



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:57 pm BST

PDB ID : 3NZJ  
Title : Crystal structure of yeast 20S proteasome in complex with ligand 2a  
Authors : Groll, M.; Gallastegui, N.; Marechal, X.; Le Ravalec, V.; Basse, N.; Richy, N.; Genin, E.; Huber, R.; Moroder, M.; Vidal, V.; Reboud-Ravaux, M.  
Deposited on : 2010-07-16  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

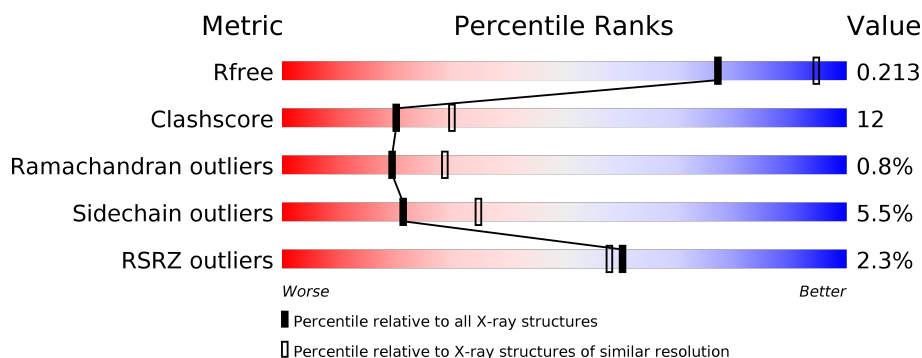
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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>0%</div> <div> <div></div> <div>82%</div> <div>17%</div> <div>•</div> </div> </div>
1	O	250	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>19%</div> <div>•</div> </div> </div>
2	B	258	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>•</div> <div>5%</div> </div> </div>
2	P	258	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>•</div> <div>5%</div> </div> </div>
3	C	254	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>•</div> <div>5%</div> </div> </div>
3	Q	254	<div> <div>10%</div> <div> <div></div> <div>62%</div> <div>30%</div> <div>•</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	261	
8	V	261	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	287	
11	Y	287	
12	L	241	
12	Z	241	
13	1	266	
13	M	266	
14	2	215	
14	N	215	
15	3	5	
15	4	5	

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 51006 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	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

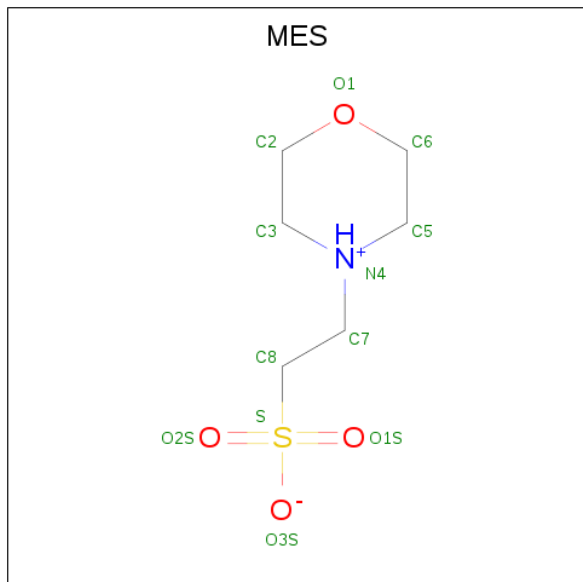
- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called TMC-95A mimic ligand 2a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	5	Total	C	N	O	0	0	0
			54	42	5	7			
15	4	5	Total	C	N	O	0	0	0
			54	42	5	7			

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
16	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	58	Total	O	0	0
			58	58		
17	B	39	Total	O	0	0
			39	39		
17	C	43	Total	O	0	0
			43	43		
17	D	38	Total	O	0	0
			38	38		
17	E	22	Total	O	0	0
			22	22		
17	F	48	Total	O	0	0
			48	48		
17	G	62	Total	O	0	0
			62	62		
17	H	51	Total	O	0	0
			51	51		

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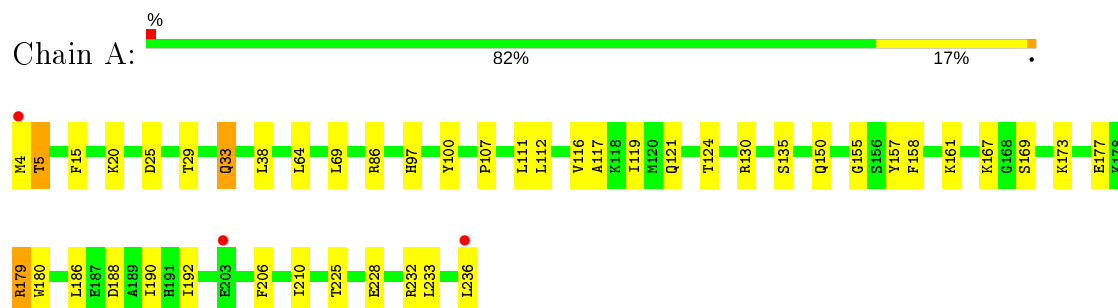
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	I	65	Total 65	O 65	0	0
17	J	52	Total 52	O 52	0	0
17	K	42	Total 42	O 42	0	0
17	L	57	Total 57	O 57	0	0
17	M	71	Total 71	O 71	0	0
17	N	61	Total 61	O 61	0	0
17	O	33	Total 33	O 33	0	0
17	P	30	Total 30	O 30	0	0
17	Q	26	Total 26	O 26	0	0
17	R	31	Total 31	O 31	0	0
17	S	19	Total 19	O 19	0	0
17	T	40	Total 40	O 40	0	0
17	U	61	Total 61	O 61	0	0
17	V	49	Total 49	O 49	0	0
17	W	61	Total 61	O 61	0	0
17	X	48	Total 48	O 48	0	0
17	Y	48	Total 48	O 48	0	0
17	Z	51	Total 51	O 51	0	0
17	1	70	Total 70	O 70	0	0
17	2	60	Total 60	O 60	0	0



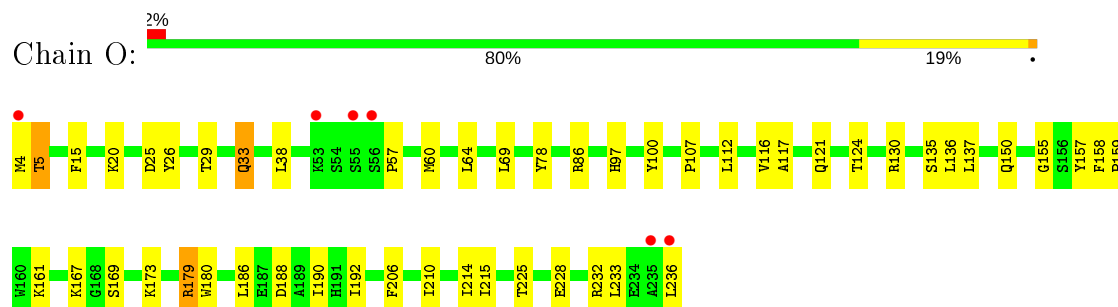
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

