5:E:188:GLU:HA	5:E:188:GLU:OE1	2.13	0.47
5:E:86:ARG:O	5:E:90:ASN:HB2	2.15	0.47
7:G:217:LYS:CE	7:G:217:LYS:HA	2.42	0.47
9:I:7:THR:CG2	9:I:110:ILE:HG13	2.45	0.47
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.49	0.47
2:P:150:THR:O	2:P:157:TYR:HA	2.15	0.47
2:P:228:GLU:O	2:P:232:ILE:HG22	2.14	0.47
8:V:18:THR:HB	8:V:30:ASN:HA	1.97	0.47
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.96	0.47
11:Y:67:GLU:OE1	11:Y:73:ARG:HA	2.14	0.47
3:C:46:VAL:HG22	3:C:146:PRO:HB2	1.96	0.47
5:E:179:THR:HG22	5:E:18(B):THR:HB	1.96	0.47
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.14	0.47
7:G:60:ASP:OD2	7:G:62:THR:OG1	2.32	0.47
14:N:10(B):LYS:O	14:N:10(B):LYS:HD3	2.14	0.47
2:P:184:MET:HE2	2:P:189:ALA:N	2.30	0.47
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.27	0.47
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.30	0.47
8:V:172:ASN:HD22	8:V:193:THR:HA	1.79	0.47
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.48	0.47
12:Z:94:PRO:HA	16:Z:198:HOH:O	2.13	0.47
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.13	0.47
3:C:62(A):ILE:HG13	3:C:63:THR:N	2.30	0.47
8:H:172:ASN:HD22	8:H:193:THR:HA	1.80	0.47
10:J:168:MET:HE3	10:X:168:MET:CE	2.45	0.47
1:O:175:PHE:O	1:O:179:ARG:HG2	2.14	0.47
4:R:227:GLU:OE2	4:R:227:GLU:N	2.36	0.47
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.78	0.47
12:Z:19:ARG:NE	12:Z:171:ASP:OD2	2.38	0.47
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.68	0.47
4:D:112:LEU:O	4:D:112:LEU:HD13	2.14	0.47
3:C:14:ILE:HB	4:D:23:GLN:HE22	1.80	0.47
5:E:28:LEU:HD12	5:E:153:PRO:HD2	1.96	0.47
7:G:197:MET:HG2	7:G:205:PHE:CE1	2.50	0.47
8:H:103:GLY:HA2	8:H:178:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:65:GLU:HA	16:R:750:HOH:O	2.13	0.47
3:Q:156:ILE:HD13	4:R:83:ALA:HB2	1.96	0.47
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.14	0.47
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.50	0.47
13:O:3:VAL:HG23	13:O:46:SER:HB3	1.97	0.47
6:F:127:ASN:ND2	6:F:127:ASN:H	2.12	0.47
11:K:86:LEU:HD13	11:K:86:LEU:C	2.35	0.47
13:M:-7:GLN:HB3	16:M:228:HOH:O	2.14	0.47
14:N:65:LEU:HG	14:N:69:GLN:NE2	2.30	0.47
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.50	0.47
6:T:68:GLN:HG2	16:T:312:HOH:O	2.14	0.47
8:V:2:THR:HG22	8:V:159:ILE:HD13	1.97	0.47
12:L:135:MET:HE2	9:W:165:ARG:NH2	2.30	0.47
9:W:29:ASN:ND2	9:W:29:ASN:N	2.63	0.47
14:1:112:THR:CG2	14:1:120:HIS:HB2	2.43	0.47
14:1:65:LEU:HG	14:1:69:GLN:HE21	1.80	0.47
2:B:176:LEU:HD23	2:B:192:LEU:HD22	1.96	0.47
2:B:176:LEU:HD23	2:B:192:LEU:CD2	2.45	0.47
9:I:110:ILE:HD12	9:I:110:ILE:O	2.15	0.47
3:Q:8:TYR:CZ	3:Q:10:ARG:HB2	2.50	0.47
4:R:189:ALA:O	4:R:193:VAL:HG23	2.16	0.47
5:S:4:PHE:CG	5:S:5:ARG:N	2.82	0.47
7:U:186:TRP:O	7:U:190:VAL:HG23	2.15	0.47
9:W:29:ASN:H	9:W:29:ASN:HD22	1.62	0.47
1:A:22:GLY:O	1:A:25:ASP:HB2	2.15	0.46
6:F:169:ARG:HB3	6:F:169:ARG:HE	1.46	0.46
7:G:35:ILE:HD11	7:G:53:LYS:HG3	1.98	0.46
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.50	0.46
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.97	0.46
4:R:86:ARG:HD3	4:R:86:ARG:HA	1.80	0.46
5:S:111:ARG:HH11	5:S:111:ARG:HG2	1.79	0.46
10:X:112:GLN:NE2	10:X:126:ALA:H	2.13	0.46
10:J:144:PRO:HG2	11:Y:207:ASN:HD21	1.80	0.46
2:B:60:GLU:HA	2:B:60:GLU:OE1	2.16	0.46
3:C:236:ILE:HA	3:C:239:GLU:HG2	1.97	0.46
13:M:104:VAL:HG13	13:M:106:GLY:O	2.14	0.46
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.44	0.46
2:B:45:GLY:HA2	2:B:146:TYR:CE1	2.51	0.46
2:P:60:GLU:OE1	2:P:60:GLU:HA	2.14	0.46
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.97	0.46
6:T:184:LEU:CD1	6:T:188:GLU:HB3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:224:LEU:HB3	7:U:228:ASN:HB2	1.96	0.46
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.15	0.46
3:C:211:GLU:O	3:C:212:ILE:HD13	2.16	0.46
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.97	0.46
3:C:69:LYS:N	16:C:277:HOH:O	2.49	0.46
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.79	0.46
6:F:184:LEU:CD1	6:F:188:GLU:HB3	2.45	0.46
7:G:203:THR:HG22	7:G:204:GLU:N	2.31	0.46
9:I:105:ASN:HB3	9:I:10(C):SER:OG	2.15	0.46
9:I:51:ASP:OD1	10:J:90(B):ARG:NH2	2.48	0.46
2:P:231:ASP:O	2:P:235:LYS:HG2	2.16	0.46
3:Q:14:ILE:HB	4:R:23:GLN:HE22	1.78	0.46
6:T:127:ASN:ND2	6:T:127:ASN:N	2.63	0.46
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.50	0.46
16:T:320:HOH:O	13:O:67:ALA:HB3	2.15	0.46
1:A:186:LEU:O	1:A:190:ILE:HG13	2.16	0.46
9:W:12:VAL:HG12	9:W:108:PRO:HB3	1.97	0.46
1:A:32:LYS:HA	1:A:32:LYS:CE	2.45	0.46
3:C:57:LYS:O	3:C:58:LEU:HB2	2.15	0.46
5:E:48:LEU:HB2	5:E:213:ALA:HB3	1.97	0.46
12:L:166:HIS:CD2	12:L:168:GLN:H	2.32	0.46
12:L:43:MET:CG	12:L:44:SER:N	2.79	0.46
2:P:38:ILE:HD13	2:P:197:LEU:HG	1.98	0.46
7:U:203:THR:HG22	7:U:204:GLU:N	2.31	0.46
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.97	0.46
9:W:101:VAL:HG23	9:W:113:PHE:HE2	1.81	0.46
9:W:110:ILE:CD1	9:W:122:ALA:O	2.63	0.46
10:X:2:ILE:O	10:X:16:SER:HA	2.16	0.46
13:O:133:MET:O	13:O:136:PRO:HD2	2.16	0.46
14:1:83:PHE:HB3	14:1:113:ILE:HD13	1.98	0.46
14:1:13:ILE:HD12	14:1:151:THR:HG22	1.97	0.46
3:C:100:ARG:O	3:C:104:GLU:N	2.49	0.46
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.96	0.46
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.31	0.46
8:H:218:ILE:HG22	8:H:219:VAL:N	2.31	0.46
9:I:29:ASN:HD22	9:I:29:ASN:H	1.63	0.46
10:J:129:TYR:O	10:J:132:PHE:HB2	2.15	0.46
12:L:147:SER:O	12:L:151:VAL:HG23	2.14	0.46
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	2.16	0.46
14:N:116:GLY:HA3	16:N:194:HOH:O	2.16	0.46
14:N:14:LEU:O	14:N:175:MET:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:215:ILE:HD11	1:O:221:PHE:HD1	1.81	0.46
2:P:176:LEU:HD23	2:P:192:LEU:HD22	1.98	0.46
2:P:185:LYS:O	2:P:188:ASP:HB2	2.15	0.46
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.81	0.46
6:T:169:ARG:O	6:T:173:LYS:HG3	2.15	0.46
8:V:103:GLY:HA2	8:V:178:MET:SD	2.56	0.46
10:X:168:MET:HA	10:X:168:MET:HE2	1.97	0.46
10:X:67:SER:O	10:X:71:ASP:N	2.49	0.46
12:Z:43:MET:CG	12:Z:44:SER:N	2.78	0.46
14:1:14:LEU:O	14:1:175:MET:HA	2.15	0.46
1:A:112:LEU:O	1:A:116:VAL:HG23	2.15	0.46
1:A:32:LYS:HE2	1:A:32:LYS:CA	2.45	0.46
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.46	0.46
11:K:137:VAL:HG21	11:K:161:ALA:HB2	1.98	0.46
14:N:65:LEU:HG	14:N:69:GLN:HE21	1.81	0.46
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.46	0.46
2:P:21(A):LYS:HE2	2:P:21(D):GLY:O	2.15	0.46
10:X:185:ARG:HH11	10:X:185:ARG:HG2	1.81	0.46
14:1:89:GLU:OE1	14:1:89:GLU:HA	2.14	0.46
2:B:228:GLU:O	2:B:232:ILE:HG22	2.15	0.46
2:B:229:ILE:O	2:B:233:LEU:HB2	2.16	0.46
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.81	0.46
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.81	0.46
8:H:18:THR:HB	8:H:30:ASN:HA	1.98	0.46
10:J:39:PRO:HG2	10:J:73:GLU:OE2	2.16	0.46
3:Q:160:TRP:NE1	4:R:59:LEU:HD23	2.31	0.46
5:S:227:GLU:CD	5:S:227:GLU:H	2.19	0.46
1:O:144:PHE:CE2	9:W:10(B):LYS:HD2	2.51	0.46
13:O:45:ILE:HG12	13:O:99:ILE:HG12	1.99	0.46
1:A:175:PHE:O	1:A:179:ARG:HG2	2.16	0.46
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.45	0.46
1:O:112:LEU:O	1:O:116:VAL:HG23	2.15	0.46
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.15	0.46
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.46	0.46
6:T:179:LEU:CD2	6:T:192:GLN:HG2	2.42	0.46
7:U:55:PRO:HG2	7:U:56:ASP:H	1.80	0.46
3:C:8:TYR:CZ	3:C:10:ARG:HB2	2.51	0.45
4:D:42:THR:C	4:D:44:GLU:H	2.19	0.45
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.96	0.45
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	2.00	0.45
14:N:161:GLN:O	14:N:164:LYS:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:258:HOH:O	3:Q:62(A):ILE:CD1	2.63	0.45
6:F:130:ARG:HG2	6:F:130:ARG:HH11	1.81	0.45
6:F:20(B):GLU:CD	6:F:20(C):LYS:HE3	2.37	0.45
6:F:42:CYS:HB2	6:F:184:LEU:O	2.16	0.45
3:Q:212:ILE:HD13	3:Q:212:ILE:N	2.30	0.45
3:C:100:ARG:NH2	16:C:278:HOH:O	2.49	0.45
10:J:39:PRO:HG2	10:J:73:GLU:CD	2.36	0.45
3:Q:236:ILE:HA	3:Q:239:GLU:HG2	1.97	0.45
4:R:56:SER:OG	4:R:57:PRO:HD2	2.16	0.45
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.81	0.45
5:S:179:THR:HG22	5:S:18(B):THR:HB	1.97	0.45
5:S:47:VAL:HG12	5:S:48:LEU:N	2.32	0.45
9:W:123:ASP:OD1	9:W:124:PHE:N	2.45	0.45
2:B:185:LYS:O	2:B:188:ASP:HB2	2.17	0.45
2:B:63:THR:HG22	2:B:63:THR:O	2.16	0.45
2:B:121:GLN:HG3	3:C:83:ALA:HB1	1.97	0.45
8:H:218:ILE:N	8:H:218:ILE:CD1	2.79	0.45
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.15	0.45
6:T:38:ILE:HG12	6:T:197:ILE:HD11	1.98	0.45
7:U:225:SER:O	7:U:226:ALA:C	2.55	0.45
7:U:227:GLU:HG2	16:U:344:HOH:O	2.16	0.45
9:W:105:ASN:HB3	9:W:10(C):SER:OG	2.16	0.45
4:D:213:SER:CB	4:D:223:ILE:HA	2.46	0.45
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.51	0.45
6:F:115:ARG:HG2	16:F:293:HOH:O	2.16	0.45
1:O:67:VAL:HG11	1:O:213:ALA:HB3	1.99	0.45
2:P:71:ASN:CG	2:P:72:ASP:H	2.16	0.45
4:R:209:GLU:HG3	4:R:230:ALA:HB2	1.98	0.45
5:S:188:GLU:OE1	5:S:188:GLU:HA	2.16	0.45
7:U:218:ASP:O	7:U:220:LYS:CB	2.64	0.45
11:Y:126:CYS:HB2	11:Y:135:TYR:CZ	2.50	0.45
12:Z:114:ASP:HB2	12:Z:118:SER:N	2.31	0.45
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.29	0.45
1:A:13:THR:O	2:B:130:ARG:HD3	2.17	0.45
2:B:88:LEU:HB3	2:B:116:LEU:HD21	1.98	0.45
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.47	0.45
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.51	0.45
3:C:238:GLN:O	3:C:242:GLU:HG3	2.16	0.45
3:C:156:ILE:HD13	4:D:83:ALA:HB2	1.99	0.45
4:D:15:PHE:HB2	5:E:23:GLN:OE1	2.17	0.45
7:G:38:LEU:CD2	7:G:197:MET:HE3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:137:MET:HE2	9:I:161:ASN:HB2	1.99	0.45
2:P:66:LYS:O	2:P:77:ALA:HA	2.17	0.45
7:U:110:ASP:HB3	7:U:149:TYR:CZ	2.52	0.45
9:W:190:LYS:HA	16:W:233:HOH:O	2.16	0.45
5:E:201:LEU:O	5:E:202:ARG:HB2	2.17	0.45
6:F:171:SER:N	16:F:308:HOH:O	2.34	0.45
7:G:17(C):LYS:HB2	7:G:17(C):LYS:HE3	1.80	0.45
10:J:168:MET:HA	10:J:168:MET:HE2	1.97	0.45
12:L:14(O):LYS:CG	12:L:14(P):PRO:HD2	2.47	0.45
12:L:17:ASP:HA	12:L:172:GLY:O	2.16	0.45
13:M:149:GLN:HE21	13:M:149:GLN:N	2.04	0.45
13:M:37:VAL:HG11	13:M:79:ILE:CD1	2.45	0.45
14:N:126:ILE:HD13	14:N:126:ILE:N	2.22	0.45
1:O:184:LEU:HB2	16:O:248:HOH:O	2.15	0.45
1:O:32:LYS:HE2	1:O:32:LYS:CA	2.45	0.45
5:S:86:ARG:HH11	5:S:86:ARG:CG	2.29	0.45
11:Y:210:ILE:HG22	11:Y:210:ILE:O	2.16	0.45
5:E:49:VAL:HG13	5:E:212:ILE:HD11	1.98	0.45
8:H:9:ASN:OD1	8:H:10:ASN:N	2.49	0.45
9:I:123:ASP:OD1	9:I:124:PHE:N	2.47	0.45
10:J:168:MET:CE	10:X:168:MET:CE	2.95	0.45
1:O:134:VAL:O	1:O:153:PRO:HG3	2.17	0.45
1:O:26:TYR:O	1:O:29:THR:HB	2.16	0.45
1:O:39:GLY:C	1:O:40:ILE:HG13	2.37	0.45
2:P:184:MET:HE3	2:P:188:ASP:HB3	1.99	0.45
3:Q:97:GLN:NE2	3:Q:97:GLN:HA	2.32	0.45
4:R:59:LEU:HD13	4:R:59:LEU:C	2.37	0.45
10:X:4:LEU:HD23	10:X:126:ALA:CB	2.46	0.45
14:1:59:VAL:HG22	14:1:82:VAL:HG12	1.98	0.45
2:B:11:ARG:O	2:B:14:ILE:HD13	2.17	0.45
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.52	0.45
4:D:122:ARG:NH1	4:D:122:ARG:HG2	2.30	0.45
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.17	0.45
4:D:170:GLU:N	4:D:170:GLU:OE1	2.50	0.45
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.47	0.45
5:E:47:VAL:HG12	5:E:48:LEU:N	2.31	0.45
14:N:92:ASP:HB2	16:N:198:HOH:O	2.17	0.45
1:O:55:SER:O	1:O:56:SER:HB2	2.17	0.45
2:P:74:ILE:C	2:P:221:GLN:HE22	2.19	0.45
3:Q:100:ARG:O	3:Q:104:GLU:N	2.47	0.45
3:Q:159:SER:O	4:R:59:LEU:HD22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:97:ASN:HD22	5:S:97:ASN:HA	1.62	0.45
6:T:28:VAL:O	6:T:32:GLU:HG3	2.17	0.45
10:X:166:MET:HA	10:X:167:PRO:HD3	1.73	0.45
11:Y:152:LEU:HD11	11:Y:187:HIS:CD2	2.52	0.45
13:O:190:LEU:CD1	13:O:190:LEU:N	2.80	0.45
2:B:21(A):LYS:HE3	2:B:21(E):VAL:HG23	1.99	0.45
6:F:169:ARG:O	6:F:173:LYS:HG3	2.17	0.45
11:K:152:LEU:HD11	11:K:187:HIS:CD2	2.52	0.45
14:N:126:ILE:H	14:N:126:ILE:CD1	2.24	0.45
2:P:176:LEU:HD23	2:P:192:LEU:CD2	2.46	0.45
2:P:229:ILE:O	2:P:233:LEU:HB2	2.16	0.45
9:W:113:PHE:HA	9:W:118:CYS:O	2.17	0.45
1:A:93:ARG:NH1	16:A:245:HOH:O	2.34	0.44
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.98	0.44
3:C:150:GLN:O	3:C:157:TYR:HA	2.17	0.44
3:C:67:VAL:HG22	3:C:77:SER:HB3	1.99	0.44
7:G:225:SER:O	7:G:226:ALA:C	2.55	0.44
9:I:55:LEU:HD21	9:I:95:TYR:CD1	2.52	0.44
12:L:-2:ASN:HA	12:L:21:ILE:O	2.16	0.44
1:O:32:LYS:HA	1:O:32:LYS:CE	2.46	0.44
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.99	0.44
8:H:123:TYR:OH	13:O:202:ASP:HB2	2.17	0.44
14:1:155:ILE:HG22	14:1:175:MET:HE2	1.99	0.44
2:B:231:ASP:O	2:B:235:LYS:HG2	2.17	0.44
2:B:235:LYS:C	2:B:237:GLY:H	2.20	0.44
4:D:23:GLN:OE1	4:D:23:GLN:HA	2.16	0.44
5:E:49:VAL:HG22	5:E:212:ILE:HD12	1.99	0.44
6:F:81:LEU:HD12	6:F:133:GLY:HA3	1.99	0.44
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.51	0.44
6:F:13:SER:HB2	7:G:130:ARG:HD3	1.98	0.44
14:N:186:ARG:O	14:N:187:LEU:HD23	2.18	0.44
1:O:147:PHE:HZ	16:O:261:HOH:O	2.00	0.44
2:P:224:PHE:H	2:P:224:PHE:HD2	1.65	0.44
5:S:160:LEU:HD13	5:S:163:THR:HB	1.99	0.44
10:X:5:GLY:O	10:X:124:TYR:HA	2.16	0.44
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.27	0.44
10:X:143:ARG:O	10:X:146:MET:HG3	2.17	0.44
12:Z:31:GLU:HA	16:Z:208:HOH:O	2.18	0.44
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.69	0.44
5:E:160:LEU:HD13	5:E:163:THR:HB	1.98	0.44
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:45:GLY:HA2	2:P:146:TYR:CE1	2.52	0.44
2:P:68:TYR:CG	2:P:89:ILE:HD13	2.52	0.44
5:S:15:PHE:H	6:T:23:GLN:NE2	2.13	0.44