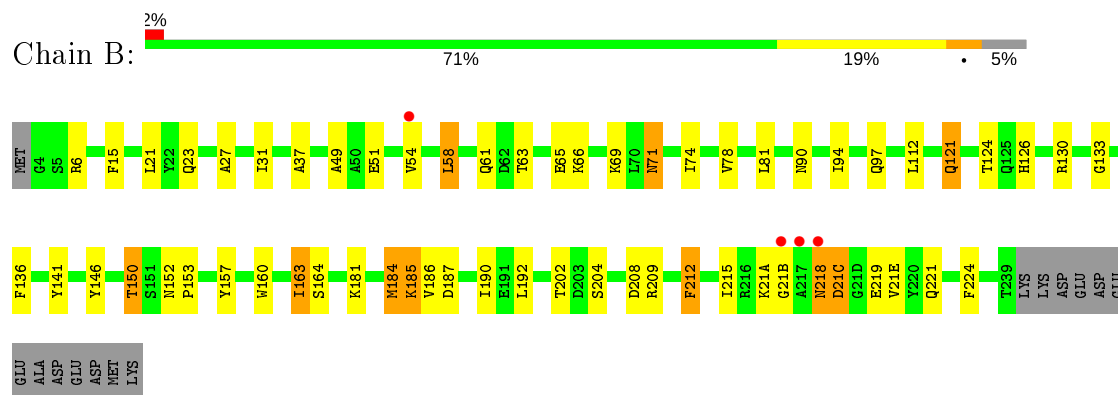
- Molecule 1: Proteasome component Y7



- Molecule 1: Proteasome component Y7

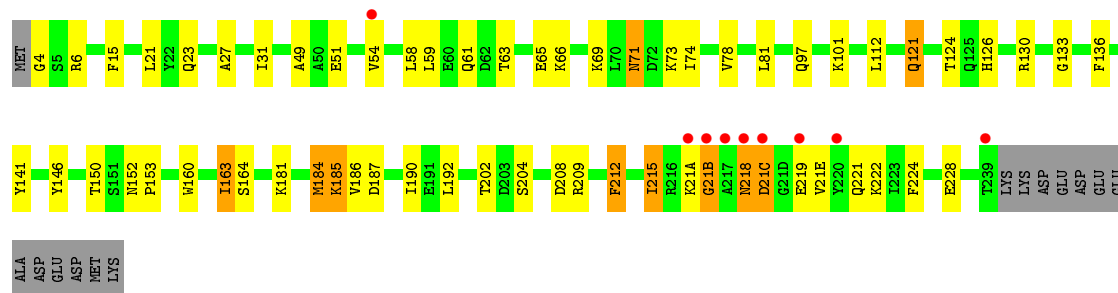


- Molecule 2: Proteasome component Y13

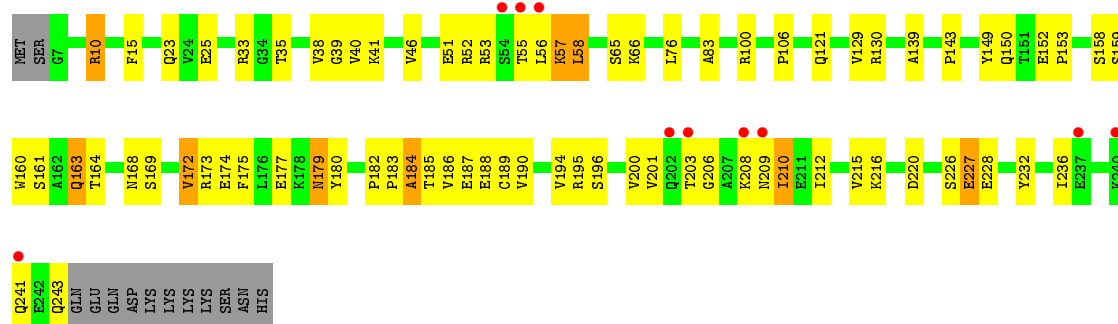


- Molecule 2: Proteasome component Y13

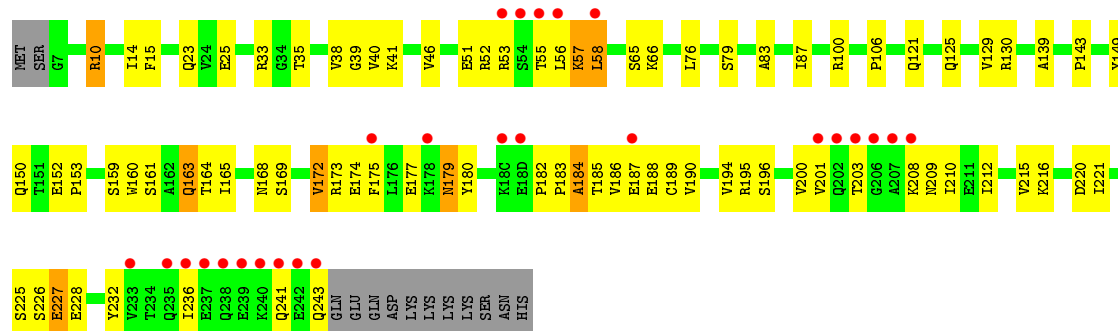




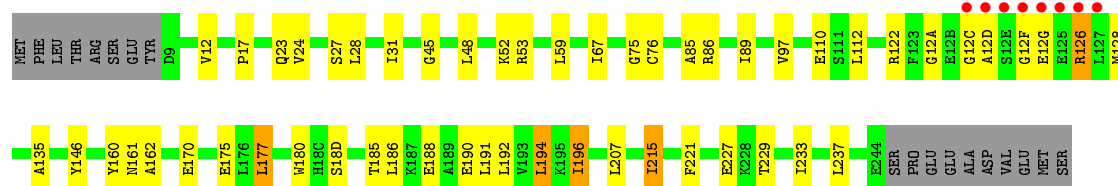
• Molecule 3: Proteasome component PRE6



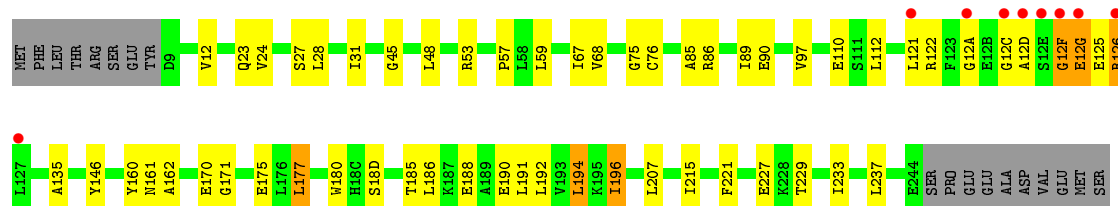
• Molecule 3: Proteasome component PRE6



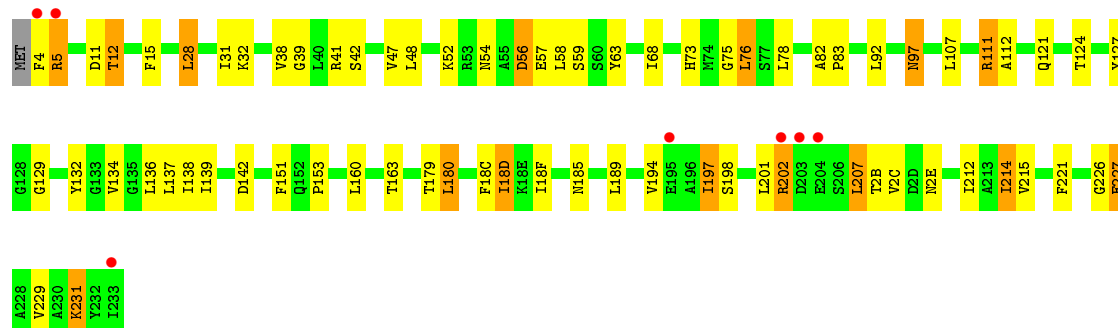
• Molecule 4: Proteasome component PUP2



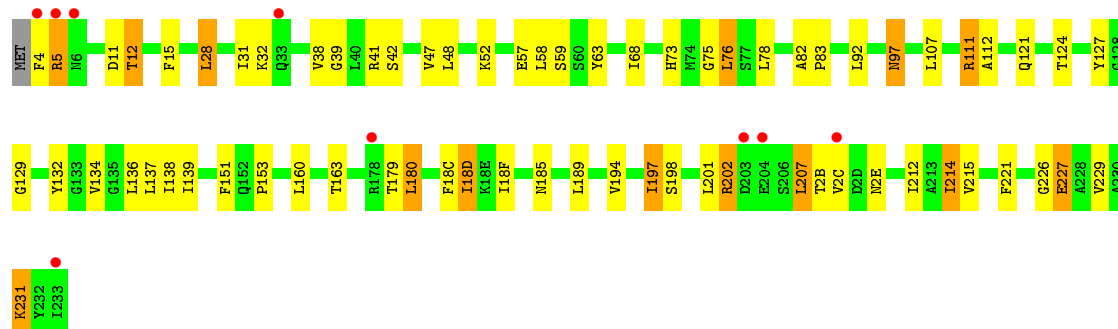
• Molecule 4: Proteasome component PUP2



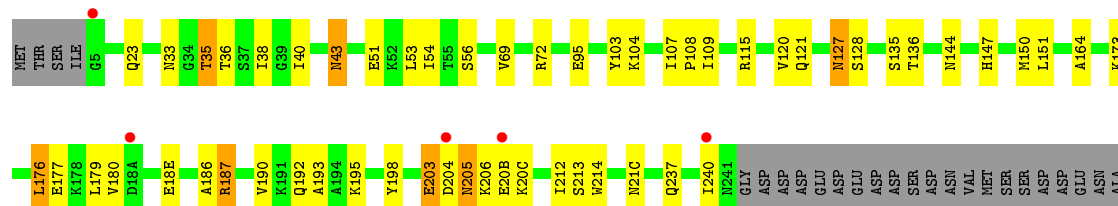
- Molecule 5: Proteasome component PRE5



- Molecule 5: Proteasome component PRE5



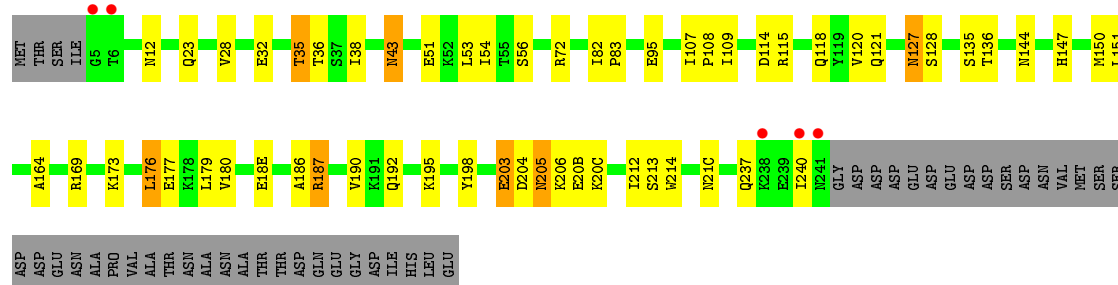
- Molecule 6: Proteasome component C1




PRO VAL  
ALA SER  
THR ILE  
ASN ASN  
ALA ALA  
ASN ALA  
THR THR  
ASP THR  
GLN GLU  
GLY GLY  
ASP ASP  
ILE ILE  
HIS HIS  
LEU LEU  
GLU GLU

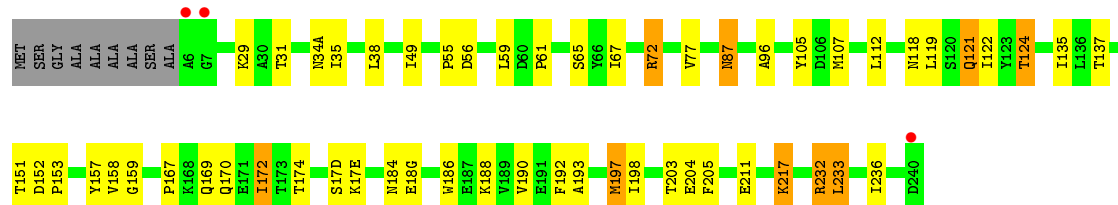
• Molecule 6: Proteasome component C1

Chain T: 



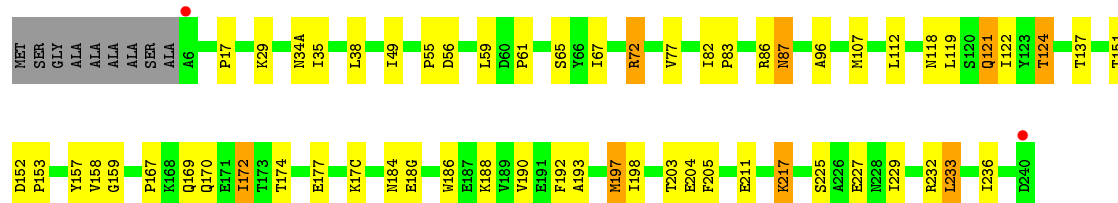
• Molecule 7: Proteasome component C7-alpha

Chain G: 



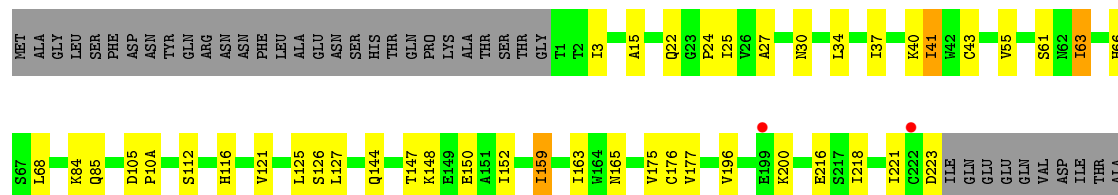
• Molecule 7: Proteasome component C7-alpha

Chain U: 

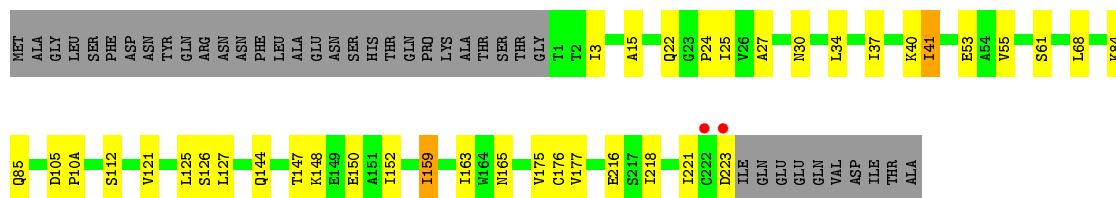


• Molecule 8: Proteasome component PUP1

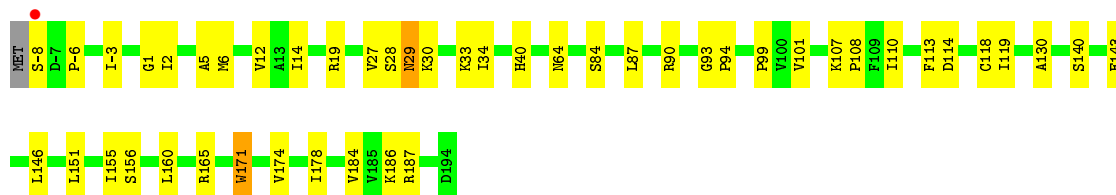
Chain H: 



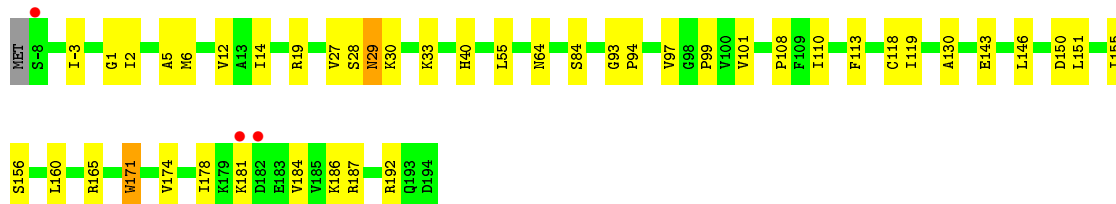
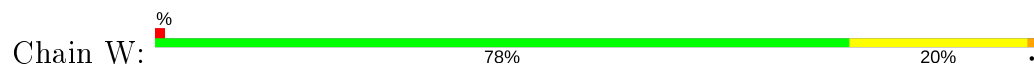
• Molecule 8: Proteasome component PUP1



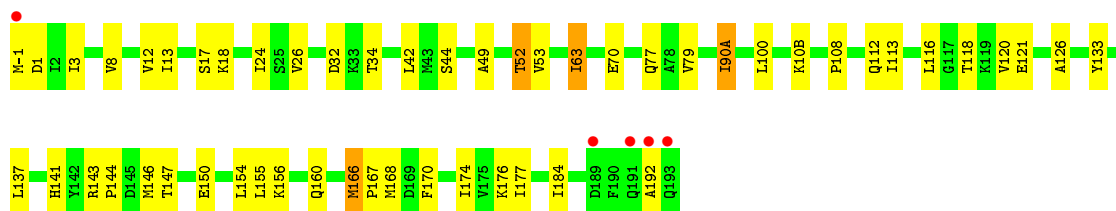
- Molecule 9: Proteasome component PUP3



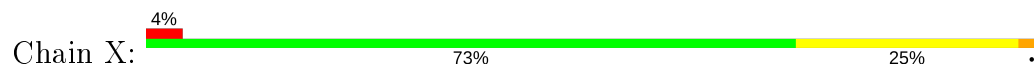
- Molecule 9: Proteasome component PUP3

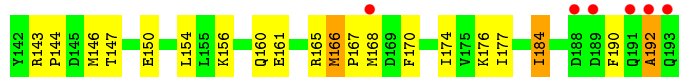


- Molecule 10: Proteasome component C11



- Molecule 10: Proteasome component C11





• Molecule 11: Proteasome component PRE2



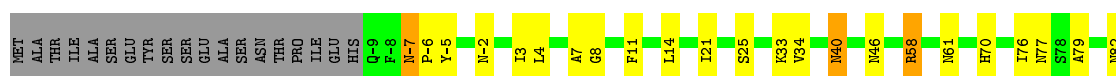
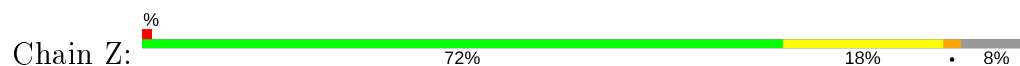
• Molecule 11: Proteasome component PRE2



• Molecule 12: Proteasome component C5

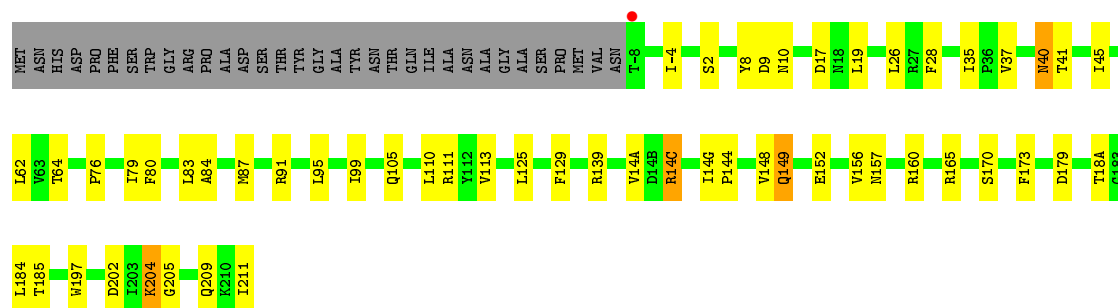


• Molecule 12: Proteasome component C5



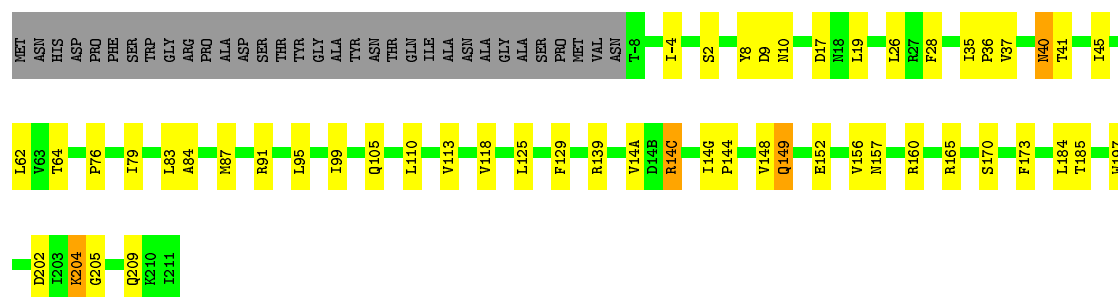
- Molecule 13: Proteasome component PRE4

Chain M:  67% 19% 12%



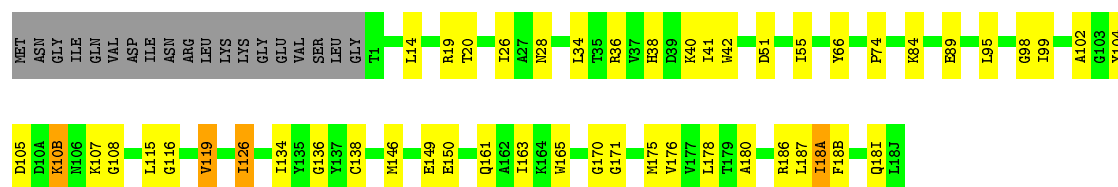
- Molecule 13: Proteasome component PRE4

Chain 1:  68% 18% 12%



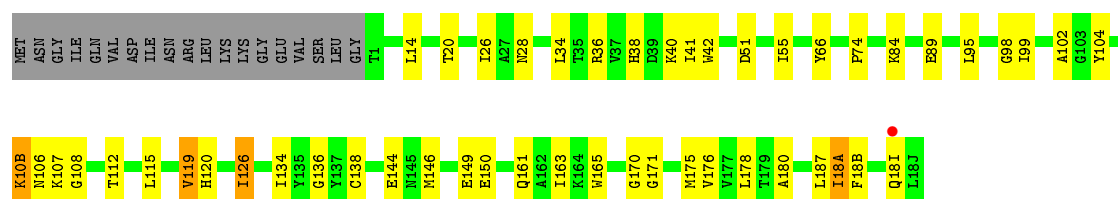
- Molecule 14: Proteasome component PRE3

Chain N:  68% 21% 9%



- Molecule 14: Proteasome component PRE3

Chain 2:  68% 21% 9%



- Molecule 15: TMC-95A mimic ligand 2a

Chain 3:  60% 40%



- Molecule 15: TMC-95A mimic ligand 2a

Chain 4:  60% 40%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.48 Å   301.13 Å   145.37 Å 90.00°   113.57°   90.00°	Depositor
Resolution (Å)	15.00 – 2.40 49.51 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (15.00-2.40) 99.7 (49.51-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.39 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.233   ,   0.249 0.213   ,   0.213	Depositor DCC
$R_{free}$ test set	20797 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	51006	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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: TY5, BOC, ABN, TRO, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.39	0/1952	0.64	0/2642
1	O	0.39	0/1952	0.64	0/2642
2	B	0.38	0/1934	0.63	0/2618
2	P	0.39	0/1934	0.63	0/2618
3	C	0.37	0/1919	0.61	0/2598
3	Q	0.37	0/1919	0.61	0/2598
4	D	0.37	0/1886	0.63	1/2541 (0.0%)
4	R	0.37	0/1886	0.63	0/2541
5	E	0.37	0/1823	0.60	0/2463
5	S	0.37	0/1823	0.61	0/2463
6	F	0.38	0/1936	0.62	0/2614
6	T	0.40	0/1936	0.62	0/2614
7	G	0.43	0/1959	0.63	0/2652
7	U	0.42	0/1959	0.63	0/2652
8	H	0.41	1/1715 (0.1%)	0.67	0/2326
8	V	0.41	0/1715	0.68	0/2326
9	I	0.41	0/1611	0.67	0/2174
9	W	0.41	0/1611	0.68	0/2174
10	J	0.41	0/1613	0.65	0/2173
10	X	0.41	0/1613	0.66	0/2173
11	K	0.41	0/1681	0.67	0/2274
11	Y	0.41	0/1681	0.67	0/2274
12	L	0.42	0/1795	0.68	0/2420
12	Z	0.42	0/1795	0.67	0/2420
13	1	0.42	0/1855	0.68	1/2514 (0.0%)
13	M	0.41	0/1855	0.68	1/2514 (0.0%)
14	2	0.40	0/1541	0.64	0/2087
14	N	0.41	0/1541	0.64	0/2087
15	3	1.25	0/4	0.49	0/4
15	4	1.15	0/4	0.53	0/4
All	All	0.40	1/50448 (0.0%)	0.65	3/68200 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1
12	L	0	1
12	Z	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	43	CYS	CB-SG	-5.11	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	95	LEU	N-CA-C	-5.74	95.49	111.00
13	M	95	LEU	N-CA-C	-5.60	95.88	111.00
4	D	128	MET	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain
1	O	78	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	36	0
1	O	1915	0	1926	40	0
2	B	1904	0	1901	60	0
2	P	1904	0	1901	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1890	0	1900	73	0
3	Q	1890	0	1900	78	0
4	D	1861	0	1836	40	0
4	R	1861	0	1836	41	0
5	E	1795	0	1797	68	0
5	S	1795	0	1797	63	0
6	F	1896	0	1886	41	0
6	T	1896	0	1886	42	0
7	G	1921	0	1910	48	0
7	U	1921	0	1910	57	0
8	H	1684	0	1688	30	0
8	V	1684	0	1688	27	0
9	I	1581	0	1574	42	0
9	W	1581	0	1574	40	0
10	J	1585	0	1590	62	0
10	X	1585	0	1590	62	0
11	K	1644	0	1595	63	0
11	Y	1644	0	1595	62	0
12	L	1757	0	1711	39	0
12	Z	1757	0	1711	40	0
13	1	1824	0	1832	41	0
13	M	1824	0	1832	42	0
14	2	1512	0	1481	42	0
14	N	1512	0	1481	45	0
15	3	54	0	44	7	0
15	4	54	0	44	7	0
16	K	12	0	13	0	0
16	Y	12	0	13	0	0
17	1	70	0	0	1	0
17	2	60	0	0	1	0
17	A	58	0	0	0	0
17	B	39	0	0	1	0
17	C	43	0	0	1	0
17	D	38	0	0	1	0
17	E	22	0	0	1	0
17	F	48	0	0	2	0
17	G	62	0	0	0	0
17	H	51	0	0	3	0
17	I	65	0	0	2	0
17	J	52	0	0	1	0
17	K	42	0	0	3	0
17	L	57	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	M	71	0	0	2	0
17	N	61	0	0	2	0
17	O	33	0	0	0	0
17	P	30	0	0	2	0
17	Q	26	0	0	2	0
17	R	31	0	0	2	0
17	S	19	0	0	1	0
17	T	40	0	0	2	0
17	U	61	0	0	3	0
17	V	49	0	0	3	0
17	W	61	0	0	1	0
17	X	48	0	0	3	0
17	Y	48	0	0	2	0
17	Z	51	0	0	3	0
All	All	51006	0	49368	1238	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 12.