5:S:214:ILE:CD1	5:S:215:VAL:N	2.74	0.44
8:V:116:HIS:HB2	16:V:545:HOH:O	2.16	0.44
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.99	0.44
14:1:4:MET:HB3	14:1:126:ILE:HG22	1.99	0.44
1:A:55:SER:O	1:A:56:SER:HB2	2.17	0.44
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.48	0.44
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.52	0.44
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.98	0.44
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.30	0.44
1:O:21(P):LYS:HB2	16:O:253:HOH:O	2.17	0.44
3:Q:31:VAL:HG11	3:Q:135:SER:HB2	2.00	0.44
3:Q:163:GLN:NE2	3:Q:173:ARG:HE	2.01	0.44
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.47	0.44
7:U:234:VAL:O	7:U:237:ALA:HB3	2.18	0.44
8:V:218:ILE:HG22	8:V:219:VAL:N	2.33	0.44
14:1:13:ILE:HD12	14:1:151:THR:CG2	2.47	0.44
1:A:136:LEU:O	1:A:150:GLN:HA	2.18	0.44
2:B:150:THR:O	2:B:157:TYR:HA	2.17	0.44
2:B:78:VAL:HG12	2:B:79:ALA:N	2.33	0.44
3:C:93:ARG:NH1	10:J:69:ARG:HA	2.32	0.44
10:J:4:LEU:HD23	10:J:126:ALA:HB2	1.98	0.44
12:L:19:ARG:HG2	12:L:21:ILE:HG23	1.99	0.44
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.66	0.44
2:P:27:ALA:O	2:P:30:SER:HB3	2.17	0.44
2:P:63:THR:HG22	2:P:63:THR:O	2.17	0.44
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.17	0.44
3:Q:87:ILE:N	3:Q:87:ILE:CD1	2.80	0.44
4:R:107:ILE:HG22	16:R:338:HOH:O	2.18	0.44
5:S:201:LEU:O	5:S:202:ARG:HB2	2.16	0.44
12:L:165:ARG:CZ	8:V:29:LYS:HE2	2.48	0.44
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.17	0.44
1:A:141:HIS:HA	1:A:146:GLY:O	2.17	0.44
1:A:67:VAL:HG11	1:A:213:ALA:HB3	1.99	0.44
3:C:206:GLY:CA	3:C:209:ASN:HD22	2.30	0.44
6:F:127:ASN:ND2	6:F:127:ASN:N	2.64	0.44
6:F:179:LEU:CD2	6:F:192:GLN:HG2	2.44	0.44
7:G:234:VAL:O	7:G:237:ALA:HB3	2.17	0.44
8:H:152:ILE:HD11	8:H:177:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:197:ARG:NH2	9:I:139:GLU:O	2.51	0.44
11:K:135:TYR:O	11:K:139:ASP:HB2	2.18	0.44
14:N:37:VAL:CG2	14:N:41:ILE:HG22	2.48	0.44
3:Q:41:LYS:HD3	3:Q:160:TRP:O	2.18	0.44
2:B:31:ILE:HD11	2:B:133:GLY:C	2.37	0.44
2:B:66:LYS:O	2:B:77:ALA:HA	2.18	0.44
4:D:189:ALA:O	4:D:193:VAL:HG23	2.17	0.44
6:F:114:ASP:O	6:F:118:GLN:HG2	2.18	0.44
6:F:50:VAL:HG12	6:F:211:GLU:HB3	1.98	0.44
11:K:31:VAL:HA	12:L:120:GLU:OE2	2.18	0.44
14:N:121:LYS:O	14:N:122:LEU:HD23	2.18	0.44
2:P:141:TYR:CG	2:P:21(E):VAL:HG21	2.53	0.44
13:O:190:LEU:HD12	13:O:190:LEU:N	2.32	0.44
1:A:130:ARG:HG2	7:G:125:GLN:HG3	2.00	0.44
1:A:21(P):LYS:N	16:A:286:HOH:O	2.43	0.44
2:B:238:ILE:O	2:B:239:THR:O	2.36	0.44
3:C:57:LYS:HG2	3:C:208:LYS:HZ1	1.83	0.44
7:G:120:SER:HA	7:G:123:TYR:CD2	2.53	0.44
8:H:175:VAL:HG12	8:H:176:CYS:N	2.33	0.44
10:J:185:ARG:HH11	10:J:185:ARG:HG2	1.82	0.44
11:K:97:MET:O	11:K:114:ASP:HA	2.17	0.44
1:O:122:GLU:C	1:O:124:THR:H	2.21	0.44
2:P:37:ALA:O	2:P:164:SER:HA	2.18	0.44
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.48	0.44
6:T:50:VAL:HG12	6:T:211:GLU:HB3	1.99	0.44
7:U:197:MET:HG2	7:U:205:PHE:CE1	2.53	0.44
8:V:159:ILE:HG22	8:V:163:ILE:CD1	2.47	0.44
15:V:500:GDT:H3	9:W:115:LEU:HD21	2.00	0.44
15:Y:500:GDT:H8	12:Z:96:TYR:CZ	2.53	0.44
7:G:49:ILE:CD1	7:G:212:VAL:HG22	2.47	0.44
9:I:186:LYS:HE2	9:I:188:TYR:CE1	2.52	0.44
9:I:191:MET:HE2	16:I:203:HOH:O	2.17	0.44
11:K:177:HIS:O	11:K:184:TRP:HA	2.17	0.44
1:O:141:HIS:HA	1:O:146:GLY:O	2.18	0.44
2:P:112:LEU:HD23	2:P:112:LEU:O	2.17	0.44
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.38	0.44
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.50	0.44
13:O:150:VAL:HG21	16:O:231:HOH:O	2.17	0.43
2:B:37:ALA:O	2:B:164:SER:HA	2.17	0.43
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.47	0.43
4:D:86:ARG:HD3	4:D:86:ARG:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:28:VAL:O	6:F:32:GLU:HG3	2.17	0.43
8:H:201:GLN:HG3	12:Z:153:LYS:HG2	2.00	0.43
9:I:16:CYS:SG	9:I:34:ILE:HG12	2.58	0.43
10:J:100:LEU:HD21	10:J:112:GLN:HG3	2.00	0.43
11:K:5:ALA:HA	11:K:13:ILE:O	2.18	0.43
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.99	0.43
8:V:22:GLN:CG	15:V:500:GDT:H36B	2.48	0.43
4:D:93:ARG:HD2	16:D:258:HOH:O	2.17	0.43
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.48	0.43
7:G:8:TYR:C	7:G:10:ARG:N	2.72	0.43
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.99	0.43
14:N:18(D):PRO:HA	14:N:18(G):TYR:CE2	2.53	0.43
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.78	0.43
3:Q:241:GLN:O	3:Q:243:GLN:N	2.46	0.43
5:S:76:LEU:O	5:S:76:LEU:HD23	2.19	0.43
1:O:58:LEU:HB3	7:U:162:ALA:O	2.19	0.43
7:U:49:ILE:CD1	7:U:212:VAL:HG22	2.48	0.43
12:L:192:LYS:HE3	8:V:195:ASN:HB3	2.00	0.43
11:Y:174:ASN:HA	11:Y:174:ASN:HD22	1.65	0.43
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.17	0.43
11:Y:65:LEU:HD12	11:Y:65:LEU:HA	1.87	0.43
12:Z:58:ARG:NH2	16:Z:244:HOH:O	2.47	0.43
2:B:224:PHE:HD2	2:B:224:PHE:H	1.64	0.43
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.53	0.43
13:M:-6:GLN:O	13:M:-6:GLN:HG3	2.17	0.43
14:N:116:GLY:CA	16:N:194:HOH:O	2.65	0.43
3:Q:238:GLN:O	3:Q:242:GLU:HG3	2.17	0.43
4:R:14:THR:HG22	4:R:15:PHE:N	2.34	0.43
6:T:130:ARG:HG2	6:T:130:ARG:HH11	1.82	0.43
6:T:13:SER:HB2	7:U:130:ARG:HD3	1.99	0.43
6:T:169:ARG:HB3	6:T:169:ARG:HE	1.47	0.43
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.32	0.43
6:T:20(B):GLU:CD	6:T:20(C):LYS:HE3	2.38	0.43
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.78	0.43
8:V:206:PHE:CZ	9:W:157:GLN:HG3	2.54	0.43
2:B:112:LEU:O	2:B:112:LEU:HD23	2.18	0.43
2:B:72:ASP:O	2:B:221:GLN:HG3	2.18	0.43
2:B:68:TYR:CG	2:B:89:ILE:HD13	2.53	0.43
3:C:147:LYS:HE2	16:C:263:HOH:O	2.18	0.43
4:D:59:LEU:C	4:D:59:LEU:HD13	2.38	0.43
7:G:130:ARG:HG3	7:G:131:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:92(A):LYS:O	13:M:92(B):MET:HB2	2.18	0.43
1:O:15:PHE:H	2:P:23:GLN:NE2	1.97	0.43
2:P:44:ASP:OD1	2:P:185:LYS:HE3	2.19	0.43
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.47	0.43
3:Q:67:VAL:HG22	3:Q:77:SER:HB3	2.00	0.43
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.18	0.43
4:R:187:LYS:O	4:R:191:LEU:HD22	2.19	0.43
10:X:100:LEU:HD21	10:X:112:GLN:HG3	2.00	0.43
2:B:172:ALA:O	2:B:176:LEU:HG	2.17	0.43
10:J:14:LEU:HD12	10:J:42:LEU:HD23	2.00	0.43
13:M:211:ILE:HD11	14:1:36:ARG:CD	2.49	0.43
3:Q:104:GLU:O	3:Q:105:ASP:HB2	2.17	0.43
3:Q:215:VAL:HG23	3:Q:221:ILE:HG13	2.01	0.43
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.84	0.43
6:T:11:SER:HB3	6:T:14:VAL:HG23	2.00	0.43
6:T:81:LEU:HD12	6:T:133:GLY:HA3	2.01	0.43
7:U:151:THR:HB	16:U:303:HOH:O	2.18	0.43
8:V:72:ARG:CG	8:V:72:ARG:HH11	2.31	0.43
10:X:143:ARG:HG2	10:X:143:ARG:HH11	1.83	0.43
12:Z:107:LYS:HA	12:Z:107:LYS:HD3	1.93	0.43
13:0:125:LEU:HA	16:0:217:HOH:O	2.17	0.43
2:B:163:ILE:HD12	2:B:164:SER:N	2.33	0.43
2:B:38:ILE:HG13	2:B:164:SER:CB	2.48	0.43
3:C:97:GLN:NE2	3:C:97:GLN:HA	2.33	0.43
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.19	0.43
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.00	0.43
8:H:43:CYS:SG	8:H:99:LEU:HB3	2.59	0.43
9:I:110:ILE:CD1	9:I:110:ILE:O	2.66	0.43
2:P:38:ILE:HG13	2:P:164:SER:CB	2.49	0.43
6:T:24:VAL:O	6:T:27:ALA:HB3	2.18	0.43
11:Y:177:HIS:O	11:Y:184:TRP:HA	2.18	0.43
11:Y:36:GLU:OE2	11:Y:184:TRP:CH2	2.72	0.43
13:0:5:SER:HB3	13:0:14:ILE:HG13	2.01	0.43
4:D:14:THR:HG22	4:D:15:PHE:N	2.33	0.43
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.53	0.43
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	2.00	0.43
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	2.01	0.43
8:H:2:THR:HG22	8:H:159:ILE:HD13	2.01	0.43
1:O:215:ILE:O	1:O:215:ILE:HG22	2.17	0.43
2:P:21(A):LYS:HE3	2:P:21(E):VAL:HG23	2.00	0.43
2:P:235:LYS:C	2:P:237:GLY:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:88:LEU:HB3	2:P:116:LEU:HD21	2.01	0.43
9:W:55:LEU:HD21	9:W:95:TYR:CD1	2.54	0.43
12:Z:19:ARG:HG2	12:Z:21:ILE:HG23	2.01	0.43
3:C:18(A):ASP:OD2	3:C:18(C):LYS:HG2	2.19	0.43
3:C:206:GLY:HA3	3:C:209:ASN:HD22	1.83	0.43
3:C:58:LEU:HD12	3:C:58:LEU:HA	1.77	0.43
5:E:162:GLY:O	5:E:163:THR:HB	2.19	0.43
10:J:5:GLY:O	10:J:124:TYR:HA	2.19	0.43
10:J:190:PHE:C	10:J:192:ALA:N	2.72	0.43
10:J:45:PHE:HD1	10:J:52:THR:HG1	1.66	0.43
1:O:13:THR:O	2:P:130:ARG:HD3	2.19	0.43
4:R:237:LEU:HD13	4:R:237:LEU:C	2.39	0.43
11:Y:105:THR:OG1	11:Y:106:GLU:HG3	2.19	0.43
11:Y:184:TRP:O	11:Y:184:TRP:CE3	2.72	0.43
2:B:184:MET:HE2	2:B:189:ALA:N	2.33	0.43
4:D:141:HIS:HA	4:D:145:GLY:O	2.19	0.43
6:F:177:GLU:OE2	7:G:57:LYS:HE2	2.19	0.43
10:J:24:ILE:O	10:X:133:TYR:OH	2.32	0.43
10:J:4:LEU:HD23	10:J:126:ALA:CB	2.49	0.43
1:O:191:HIS:CE1	1:O:236:LEU:HA	2.53	0.43
2:P:31:ILE:HD11	2:P:133:GLY:C	2.40	0.43
2:P:14:ILE:HB	3:Q:23:GLN:NE2	2.33	0.43
4:R:213:SER:CB	4:R:223:ILE:HA	2.48	0.43
7:U:171:GLU:N	7:U:171:GLU:OE1	2.51	0.43
12:Z:43:MET:CB	12:Z:101:ILE:HG22	2.46	0.43
1:A:110:LYS:HG2	16:A:246:HOH:O	2.18	0.43
3:C:220:ASP:HA	16:C:290:HOH:O	2.19	0.43
4:D:40:ILE:HG13	4:D:193:VAL:HG22	2.00	0.43
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.48	0.43
11:K:197:TRP:HA	11:K:197:TRP:CE3	2.54	0.43
1:O:43:THR:HG23	1:O:184:LEU:O	2.18	0.43
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.54	0.43
4:R:207:LEU:HD21	4:R:233:ILE:HG12	2.01	0.43
4:R:23:GLN:OE1	4:R:23:GLN:HA	2.18	0.43
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.84	0.43
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.19	0.43
7:U:18(H):GLU:N	7:U:18(H):GLU:CD	2.73	0.43
7:U:35:ILE:HD11	7:U:53:LYS:HG3	2.00	0.43
9:W:7:THR:HG23	9:W:110:ILE:HG13	2.01	0.43
9:W:-2:ASN:HA	9:W:21:GLY:O	2.19	0.43
11:Y:97:MET:O	11:Y:114:ASP:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:0:187:LYS:HB3	13:0:190:LEU:HD11	2.01	0.42
3:C:159:SER:O	4:D:59:LEU:HD22	2.18	0.42
3:C:195:ARG:HG3	3:C:236:ILE:HD13	2.01	0.42
3:C:215:VAL:HG23	3:C:221:ILE:HG13	2.01	0.42
7:G:186:TRP:O	7:G:190:VAL:HG23	2.19	0.42
9:I:27:VAL:HG13	16:J:232:HOH:O	2.19	0.42
11:K:105:THR:OG1	11:K:106:GLU:HG3	2.19	0.42
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.53	0.42
13:M:150:VAL:HG21	16:M:266:HOH:O	2.18	0.42
14:N:146:MET:HE2	14:N:150:GLU:O	2.18	0.42
1:O:67:VAL:HB	1:O:223:LYS:HZ2	1.82	0.42
5:S:220:PRO:O	5:S:221:PHE:C	2.56	0.42
6:T:177:GLU:OE2	7:U:57:LYS:HE2	2.19	0.42
7:U:168:LYS:O	7:U:172:ILE:HG12	2.19	0.42
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.48	0.42
5:E:97:ASN:HA	5:E:97:ASN:HD22	1.64	0.42
6:F:122:ALA:HA	6:F:125:LEU:CD1	2.43	0.42
7:G:171:GLU:OE1	7:G:171:GLU:N	2.52	0.42
8:H:10:ASN:ND2	8:H:179:GLU:HG2	2.34	0.42
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.53	0.42
11:K:156:LYS:HB2	11:K:175:LEU:HD11	2.01	0.42
13:M:5:SER:HB3	13:M:14:ILE:HG13	2.00	0.42
13:M:187:LYS:HB3	13:M:190:LEU:HD11	2.00	0.42
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.77	0.42
4:R:191:LEU:HD12	4:R:237:LEU:HB2	1.99	0.42
5:S:226:GLY:O	5:S:227:GLU:C	2.57	0.42
10:X:190:PHE:C	10:X:192:ALA:N	2.72	0.42
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	2.01	0.42
1:A:202:VAL:HG21	1:A:206:PHE:CE1	2.54	0.42
2:B:44:ASP:OD1	2:B:185:LYS:HE3	2.20	0.42
3:C:41:LYS:HD3	3:C:160:TRP:O	2.18	0.42
4:D:209:GLU:HG3	4:D:230:ALA:HB2	2.01	0.42
7:G:188:LYS:HA	7:G:188:LYS:HD3	1.89	0.42
7:G:211:GLU:HA	16:G:260:HOH:O	2.18	0.42
8:H:112:SER:OG	8:H:120:ASP:HB2	2.19	0.42
9:I:-2:ASN:HA	9:I:21:GLY:O	2.19	0.42
2:P:172:ALA:O	2:P:176:LEU:HG	2.19	0.42
3:Q:206:GLY:CA	3:Q:209:ASN:HD22	2.32	0.42
7:U:48:VAL:O	7:U:48:VAL:HG23	2.20	0.42
8:V:159:ILE:O	8:V:163:ILE:HD12	2.19	0.42
1:A:39:GLY:C	1:A:40:ILE:HG13	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:THR:N	16:C:260:HOH:O	2.50	0.42
3:C:73:HIS:CE1	3:C:106:PRO:HB2	2.54	0.42
10:J:168:MET:CE	10:X:168:MET:HE3	2.48	0.42
2:P:202:THR:CG2	2:P:204:SER:HB2	2.49	0.42
4:R:122:ARG:HG2	4:R:122:ARG:NH1	2.33	0.42
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.49	0.42
12:Z:14(H):GLY:O	12:Z:1(I):ASN:N	2.53	0.42
13:O:157:ASN:HB3	16:O:250:HOH:O	2.19	0.42
1:A:173:LYS:O	1:A:177:GLU:HG3	2.20	0.42
4:D:97:VAL:HG21	11:K:65:LEU:CD1	2.44	0.42
2:B:144:ARG:HG3	10:J:72:TYR:CZ	2.55	0.42
11:K:36:GLU:OE2	11:K:184:TRP:CH2	2.73	0.42
12:L:43:MET:CB	12:L:101:ILE:HG22	2.48	0.42
14:N:30:VAL:HG11	13:O:199:PHE:HE2	1.84	0.42
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	2.02	0.42
6:T:115:ARG:HG2	16:T:315:HOH:O	2.19	0.42
8:V:218:ILE:CD1	8:V:218:ILE:N	2.83	0.42
12:Z:14(O):LYS:CG	12:Z:14(P):PRO:HD2	2.49	0.42
3:C:36:CYS:H	3:C:51:GLU:CG	2.33	0.42
5:E:220:PRO:O	5:E:221:PHE:C	2.58	0.42
16:E:238:HOH:O	6:F:12:ASN:HB2	2.19	0.42
12:L:113:PHE:CD1	12:L:113:PHE:N	2.87	0.42
1:O:15:PHE:N	2:P:23:GLN:HE22	1.98	0.42
3:Q:36:CYS:H	3:Q:51:GLU:CG	2.33	0.42
4:R:40:ILE:HG13	4:R:193:VAL:HG22	2.00	0.42
5:S:107:LEU:HA	16:S:253:HOH:O	2.19	0.42
5:S:162:GLY:O	5:S:163:THR:HB	2.19	0.42
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.49	0.42
8:V:10:ASN:ND2	8:V:179:GLU:HG2	2.35	0.42
8:V:9:ASN:OD1	8:V:10:ASN:N	2.52	0.42
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.46	0.42
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	2.02	0.42
14:1:146:MET:HB3	14:1:150:GLU:HB2	2.02	0.42
2:B:186:VAL:HG21	2:B:216:ARG:CD	2.46	0.42
6:F:11:SER:HB3	6:F:14:VAL:HG23	2.00	0.42
10:J:166:MET:HA	10:J:167:PRO:HD3	1.73	0.42
12:L:114:ASP:HB2	12:L:118:SER:N	2.34	0.42
12:L:14(H):GLY:O	12:L:1(I):ASN:N	2.53	0.42
12:L:30:TYR:CZ	12:L:32:PRO:HG3	2.55	0.42
13:M:190:LEU:N	13:M:190:LEU:CD1	2.83	0.42
1:O:136:LEU:O	1:O:150:GLN:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:173:LYS:O	1:O:177:GLU:HG3	2.20	0.42
7:U:63:THR:HG21	16:U:325:HOH:O	2.19	0.42