All (1238) 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)
7:U:96:ALA:HA	7:U:107:MET:HE2	1.31	1.12
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.13	1.09
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.11	1.08
2:P:202:THR:HG22	2:P:204:SER:H	1.21	1.06
7:G:96:ALA:HA	7:G:107:MET:HE2	1.33	1.05
2:B:202:THR:HG22	2:B:204:SER:H	1.22	1.03
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.26	0.99
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.11	0.99
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.09	0.99
2:B:15:PHE:H	3:C:23:GLN:HE22	1.04	0.95
10:J:133:TYR:HE1	17:X:876:HOH:O	1.49	0.95
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.47	0.94
10:J:133:TYR:HD1	17:Y:593:HOH:O	1.48	0.94
5:S:15:PHE:H	6:T:23:GLN:HE22	1.12	0.94
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.34	0.92
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.50	0.92
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.53	0.91
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.52	0.91
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:65:SER:HB2	17:Q:303:HOH:O	1.69	0.91
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.52	0.90
14:2:107:LYS:HG2	14:2:108:GLY:H	1.36	0.90
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.55	0.89
5:E:12:THR:HG21	5:E:124:THR:HA	1.55	0.89
5:E:207:LEU:HD23	5:E:207:LEU:H	1.37	0.89
5:E:15:PHE:H	6:F:23:GLN:HE22	1.15	0.89
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.37	0.89
5:S:207:LEU:HD23	5:S:207:LEU:H	1.37	0.88
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	1.84	0.88
10:J:-1:MET:HG2	10:J:1:ASP:H	1.38	0.88
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.38	0.88
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	1.88	0.88
11:K:40:PHE:HB3	11:K:73:ARG:NH2	1.88	0.87
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.20	0.86
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.73	0.86
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.20	0.86
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.82	0.86
14:N:107:LYS:HG2	14:N:108:GLY:H	1.38	0.86
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.74	0.86
1:O:15:PHE:H	2:P:23:GLN:HE22	1.22	0.85
3:C:185:THR:HG22	3:C:187:GLU:H	1.41	0.85
5:S:12:THR:HG21	5:S:124:THR:HA	1.57	0.85
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.57	0.84
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.40	0.84
11:Y:40:PHE:HB3	11:Y:73:ARG:HH21	1.40	0.84
10:X:-1:MET:HG2	10:X:1:ASP:H	1.40	0.84
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.27	0.83
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.21	0.83
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.79	0.83
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.78	0.82
11:K:40:PHE:HB3	11:K:73:ARG:HH21	1.39	0.82
11:K:207:ASN:ND2	10:X:144:PRO:HG3	1.94	0.82
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	1.94	0.82
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.92	0.81
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.80	0.81
11:K:180:GLU:HB3	17:K:924:HOH:O	1.80	0.81
11:K:208:ASN:ND2	9:W:29:ASN:HD21	1.79	0.81
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.45	0.80
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.80	0.80
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.46	0.80
1:A:124:THR:CG2	2:B:130:ARG:HH21	1.95	0.80
2:B:163:ILE:HG13	2:B:164:SER:N	1.98	0.79
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.29	0.79
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.46	0.79
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.64	0.79
2:P:163:ILE:HG13	2:P:164:SER:N	1.98	0.79
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.95	0.79
1:A:15:PHE:H	2:B:23:GLN:HE22	1.30	0.79
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.65	0.78
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.64	0.78
6:F:35:THR:HG21	6:F:51:GLU:O	1.84	0.78
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.81	0.77
6:T:35:THR:HG21	6:T:51:GLU:O	1.85	0.77
13:I:157:ASN:ND2	13:I:160:ARG:HH11	1.82	0.77
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.49	0.77
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.98	0.77
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.32	0.77
3:C:185:THR:HB	3:C:188:GLU:HG2	1.65	0.77
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.47	0.77
2:P:163:ILE:HG13	2:P:164:SER:H	1.50	0.77
11:Y:10(B):LYS:N	11:Y:10(B):LYS:HD2	1.96	0.77
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.67	0.76
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.66	0.76
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.67	0.76
12:L:166:HIS:HD2	12:L:168:GLN:H	1.33	0.76
11:Y:45:MET:HB2	15:4:5:ABN:H5	1.67	0.76
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.31	0.76
9:W:27:VAL:HG13	17:X:622:HOH:O	1.85	0.76
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.66	0.76
3:Q:163:GLN:HA	3:Q:163:GLN:HE21	1.51	0.76
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.68	0.76
10:J:144:PRO:HG3	11:Y:207:ASN:ND2	2.01	0.76
8:H:165:ASN:HD22	13:I:139:ARG:HH11	1.31	0.75
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.31	0.75
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.35	0.75
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.16	0.75
2:B:163:ILE:HG13	2:B:164:SER:H	1.48	0.75
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG12	1.68	0.75
7:G:217:LYS:HE3	7:G:217:LYS:HA	1.69	0.75
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:SER:HB2	17:C:274:HOH:O	1.86	0.74
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.16	0.74
9:I:29:ASN:HD21	11:Y:208:ASN:ND2	1.85	0.74
3:C:15:PHE:H	4:D:23:GLN:HE22	1.35	0.74
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.53	0.74
6:T:127:ASN:HD22	6:T:127:ASN:C	1.91	0.74
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.53	0.73
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.68	0.73
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.68	0.73
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.18	0.73
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.69	0.73
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.34	0.73
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.71	0.73
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.54	0.73
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.68	0.73
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.54	0.73
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.71	0.73
6:T:127:ASN:HD22	6:T:128:SER:N	1.87	0.73
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.04	0.72
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.24	0.72
11:K:45:MET:HB2	15:3:5:ABN:H5	1.71	0.72
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.71	0.72
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.55	0.72
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.01	0.72
11:K:208:ASN:HB3	17:K:776:HOH:O	1.89	0.72
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.05	0.72
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.05	0.72
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.04	0.72
6:F:127:ASN:HD22	6:F:127:ASN:C	1.92	0.72
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.55	0.72
4:R:207:LEU:CD2	4:R:233:ILE:HD12	2.20	0.72
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.25	0.71
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.72	0.71
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.72	0.71
9:W:192:ARG:HG3	17:W:201:HOH:O	1.89	0.71
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.20	0.71
11:Y:99:THR:HG22	11:Y:113:VAL:O	1.89	0.71
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.55	0.71
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.54	0.71
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.73	0.71
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.71	0.71
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.56	0.71
10:X:90(A):ILE:O	10:X:90(A):ILE:HD13	1.90	0.71
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.39	0.71
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.21	0.71
10:J:-1:MET:HG2	10:J:1:ASP:N	2.05	0.71
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.56	0.71
10:J:90(A):ILE:O	10:J:90(A):ILE:HD13	1.90	0.71
4:R:207:LEU:HD21	4:R:233:ILE:HD12	1.71	0.70
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.26	0.70
5:S:214:ILE:HG13	5:S:215:VAL:N	2.07	0.70
5:E:198:SER:HA	5:E:201:LEU:HG	1.74	0.70
12:L:98:HIS:HD2	17:L:199:HOH:O	1.73	0.70
2:P:121:GLN:O	2:P:124:THR:HB	1.89	0.70
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.73	0.70
2:B:202:THR:HG22	2:B:204:SER:N	2.04	0.70
6:F:127:ASN:HD22	6:F:128:SER:N	1.90	0.70
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.74	0.70
3:C:163:GLN:NE2	3:C:164:THR:H	1.90	0.69
7:U:227:GLU:HG2	17:U:1255:HOH:O	1.91	0.69
2:B:121:GLN:O	2:B:124:THR:HB	1.92	0.69
10:X:-1:MET:HG2	10:X:1:ASP:N	2.06	0.69
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.21	0.69
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.40	0.69
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.05	0.69
14:2:34:LEU:HD13	14:2:176:VAL:HG23	1.74	0.69
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.22	0.69
4:D:207:LEU:CD2	4:D:233:ILE:HD12	2.22	0.69
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.57	0.69
7:U:96:ALA:CA	7:U:107:MET:HE2	2.18	0.69
4:R:121:LEU:HB2	17:R:853:HOH:O	1.92	0.69
5:S:198:SER:HA	5:S:201:LEU:HG	1.75	0.68
6:T:237:GLN:O	6:T:240:ILE:HG22	1.93	0.68
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.05	0.68
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.27	0.68
5:S:132:TYR:O	5:S:153:PRO:HB3	1.93	0.68
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.23	0.68
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.74	0.68
3:C:232:TYR:O	3:C:236:ILE:HG13	1.92	0.68
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.23	0.68
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.75	0.68
11:K:99:THR:HG22	11:K:113:VAL:O	1.92	0.68
4:D:207:LEU:HD21	4:D:233:ILE:HD12	1.75	0.68
5:E:214:ILE:HG13	5:E:215:VAL:N	2.07	0.68
1:O:97:HIS:HD2	8:V:61:SER:OG	1.76	0.68
6:F:237:GLN:O	6:F:240:ILE:HG22	1.94	0.68
11:K:142:TYR:O	11:K:143:LYS:HD2	1.94	0.68
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.94	0.68
2:P:202:THR:HG22	2:P:204:SER:N	2.03	0.68
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.76	0.67
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.75	0.67
10:X:32:ASP:OD2	10:X:34:THR:HG22	1.95	0.67
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.58	0.67
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.93	0.67
3:Q:232:TYR:O	3:Q:236:ILE:HG13	1.94	0.67
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.77	0.67
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.30	0.67
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.08	0.67
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.94	0.67
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.76	0.67
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.77	0.67
9:I:6:MET:HE3	9:I:155:ILE:HA	1.77	0.67
2:B:185:LYS:HE2	2:B:187:ASP:OD1	1.95	0.66
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.58	0.66
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.11	0.66
14:2:107:LYS:HG2	14:2:108:GLY:N	2.09	0.66
4:D:31:ILE:HD13	4:D:135:ALA:HB2	1.76	0.66
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.93	0.66
1:O:121:GLN:O	1:O:124:THR:HB	1.96	0.66
9:I:6:MET:HE3	9:I:155:ILE:HD12	1.76	0.66
10:J:32:ASP:OD2	10:J:34:THR:HG22	1.96	0.66
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.78	0.66
7:G:96:ALA:CA	7:G:107:MET:HE2	2.19	0.65
10:X:10(B):LYS:NZ	10:X:10(B):LYS:HB2	2.10	0.65
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.31	0.65
1:A:121:GLN:O	1:A:124:THR:HB	1.95	0.65
11:K:38:ASN:O	11:K:40:PHE:N	2.30	0.65
14:N:107:LYS:HG2	14:N:108:GLY:N	2.10	0.65
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.95	0.65
10:J:156:LYS:O	10:J:160:GLN:HG3	1.97	0.65
9:W:6:MET:HE3	9:W:155:ILE:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:40:ASN:HD22	13:1:40:ASN:H	1.44	0.65
13:M:40:ASN:H	13:M:40:ASN:HD22	1.44	0.65
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.43	0.64
5:E:132:TYR:O	5:E:153:PRO:HB3	1.96	0.64
2:B:160:TRP:CE2	2:B:163:ILE:HD13	2.33	0.64
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.27	0.64
7:G:121:GLN:O	7:G:124:THR:HB	1.97	0.64
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.44	0.64
11:Y:38:ASN:O	11:Y:40:PHE:N	2.31	0.64
9:I:90:ARG:HD2	17:I:1159:HOH:O	1.96	0.64
2:P:160:TRP:CE2	2:P:163:ILE:HD13	2.33	0.64
5:E:15:PHE:H	6:F:23:GLN:NE2	1.94	0.64
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.12	0.64
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.27	0.64
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.11	0.64
3:C:186:VAL:O	3:C:190:VAL:HG23	1.98	0.63
11:K:12:ILE:HG21	11:K:110:ILE:HD11	1.80	0.63
4:R:186:LEU:O	4:R:190:GLU:HG3	1.98	0.63
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.82	0.62
3:Q:186:VAL:O	3:Q:190:VAL:HG23	1.99	0.62
9:W:6:MET:HE3	9:W:155:ILE:HD12	1.81	0.62
13:1:14(A):VAL:O	13:1:14(A):VAL:HG23	2.00	0.62
3:Q:190:VAL:O	3:Q:194:VAL:HG23	1.98	0.62
4:D:186:LEU:O	4:D:190:GLU:HG3	1.97	0.62
10:X:90(A):ILE:HG13	10:X:116:LEU:HD23	1.81	0.62
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.81	0.62
5:E:226:GLY:O	5:E:229:VAL:HG22	2.00	0.62
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.12	0.62
3:Q:195:ARG:CG	3:Q:236:ILE:HD13	2.27	0.62
4:R:207:LEU:C	4:R:207:LEU:HD23	2.19	0.62
3:C:175:PHE:O	3:C:179:ASN:HB2	1.99	0.62
3:C:57:LYS:O	3:C:58:LEU:HB2	1.99	0.62
1:A:97:HIS:HD2	8:H:61:SER:OG	1.81	0.62
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.81	0.62
11:K:208:ASN:HD21	9:W:29:ASN:HD21	1.46	0.62
10:J:90(A):ILE:HG13	10:J:116:LEU:HD23	1.82	0.61
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.65	0.61
2:P:185:LYS:HE2	2:P:187:ASP:OD1	1.99	0.61
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.83	0.61
8:V:126:SER:O	8:V:127:LEU:HD23	2.00	0.61
5:E:207:LEU:CD2	5:E:207:LEU:H	2.10	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:85:ALA:O	4:R:89:ILE:HG12	2.00	0.61
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.00	0.61
12:Z:96:TYR:CE1	15:4:2:TY5:H49	2.36	0.61
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.66	0.61
13:1:37:VAL:HG11	13:1:79:ILE:HD13	1.82	0.61
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.82	0.61
5:S:226:GLY:O	5:S:229:VAL:HG22	2.01	0.61
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.66	0.61
7:G:59:LEU:O	7:G:61:PRO:HD3	2.01	0.61
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.83	0.61
7:G:233:LEU:O	7:G:236:ILE:HG13	2.01	0.61
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.64	0.61
6:T:109:ILE:HD13	6:T:109:ILE:N	2.16	0.61
3:C:190:VAL:O	3:C:194:VAL:HG23	2.00	0.61
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.31	0.61
13:M:-4:ILE:HD13	14:N:115:LEU:HB3	1.83	0.61
10:X:156:LYS:O	10:X:160:GLN:HG3	2.00	0.61
8:H:126:SER:O	8:H:127:LEU:HD23	2.00	0.61
11:Y:12:ILE:HG21	11:Y:110:ILE:HD11	1.82	0.60
10:J:168:MET:HE1	10:X:167:PRO:CB	2.31	0.60
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.01	0.60
3:C:163:GLN:CA	3:C:163:GLN:HE21	2.14	0.60
5:E:38:VAL:HG23	5:E:197:ILE:HD12	1.83	0.60
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.63	0.60
14:2:18(A):ILE:HD13	14:2:18(B):PHE:N	2.17	0.60
5:E:18(D):ILE:O	5:E:18(D):ILE:HD13	2.01	0.60
4:D:229:THR:O	4:D:233:ILE:HG12	2.02	0.60
10:J:133:TYR:CE1	17:X:876:HOH:O	2.37	0.60
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	2.01	0.60
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.82	0.60
2:B:112:LEU:C	2:B:112:LEU:HD23	2.22	0.60
14:N:126:ILE:HD13	14:N:126:ILE:H	1.66	0.60
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.83	0.60
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.34	0.60
8:H:218:ILE:N	8:H:218:ILE:HD12	2.17	0.60
14:N:18(A):ILE:HD13	14:N:18(B):PHE:N	2.17	0.60
5:S:207:LEU:H	5:S:207:LEU:CD2	2.10	0.60
3:C:41:LYS:HG2	3:C:161:SER:O	2.02	0.60
3:C:163:GLN:HE21	3:C:164:THR:H	1.50	0.60
3:C:195:ARG:CG	3:C:236:ILE:HD13	2.28	0.60
4:D:85:ALA:O	4:D:89:ILE:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:112:GLN:NE2	10:J:126:ALA:H	2.00	0.60
11:K:73:ARG:NH2	11:K:104:TYR:O	2.34	0.60
7:U:233:LEU:O	7:U:236:ILE:HG13	2.01	0.60
10:X:112:GLN:NE2	10:X:126:ALA:H	2.00	0.60
4:R:229:THR:O	4:R:233:ILE:HG12	2.02	0.59
14:2:126:ILE:H	14:2:126:ILE:HD13	1.66	0.59
4:D:207:LEU:HD23	4:D:207:LEU:C	2.21	0.59
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.37	0.59
5:S:38:VAL:HG23	5:S:197:ILE:HD12	1.84	0.59
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.32	0.59
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.37	0.59
5:S:15:PHE:H	6:T:23:GLN:NE2	1.93	0.59
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.67	0.59
8:V:218:ILE:HD12	8:V:218:ILE:N	2.18	0.59
5:S:18(D):ILE:HD13	5:S:18(D):ILE:O	2.02	0.59
10:X:52:THR:HG22	10:X:53:VAL:N	2.18	0.58
10:J:52:THR:HG22	10:J:53:VAL:N	2.18	0.58
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.85	0.58
12:L:114:ASP:CB	12:L:118:SER:HB3	2.32	0.58
7:U:107:MET:CE	7:U:112:LEU:HD13	2.34	0.58
12:L:96:TYR:CE1	15:3:2:TY5:H49	2.38	0.58
11:Y:1:THR:OG1	15:4:5:ABN:H2A	2.04	0.58
1:A:188:ASP:O	1:A:192:ILE:HG12	2.04	0.58
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.86	0.58
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.00	0.58
10:J:167:PRO:CB	10:X:168:MET:HE1	2.34	0.58
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.86	0.58
13:1:-4:ILE:HD13	14:2:115:LEU:HB3	1.86	0.58
14:N:98:GLY:C	14:N:99:ILE:HD13	2.24	0.58
7:U:121:GLN:O	7:U:124:THR:HB	2.02	0.58
12:Z:114:ASP:CB	12:Z:118:SER:HB3	2.33	0.58
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.86	0.57
2:P:185:LYS:HD3	2:P:186:VAL:N	2.19	0.57
11:Y:4:LEU:CD1	11:Y:15:ALA:HB3	2.34	0.57
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.99	0.57
7:U:59:LEU:O	7:U:61:PRO:HD3	2.04	0.57
4:R:207:LEU:HD21	4:R:233:ILE:CD1	2.33	0.57
14:2:107:LYS:CG	14:2:108:GLY:H	2.14	0.57
3:C:185:THR:HG22	3:C:187:GLU:N	2.14	0.57
2:P:112:LEU:HD23	2:P:112:LEU:C	2.24	0.57
14:2:51:ASP:O	14:2:55:ILE:HD12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:51:ASP:O	14:N:55:ILE:HD12	2.05	0.57
3:C:46:VAL:O	3:C:215:VAL:HG12	2.05	0.57
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.70	0.57
6:F:69:VAL:HG12	17:F:319:HOH:O	2.04	0.57
10:J:13:ILE:N	10:J:13:ILE:HD12	2.20	0.57
11:K:1:THR:OG1	15:3:5:ABN:H2A	2.04	0.57
2:B:185:LYS:HD3	2:B:186:VAL:N	2.19	0.57
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.86	0.56
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.53	0.56
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.87	0.56
3:C:241:GLN:C	3:C:243:GLN:H	2.07	0.56
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.86	0.56
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.39	0.56
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.86	0.56
12:L:148:VAL:O	12:L:152:ILE:HG12	2.05	0.56
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.85	0.56
7:U:77:VAL:CG1	7:U:137:THR:HB	2.34	0.56
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.87	0.56
9:I:29:ASN:HD21	11:Y:208:ASN:HD21	1.53	0.56
10:J:24:ILE:O	10:X:133:TYR:OH	2.20	0.56
3:Q:241:GLN:C	3:Q:243:GLN:H	2.07	0.56
13:M:19:LEU:HD12	13:M:28:PHE:O	2.05	0.56
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.52	0.56
13:1:19:LEU:HD12	13:1:28:PHE:O	2.06	0.56
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.88	0.56
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.74	0.56
13:1:37:VAL:HG11	13:1:79:ILE:CD1	2.36	0.56
14:2:146:MET:HE3	14:2:150:GLU:HB3	1.88	0.56
4:D:207:LEU:HD21	4:D:233:ILE:CD1	2.35	0.56
11:K:10(B):LYS:CD	11:K:10(B):LYS:N	2.63	0.56
12:L:145:TYR:CD1	12:L:146:LEU:N	2.73	0.56
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.54	0.55
5:E:76:LEU:O	5:E:76:LEU:HD23	2.07	0.55
9:I:113:PHE:HA	9:I:118:CYS:O	2.05	0.55
1:O:60:MET:HE1	17:U:400:HOH:O	2.06	0.55
11:K:12:ILE:HB	11:K:178:VAL:HB	1.89	0.55
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.87	0.55
11:K:140:SER:OG	10:X:137:LEU:HD21	2.07	0.55
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.86	0.55
7:U:172:ILE:HD13	7:U:197:MET:CE	2.37	0.55
14:N:105:ASP:HB2	17:N:775:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.41	0.55
13:M:37:VAL:HG11	13:M:79:ILE:HD13	1.88	0.55
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.88	0.55
8:V:34:LEU:HB2	17:V:578:HOH:O	2.06	0.55
4:D:175:GLU:HB3	4:D:196:ILE:HD13	1.89	0.55
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.89	0.55
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.07	0.55
6:T:147:HIS:HD2	17:T:282:HOH:O	1.88	0.55
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.89	0.55
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.54	0.55
7:G:77:VAL:CG1	7:G:137:THR:HB	2.37	0.55
10:J:133:TYR:OH	10:X:24:ILE:O	2.24	0.55
10:X:13:ILE:N	10:X:13:ILE:HD12	2.22	0.55
14:2:98:GLY:C	14:2:99:ILE:HD13	2.27	0.55
5:E:78:LEU:HD12	5:E:78:LEU:C	2.27	0.55
9:W:178:ILE:HG23	9:W:184:VAL:HG22	1.89	0.55
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.42	0.55
10:J:10(B):LYS:HB2	10:J:10(B):LYS:HZ2	1.70	0.55
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.36	0.55
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.89	0.55
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.54	0.55
13:1:148:VAL:HG23	17:1:182:HOH:O	2.07	0.54
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.89	0.54
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.72	0.54
1:O:4:MET:SD	1:O:5:THR:N	2.67	0.54
5:S:76:LEU:O	5:S:76:LEU:HD23	2.07	0.54
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.89	0.54
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.89	0.54
12:L:96:TYR:CD1	15:3:2:TY5:H49	2.42	0.54
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.23	0.54
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.38	0.54
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.54	0.54
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.89	0.54
6:T:127:ASN:ND2	6:T:127:ASN:C	2.61	0.54
6:T:187:ARG:HG3	6:T:187:ARG:HH11	1.72	0.54
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.72	0.54
7:G:172:ILE:HD13	7:G:197:MET:CE	2.37	0.54
9:I:12:VAL:HG23	9:I:178:ILE:HB	1.88	0.54
10:X:52:THR:CG2	10:X:53:VAL:N	2.71	0.54
12:L:123:GLN:HG3	12:L:145:TYR:OH	2.08	0.54
8:V:148:LYS:O	8:V:152:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:221:ILE:HD12	9:W:40:HIS:HA	1.90	0.54
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.54	0.54
1:O:188:ASP:O	1:O:192:ILE:HG12	2.07	0.54
3:Q:195:ARG:HG3	3:Q:236:ILE:CD1	2.34	0.54
11:Y:31:VAL:HG11	15:4:5:ABN:H3	1.90	0.54
2:B:181:LYS:O	2:B:184:MET:HG3	2.08	0.54
10:J:141:HIS:HB2	10:J:154:LEU:HD11	1.90	0.54
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.89	0.54
17:V:1181:HOH:O	9:W:150:ASP:HA	2.06	0.54
12:Z:96:TYR:CD1	15:4:2:TY5:H49	2.43	0.54
14:2:176:VAL:HG12	14:2:178:LEU:CD1	2.37	0.54
1:A:206:PHE:CE1	1:A:210:ILE:HD11	2.43	0.54
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.90	0.54
7:G:107:MET:CE	7:G:112:LEU:HD13	2.37	0.54
14:N:176:VAL:HG12	14:N:178:LEU:CD1	2.38	0.54
3:Q:41:LYS:HG2	3:Q:161:SER:O	2.07	0.54
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.89	0.54
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.44	0.54
12:Z:99:THR:CG2	17:Z:231:HOH:O	2.56	0.54
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.89	0.53
11:K:40:PHE:CB	11:K:73:ARG:NH2	2.66	0.53
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.43	0.53
5:E:73:HIS:HE1	5:E:107:LEU:O	1.92	0.53
1:O:159:PRO:O	2:P:59:LEU:HD12	2.08	0.53
5:S:78:LEU:HD12	5:S:78:LEU:C	2.29	0.53
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.38	0.53
9:W:113:PHE:HA	9:W:118:CYS:O	2.07	0.53
11:K:208:ASN:O	9:W:30:LYS:NZ	2.41	0.53
3:C:195:ARG:HG3	3:C:236:ILE:CD1	2.33	0.53
11:K:31:VAL:HG11	15:3:5:ABN:H3	1.90	0.53
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.91	0.53
6:F:109:ILE:HD13	6:F:109:ILE:N	2.22	0.53
11:K:31:VAL:HG11	15:3:5:ABN:C3	2.39	0.53
14:2:10(B):LYS:C	14:2:10(B):LYS:HD3	2.29	0.53
12:Z:148:VAL:O	12:Z:152:ILE:HG12	2.09	0.53
4:D:192:LEU:O	4:D:196:ILE:HG13	2.09	0.53
4:D:194:LEU:HG	4:D:233:ILE:HD13	1.91	0.53
10:J:133:TYR:CE2	10:J:166:MET:HG2	2.43	0.53
5:S:73:HIS:HE1	5:S:107:LEU:O	1.91	0.53
9:W:12:VAL:HG23	9:W:178:ILE:HB	1.90	0.53
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	2.04	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.43	0.53
10:J:52:THR:CG2	10:J:53:VAL:N	2.70	0.53
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.43	0.53
6:F:173:LYS:O	6:F:177:GLU:HG3	2.09	0.53
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.39	0.53
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.90	0.53
1:A:4:MET:SD	1:A:5:THR:N	2.67	0.53
5:E:160:LEU:HD13	5:E:163:THR:HB	1.91	0.53
7:G:198:ILE:HG23	7:G:203:THR:O	2.07	0.53
5:S:160:LEU:HD13	5:S:163:THR:HB	1.91	0.53
7:U:198:ILE:HG23	7:U:203:THR:O	2.08	0.53
8:V:175:VAL:HG12	8:V:176:CYS:N	2.24	0.53
11:Y:143:LYS:HB2	11:Y:146:LEU:HD11	1.89	0.53
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.90	0.53
9:I:178:ILE:HG23	9:I:184:VAL:HG22	1.91	0.53
10:J:42:LEU:HB2	10:J:184:ILE:HD13	1.91	0.53
2:P:215:ILE:HD13	2:P:221:GLN:HG2	1.91	0.53
6:T:203:GLU:O	6:T:206:LYS:HD2	2.09	0.53
10:X:141:HIS:HB2	10:X:154:LEU:HD11	1.89	0.53
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	2.09	0.53
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.10	0.52
11:Y:31:VAL:HG11	15:4:5:ABN:C3	2.39	0.52
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.25	0.52
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.09	0.52
5:S:52:LYS:HB3	5:S:63:TYR:HB3	1.90	0.52
11:Y:45:MET:CB	15:4:5:ABN:H5	2.36	0.52
11:K:143:LYS:HB2	11:K:146:LEU:HD11	1.90	0.52
12:L:185:ARG:NH1	17:L:1161:HOH:O	2.35	0.52
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.29	0.52
5:E:194:VAL:O	5:E:197:ILE:HG22	2.09	0.52