7:U:70:ILE:HG21	7:U:112:LEU:HD21	2.01	0.42
10:X:113:ILE:CG1	10:X:119:LYS:HG3	2.49	0.42
11:Y:137:VAL:HG21	11:Y:161:ALA:HB2	2.02	0.42
11:Y:197:TRP:HA	11:Y:197:TRP:CE3	2.54	0.42
1:A:88:LEU:HG	1:A:132:PHE:CE2	2.55	0.42
1:A:191:HIS:CE1	1:A:236:LEU:HA	2.53	0.42
1:A:58:LEU:HD12	7:G:173:THR:HG23	2.01	0.42
3:C:212:ILE:HD13	3:C:212:ILE:N	2.35	0.42
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.83	0.42
9:I:12:VAL:HG12	9:I:108:PRO:HB3	2.02	0.42
9:I:113:PHE:HA	9:I:118:CYS:O	2.19	0.42
9:I:22:SER:O	9:I:23:GLN:HB2	2.20	0.42
13:M:202:ASP:HB2	8:V:123:TYR:OH	2.19	0.42
8:V:175:VAL:HG12	8:V:176:CYS:N	2.34	0.42
12:L:14(C):GLN:HG2	8:V:210:THR:HG21	2.01	0.42
9:W:124:PHE:O	9:W:125:ILE:HD13	2.19	0.42
8:H:167:LEU:HD22	12:Z:167:ILE:O	2.20	0.42
2:B:202:THR:CG2	2:B:204:SER:HB2	2.50	0.42
2:B:6:ARG:HD2	4:D:9:ASP:N	2.34	0.42
13:M:42:VAL:HG23	13:M:178:ILE:HD11	2.01	0.42
1:O:57:PRO:HG2	7:U:177:GLU:HG2	2.01	0.42
1:O:8:TYR:HD2	7:U:128:TYR:HB3	1.84	0.42
2:P:137:ILE:CD1	2:P:165:VAL:HG22	2.48	0.42
2:P:238:ILE:O	2:P:239:THR:O	2.38	0.42
5:S:111:ARG:NH1	5:S:111:ARG:HG2	2.35	0.42
9:W:16:CYS:SG	9:W:34:ILE:HG12	2.59	0.42
14:1:146:MET:HE1	16:1:230:HOH:O	2.20	0.42
14:1:161:GLN:O	14:1:164:LYS:HB3	2.20	0.42
14:1:18(D):PRO:HA	14:1:18(G):TYR:CE2	2.55	0.42
2:B:235:LYS:C	2:B:237:GLY:N	2.73	0.42
16:G:249:HOH:O	8:H:82:MET:HA	2.20	0.42
10:J:133:TYR:OH	10:X:24:ILE:HG13	2.20	0.42
14:N:155:ILE:HG22	14:N:175:MET:HE2	2.01	0.42
14:N:4:MET:HB3	14:N:126:ILE:HG22	2.02	0.42
6:T:42:CYS:HB2	6:T:184:LEU:O	2.19	0.42
6:T:194:ALA:O	6:T:198:TYR:HD1	2.02	0.42
7:U:217:LYS:HA	7:U:217:LYS:CE	2.41	0.42
11:Y:75:SER:HA	11:Y:105:THR:HG21	2.02	0.42
11:Y:2:THR:HG22	11:Y:159:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Y:500:GDT:H36A	12:Z:114:ASP:OD2	2.20	0.42
12:Z:11:PHE:CE1	12:Z:148:VAL:HA	2.55	0.42
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.32	0.42
1:A:134:VAL:O	1:A:153:PRO:HG3	2.20	0.41
1:A:179:ARG:CB	1:A:179:ARG:HH11	2.28	0.41
1:A:215:ILE:O	1:A:215:ILE:HG22	2.19	0.41
3:C:38:VAL:HG22	3:C:39:GLY:N	2.35	0.41
4:D:156:THR:HG22	5:E:83:PRO:HD3	2.02	0.41
10:J:2:ILE:O	10:J:16:SER:HA	2.20	0.41
1:O:29:THR:O	1:O:33:GLN:HG2	2.19	0.41
1:O:88:LEU:HG	1:O:132:PHE:CE2	2.54	0.41
3:Q:206:GLY:HA3	3:Q:209:ASN:HD22	1.85	0.41
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.20	0.41
3:Q:62(A):ILE:O	3:Q:63:THR:C	2.58	0.41
7:U:60:ASP:OD2	7:U:62:THR:OG1	2.36	0.41
9:W:164:ASP:HA	16:W:213:HOH:O	2.20	0.41
11:Y:138:LEU:HD12	11:Y:154:LEU:HG	2.01	0.41
11:Y:17:ASP:CG	11:Y:33:LYS:HZ2	2.23	0.41
13:O:201:LYS:HG3	13:O:202:ASP:OD2	2.20	0.41
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.35	0.41
3:C:55:THR:C	3:C:56:LEU:HD22	2.41	0.41
5:E:15:PHE:H	6:F:23:GLN:NE2	2.17	0.41
7:G:110:ASP:N	7:G:110:ASP:OD2	2.53	0.41
7:G:48:VAL:HG23	7:G:48:VAL:O	2.20	0.41
10:J:143:ARG:HG2	10:J:143:ARG:HH11	1.85	0.41
10:J:35:ARG:HA	10:J:35:ARG:HD3	1.78	0.41
12:L:153:LYS:HG2	8:V:201:GLN:HG3	2.01	0.41
13:M:17:ASP:HA	13:M:173:PHE:HA	2.02	0.41
13:M:1:THR:OG1	13:M:2:SER:N	2.52	0.41
6:T:202:HIS:O	6:T:202:HIS:CG	2.73	0.41
6:T:21(B):THR:O	6:T:21(C):ASN:CB	2.67	0.41
8:V:112:SER:OG	8:V:120:ASP:HB2	2.20	0.41
9:W:81:GLN:NE2	9:W:81:GLN:HA	2.34	0.41
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:N	2.68	0.41
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.87	0.41
14:1:126:ILE:CD1	14:1:126:ILE:H	2.26	0.41
14:1:126:ILE:N	14:1:126:ILE:HD13	2.24	0.41
4:D:191:LEU:HD12	4:D:237:LEU:HB2	2.02	0.41
11:K:138:LEU:HD12	11:K:154:LEU:HG	2.01	0.41
11:K:52:CYS:O	11:K:56:GLU:HB2	2.21	0.41
3:Q:18(A):ASP:OD2	3:Q:18(C):LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:170:GLU:N	4:R:170:GLU:OE1	2.53	0.41
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.55	0.41
9:W:93:GLY:C	16:W:215:HOH:O	2.59	0.41
10:X:46:ALA:HA	16:X:223:HOH:O	2.19	0.41
13:O:-5:PRO:HD3	13:O:96:TRP:CE2	2.56	0.41
14:1:55:ILE:HD11	14:1:95:LEU:HD22	2.01	0.41
1:A:142:ASP:OD1	1:A:145:ASN:HB2	2.20	0.41
3:C:104:GLU:O	3:C:105:ASP:HB2	2.19	0.41
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.20	0.41
9:I:137:MET:HE1	9:I:141:LEU:HD11	2.02	0.41
10:J:-1:MET:CG	10:J:1:ASP:N	2.81	0.41
12:L:11:PHE:CE1	12:L:148:VAL:HA	2.55	0.41
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	2.02	0.41
3:Q:72:SER:O	3:Q:221:ILE:HD12	2.20	0.41
4:R:141:HIS:HA	4:R:145:GLY:O	2.21	0.41
5:S:28:LEU:HD12	5:S:153:PRO:HD2	2.02	0.41
6:T:31:VAL:HG11	6:T:135:SER:HB2	2.02	0.41
9:W:61:TYR:C	9:W:61:TYR:CD1	2.94	0.41
14:1:20:THR:OG1	14:1:28:ASN:HB3	2.21	0.41
2:B:107:ILE:HG23	2:B:107:ILE:O	2.20	0.41
3:C:134:VAL:HG12	3:C:135:SER:N	2.35	0.41
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.85	0.41
4:D:237:LEU:C	4:D:237:LEU:HD13	2.41	0.41
4:D:39:GLY:O	4:D:162:ALA:HA	2.20	0.41
5:E:86:ARG:HH11	5:E:86:ARG:CG	2.33	0.41
6:F:240:ILE:O	6:F:240:ILE:HD12	2.19	0.41
8:H:22:GLN:CG	15:H:500:GDT:H36B	2.50	0.41
8:H:25:ILE:N	8:H:25:ILE:CD1	2.84	0.41
11:K:174:ASN:HD22	11:K:174:ASN:HA	1.65	0.41
12:L:31:GLU:OE1	13:M:120:TYR:HA	2.21	0.41
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.19	0.41
3:Q:150:GLN:HE21	3:Q:150:GLN:HB3	1.68	0.41
4:R:117:CYS:HG	4:R:157:PHE:HD2	1.66	0.41
4:R:179:GLU:O	4:R:18(C):HIS:HD2	2.04	0.41
11:K:210:ILE:HD13	9:W:30:LYS:NZ	2.35	0.41
9:W:51:ASP:OD1	10:X:90(B):ARG:NH2	2.53	0.41
12:Z:43:MET:HG2	12:Z:44:SER:N	2.34	0.41
1:A:43:THR:HG23	1:A:184:LEU:O	2.19	0.41
2:B:191:GLU:O	2:B:195:LYS:HG2	2.20	0.41
2:B:141:TYR:CG	2:B:21(E):VAL:HG21	2.54	0.41
4:D:123:PHE:CE2	4:D:131:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:237:LEU:O	4:D:241:GLU:HG3	2.20	0.41
6:F:31:VAL:HG11	6:F:135:SER:HB2	2.03	0.41
6:F:24:VAL:O	6:F:27:ALA:HB3	2.19	0.41
7:G:191:GLU:CG	7:G:232:ARG:HG3	2.50	0.41
9:I:-2:ASN:HB3	16:I:200:HOH:O	2.20	0.41
2:B:97:GLN:OE1	9:I:64:ASN:HB3	2.20	0.41
12:L:4:LEU:HD13	12:L:138:LEU:HD21	2.01	0.41
2:P:21:LEU:O	2:P:25:GLU:HG2	2.20	0.41
4:R:12:VAL:HG13	4:R:12(B):GLU:OE1	2.20	0.41
4:R:237:LEU:O	4:R:241:GLU:HG3	2.20	0.41
6:T:109:ILE:HD13	6:T:109:ILE:H	1.84	0.41
8:V:29:LYS:NZ	9:W:139:GLU:OE2	2.54	0.41
3:Q:93:ARG:NH1	10:X:69:ARG:HA	2.36	0.41
13:O:-3:VAL:HG12	13:O:49:ILE:CG1	2.50	0.41
1:A:29:THR:O	1:A:33:GLN:HG2	2.20	0.41
1:A:38:LEU:HD12	1:A:38:LEU:C	2.41	0.41
3:C:163:GLN:HA	3:C:163:GLN:NE2	2.34	0.41
8:H:206:PHE:CZ	9:I:157:GLN:HG3	2.56	0.41
13:M:177:ILE:C	13:M:178:ILE:HD13	2.41	0.41
13:M:177:ILE:O	13:M:178:ILE:HD13	2.20	0.41
1:O:212:LEU:HD22	1:O:224:LEU:HD12	2.02	0.41
1:O:161:LYS:HG3	2:P:58:LEU:O	2.20	0.41
5:S:86:ARG:NH1	5:S:86:ARG:HG3	2.32	0.41
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.51	0.41
12:Z:22:THR:O	12:Z:23:ASP:HB2	2.20	0.41
14:1:143:ARG:O	14:1:146:MET:HG3	2.21	0.41
14:1:67:THR:O	14:1:68:SER:C	2.58	0.41
1:A:4:MET:O	1:A:5:THR:O	2.39	0.41
2:B:97:GLN:NE2	2:B:97:GLN:HA	2.35	0.41
4:D:207:LEU:HD21	4:D:233:ILE:HG12	2.02	0.41
6:F:194:ALA:O	6:F:198:TYR:HD1	2.03	0.41
6:F:26:TYR:O	6:F:29:LYS:HB2	2.21	0.41
9:I:110:ILE:CD1	9:I:122:ALA:O	2.69	0.41
9:I:137:MET:CE	9:I:141:LEU:HD11	2.51	0.41
14:N:136:GLY:O	14:N:140:LYS:HG2	2.21	0.41
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.51	0.41
5:S:24:VAL:O	5:S:27:ALA:HB3	2.21	0.41
7:U:130:ARG:HG3	7:U:131:PRO:O	2.21	0.41
7:U:191:GLU:CG	7:U:232:ARG:HG3	2.51	0.41
8:V:43:CYS:SG	8:V:99:LEU:HB3	2.60	0.41
10:X:18:LYS:HD3	10:X:174:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.33	0.41
11:Y:52:CYS:O	11:Y:56:GLU:HB2	2.20	0.41
3:C:31:VAL:HG11	3:C:135:SER:HB2	2.02	0.41
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.51	0.41
7:G:191:GLU:HG3	7:G:232:ARG:HG3	2.02	0.41
7:G:218:ASP:O	7:G:220:LYS:CB	2.66	0.41
11:K:100:MET:HA	11:K:111:TYR:O	2.21	0.41
14:N:132:THR:HA	14:N:135:TYR:CD2	2.55	0.41
14:N:36:ARG:CD	13:O:211:ILE:HD11	2.51	0.41
2:P:44:ASP:N	2:P:44:ASP:OD2	2.52	0.41
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	2.02	0.41
8:V:139:GLU:OE2	8:V:139:GLU:HA	2.21	0.41
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.82	0.41
11:Y:100:MET:HA	11:Y:111:TYR:O	2.21	0.41
12:Z:76:ILE:HG22	16:Z:229:HOH:O	2.21	0.41
1:A:26:TYR:O	1:A:29:THR:HB	2.21	0.41
2:B:144:ARG:CZ	2:B:14(A):TYR:CE2	3.04	0.41
2:B:184:MET:HE3	2:B:188:ASP:HB3	2.02	0.41
3:C:163:GLN:NE2	3:C:164:THR:N	2.52	0.41
4:D:179:GLU:O	4:D:18(C):HIS:HD2	2.03	0.41
6:F:38:ILE:HG12	6:F:197:ILE:HD11	2.03	0.41
7:G:107:MET:HA	7:G:108:PRO:HD3	1.92	0.41
8:H:72:ARG:NH1	8:H:72:ARG:HG3	2.34	0.41
10:J:90(A):ILE:HD12	10:J:90(A):ILE:HA	1.87	0.41
14:N:146:MET:HB3	14:N:150:GLU:HB2	2.03	0.41
3:Q:150:GLN:O	3:Q:157:TYR:HA	2.21	0.41
4:R:112:LEU:O	4:R:112:LEU:HD13	2.21	0.41
7:U:29:LYS:HA	7:U:29:LYS:HD2	1.88	0.41
8:V:170:GLY:O	8:V:171:SER:HB2	2.21	0.41
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.35	0.41
1:A:122:GLU:C	1:A:124:THR:H	2.23	0.41
1:A:13:THR:HG22	1:A:21:LEU:HD22	2.02	0.41
2:B:44:ASP:N	2:B:44:ASP:OD2	2.53	0.41
3:C:106:PRO:HG2	3:C:143:PRO:HG3	2.02	0.41
16:B:254:HOH:O	3:C:62(A):ILE:CD1	2.63	0.41
3:C:72:SER:O	3:C:221:ILE:HD12	2.20	0.41
10:J:143:ARG:HB2	10:J:146:MET:HG3	2.03	0.41
14:N:143:ARG:O	14:N:146:MET:HG3	2.21	0.41
14:N:67:THR:O	14:N:68:SER:C	2.60	0.41
14:N:55:ILE:HD11	14:N:95:LEU:HD22	2.03	0.41
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:70:ILE:HB	4:R:74:ILE:HG22	2.03	0.41
7:U:112:LEU:O	7:U:116:MET:HG2	2.20	0.41
13:0:112:TYR:HE1	13:0:127:THR:HG22	1.86	0.40
6:F:217:LEU:HA	6:F:217:LEU:HD12	1.90	0.40
6:F:21(B):THR:O	6:F:21(C):ASN:CB	2.69	0.40
10:J:112:GLN:NE2	10:J:126:ALA:N	2.69	0.40
13:M:193:GLU:HA	13:M:193:GLU:OE2	2.21	0.40
1:O:4:MET:O	1:O:5:THR:O	2.39	0.40
2:P:191:GLU:O	2:P:195:LYS:HG2	2.20	0.40
2:P:38:ILE:HG22	2:P:39:GLY:N	2.36	0.40
3:Q:136:THR:O	3:Q:150:GLN:HA	2.21	0.40
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.52	0.40
5:S:214:ILE:HD12	5:S:214:ILE:C	2.41	0.40
6:T:109:ILE:HB	6:T:110:PRO:HD3	2.02	0.40
8:V:152:ILE:HD11	8:V:177:VAL:HG21	2.02	0.40
16:V:540:HOH:O	9:W:150:ASP:HA	2.21	0.40
14:1:55:ILE:HD11	14:1:95:LEU:CD2	2.50	0.40
3:C:201:VAL:HG21	3:C:210:ILE:CD1	2.46	0.40
4:D:46:VAL:HG11	4:D:139:ALA:HB1	2.03	0.40
6:F:202:HIS:O	6:F:202:HIS:CG	2.73	0.40
8:H:156:SER:O	8:H:160:GLN:HG3	2.22	0.40
1:O:179:ARG:HH11	1:O:179:ARG:CB	2.27	0.40
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.56	0.40
3:Q:90:GLU:OE2	3:Q:90:GLU:HA	2.21	0.40
4:R:39:GLY:O	4:R:162:ALA:HA	2.21	0.40
5:S:179:THR:O	5:S:179:THR:HG22	2.21	0.40
6:T:26:TYR:O	6:T:29:LYS:HB2	2.22	0.40
14:1:37:VAL:CG2	14:1:41:ILE:HG22	2.51	0.40
2:B:137:ILE:CD1	2:B:165:VAL:HG22	2.52	0.40
3:C:62(A):ILE:O	3:C:63:THR:C	2.59	0.40
4:D:187:LYS:O	4:D:191:LEU:HD22	2.21	0.40
10:J:143:ARG:O	10:J:146:MET:HG3	2.21	0.40
10:J:66:TYR:CE2	10:J:74:LEU:HG	2.56	0.40
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.87	0.40
13:M:17:ASP:C	13:M:17:ASP:OD2	2.59	0.40
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.21	0.40
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.22	0.40
4:R:18(C):HIS:O	4:R:18(E):SER:N	2.54	0.40
9:W:110:ILE:O	9:W:110:ILE:CD1	2.70	0.40
9:W:143:GLU:HA	9:W:144:PRO:HD3	1.88	0.40
3:C:46:VAL:O	3:C:215:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.57	0.40
11:K:4:LEU:CD1	11:K:159:ILE:HG12	2.51	0.40
14:N:32:ASP:OD1	14:N:186:ARG:NH2	2.54	0.40
8:H:118:SER:HB3	14:N:50:ALA:N	2.37	0.40
1:O:185:GLU:OE1	1:O:187:GLU:HB2	2.22	0.40
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.37	0.40
1:O:17:PRO:HA	2:P:26:TYR:CE1	2.57	0.40
10:X:135:PHE:HZ	16:X:213:HOH:O	2.04	0.40
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.57	0.40
4:D:82:THR:N	16:D:256:HOH:O	2.55	0.40
11:K:67:GLU:CG	11:K:73:ARG:HA	2.52	0.40
3:Q:163:GLN:HA	3:Q:163:GLN:NE2	2.36	0.40
4:R:197:LEU:O	4:R:201:MET:HG3	2.21	0.40
7:U:8:TYR:C	7:U:10:ARG:N	2.73	0.40
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.04	0.40
10:X:155:LEU:HA	10:X:155:LEU:HD23	1.85	0.40
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:HH11	1.87	0.40
12:Z:9:GLU:O	12:Z:107:LYS:HA	2.21	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%)	228 (92%)	15 (6%)	5 (2%)	7	19
1	O	248/250 (99%)	228 (92%)	16 (6%)	4 (2%)	9	24
2	B	242/258 (94%)	220 (91%)	19 (8%)	3 (1%)	13	32
2	P	242/258 (94%)	219 (90%)	19 (8%)	4 (2%)	9	23
3	C	239/254 (94%)	215 (90%)	18 (8%)	6 (2%)	5	14
3	Q	239/254 (94%)	217 (91%)	17 (7%)	5 (2%)	7	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	240/260 (92%)	215 (90%)	20 (8%)	5 (2%)	7	18
4	R	240/260 (92%)	216 (90%)	18 (8%)	6 (2%)	5	14
5	E	231/234 (99%)	210 (91%)	15 (6%)	6 (3%)	5	13
5	S	231/234 (99%)	210 (91%)	16 (7%)	5 (2%)	6	17
6	F	242/287 (84%)	228 (94%)	12 (5%)	2 (1%)	19	43
6	T	242/287 (84%)	226 (93%)	14 (6%)	2 (1%)	19	43
7	G	241/252 (96%)	225 (93%)	13 (5%)	3 (1%)	13	32
7	U	241/252 (96%)	225 (93%)	13 (5%)	3 (1%)	13	32
8	H	220/232 (95%)	203 (92%)	13 (6%)	4 (2%)	8	21
8	V	220/232 (95%)	204 (93%)	12 (6%)	4 (2%)	8	21
9	I	202/205 (98%)	192 (95%)	9 (4%)	1 (0%)	29	54
9	W	202/205 (98%)	190 (94%)	10 (5%)	2 (1%)	15	37
10	J	196/198 (99%)	184 (94%)	10 (5%)	2 (1%)	15	37
10	X	196/198 (99%)	184 (94%)	10 (5%)	2 (1%)	15	37
11	K	210/212 (99%)	192 (91%)	17 (8%)	1 (0%)	29	54
11	Y	210/212 (99%)	193 (92%)	16 (8%)	1 (0%)	29	54
12	L	220/241 (91%)	208 (94%)	11 (5%)	1 (0%)	29	54
12	Z	220/241 (91%)	208 (94%)	11 (5%)	1 (0%)	29	54
13	O	231/266 (87%)	212 (92%)	18 (8%)	1 (0%)	34	60
13	M	231/266 (87%)	213 (92%)	17 (7%)	1 (0%)	34	60
14	1	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
All	All	6312/6690 (94%)	5840 (92%)	392 (6%)	80 (1%)	12	30

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	56	SER
3	C	58	LEU
4	D	12(G)	GLU
6	F	64	ASN
7	G	220	LYS
10	J	192	ALA

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Mol	Chain	Res	Type
1	O	5	THR
1	O	56	SER
3	Q	58	LEU
4	R	12(G)	GLU
5	S	202	ARG
6	T	64	ASN
7	U	220	LYS
10	X	192	ALA
1	A	167	LYS
2	B	54	VAL
2	B	21(C)	ASP
3	C	183	PRO
3	C	203	THR
4	D	18(D)	SER
5	E	5	ARG
5	E	180	LEU
5	E	202	ARG
5	E	227	GLU
5	E	231	LYS
7	G	184	ASN
11	K	39	PRO
12	L	14(I)	THR
1	O	167	LYS
2	P	54	VAL
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	203	THR
4	R	18(D)	SER
5	S	5	ARG
5	S	227	GLU
5	S	231	LYS
7	U	184	ASN
11	Y	39	PRO
12	Z	14(I)	THR
3	C	184	ALA
4	D	128	MET
7	G	239	GLN
8	H	10(A)	PRO
13	M	96	TRP
1	O	204	GLY
3	Q	184	ALA
4	R	128	MET

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Mol	Chain	Res	Type
5	S	180	LEU
7	U	239	GLN
8	V	10(A)	PRO
1	A	204	GLY
4	D	12(C)	GLY
6	F	205	ASN
9	I	93	GLY
4	R	12(C)	GLY
6	T	205	ASN
8	V	91	GLN
9	W	93	GLY
3	C	179	ASN
5	E	18(A)	ASP
8	H	91	GLN
3	Q	179	ASN
8	V	171	SER
9	W	23	GLN
13	O	96	TRP
3	C	242	GLU
8	H	171	SER
2	P	6	ARG
4	R	11	GLY
4	R	12(E)	SER
8	H	180	ILE
10	J	8	VAL
10	X	8	VAL
2	B	21(B)	GLY
2	P	21(B)	GLY
8	V	180	ILE
1	A	22	GLY
4	D	11	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/209 (100%)	201 (96%)	8 (4%)	33 62
1	O	209/209 (100%)	200 (96%)	9 (4%)	29 57
2	B	203/216 (94%)	187 (92%)	16 (8%)	12 28
2	P	203/216 (94%)	186 (92%)	17 (8%)	11 25
3	C	213/226 (94%)	200 (94%)	13 (6%)	18 41
3	Q	213/226 (94%)	200 (94%)	13 (6%)	18 41
4	D	198/215 (92%)	188 (95%)	10 (5%)	24 50
4	R	198/215 (92%)	187 (94%)	11 (6%)	21 45
5	E	192/193 (100%)	174 (91%)	18 (9%)	8 20
5	S	192/193 (100%)	173 (90%)	19 (10%)	8 18
6	F	201/238 (84%)	180 (90%)	21 (10%)	7 16
6	T	201/238 (84%)	181 (90%)	20 (10%)	7 18
7	G	207/210 (99%)	192 (93%)	15 (7%)	14 34
7	U	207/210 (99%)	192 (93%)	15 (7%)	14 34
8	H	181/190 (95%)	174 (96%)	7 (4%)	32 61
8	V	181/190 (95%)	174 (96%)	7 (4%)	32 61
9	I	172/173 (99%)	166 (96%)	6 (4%)	36 65
9	W	172/173 (99%)	166 (96%)	6 (4%)	36 65
10	J	175/175 (100%)	165 (94%)	10 (6%)	20 44
10	X	175/175 (100%)	164 (94%)	11 (6%)	18 40
11	K	169/169 (100%)	158 (94%)	11 (6%)	17 38
11	Y	169/169 (100%)	158 (94%)	11 (6%)	17 38
12	L	185/201 (92%)	174 (94%)	11 (6%)	19 43
12	Z	185/201 (92%)	174 (94%)	11 (6%)	19 43
13	O	199/224 (89%)	187 (94%)	12 (6%)	19 42
13	M	199/224 (89%)	188 (94%)	11 (6%)	21 46
14	I	162/162 (100%)	151 (93%)	11 (7%)	16 36
14	N	162/162 (100%)	151 (93%)	11 (7%)	16 36
All	All	5332/5602 (95%)	4991 (94%)	341 (6%)	17 39