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.90	0.52
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.44	0.52
13:1:149:GLN:H	13:1:149:GLN:NE2	2.07	0.52
2:B:121:GLN:HG3	3:C:83:ALA:HB1	1.92	0.52
5:E:207:LEU:HD23	5:E:207:LEU:N	2.17	0.52
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.10	0.52
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.91	0.52
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.74	0.52
11:Y:40:PHE:CB	11:Y:73:ARG:NH2	2.66	0.52
3:C:57:LYS:HD2	3:C:58:LEU:N	2.24	0.52
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.91	0.52
3:C:169:SER:HA	3:C:172:VAL:CG1	2.40	0.52
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.39	0.52
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.90	0.52
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.10	0.52
11:K:180:GLU:N	17:K:924:HOH:O	2.42	0.52
1:O:206:PHE:CE1	1:O:210:ILE:HD11	2.45	0.52
13:1:40:ASN:HD22	13:1:40:ASN:N	2.05	0.51
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.91	0.51
3:C:227:GLU:OE1	3:C:227:GLU:N	2.41	0.51
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.75	0.51
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.45	0.51
14:N:34:LEU:CD1	14:N:176:VAL:HG23	2.39	0.51
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.40	0.51
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.25	0.51
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.40	0.51
4:R:194:LEU:HG	4:R:233:ILE:HD13	1.92	0.51
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.92	0.51
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.92	0.51
9:I:6:MET:CE	9:I:155:ILE:HA	2.41	0.51
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.05	0.51
10:X:133:TYR:CE2	10:X:166:MET:HG2	2.44	0.51
11:Y:179:THR:HB	17:Y:812:HOH:O	2.10	0.51
14:2:34:LEU:CD1	14:2:176:VAL:HG23	2.41	0.51
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.75	0.51
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.57	0.51
3:C:40:VAL:HG23	3:C:189:CYS:SG	2.51	0.51
3:C:41:LYS:HD3	3:C:161:SER:HA	1.93	0.51
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.43	0.51
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.90	0.51
17:T:284:HOH:O	7:U:86:ARG:HD2	2.10	0.51
10:J:168:MET:CE	10:X:168:MET:CE	2.89	0.51
7:G:107:MET:HE1	7:G:112:LEU:HD13	1.93	0.51
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.93	0.51
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.45	0.51
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.11	0.51
7:G:96:ALA:HA	7:G:107:MET:CE	2.23	0.51
12:Z:134:ILE:HD11	12:Z:162:ALA:HB2	1.92	0.51
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.92	0.51
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.24	0.51
8:V:53:GLU:HB2	17:V:1327:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.41	0.51
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.75	0.51
2:P:27:ALA:O	2:P:31:ILE:HG12	2.11	0.51
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.93	0.51
9:I:27:VAL:HG13	17:J:898:HOH:O	2.10	0.51
11:K:4:LEU:HD13	11:K:15:ALA:O	2.11	0.51
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.75	0.51
6:T:173:LYS:O	6:T:177:GLU:HG3	2.11	0.51
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.46	0.50
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.92	0.50
13:M:149:GLN:NE2	13:M:149:GLN:H	2.10	0.50
13:M:17:ASP:HA	13:M:173:PHE:CB	2.41	0.50
14:N:99:ILE:HD13	14:N:99:ILE:N	2.26	0.50
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.92	0.50
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.41	0.50
3:Q:40:VAL:HG23	3:Q:189:CYS:SG	2.51	0.50
5:S:227:GLU:CD	5:S:227:GLU:H	2.13	0.50
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.94	0.50
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.92	0.50
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.92	0.50
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.93	0.50
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.27	0.50
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.45	0.50
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.11	0.50
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.76	0.50
8:H:148:LYS:O	8:H:152:ILE:HG12	2.11	0.50
7:U:96:ALA:HA	7:U:107:MET:CE	2.22	0.50
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.26	0.50
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.23	0.50
8:H:41:ILE:HD13	8:H:41:ILE:N	2.27	0.50
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.11	0.50
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.47	0.50
7:G:77:VAL:HG12	7:G:137:THR:HB	1.93	0.50
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.76	0.50
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.93	0.50
12:L:21:ILE:HD12	12:L:21:ILE:C	2.30	0.50
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.94	0.50
7:U:77:VAL:HG12	7:U:137:THR:HB	1.92	0.50
13:M:37:VAL:HG11	13:M:79:ILE:CD1	2.42	0.50
9:W:6:MET:CE	9:W:155:ILE:HA	2.41	0.50
13:I:76:PRO:HD2	13:I:105:GLN:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:GLU:CD	3:C:227:GLU:H	2.15	0.50
5:E:227:GLU:CD	5:E:227:GLU:H	2.14	0.50
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	1.93	0.50
11:K:40:PHE:CB	11:K:73:ARG:HH21	2.18	0.50
1:O:33:GLN:HA	1:O:33:GLN:HE21	1.77	0.50
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.93	0.50
10:X:52:THR:HG22	10:X:53:VAL:HG23	1.93	0.50
13:1:17:ASP:HA	13:1:173:PHE:CB	2.42	0.49
3:C:152:GLU:HB2	3:C:153:PRO:HD2	1.94	0.49
5:E:18(C):PHE:HA	5:E:18(F):ILE:CG1	2.39	0.49
12:L:93:PHE:N	12:L:94:PRO:HD3	2.27	0.49
2:P:181:LYS:O	2:P:184:MET:HG3	2.11	0.49
5:S:194:VAL:O	5:S:197:ILE:HG22	2.12	0.49
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.41	0.49
10:J:52:THR:HG22	10:J:53:VAL:H	1.77	0.49
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.26	0.49
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.47	0.49
14:2:134:ILE:HD12	14:2:138:CYS:SG	2.51	0.49
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.77	0.49
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.94	0.49
4:R:53:ARG:HG2	4:R:53:ARG:O	2.12	0.49
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.27	0.49
11:Y:4:LEU:HD13	11:Y:15:ALA:O	2.12	0.49
17:R:886:HOH:O	12:Z:70:HIS:HE1	1.95	0.49
7:G:87:ASN:HD22	7:G:87:ASN:C	2.16	0.49
5:S:207:LEU:N	5:S:207:LEU:HD23	2.17	0.49
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.35	0.49
6:T:186:ALA:O	6:T:190:VAL:HG23	2.12	0.49
9:W:84:SER:OG	9:W:119:ILE:HD11	2.11	0.49
12:Z:21:ILE:HD12	12:Z:21:ILE:C	2.33	0.49
5:E:12:THR:CG2	5:E:124:THR:HA	2.35	0.49
8:H:175:VAL:HG12	8:H:176:CYS:N	2.26	0.49
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.47	0.49
5:S:107:LEU:HD11	5:S:111:ARG:HG2	1.94	0.49
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.12	0.49
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.12	0.49
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.12	0.49
4:D:112:LEU:C	4:D:112:LEU:HD13	2.33	0.49
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.27	0.49
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.15	0.49
7:U:118:ASN:O	7:U:122:ILE:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:5:ALA:HB2	9:W:14:ILE:CD1	2.42	0.49
6:F:203:GLU:O	6:F:206:LYS:HD2	2.11	0.49
14:N:107:LYS:CG	14:N:108:GLY:H	2.14	0.49
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.95	0.49
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.47	0.49
10:J:113:ILE:HA	10:J:118:THR:O	2.13	0.49
2:B:78:VAL:HG22	2:B:136:PHE:CE2	2.48	0.49
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.95	0.49
11:K:36:GLU:HG2	11:K:184:TRP:CZ2	2.48	0.49
8:V:41:ILE:HD13	8:V:41:ILE:N	2.27	0.49
9:I:84:SER:OG	9:I:119:ILE:HD11	2.13	0.49
12:L:1:GLY:N	17:L:755:HOH:O	2.45	0.49
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.94	0.48
6:F:127:ASN:ND2	6:F:127:ASN:C	2.61	0.48
9:W:101:VAL:O	9:W:110:ILE:HA	2.13	0.48
10:J:52:THR:HG22	10:J:53:VAL:HG23	1.94	0.48
11:K:12:ILE:CG2	11:K:110:ILE:HD11	2.42	0.48
12:L:134:ILE:HD11	12:L:162:ALA:HB2	1.95	0.48
2:P:78:VAL:HG22	2:P:136:PHE:CE2	2.47	0.48
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.13	0.48
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.95	0.48
6:T:35:THR:CG2	6:T:51:GLU:O	2.60	0.48
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.34	0.48
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.33	0.48
14:2:40:LYS:C	14:2:41:ILE:HD13	2.34	0.48
11:K:45:MET:CB	15:3:5:ABN:H5	2.41	0.48
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.77	0.48
7:G:197:MET:HG2	7:G:205:PHE:CE1	2.49	0.48
11:K:86:LEU:HD13	11:K:86:LEU:C	2.33	0.48
12:L:79:ALA:O	12:L:83:ILE:HG13	2.13	0.48
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.13	0.48
3:C:163:GLN:HE21	3:C:164:THR:N	2.11	0.48
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.25	0.48
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.03	0.48
5:S:231:LYS:H	5:S:231:LYS:HD2	1.77	0.48
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:N	2.65	0.48
12:Z:79:ALA:O	12:Z:83:ILE:HG13	2.14	0.48
3:C:173:ARG:O	3:C:177:GLU:HG3	2.14	0.48
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.95	0.48
3:Q:163:GLN:HA	3:Q:163:GLN:NE2	2.24	0.48
6:F:186:ALA:O	6:F:190:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.62	0.48
13:1:14(C):ARG:CG	13:1:14(C):ARG:HH11	2.26	0.48
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.49	0.48
6:F:53:LEU:HD13	6:F:20(C):LYS:HD2	1.96	0.48
11:K:142:TYR:C	11:K:143:LYS:HD2	2.33	0.48
11:K:4:LEU:C	11:K:4:LEU:HD22	2.34	0.48
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.49	0.48
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.95	0.48
5:E:231:LYS:HD2	5:E:231:LYS:H	1.78	0.48
7:G:186:TRP:O	7:G:190:VAL:HG23	2.13	0.48
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.96	0.48
5:S:12:THR:CG2	5:S:124:THR:HA	2.36	0.48
3:C:163:GLN:HA	3:C:163:GLN:NE2	2.25	0.48
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.14	0.48
13:M:40:ASN:HD22	13:M:40:ASN:N	2.05	0.48
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	1.94	0.48
5:S:15:PHE:N	6:T:23:GLN:HE22	1.95	0.48
11:Y:36:GLU:HG2	11:Y:184:TRP:CZ2	2.49	0.48
7:G:118:ASN:O	7:G:122:ILE:HD12	2.13	0.47
9:I:114:ASP:HB2	17:I:851:HOH:O	2.14	0.47
3:Q:160:TRP:CZ2	4:R:59:LEU:HD23	2.49	0.47
7:U:49:ILE:HD12	7:U:193:ALA:CB	2.44	0.47
9:I:30:LYS:NZ	11:Y:208:ASN:O	2.46	0.47
4:D:185:THR:OG1	4:D:188:GLU:HG3	2.14	0.47
2:P:63:THR:HG22	2:P:63:THR:O	2.14	0.47
7:U:186:TRP:O	7:U:190:VAL:HG23	2.15	0.47
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.95	0.47
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.96	0.47
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.96	0.47
6:T:72:ARG:HD2	13:1:64:THR:OG1	2.14	0.47
7:U:87:ASN:HD22	7:U:87:ASN:C	2.17	0.47
10:X:52:THR:HG22	10:X:53:VAL:H	1.78	0.47
10:X:90(A):ILE:HG13	10:X:116:LEU:CD2	2.45	0.47
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.27	0.47
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.50	0.47
4:R:192:LEU:O	4:R:196:ILE:HG13	2.15	0.47
10:X:10(B):LYS:HB2	10:X:10(B):LYS:HZ2	1.77	0.47
11:Y:12:ILE:CG2	11:Y:110:ILE:HD11	2.44	0.47
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.79	0.47
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.44	0.47
10:J:168:MET:CE	10:X:168:MET:HE3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:O	1:A:116:VAL:HG23	2.15	0.47
2:B:63:THR:HG22	2:B:63:THR:O	2.15	0.47
5:E:142:ASP:HB2	17:M:885:HOH:O	2.15	0.47
5:E:2(C):VAL:O	5:E:226:GLY:HA2	2.14	0.47
8:H:34:LEU:HB2	17:H:540:HOH:O	2.13	0.47
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.96	0.47
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.35	0.47
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.15	0.47
9:I:101:VAL:O	9:I:110:ILE:HA	2.15	0.47
4:R:24:VAL:O	4:R:27:SER:HB3	2.15	0.47
10:X:113:ILE:HA	10:X:118:THR:O	2.15	0.47
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.15	0.47
12:L:113:PHE:CD1	12:L:113:PHE:N	2.82	0.47
14:N:40:LYS:O	14:N:41:ILE:HD13	2.15	0.47
2:B:27:ALA:O	2:B:31:ILE:HG12	2.15	0.47
3:C:182:PRO:O	3:C:184:ALA:N	2.48	0.47
3:C:46:VAL:HG11	3:C:139:ALA:HB1	1.97	0.47
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.80	0.47
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.30	0.47
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.50	0.47
6:T:53:LEU:HD13	6:T:20(C):LYS:HD2	1.96	0.47
12:L:135:MET:CE	9:W:165:ARG:NH2	2.78	0.47
13:1:184:LEU:HD23	13:1:185:THR:N	2.30	0.47
13:1:35:ILE:N	13:1:35:ILE:HD12	2.29	0.47
2:B:185:LYS:CD	2:B:187:ASP:H	2.28	0.47
10:J:133:TYR:CZ	10:J:166:MET:HG2	2.50	0.47
7:U:192:PHE:C	7:U:192:PHE:CD1	2.87	0.47
10:J:137:LEU:HD21	11:Y:140:SER:OG	2.14	0.47
1:A:150:GLN:O	1:A:157:TYR:HA	2.14	0.46
5:E:28:LEU:HA	5:E:31:ILE:HD12	1.97	0.46
6:F:33:ASN:HB2	17:F:1331:HOH:O	2.15	0.46
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.98	0.46
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.96	0.46
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.50	0.46
17:P:462:HOH:O	3:Q:87:ILE:HD11	2.16	0.46
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.97	0.46