All (341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	65	SER
1	A	10(A)	ILE
1	A	124	THR
1	A	158	PHE
1	A	179	ARG
1	A	215	ILE
2	B	8	TYR
2	B	14	ILE
2	B	58	LEU
2	B	71	ASN
2	B	87	ILE
2	B	104	ASN
2	B	116	LEU
2	B	121	GLN
2	B	144	ARG
2	B	150	THR
2	B	163	ILE
2	B	198	SER
2	B	206	THR
2	B	212	PHE
2	B	218	ASN
2	B	224	PHE
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	66	LYS
3	C	87	ILE
3	C	100	ARG
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	163	GLN
3	C	174	GLU
3	C	208	LYS
3	C	227	GLU
4	D	28	LEU
4	D	40	ILE
4	D	107	ILE
4	D	126	ARG
4	D	14(A)	ASP
4	D	170	GLU

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Mol	Chain	Res	Type
4	D	177	LEU
4	D	194	LEU
4	D	215	ILE
4	D	244	GLU
5	E	12	THR
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	111	ARG
5	E	121	GLN
5	E	18(D)	ILE
5	E	18(F)	ILE
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	2(C)	VAL
5	E	214	ILE
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	35	THR
6	F	43	ASN
6	F	56	SER
6	F	74	ILE
6	F	98	SER
6	F	105	THR
6	F	109	ILE
6	F	121	GLN
6	F	127	ASN
6	F	135	SER
6	F	144	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
6	F	21(C)	ASN

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Mol	Chain	Res	Type
6	F	240	ILE
7	G	14	ILE
7	G	34(A)	ASN
7	G	38	LEU
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	169	GLN
7	G	184	ASN
7	G	197	MET
7	G	204	GLU
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	25	ILE
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	144	GLN
8	H	197	ARG
8	H	218	ILE
9	I	29	ASN
9	I	110	ILE
9	I	125	ILE
9	I	135	PHE
9	I	160	LEU
9	I	171	TRP
10	J	6	ILE
10	J	24	ILE
10	J	70	GLU
10	J	77	GLN
10	J	90(A)	ILE
10	J	115	TYR
10	J	121	GLU
10	J	133	TYR
10	J	155	LEU
10	J	166	MET
11	K	4	LEU
11	K	9	GLN
11	K	39	PRO

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Mol	Chain	Res	Type
11	K	74	ILE
11	K	87	VAL
11	K	100	MET
11	K	101	ILE
11	K	104	TYR
11	K	10(B)	LYS
11	K	110	ILE
11	K	210	ILE
12	L	-7	ASN
12	L	14	LEU
12	L	40	ASN
12	L	58	ARG
12	L	70(A)	ASN
12	L	99	THR
12	L	114	ASP
12	L	120	GLU
12	L	138	LEU
12	L	1(I)	ASN
12	L	145	TYR
13	M	40	ASN
13	M	62	LEU
13	M	65	GLU
13	M	91	ARG
13	M	115	LEU
13	M	129	PHE
13	M	14(C)	ARG
13	M	14(G)	ILE
13	M	149	GLN
13	M	203	ILE
13	M	204	LYS
14	N	20	THR
14	N	36	ARG
14	N	55	ILE
14	N	84	LYS
14	N	89	GLU
14	N	10(A)	ASP
14	N	115	LEU
14	N	119	VAL
14	N	126	ILE
14	N	178	LEU
14	N	18(I)	GLN
1	O	32	LYS

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Mol	Chain	Res	Type
1	O	33	GLN
1	O	64	LEU
1	O	65	SER
1	O	10(A)	ILE
1	O	124	THR
1	O	158	PHE
1	O	179	ARG
1	O	215	ILE
2	P	8	TYR
2	P	14	ILE
2	P	58	LEU
2	P	71	ASN
2	P	87	ILE
2	P	104	ASN
2	P	116	LEU
2	P	121	GLN
2	P	144	ARG
2	P	150	THR
2	P	156	ASN
2	P	163	ILE
2	P	198	SER
2	P	206	THR
2	P	212	PHE
2	P	218	ASN
2	P	224	PHE
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	66	LYS
3	Q	87	ILE
3	Q	100	ARG
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	163	GLN
3	Q	174	GLU
3	Q	208	LYS
3	Q	227	GLU
4	R	28	LEU
4	R	40	ILE
4	R	107	ILE
4	R	126	ARG

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Mol	Chain	Res	Type
4	R	14(A)	ASP
4	R	170	GLU
4	R	177	LEU
4	R	194	LEU
4	R	196	ILE
4	R	215	ILE
4	R	244	GLU
5	S	12	THR
5	S	28	LEU
5	S	32	LYS
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	104	ASN
5	S	111	ARG
5	S	121	GLN
5	S	18(D)	ILE
5	S	18(F)	ILE
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	2(C)	VAL
5	S	214	ILE
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	35	THR
6	T	43	ASN
6	T	56	SER
6	T	74	ILE
6	T	98	SER
6	T	105	THR
6	T	109	ILE
6	T	121	GLN
6	T	127	ASN
6	T	135	SER
6	T	169	ARG
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP

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Mol	Chain	Res	Type
6	T	205	ASN
6	T	214	TRP
6	T	21(C)	ASN
6	T	240	ILE
7	U	14	ILE
7	U	34(A)	ASN
7	U	38	LEU
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	169	GLN
7	U	184	ASN
7	U	197	MET
7	U	204	GLU
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	25	ILE
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	144	GLN
8	V	197	ARG
8	V	218	ILE
9	W	29	ASN
9	W	90	ARG
9	W	110	ILE
9	W	125	ILE
9	W	160	LEU
9	W	171	TRP
10	X	6	ILE
10	X	24	ILE
10	X	34	THR
10	X	70	GLU
10	X	77	GLN
10	X	90(A)	ILE
10	X	115	TYR
10	X	121	GLU
10	X	133	TYR
10	X	155	LEU

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Mol	Chain	Res	Type
10	X	166	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	39	PRO
11	Y	74	ILE
11	Y	87	VAL
11	Y	100	MET
11	Y	101	ILE
11	Y	104	TYR
11	Y	10(B)	LYS
11	Y	110	ILE
11	Y	210	ILE
12	Z	-7	ASN
12	Z	14	LEU
12	Z	40	ASN
12	Z	58	ARG
12	Z	70(A)	ASN
12	Z	99	THR
12	Z	114	ASP
12	Z	120	GLU
12	Z	138	LEU
12	Z	1(I)	ASN
12	Z	145	TYR
13	0	39	ASP
13	0	40	ASN
13	0	62	LEU
13	0	65	GLU
13	0	91	ARG
13	0	115	LEU
13	0	129	PHE
13	0	14(C)	ARG
13	0	14(G)	ILE
13	0	149	GLN
13	0	203	ILE
13	0	204	LYS
14	1	20	THR
14	1	36	ARG
14	1	55	ILE
14	1	84	LYS
14	1	89	GLU
14	1	10(A)	ASP
14	1	115	LEU

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Mol	Chain	Res	Type
14	1	119	VAL
14	1	126	ILE
14	1	178	LEU
14	1	18(I)	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (202) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
1	A	191	HIS
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	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	114	GLN
4	D	161	ASN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	73	HIS
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	156	ASN
5	E	185	ASN

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Mol	Chain	Res	Type
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
7	G	11	HIS
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	10	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
9	I	29	ASN
9	I	64	ASN
9	I	81	GLN
9	I	145	ASN
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
10	J	193	GLN
11	K	85	ASN
11	K	131	GLN

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Mol	Chain	Res	Type
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	82	ASN
12	L	1(I)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	69	GLN
14	N	145	ASN
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
1	O	191	HIS
2	P	23	GLN
2	P	71	ASN
2	P	95	HIS
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

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Mol	Chain	Res	Type
3	Q	209	ASN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	114	GLN
4	R	161	ASN
4	R	211	GLN
4	R	218	GLN
4	R	226	ASN
5	S	73	HIS
5	S	97	ASN
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	156	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	192	GLN
7	U	11	HIS
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	18(C)	HIS
7	U	184	ASN
7	U	228	ASN
8	V	10	ASN
8	V	30	ASN
8	V	66	HIS
8	V	91	GLN
8	V	144	GLN
8	V	165	ASN

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Mol	Chain	Res	Type
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	64	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
10	X	193	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	-2	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	84	GLN
12	Z	85	HIS
12	Z	1(I)	ASN
12	Z	166	HIS
13	0	10	ASN
13	0	18	ASN
13	0	40	ASN
13	0	89	GLN
13	0	93	ASN
13	0	149	GLN
13	0	157	ASN
13	0	172	ASN
13	0	191	GLN
14	1	69	GLN
14	1	145	ASN
14	1	161	GLN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	GDT	V	500	8	36,37,37	2.25	3 (8%)	41,46,46	1.74	8 (19%)
15	GDT	H	500	8	36,37,37	2.16	3 (8%)	41,46,46	1.75	8 (19%)
15	GDT	Y	500	11	36,37,37	1.90	1 (2%)	41,46,46	1.94	8 (19%)
15	GDT	K	500	11	36,37,37	2.09	3 (8%)	41,46,46	1.86	8 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GDT	V	500	8	-	11/50/50/50	0/0/1/1
15	GDT	H	500	8	-	11/50/50/50	0/0/1/1
15	GDT	Y	500	11	-	9/50/50/50	0/0/1/1
15	GDT	K	500	11	-	9/50/50/50	0/0/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	500	GDT	C26-C27	11.42	1.59	1.32
15	H	500	GDT	C26-C27	11.17	1.58	1.32
15	K	500	GDT	C26-C27	10.81	1.57	1.32
15	Y	500	GDT	C26-C27	9.52	1.54	1.32
15	V	500	GDT	C14-N13	3.12	1.52	1.45
15	H	500	GDT	C14-N13	2.74	1.51	1.45
15	V	500	GDT	C31-N30	2.53	1.39	1.34
15	K	500	GDT	C22-N23	-2.38	1.40	1.46
15	H	500	GDT	C31-N30	2.29	1.39	1.34
15	K	500	GDT	C14-N13	2.04	1.50	1.45

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Y	500	GDT	C26-C24-N23	7.07	128.30	114.97
15	K	500	GDT	C26-C24-N23	6.74	127.67	114.97
15	Y	500	GDT	C27-C26-C24	-6.00	107.68	122.69
15	V	500	GDT	C26-C24-N23	5.81	125.91	114.97
15	H	500	GDT	C26-C24-N23	5.48	125.30	114.97
15	K	500	GDT	C27-C26-C24	-5.46	109.04	122.69
15	H	500	GDT	C27-C26-C24	-4.59	111.21	122.69
15	V	500	GDT	C27-C26-C24	-4.35	111.81	122.69
15	Y	500	GDT	O25-C24-C26	-3.87	114.21	123.03
15	K	500	GDT	O25-C24-C26	-3.75	114.47	123.03
15	H	500	GDT	C1-C12-N13	3.68	121.64	114.56
15	V	500	GDT	C1-C12-N13	3.65	121.58	114.56
15	V	500	GDT	O25-C24-C26	-3.37	115.34	123.03
15	H	500	GDT	C22-N23-C24	3.30	127.37	122.54
15	V	500	GDT	C22-N23-C24	3.12	127.11	122.54
15	K	500	GDT	C1-C12-N13	2.98	120.30	114.56
15	Y	500	GDT	C1-C12-N13	2.96	120.25	114.56
15	H	500	GDT	O25-C24-C26	-2.96	116.29	123.03
15	Y	500	GDT	O25-C24-N23	-2.87	117.49	122.23
15	H	500	GDT	O37-C12-C1	-2.75	116.75	123.03
15	K	500	GDT	C22-N23-C24	2.67	126.46	122.54
15	K	500	GDT	O25-C24-N23	-2.66	117.83	122.23
15	Y	500	GDT	C22-N23-C24	2.61	126.37	122.54
15	Y	500	GDT	C28-N30-C31	-2.55	119.34	122.97
15	H	500	GDT	C3-C2-C1	-2.44	118.58	124.67
15	K	500	GDT	C28-N30-C31	-2.40	119.56	122.97
15	V	500	GDT	O37-C12-C1	-2.40	117.56	123.03
15	Y	500	GDT	O37-C12-C1	-2.39	117.59	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	H	500	GDT	O25-C24-N23	-2.31	118.41	122.23
15	V	500	GDT	C3-C2-C1	-2.30	118.94	124.67
15	K	500	GDT	O37-C12-C1	-2.28	117.83	123.03
15	V	500	GDT	O25-C24-N23	-2.11	118.75	122.23

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	V	500	GDT	N16-C17-C18-C19
15	V	500	GDT	C26-C27-C28-N30
15	V	500	GDT	C24-C26-C27-C28
15	V	500	GDT	C26-C24-N23-C22
15	V	500	GDT	O25-C24-N23-C22
15	H	500	GDT	N16-C17-C18-C19
15	H	500	GDT	C26-C27-C28-N30
15	H	500	GDT	C24-C26-C27-C28
15	H	500	GDT	C26-C24-N23-C22
15	H	500	GDT	O25-C24-N23-C22
15	H	500	GDT	O20-C19-C21-C22
15	Y	500	GDT	C26-C27-C28-N30
15	Y	500	GDT	C24-C26-C27-C28
15	Y	500	GDT	C26-C24-N23-C22
15	Y	500	GDT	O25-C24-N23-C22
15	K	500	GDT	C26-C27-C28-N30
15	K	500	GDT	C24-C26-C27-C28
15	K	500	GDT	C26-C24-N23-C22
15	K	500	GDT	O25-C24-N23-C22
15	V	500	GDT	C26-C27-C28-C29
15	H	500	GDT	C26-C27-C28-C29
15	Y	500	GDT	C26-C27-C28-C29
15	K	500	GDT	C26-C27-C28-C29
15	K	500	GDT	N23-C24-C26-C27
15	V	500	GDT	C4-C5-C6-C7
15	H	500	GDT	C4-C5-C6-C7
15	Y	500	GDT	O25-C24-C26-C27
15	K	500	GDT	O25-C24-C26-C27
15	Y	500	GDT	N23-C24-C26-C27
15	V	500	GDT	C31-C17-C18-C19
15	H	500	GDT	C31-C17-C18-C19
15	V	500	GDT	O20-C19-C21-C22
15	H	500	GDT	C18-C19-C21-C22

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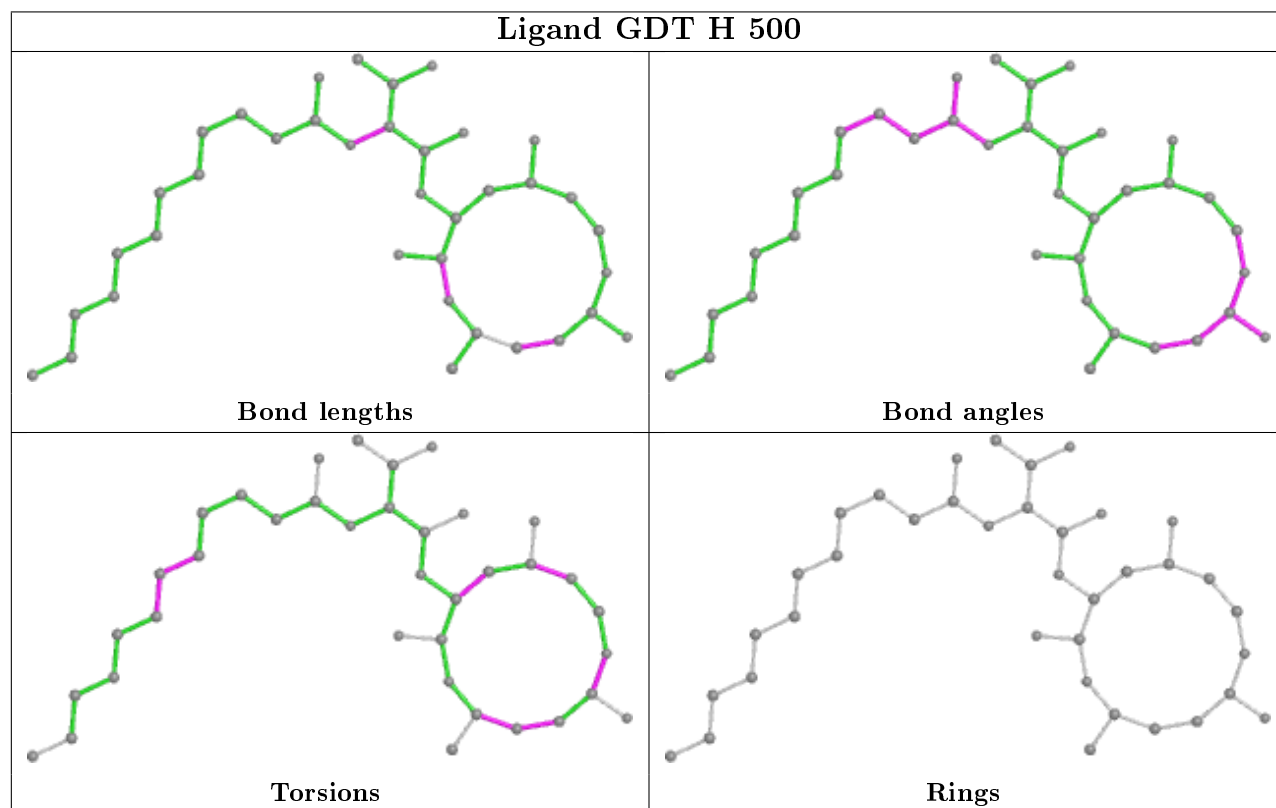
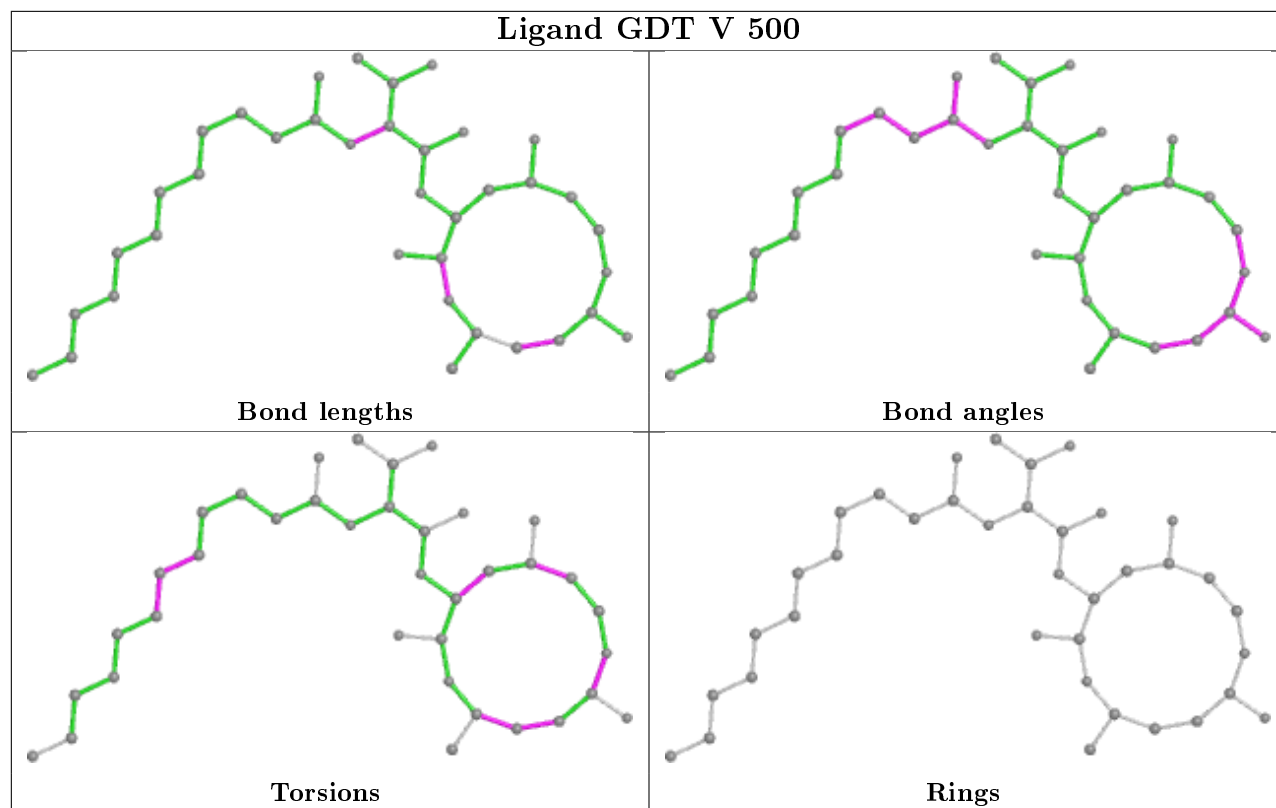
Mol	Chain	Res	Type	Atoms
15	V	500	GDT	C3-C4-C5-C6
15	Y	500	GDT	C17-C18-C19-O20
15	K	500	GDT	C31-C17-C18-C19
15	H	500	GDT	C3-C4-C5-C6
15	V	500	GDT	C18-C19-C21-C22
15	Y	500	GDT	O20-C19-C21-C22
15	K	500	GDT	O20-C19-C21-C22