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.50	0.46
13:M:14(C):ARG:CG	13:M:14(C):ARG:HH11	2.26	0.46
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.40	0.46
14:2:40:LYS:O	14:2:41:ILE:HD13	2.15	0.46
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.13	0.46
13:M:35:ILE:N	13:M:35:ILE:HD12	2.30	0.46
2:P:160:TRP:CD2	2:P:163:ILE:HD13	2.50	0.46
5:S:134:VAL:O	5:S:153:PRO:HG3	2.15	0.46
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.97	0.46
2:B:71:ASN:HD22	2:B:71:ASN:HA	1.53	0.46
3:C:160:TRP:CZ2	4:D:59:LEU:HD23	2.49	0.46
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.45	0.46
14:N:26:ILE:HG13	13:1:165:ARG:C	2.35	0.46
8:V:40:LYS:C	8:V:41:ILE:HD13	2.36	0.46
4:D:24:VAL:O	4:D:27:SER:HB3	2.15	0.46
7:G:192:PHE:CD1	7:G:192:PHE:C	2.87	0.46
8:H:40:LYS:C	8:H:41:ILE:HD13	2.36	0.46
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.80	0.46
10:J:90(A):ILE:HG13	10:J:116:LEU:CD2	2.45	0.46
1:O:150:GLN:O	1:O:157:TYR:HA	2.16	0.46
7:U:203:THR:HG22	7:U:204:GLU:N	2.31	0.46
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.14	0.46
5:E:38:VAL:HG12	5:E:39:GLY:N	2.31	0.46
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.97	0.46
3:Q:182:PRO:O	3:Q:184:ALA:N	2.49	0.46
1:A:177:GLU:HG2	2:B:58:LEU:HD21	1.97	0.46
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.99	0.46
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.16	0.46
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.51	0.46
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.46	0.46
5:S:2(C):VAL:O	5:S:226:GLY:HA2	2.16	0.46
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.30	0.46
13:1:83:LEU:O	13:1:87:MET:HG2	2.15	0.46
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.53	0.46
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.63	0.46
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.51	0.46
7:G:49:ILE:HD12	7:G:193:ALA:CB	2.46	0.46
7:G:203:THR:HG22	7:G:204:GLU:N	2.31	0.46
10:J:13:ILE:HG21	10:J:155:LEU:HD12	1.99	0.46
10:J:168:MET:HE2	10:X:168:MET:HE2	1.98	0.46
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.97	0.46
14:N:126:ILE:HD13	14:N:126:ILE:N	2.32	0.46
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.30	0.46
14:2:99:ILE:N	14:2:99:ILE:HD13	2.30	0.45
2:B:15:PHE:H	3:C:23:GLN:NE2	1.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:VAL:O	2:B:190:ILE:HG13	2.16	0.45
2:B:71:ASN:HB3	2:B:74:ILE:H	1.81	0.45
3:C:228:GLU:O	3:C:232:TYR:HD1	1.99	0.45
2:P:186:VAL:O	2:P:190:ILE:HG13	2.15	0.45
5:S:41:ARG:NH1	5:S:42:SER:O	2.48	0.45
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.78	0.45
3:C:38:VAL:HG22	3:C:39:GLY:N	2.31	0.45
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.98	0.45
9:I:12:VAL:CG2	9:I:178:ILE:HB	2.46	0.45
1:O:112:LEU:O	1:O:116:VAL:HG23	2.16	0.45
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.32	0.45
7:U:67:ILE:HD12	7:U:211:GLU:CG	2.36	0.45
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.99	0.45
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.84	0.45
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.98	0.45
2:B:181:LYS:HG3	2:B:184:MET:HG3	1.99	0.45
7:G:55:PRO:HG2	7:G:56:ASP:H	1.81	0.45
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.98	0.45
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.81	0.45
7:U:38:LEU:HD23	7:U:197:MET:HE3	1.99	0.45
10:X:3:ILE:HG22	10:X:100:LEU:CD1	2.47	0.45
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.99	0.45
11:Y:40:PHE:CB	11:Y:73:ARG:HH21	2.19	0.45
5:E:47:VAL:HG22	5:E:214:ILE:HD12	1.97	0.45
8:H:15:ALA:C	8:H:159:ILE:HD11	2.37	0.45
9:I:5:ALA:HB2	9:I:14:ILE:CD1	2.46	0.45
4:D:53:ARG:HG2	4:D:53:ARG:O	2.15	0.45
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.98	0.45
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.97	0.45
3:Q:152:GLU:HB2	3:Q:153:PRO:CD	2.46	0.45
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.97	0.45
3:C:152:GLU:HB2	3:C:153:PRO:CD	2.46	0.45
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.97	0.45
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.78	0.45
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.16	0.45
11:K:195:LEU:O	11:K:199:VAL:HG23	2.17	0.45
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.97	0.45
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.17	0.45
4:R:175:GLU:HB3	4:R:196:ILE:HD13	1.99	0.45
4:D:162:ALA:HB3	5:E:58:LEU:HD23	1.99	0.45
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:8:SER:O	9:I:6:PRO:HD3	2.17	0.45
8:V:25:ILE:HD12	8:V:25:ILE:N	2.32	0.45
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.97	0.45
5:E:76:LEU:C	5:E:76:LEU:HD23	2.37	0.45
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.52	0.45
2:P:71:ASN:HB3	2:P:74:ILE:H	1.82	0.45
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.98	0.45
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.98	0.45
12:Z:58:ARG:HH11	12:Z:58:ARG:HG2	1.82	0.45
4:D:17:PRO:HD2	17:D:1171:HOH:O	2.15	0.45
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.52	0.45
12:L:166:HIS:CD2	12:L:168:GLN:H	2.23	0.45
13:M:148:VAL:HG23	17:M:502:HOH:O	2.15	0.45
13:M:152:GLU:O	13:M:156:VAL:HG23	2.17	0.45
13:M:83:LEU:O	13:M:87:MET:HG2	2.17	0.45
10:J:133:TYR:OH	10:X:24:ILE:HG13	2.16	0.45
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.80	0.45
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.99	0.45
10:J:12:VAL:C	10:J:13:ILE:HD12	2.37	0.45
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.47	0.45
14:N:134:ILE:HD12	14:N:138:CYS:SG	2.57	0.45
8:V:15:ALA:C	8:V:159:ILE:HD11	2.38	0.45
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.29	0.45
8:H:84:LYS:HG3	8:H:85:GLN:N	2.32	0.44
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.32	0.44
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.32	0.44
10:J:24:ILE:HG13	10:X:133:TYR:OH	2.17	0.44
2:B:202:THR:CG2	2:B:204:SER:HB2	2.47	0.44
4:D:227:GLU:OE2	4:D:227:GLU:N	2.47	0.44
9:I:5:ALA:HB2	9:I:14:ILE:HD12	1.99	0.44
10:J:143:ARG:HB2	10:J:146:MET:HG3	1.99	0.44
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.99	0.44
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.80	0.44
5:S:47:VAL:HG22	5:S:214:ILE:HD12	1.99	0.44
7:U:55:PRO:HG2	7:U:56:ASP:H	1.81	0.44
10:X:133:TYR:CZ	10:X:166:MET:HG2	2.53	0.44
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.23	0.44
13:1:9:ASP:OD1	13:1:10:ASN:N	2.50	0.44
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.51	0.44
8:H:63:ILE:HD13	8:H:63:ILE:HA	1.81	0.44
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:40:ASN:ND2	13:M:40:ASN:H	2.14	0.44
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.52	0.44
2:P:185:LYS:CD	2:P:187:ASP:H	2.30	0.44
2:P:202:THR:CG2	2:P:204:SER:HB2	2.48	0.44
5:S:201:LEU:O	5:S:202:ARG:HB2	2.17	0.44
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.80	0.44
12:Z:114:ASP:HB3	12:Z:118:SER:H	1.82	0.44
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.48	0.44
10:J:13:ILE:N	10:J:13:ILE:CD1	2.81	0.44
11:K:45:MET:HB3	11:K:52:CYS:HB3	1.99	0.44
6:T:176:LEU:O	6:T:180:VAL:HG23	2.17	0.44
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.98	0.44
14:2:126:ILE:N	14:2:126:ILE:HD13	2.30	0.44
2:B:51:GLU:OE2	2:B:209:ARG:NH2	2.47	0.44
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.53	0.44
7:G:158:VAL:HG22	7:G:159:GLY:N	2.32	0.44
14:N:40:LYS:C	14:N:41:ILE:HD13	2.38	0.44
3:Q:228:GLU:O	3:Q:232:TYR:HD1	2.00	0.44
5:S:38:VAL:HG12	5:S:39:GLY:N	2.31	0.44
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.99	0.44
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.81	0.44
13:1:14(G):ILE:HB	13:1:144:PRO:CD	2.48	0.44
3:C:76:LEU:HD23	3:C:76:LEU:C	2.38	0.44
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.33	0.44
13:M:211:ILE:HD11	17:2:193:HOH:O	2.18	0.44
4:R:12(D):ALA:HA	5:S:129:GLY:HA2	1.99	0.44
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.48	0.44
7:U:197:MET:HG2	7:U:205:PHE:CE1	2.52	0.44
9:W:5:ALA:HB2	9:W:14:ILE:HD12	1.99	0.44
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.99	0.44
8:H:25:ILE:N	8:H:25:ILE:HD12	2.32	0.44
10:J:168:MET:HG2	10:X:168:MET:CE	2.48	0.44
14:N:186:ARG:HD3	17:N:933:HOH:O	2.16	0.44
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.99	0.44
10:X:166:MET:HA	10:X:167:PRO:HD3	1.76	0.44
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.00	0.44
13:1:40:ASN:ND2	13:1:40:ASN:H	2.13	0.44
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.53	0.44
5:E:134:VAL:O	5:E:153:PRO:HG3	2.17	0.44
8:H:221:ILE:HD12	9:I:40:HIS:HA	2.00	0.44
10:J:3:ILE:HG22	10:J:100:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:147:SER:O	11:K:148:VAL:C	2.55	0.44
5:S:227:GLU:N	5:S:227:GLU:CD	2.71	0.44
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.18	0.44
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.48	0.44
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.27	0.44
9:W:84:SER:CB	9:W:119:ILE:HD11	2.48	0.44
3:C:164:THR:HG21	3:C:172:VAL:HG13	2.00	0.44
7:G:65:SER:HA	7:G:211:GLU:OE2	2.18	0.44
10:J:168:MET:CE	10:X:168:MET:HG2	2.48	0.44
13:M:184:LEU:HD23	13:M:185:THR:N	2.32	0.44
4:R:112:LEU:C	4:R:112:LEU:HD13	2.39	0.44
5:S:28:LEU:HA	5:S:31:ILE:HD12	2.00	0.44
1:A:69:LEU:HD23	1:A:69:LEU:C	2.38	0.43
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.99	0.43
7:G:87:ASN:ND2	7:G:87:ASN:C	2.72	0.43
8:H:116:HIS:HE1	17:H:762:HOH:O	2.00	0.43
9:I:28:SER:HB2	10:J:120:VAL:HG21	2.00	0.43
11:K:38:ASN:OD1	11:K:38:ASN:C	2.55	0.43
13:M:45:ILE:HG12	13:M:99:ILE:HG12	2.00	0.43
1:O:124:THR:HG22	2:P:130:ARG:NH2	2.10	0.43
6:T:136:THR:O	6:T:150:MET:HA	2.18	0.43
5:E:201:LEU:O	5:E:202:ARG:HB2	2.18	0.43
6:F:176:LEU:O	6:F:180:VAL:HG23	2.17	0.43
6:F:212:ILE:HG22	6:F:213:SER:N	2.34	0.43
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.14	0.43
10:J:12:VAL:HG23	10:J:108:PRO:HB2	2.00	0.43
14:N:161:GLN:NE2	14:N:165:TRP:HE1	2.16	0.43
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.48	0.43
4:R:86:ARG:HD3	4:R:86:ARG:HA	1.87	0.43
14:N:14:LEU:O	14:N:175:MET:HA	2.18	0.43
1:O:100:TYR:CG	1:O:107:PRO:HB3	2.53	0.43
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.54	0.43
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.42	0.43
11:Y:45:MET:HB3	11:Y:52:CYS:HB3	2.00	0.43
14:2:14:LEU:O	14:2:175:MET:HA	2.18	0.43
5:E:15:PHE:N	6:F:23:GLN:HE22	1.97	0.43
4:R:90:GLU:OE1	11:Y:69:ARG:HD2	2.18	0.43
17:S:656:HOH:O	6:T:12:ASN:HB2	2.18	0.43
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.19	0.43
3:Q:163:GLN:HE21	3:Q:164:THR:N	2.14	0.43
5:S:76:LEU:HA	5:S:137:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:212:ILE:HG22	6:T:213:SER:N	2.34	0.43
7:U:34(A):ASN:HA	7:U:167:PRO:HG2	2.01	0.43
12:Z:99:THR:HG22	17:Z:231:HOH:O	2.18	0.43
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.49	0.43
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.99	0.43
10:X:17:SER:HB2	10:X:170:PHE:HB2	2.00	0.43
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.16	0.43
13:1:35:ILE:HA	13:1:36:PRO:HD3	1.86	0.43
14:2:38:HIS:HB3	14:2:41:ILE:HG12	2.00	0.43
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.18	0.43
3:C:35:THR:HB	3:C:51:GLU:HG3	2.00	0.43
5:E:227:GLU:CD	5:E:227:GLU:N	2.71	0.43
5:E:41:ARG:NH1	5:E:42:SER:O	2.50	0.43
13:M:202:ASP:O	13:M:204:LYS:HD3	2.18	0.43
14:N:38:HIS:HB3	14:N:41:ILE:HG12	1.99	0.43
10:X:146:MET:HE3	10:X:150:GLU:HB3	2.01	0.43
11:Y:67:GLU:HG2	11:Y:73:ARG:HA	2.01	0.43
1:A:177:GLU:CG	2:B:58:LEU:CD2	2.94	0.43
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.54	0.43
10:J:17:SER:HB2	10:J:170:PHE:HB2	2.01	0.43
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.19	0.43
6:T:35:THR:CG2	6:T:36:THR:N	2.82	0.43
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.18	0.43
13:1:205:GLY:HA3	13:1:209:GLN:HB3	2.00	0.43
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.54	0.43
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.19	0.43
3:Q:79:SER:OG	3:Q:165:ILE:HG13	2.19	0.43
4:R:227:GLU:OE2	4:R:227:GLU:N	2.48	0.43
14:N:26:ILE:HG13	13:1:165:ARG:O	2.19	0.42
13:1:202:ASP:O	13:1:204:LYS:HD3	2.19	0.42
2:B:90:ASN:O	2:B:94:ILE:HG12	2.18	0.42
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.49	0.42
5:E:214:ILE:HG13	5:E:215:VAL:H	1.81	0.42
9:I:28:SER:CB	10:J:120:VAL:HG21	2.49	0.42
13:M:9:ASP:OD1	13:M:10:ASN:N	2.51	0.42
1:O:233:LEU:O	1:O:236:LEU:HB2	2.19	0.42
5:S:179:THR:O	5:S:179:THR:HG22	2.18	0.42
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.19	0.42
13:1:40:ASN:ND2	13:1:40:ASN:N	2.66	0.42
13:1:45:ILE:HG12	13:1:99:ILE:HG12	2.01	0.42
1:A:100:TYR:CG	1:A:107:PRO:HB3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:O	1:A:190:ILE:HG13	2.19	0.42
8:H:159:ILE:HG22	8:H:163:ILE:HD12	2.00	0.42
9:I:155:ILE:HG23	9:I:156:SER:N	2.34	0.42
2:P:202:THR:HG21	2:P:204:SER:HB2	2.01	0.42
5:S:76:LEU:HD23	5:S:76:LEU:C	2.39	0.42
7:U:87:ASN:ND2	7:U:87:ASN:C	2.72	0.42
11:Y:147:SER:O	11:Y:148:VAL:C	2.57	0.42
4:D:170:GLU:N	4:D:170:GLU:OE1	2.49	0.42
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.20	0.42