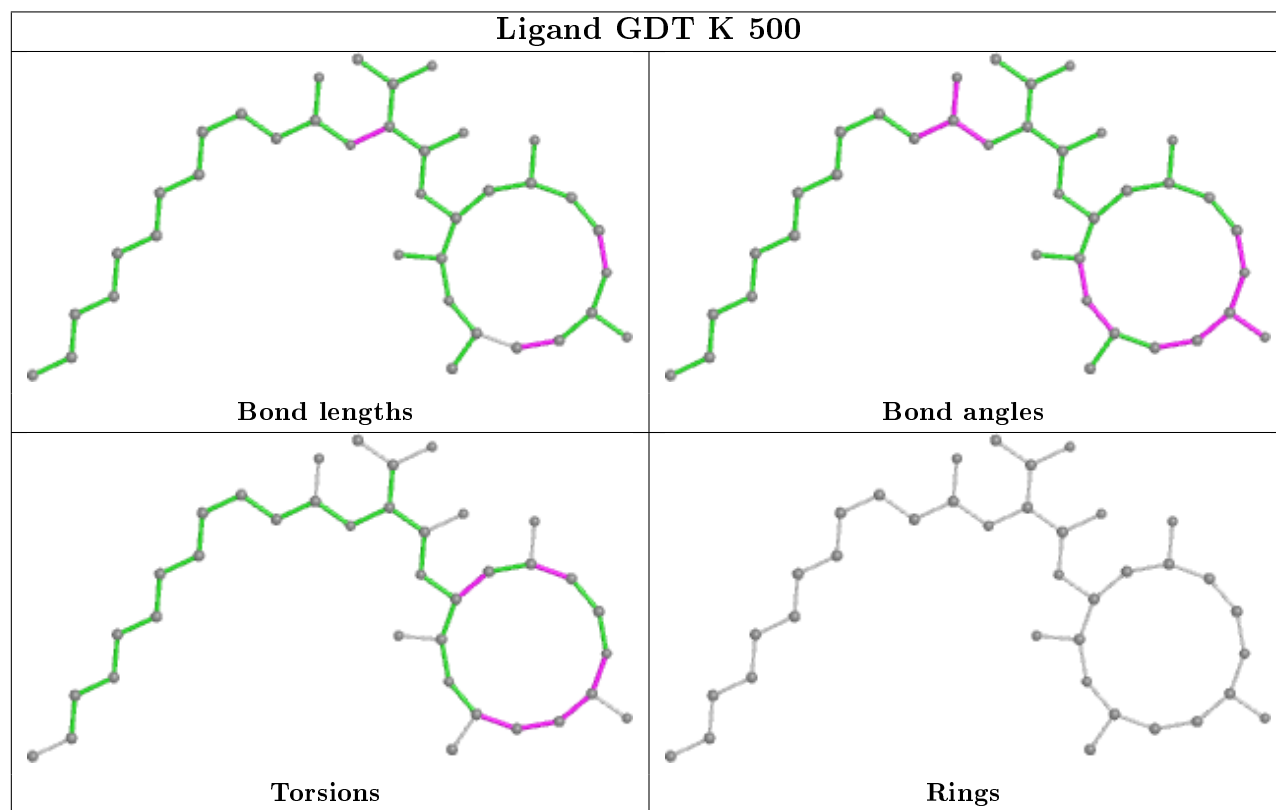
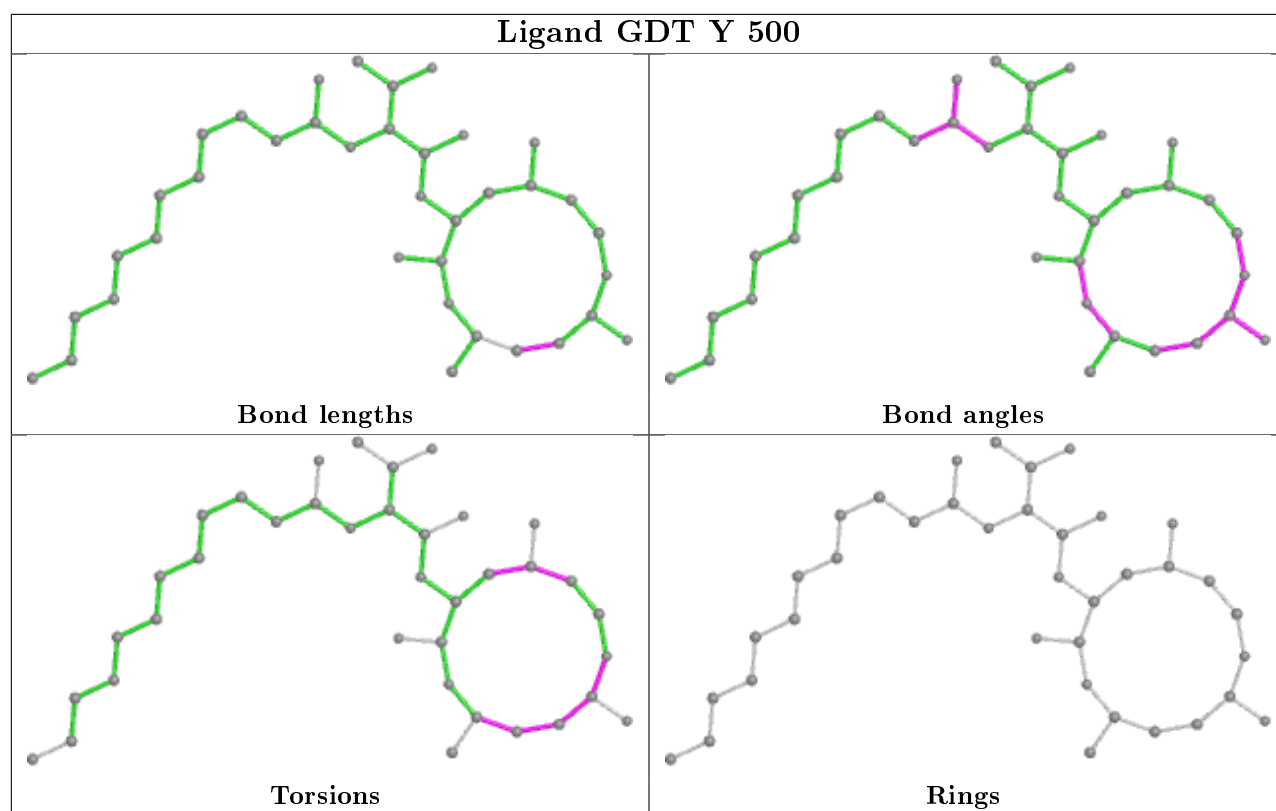
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	V	500	GDT	3	0
15	H	500	GDT	2	0
15	Y	500	GDT	4	0
15	K	500	GDT	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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%)	0.06	6 (2%) 59 60	34, 52, 82, 108	0
1	O	250/250 (100%)	0.23	16 (6%) 19 18	37, 60, 85, 105	0
2	B	244/258 (94%)	0.23	11 (4%) 33 31	34, 58, 92, 117	0
2	P	244/258 (94%)	0.26	16 (6%) 18 16	38, 58, 92, 117	0
3	C	241/254 (94%)	0.35	14 (5%) 23 22	35, 62, 106, 123	0
3	Q	241/254 (94%)	0.65	34 (14%) 2 1	41, 66, 110, 124	0
4	D	242/260 (93%)	0.24	9 (3%) 41 41	39, 58, 90, 123	0
4	R	242/260 (93%)	0.33	15 (6%) 20 19	42, 62, 94, 125	0
5	E	233/234 (99%)	0.23	13 (5%) 24 23	37, 58, 84, 108	0
5	S	233/234 (99%)	0.27	15 (6%) 19 18	32, 58, 88, 107	0
6	F	244/287 (85%)	0.09	9 (3%) 41 41	32, 53, 88, 102	0
6	T	244/287 (85%)	0.10	10 (4%) 37 36	29, 52, 87, 105	0
7	G	243/252 (96%)	-0.02	9 (3%) 41 41	29, 48, 78, 113	0
7	U	243/252 (96%)	0.01	6 (2%) 57 59	33, 52, 78, 112	0
8	H	222/232 (95%)	-0.16	2 (0%) 84 85	27, 43, 64, 106	0
8	V	222/232 (95%)	-0.20	3 (1%) 75 77	28, 46, 64, 109	0
9	I	204/205 (99%)	-0.06	3 (1%) 73 76	31, 50, 66, 79	0
9	W	204/205 (99%)	0.01	2 (0%) 82 83	31, 48, 66, 78	0
10	J	198/198 (100%)	-0.04	5 (2%) 57 59	33, 49, 70, 119	0
10	X	198/198 (100%)	-0.02	6 (3%) 50 51	36, 49, 69, 124	0
11	K	212/212 (100%)	0.12	5 (2%) 59 60	30, 51, 78, 85	0
11	Y	212/212 (100%)	0.10	8 (3%) 40 39	33, 54, 76, 85	0
12	L	222/241 (92%)	-0.04	6 (2%) 54 55	32, 50, 74, 90	0
12	Z	222/241 (92%)	0.05	4 (1%) 68 70	37, 50, 74, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	0	233/266 (87%)	-0.19	1 (0%) 92 93	29, 44, 61, 69	0
13	M	233/266 (87%)	-0.19	2 (0%) 84 85	27, 45, 60, 69	0
14	1	196/196 (100%)	-0.16	3 (1%) 73 76	32, 42, 62, 84	0
14	N	196/196 (100%)	-0.20	2 (1%) 82 83	28, 41, 63, 83	0
All	All	6368/6690 (95%)	0.08	235 (3%) 41 41	27, 52, 85, 125	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	12(E)	SER	10.1
4	R	12(F)	GLY	9.8
4	D	12(D)	ALA	9.5
10	X	193	GLN	8.2
3	Q	236	ILE	8.1
4	R	12(C)	GLY	7.9
10	J	192	ALA	7.5
10	X	192	ALA	7.5
4	D	12(E)	SER	7.4
4	R	12(D)	ALA	7.3
7	G	240	ASP	7.3
4	D	12(C)	GLY	7.3
6	F	5	GLY	6.3
1	A	236	LEU	6.3
4	D	12(F)	GLY	6.1
2	B	218	ASN	6.1
3	Q	203	THR	6.0
1	O	235	ALA	5.9
6	T	240	ILE	5.9
7	U	240	ASP	5.8
8	V	223	ASP	5.8
10	J	191	GLN	5.7
3	C	55	THR	5.6
13	M	-8	THR	5.6
3	Q	240	LYS	5.6
3	Q	243	GLN	5.6
1	O	236	LEU	5.5
10	X	191	GLN	5.4
9	W	-8	SER	5.4
2	P	218	ASN	5.3
10	J	193	GLN	5.1
5	S	233	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
6	F	240	ILE	5.0
13	0	-8	THR	4.8
7	U	6	ALA	4.8
2	P	21(C)	ASP	4.8
5	S	5	ARG	4.8
12	L	145	TYR	4.6
2	B	21(A)	LYS	4.5
2	P	217	ALA	4.5
5	S	207	LEU	4.5
11	K	181	ASP	4.4
7	G	6	ALA	4.4
1	O	5	THR	4.4
3	C	236	ILE	4.3
2	B	217	ALA	4.3
12	Z	145	TYR	4.2
3	Q	55	THR	4.2
3	Q	239	GLU	4.1
1	O	206	PHE	4.1
1	A	5	THR	4.1
5	E	233	ILE	4.1
5	E	203	ASP	4.1
5	S	204	GLU	4.0
12	Z	14(W)	LYS	4.0
4	R	126	ARG	3.9
6	F	6	THR	3.9
2	P	21(A)	LYS	3.9
4	D	126	ARG	3.9
3	Q	206	GLY	3.8
2	B	54	VAL	3.8
2	B	21(C)	ASP	3.8
3	C	233	VAL	3.7
3	Q	202	GLN	3.7
3	Q	229	ILE	3.7
2	P	236	THR	3.7
3	Q	56	LEU	3.6
4	D	10	ARG	3.6
3	Q	238	GLN	3.6
4	R	9	ASP	3.5
3	Q	210	ILE	3.5
11	K	104	TYR	3.5
11	Y	145	ASP	3.5
7	G	8	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
8	H	223	ASP	3.4
2	B	229	ILE	3.4
5	S	178	ARG	3.4
5	S	203	ASP	3.4
3	Q	178	LYS	3.3
3	Q	241	GLN	3.3
2	P	21(B)	GLY	3.3
5	S	127	TYR	3.3
3	C	241	GLN	3.3
2	P	220	TYR	3.3
2	P	219	GLU	3.2
3	Q	237	GLU	3.2
5	S	4	PHE	3.2
11	Y	104	TYR	3.2
4	D	127	LEU	3.2
12	L	14(W)	LYS	3.2
3	Q	242	GLU	3.1
3	C	237	GLU	3.1
3	C	243	GLN	3.1
3	Q	191	LYS	3.1
3	Q	233	VAL	3.1
12	L	-9	GLN	3.1
1	O	179	ARG	3.0
2	P	233	LEU	3.0
4	R	12(G)	GLU	3.0
7	U	8	TYR	2.9
3	C	43	LYS	2.9
11	K	143	LYS	2.9
1	O	234	GLU	2.9
12	L	182	ASP	2.9
10	X	92	ARG	2.9
3	C	56	LEU	2.8
5	E	189	LEU	2.8
5	E	5	ARG	2.8
6	T	228	LEU	2.8
14	N	18(J)	LEU	2.8
5	E	4	PHE	2.8
1	O	198	LYS	2.8
6	T	18(D)	PRO	2.8
5	E	217	LYS	2.8
12	L	14(J)	GLY	2.8
3	C	240	LYS	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
11	Y	10(A)	ARG	2.8
2	B	21(B)	GLY	2.7
4	R	242	ALA	2.7
5	S	229	VAL	2.7
6	F	18(E)	GLU	2.7
3	Q	18(D)	GLU	2.7
7	G	18(A)	ILE	2.7
3	Q	196	SER	2.7
2	P	239	THR	2.7
9	I	181	LYS	2.7
5	S	227	GLU	2.7
11	Y	93	ALA	2.7
2	P	54	VAL	2.7
1	O	232	ARG	2.7
2	P	6	ARG	2.7
9	I	182	ASP	2.7
5	E	207	LEU	2.6
3	Q	18(B)	ARG	2.6
3	Q	232	TYR	2.6
1	O	202	VAL	2.6
12	Z	-9	GLN	2.6
5	S	202	ARG	2.6
14	1	18(I)	GLN	2.6
1	O	21(P)	LYS	2.6
10	X	-1	MET	2.6
3	Q	198	LEU	2.6
6	T	238	LYS	2.5
8	H	222	CYS	2.5
4	R	240	LYS	2.5
4	R	243	ALA	2.5
5	E	178	ARG	2.5
12	Z	14(K)	LYS	2.5
12	L	14(M)	VAL	2.5
10	J	92	ARG	2.5
3	C	203	THR	2.5
5	E	204	GLU	2.5
11	K	180	GLU	2.4
7	G	17(D)	SER	2.4
9	I	-8	SER	2.4
6	F	18(D)	PRO	2.4
1	O	233	LEU	2.4
4	D	12(G)	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	R	125	GLU	2.4
7	U	239	GLN	2.4
3	Q	201	VAL	2.4
5	S	195	GLU	2.4
7	U	17(E)	LYS	2.4
2	B	236	THR	2.4
3	Q	224	LEU	2.4
2	P	21(D)	GLY	2.4
6	T	233	ILE	2.4
3	Q	200	VAL	2.4
5	E	127	TYR	2.3
14	1	18(J)	LEU	2.3
5	S	197	ILE	2.3
6	T	180	VAL	2.3
13	M	92(B)	MET	2.3
1	O	205	GLU	2.3
5	E	201	LEU	2.3
1	A	200	SER	2.3
6	F	228	LEU	2.3
3	C	178	LYS	2.3
4	R	235	LYS	2.3
4	D	179	GLU	2.3
4	R	127	LEU	2.3
3	Q	18(C)	LYS	2.3
3	Q	187	GLU	2.3
3	Q	194	VAL	2.3
1	O	195	LEU	2.2
5	S	201	LEU	2.2
3	C	239	GLU	2.2
3	Q	207	ALA	2.2
1	A	4	MET	2.2
3	Q	184	ALA	2.2
1	O	210	ILE	2.2
11	Y	144	TRP	2.2
1	O	197	LEU	2.2
4	R	194	LEU	2.2
6	T	184	LEU	2.2
8	V	222	CYS	2.2
3	C	52	ARG	2.2
6	F	184	LEU	2.2
1	A	235	ALA	2.2
7	G	239	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
11	Y	180	GLU	2.1
5	E	18(D)	ILE	2.1
6	F	180	VAL	2.1
11	Y	148	VAL	2.1
14	N	18(I)	GLN	2.1
9	W	181	LYS	2.1
6	T	235	PHE	2.1
2	B	20(B)	ALA	2.1
4	R	231	GLU	2.1
1	A	204	GLY	2.1
2	B	222	LYS	2.1
3	Q	14(B)	ASP	2.1
10	X	93	ARG	2.1
11	Y	181	ASP	2.1
2	P	186	VAL	2.1
5	E	194	VAL	2.1
7	G	236	ILE	2.1
2	P	7	ARG	2.1
3	C	53	ARG	2.1
7	G	18(H)	GLU	2.1
3	Q	40	VAL	2.1
8	V	219	VAL	2.1
1	O	6	ASP	2.1
7	G	7	GLY	2.1
10	J	149	GLU	2.1
2	P	180	TYR	2.0
5	S	231	LYS	2.0
7	U	188	LYS	2.0
2	B	220	TYR	2.0
11	K	93	ALA	2.0
3	Q	179	ASN	2.0
6	F	238	LYS	2.0
6	T	241	ASN	2.0
14	1	107	LYS	2.0
6	T	18(E)	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

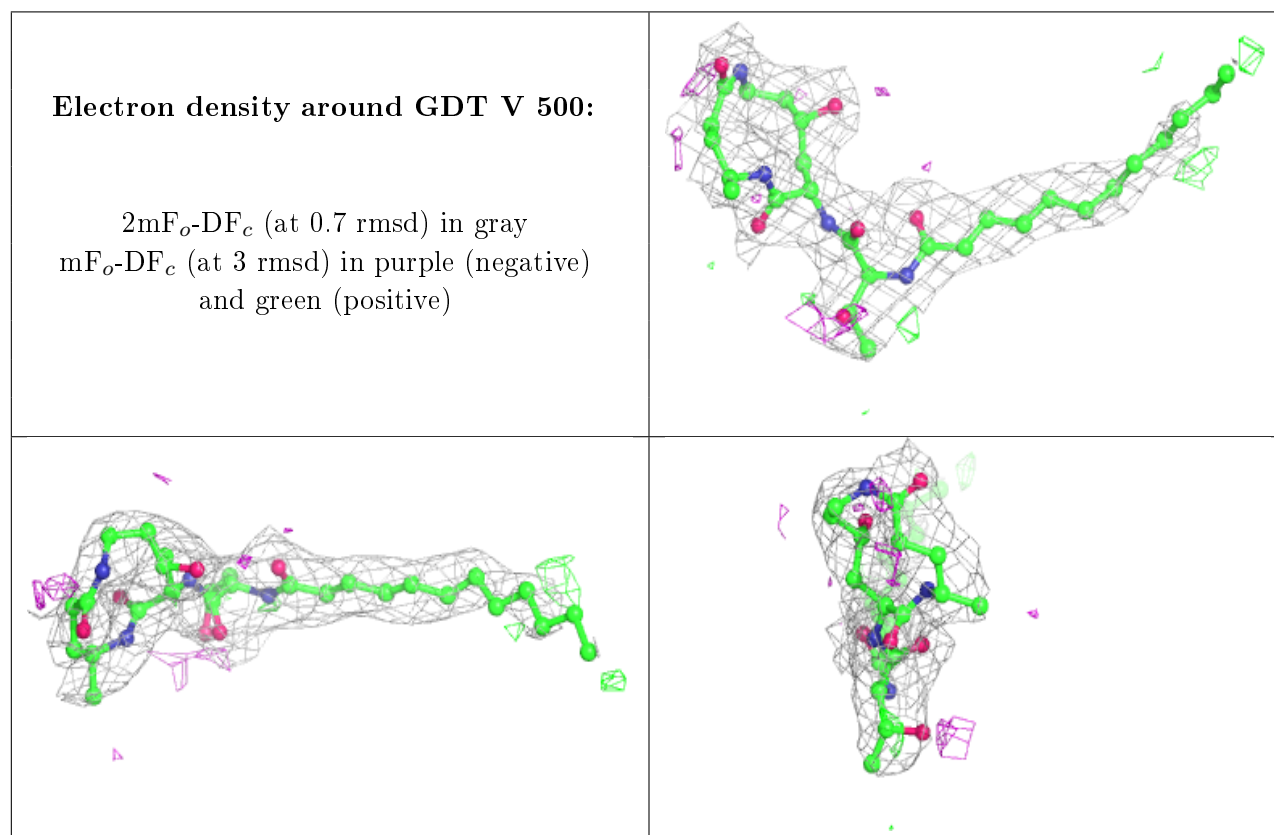
There are no carbohydrates in this entry.

## 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.

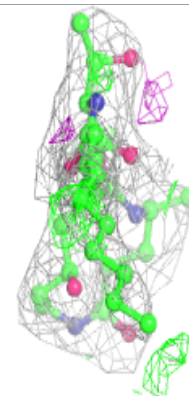
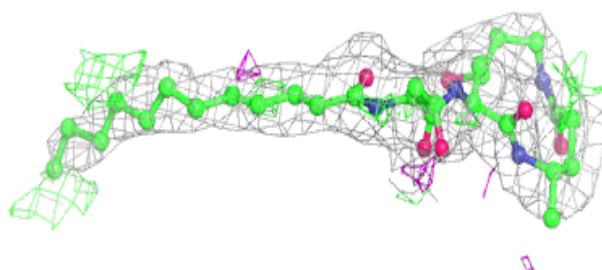
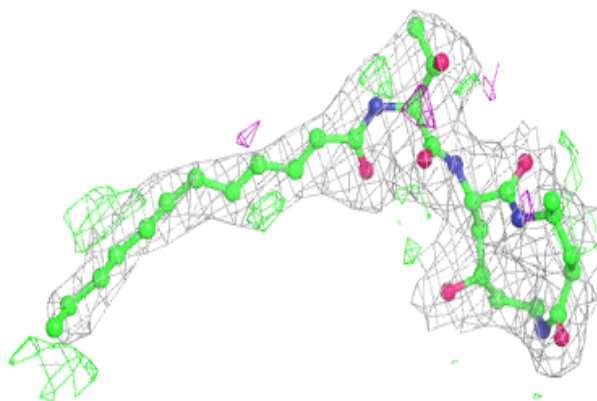
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	GDT	V	500	37/37	0.88	0.24	35,40,62,63	0
15	GDT	H	500	37/37	0.89	0.23	31,35,53,53	0
15	GDT	Y	500	37/37	0.93	0.19	39,44,55,56	0
15	GDT	K	500	37/37	0.94	0.19	31,41,46,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

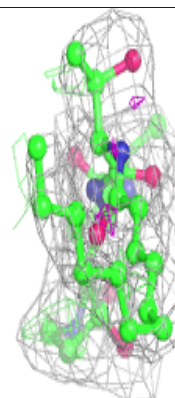
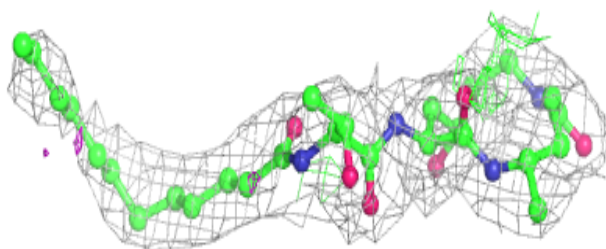
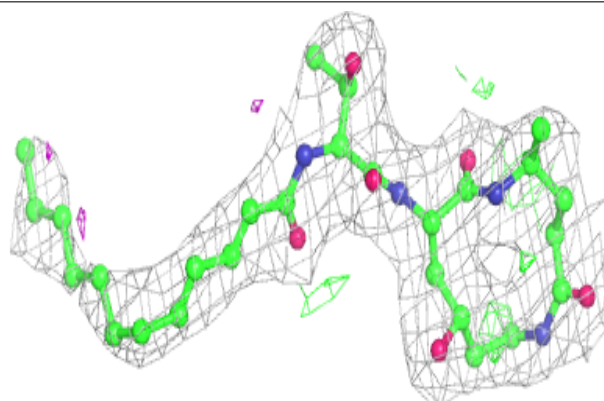


**Electron density around GDT H 500:**

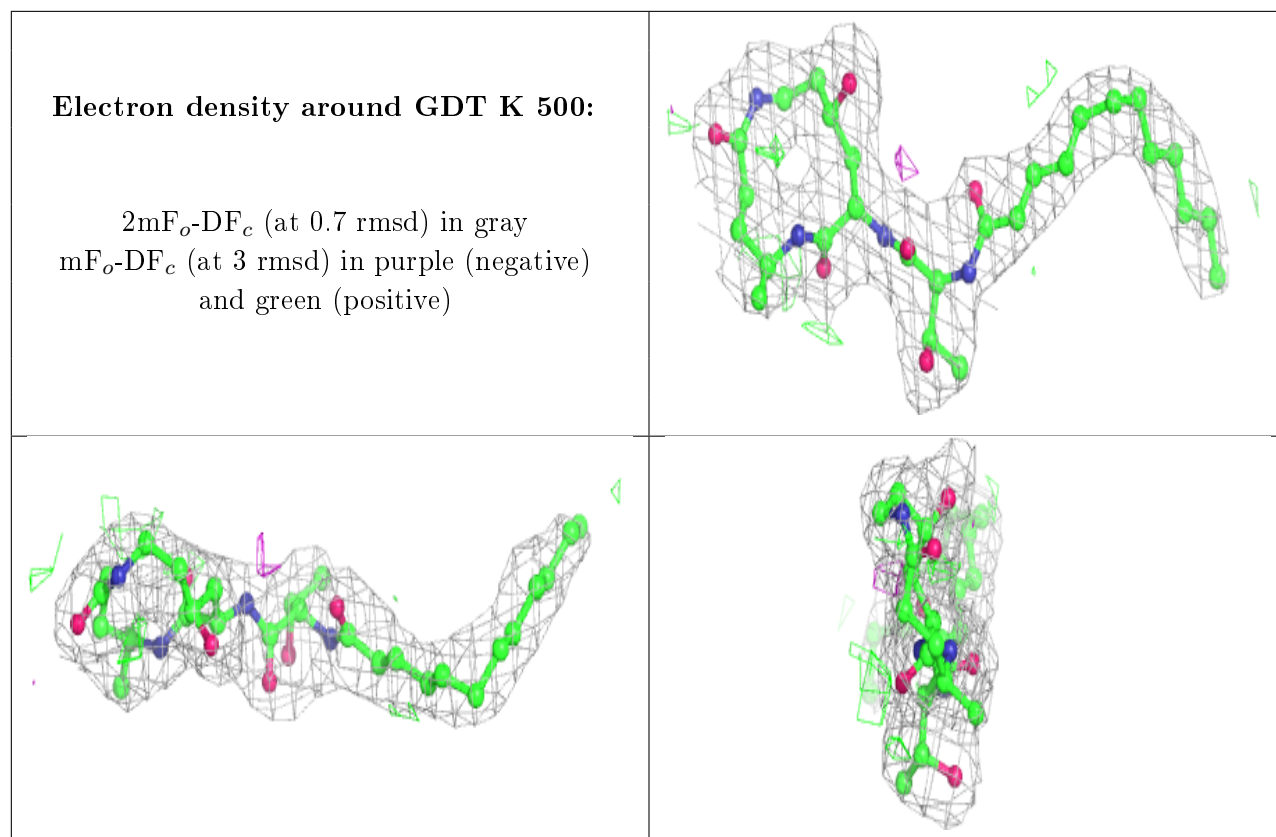
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around GDT Y 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.