6:F:43:ASN:N	6:F:43:ASN:HD22	2.17	0.42
11:K:99:THR:CG2	11:K:113:VAL:HB	2.50	0.42
11:K:36:GLU:O	11:K:37:ILE:C	2.57	0.42
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.49	0.42
7:U:65:SER:HA	7:U:211:GLU:OE2	2.19	0.42
7:U:225:SER:O	7:U:229:ILE:HG13	2.19	0.42
9:W:6:MET:HB3	9:W:151:LEU:HD11	2.00	0.42
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.50	0.42
12:Z:90:LYS:HE3	12:Z:93:PHE:O	2.20	0.42
12:Z:99:THR:HG23	17:Z:231:HOH:O	2.18	0.42
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.20	0.42
1:A:169:SER:O	1:A:173:LYS:HG3	2.19	0.42
2:B:6:ARG:HG3	2:B:6:ARG:HH11	1.84	0.42
5:E:179:THR:O	5:E:179:THR:HG22	2.19	0.42
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.50	0.42
9:I:6:MET:HB3	9:I:151:LEU:HD11	2.00	0.42
10:J:63:ILE:HD11	10:J:79:VAL:HG13	2.00	0.42
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.33	0.42
17:E:1080:HOH:O	12:L:64:LYS:HE3	2.19	0.42
3:Q:168:ASN:O	3:Q:172:VAL:HG12	2.20	0.42
8:V:152:ILE:HD11	8:V:177:VAL:CG2	2.49	0.42
9:W:12:VAL:CG2	9:W:178:ILE:HB	2.49	0.42
10:X:143:ARG:HB2	10:X:146:MET:HG3	2.00	0.42
10:X:42:LEU:HB2	10:X:184:ILE:HD13	2.01	0.42
12:Z:40:ASN:HA	12:Z:40:ASN:HD22	1.69	0.42
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.15	0.42
1:A:38:LEU:HD12	1:A:38:LEU:C	2.40	0.42
6:F:136:THR:O	6:F:150:MET:HA	2.20	0.42
6:F:35:THR:CG2	6:F:51:GLU:O	2.60	0.42
12:L:76:ILE:HG23	12:L:77:ASN:N	2.35	0.42
1:O:29:THR:O	1:O:33:GLN:HG2	2.20	0.42
1:O:38:LEU:HD12	1:O:38:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:181:LYS:HG3	2:P:184:MET:HG3	2.00	0.42
6:T:82:ILE:HB	6:T:83:PRO:HD3	2.01	0.42
11:Y:35:ILE:HD11	11:Y:37:ILE:HD13	2.02	0.42
2:B:202:THR:HG21	2:B:204:SER:HB2	2.01	0.42
9:I:14:ILE:HG13	9:I:34:ILE:HD13	2.00	0.42
10:J:63:ILE:CD1	10:J:79:VAL:HG13	2.49	0.42
1:O:214:ILE:C	1:O:215:ILE:HD13	2.40	0.42
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.54	0.42
4:R:170:GLU:OE1	4:R:170:GLU:N	2.48	0.42
7:U:29:LYS:HA	7:U:29:LYS:HD2	1.85	0.42
9:W:119:ILE:N	9:W:119:ILE:HD12	2.34	0.42
2:B:150:THR:O	2:B:157:TYR:HA	2.20	0.42
9:I:2:ILE:HG21	9:I:130:ALA:HB3	2.01	0.42
12:L:114:ASP:HB3	12:L:118:SER:H	1.84	0.42
1:O:69:LEU:HD23	1:O:69:LEU:C	2.40	0.42
6:T:43:ASN:HD22	6:T:43:ASN:N	2.18	0.42
7:U:49:ILE:HD12	7:U:193:ALA:HB1	2.02	0.42
8:V:84:LYS:HG3	8:V:85:GLN:N	2.34	0.42
9:W:19:ARG:HB2	9:W:171:TRP:HB2	2.02	0.42
10:X:112:GLN:HE22	10:X:126:ALA:H	1.66	0.42
11:Y:36:GLU:O	11:Y:37:ILE:C	2.57	0.42
2:B:224:PHE:HD2	2:B:224:PHE:H	1.67	0.42
5:E:54:ASN:ND2	5:E:56:ASP:O	2.53	0.42
5:E:76:LEU:HA	5:E:137:LEU:O	2.19	0.42
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	2.02	0.42
11:K:44:THR:OG1	11:K:100:MET:HB2	2.19	0.42
11:K:5:ALA:HA	11:K:13:ILE:O	2.20	0.42
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.55	0.42
5:S:82:ALA:HB3	5:S:83:PRO:HD3	2.01	0.42
7:U:107:MET:HE1	7:U:112:LEU:HD13	2.00	0.42
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.55	0.42
8:H:165:ASN:ND2	13:I:139:ARG:HH11	2.08	0.42
1:A:233:LEU:O	1:A:236:LEU:HB2	2.20	0.42
5:E:4:PHE:CG	5:E:5:ARG:N	2.88	0.42
7:G:31:THR:HG21	7:G:135:ILE:HG13	2.02	0.42
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.86	0.42
3:Q:159:SER:HB2	17:Q:1140:HOH:O	2.20	0.42
5:S:214:ILE:HG13	5:S:215:VAL:H	1.83	0.42
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.20	0.42
8:V:175:VAL:CG1	8:V:176:CYS:N	2.83	0.42
8:H:22:GLN:HG3	8:H:27:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:87:LEU:HD11	9:I:99:PRO:HG2	2.01	0.41
10:J:112:GLN:HE22	10:J:126:ALA:H	1.66	0.41
13:M:40:ASN:ND2	13:M:40:ASN:N	2.67	0.41
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	2.02	0.41
3:Q:35:THR:HB	3:Q:51:GLU:HG3	2.02	0.41
8:V:216:GLU:HG3	9:W:187:ARG:HG2	2.01	0.41
1:O:97:HIS:CD2	8:V:61:SER:OG	2.63	0.41
10:X:12:VAL:C	10:X:13:ILE:HD12	2.41	0.41
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.20	0.41
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.20	0.41
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.85	0.41
5:E:138:ILE:N	5:E:138:ILE:HD12	2.36	0.41
8:H:41:ILE:N	8:H:41:ILE:CD1	2.83	0.41
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.49	0.41
12:L:-2:ASN:HA	12:L:21:ILE:O	2.19	0.41
2:P:6:ARG:HG3	2:P:6:ARG:HH11	1.85	0.41
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.85	0.41
3:Q:76:LEU:HD23	3:Q:76:LEU:C	2.40	0.41
11:Y:191:ASP:OD2	11:Y:193:GLY:N	2.53	0.41
13:1:152:GLU:O	13:1:156:VAL:HG23	2.20	0.41
4:D:86:ARG:HD3	4:D:86:ARG:HA	1.87	0.41
13:M:165:ARG:C	14:2:26:ILE:HG13	2.41	0.41
1:O:186:LEU:O	1:O:190:ILE:HG13	2.20	0.41
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.33	0.41
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.51	0.41
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.85	0.41
11:Y:50:ALA:CB	12:Z:116:VAL:HG23	2.50	0.41
2:B:185:LYS:HD3	2:B:187:ASP:H	1.85	0.41
6:F:35:THR:CG2	6:F:36:THR:N	2.81	0.41
11:K:67:GLU:HG2	11:K:73:ARG:HA	2.01	0.41
2:P:146:TYR:OH	2:P:21(A):LYS:HB2	2.19	0.41
6:T:28:VAL:O	6:T:32:GLU:HG3	2.19	0.41
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.23	0.41
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.50	0.41
1:A:173:LYS:O	1:A:177:GLU:HG3	2.20	0.41
6:F:120:VAL:HG21	6:F:151:LEU:HD21	2.02	0.41
7:G:72:ARG:HH11	7:G:72:ARG:HB2	1.85	0.41
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.18	0.41
14:N:19:ARG:NE	14:N:26:ILE:HD13	2.35	0.41
2:P:51:GLU:OE2	2:P:209:ARG:NH2	2.48	0.41
2:P:71:ASN:HB3	2:P:73:LYS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.20	0.41
4:R:170:GLU:HG2	4:R:171:GLY:N	2.35	0.41
9:W:2:ILE:HG21	9:W:130:ALA:HB3	2.03	0.41
10:X:190:PHE:C	10:X:192:ALA:H	2.24	0.41
14:2:106:ASN:O	14:2:107:LYS:HB3	2.21	0.41
1:A:29:THR:O	1:A:33:GLN:HG2	2.21	0.41
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.35	0.41
4:D:215:ILE:O	4:D:215:ILE:HD13	2.20	0.41
7:G:56:ASP:HB3	7:G:59:LEU:HG	2.03	0.41
10:J:166:MET:HA	10:J:167:PRO:HD3	1.76	0.41
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.19	0.41
4:R:68:VAL:HG21	4:R:89:ILE:HD12	2.02	0.41
9:W:93:GLY:N	9:W:94:PRO:CD	2.83	0.41
2:B:224:PHE:CD2	2:B:224:PHE:N	2.89	0.41
9:I:84:SER:CB	9:I:119:ILE:HD11	2.50	0.41
9:I:119:ILE:HD12	9:I:119:ILE:N	2.36	0.41
13:M:-4:ILE:HD12	14:N:116:GLY:HA2	2.02	0.41
1:O:169:SER:O	1:O:173:LYS:HG3	2.21	0.41
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.76	0.41
7:U:158:VAL:HG22	7:U:159:GLY:N	2.35	0.41
13:1:113:VAL:HA	13:1:118:VAL:O	2.21	0.41
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.20	0.41
3:C:163:GLN:CA	3:C:163:GLN:NE2	2.83	0.41
3:C:175:PHE:CZ	3:C:195:ARG:HB3	2.55	0.41
11:K:13:ILE:HD12	11:K:152:LEU:HD23	2.02	0.41
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.25	0.41
1:O:117:ALA:HB1	1:O:155:GLY:O	2.20	0.41
2:P:97:GLN:NE2	17:P:299:HOH:O	2.50	0.41
5:S:4:PHE:CG	5:S:5:ARG:N	2.88	0.41
8:V:22:GLN:HG3	8:V:27:ALA:HB2	2.02	0.41
10:J:168:MET:HG2	10:X:168:MET:HE3	2.02	0.41
10:X:3:ILE:HD13	10:X:3:ILE:HA	1.94	0.41
14:2:112:THR:HG22	14:2:120:HIS:HB2	2.03	0.41
2:B:146:TYR:OH	2:B:21(A):LYS:HB2	2.21	0.41
7:G:38:LEU:C	7:G:38:LEU:HD12	2.42	0.41
8:H:152:ILE:HD11	8:H:177:VAL:CG2	2.51	0.41
8:H:196:VAL:HG23	17:H:520:HOH:O	2.20	0.41
9:I:19:ARG:HB2	9:I:171:TRP:HB2	2.03	0.41
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.56	0.41
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.21	0.41
10:X:90(B):ARG:HG2	10:X:90(B):ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:ASN:O	3:C:172:VAL:HG12	2.21	0.41
10:J:44:SER:OG	10:J:100:LEU:HB2	2.21	0.41
11:K:10(A):ARG:HB3	11:K:10(B):LYS:HE3	2.02	0.41
2:P:222:LYS:NZ	2:P:228:GLU:OE2	2.53	0.41
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.20	0.41
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.03	0.41
9:W:155:ILE:HG23	9:W:156:SER:N	2.35	0.41
1:A:117:ALA:HB1	1:A:155:GLY:O	2.20	0.41
17:B:565:HOH:O	3:C:33:ARG:HD2	2.20	0.41
3:Q:241:GLN:C	3:Q:243:GLN:N	2.74	0.41
6:T:38:ILE:HG22	6:T:164:ALA:HB2	2.03	0.41
7:U:56:ASP:HB3	7:U:59:LEU:HG	2.02	0.41
9:W:181:LYS:HE3	9:W:181:LYS:HB3	1.93	0.41
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.21	0.40
11:K:37:ILE:HB	11:K:41:LEU:HB3	2.03	0.40
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.56	0.40
1:O:136:LEU:O	1:O:150:GLN:HA	2.22	0.40
2:P:224:PHE:H	2:P:224:PHE:HD2	1.67	0.40
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.86	0.40
6:T:120:VAL:HG21	6:T:151:LEU:HD21	2.02	0.40
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.35	0.40
6:F:103:TYR:O	6:F:104:LYS:HB3	2.22	0.40
7:G:232:ARG:NE	7:G:232:ARG:HA	2.36	0.40
2:P:224:PHE:N	2:P:224:PHE:CD2	2.89	0.40
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.35	0.40
3:Q:215:VAL:HG23	3:Q:221:ILE:HG13	2.03	0.40
3:C:158:SER:CB	4:D:59:LEU:HD21	2.52	0.40
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.51	0.40
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.34	0.40
4:D:59:LEU:C	4:D:59:LEU:HD13	2.41	0.40
4:D:177:LEU:CD2	5:E:58:LEU:HD13	2.48	0.40
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.50	0.40
7:G:29:LYS:HD2	7:G:29:LYS:HA	1.85	0.40
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.02	0.40
8:H:200:LYS:HE3	9:I:140:SER:O	2.22	0.40
3:Q:163:GLN:NE2	3:Q:163:GLN:CA	2.82	0.40
3:Q:175:PHE:CZ	3:Q:195:ARG:HB3	2.56	0.40
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.91	0.40
5:S:138:ILE:HD12	5:S:138:ILE:N	2.36	0.40
6:T:114:ASP:O	6:T:118:GLN:HG2	2.21	0.40
7:U:82:ILE:HG22	7:U:83:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:159:ILE:HG22	8:V:163:ILE:HD12	2.03	0.40
9:W:28:SER:CB	10:X:120:VAL:HG21	2.51	0.40
10:J:24:ILE:CG1	10:X:133:TYR:OH	2.69	0.40
11:Y:105:THR:HB	11:Y:10(B):LYS:CD	2.51	0.40
2:B:37:ALA:O	2:B:164:SER:HA	2.22	0.40
6:F:40:ILE:HD12	6:F:193:ALA:HB2	2.02	0.40
9:I:93:GLY:N	9:I:94:PRO:CD	2.84	0.40
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.86	0.40
11:K:16:VAL:HG21	11:K:34:VAL:HG23	2.03	0.40
11:K:208:ASN:HD21	9:W:29:ASN:ND2	2.17	0.40
12:L:90:LYS:HE3	12:L:93:PHE:O	2.22	0.40
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.21	0.40
1:O:137:LEU:HA	1:O:137:LEU:HD23	1.91	0.40
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.60	0.40
3:Q:225:SER:OG	3:Q:228:GLU:HG3	2.22	0.40
7:U:35:ILE:HD11	17:U:1201:HOH:O	2.21	0.40
7:U:72:ARG:HB2	7:U:72:ARG:HH11	1.85	0.40
9:W:28:SER:HB2	10:X:120:VAL:HG21	2.04	0.40
10:X:137:LEU:HD23	10:X:137:LEU:HA	1.94	0.40
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.03	0.40
1:A:111:LEU:HA	1:A:111:LEU:HD23	1.85	0.40
3:C:206:GLY:HA3	3:C:209:ASN:HB2	2.04	0.40
3:C:241:GLN:C	3:C:243:GLN:N	2.74	0.40
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.36	0.40
2:P:71:ASN:HA	2:P:71:ASN:HD22	1.53	0.40
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.51	0.40
2:P:6:ARG:HB2	5:S:127:TYR:OH	2.22	0.40
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.56	0.40
10:J:26:VAL:HG23	10:X:165:ARG:O	2.22	0.40
11:Y:10(A):ARG:HB3	11:Y:10(B):LYS:HE3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	236 (95%)	10 (4%)	2 (1%)	19	29
1	O	248/250 (99%)	236 (95%)	10 (4%)	2 (1%)	19	29
2	B	242/258 (94%)	222 (92%)	16 (7%)	4 (2%)	9	11
2	P	242/258 (94%)	224 (93%)	14 (6%)	4 (2%)	9	11
3	C	239/254 (94%)	224 (94%)	9 (4%)	6 (2%)	5	6
3	Q	239/254 (94%)	222 (93%)	11 (5%)	6 (2%)	5	6
4	D	240/260 (92%)	228 (95%)	8 (3%)	4 (2%)	9	11
4	R	240/260 (92%)	228 (95%)	8 (3%)	4 (2%)	9	11
5	E	231/234 (99%)	213 (92%)	15 (6%)	3 (1%)	12	17
5	S	231/234 (99%)	213 (92%)	15 (6%)	3 (1%)	12	17
6	F	242/288 (84%)	234 (97%)	7 (3%)	1 (0%)	34	48
6	T	242/288 (84%)	233 (96%)	8 (3%)	1 (0%)	34	48
7	G	241/252 (96%)	232 (96%)	9 (4%)	0	100	100
7	U	241/252 (96%)	232 (96%)	9 (4%)	0	100	100
8	H	220/261 (84%)	209 (95%)	11 (5%)	0	100	100
8	V	220/261 (84%)	210 (96%)	10 (4%)	0	100	100
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	196/198 (99%)	187 (95%)	6 (3%)	3 (2%)	10	14
10	X	196/198 (99%)	187 (95%)	6 (3%)	3 (2%)	10	14
11	K	210/287 (73%)	204 (97%)	5 (2%)	1 (0%)	29	41
11	Y	210/287 (73%)	204 (97%)	5 (2%)	1 (0%)	29	41
12	L	220/241 (91%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/241 (91%)	214 (97%)	6 (3%)	0	100	100
13	1	231/266 (87%)	220 (95%)	10 (4%)	1 (0%)	34	48
13	M	231/266 (87%)	220 (95%)	10 (4%)	1 (0%)	34	48
14	2	194/215 (90%)	184 (95%)	10 (5%)	0	100	100
14	N	194/215 (90%)	185 (95%)	9 (5%)	0	100	100
15	3	1/5 (20%)	1 (100%)	0	0	100	100
15	4	1/5 (20%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6314/6948 (91%)	6009 (95%)	255 (4%)	50 (1%)	19	29

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21(C)	ASP
3	C	58	LEU
4	D	12(G)	GLU
11	K	39	PRO
2	P	21(C)	ASP
3	Q	58	LEU
4	R	12(G)	GLU
11	Y	39	PRO
1	A	5	THR
2	B	54	VAL
2	B	21(B)	GLY
3	C	203	THR
4	D	18(D)	SER
5	E	5	ARG
5	E	202	ARG
10	J	192	ALA
1	O	5	THR
2	P	54	VAL
2	P	21(B)	GLY
3	Q	203	THR
4	R	18(D)	SER
5	S	5	ARG
5	S	202	ARG
10	X	192	ALA
1	A	167	LYS
2	B	184	MET
3	C	183	PRO
4	D	12(C)	GLY
4	D	12(F)	GLY
6	F	205	ASN
1	O	167	LYS
3	Q	183	PRO
3	Q	184	ALA
4	R	12(C)	GLY
4	R	12(F)	GLY
6	T	205	ASN
3	C	179	ASN

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Mol	Chain	Res	Type
3	C	184	ALA
5	E	180	LEU
2	P	184	MET
3	Q	179	ASN
5	S	180	LEU
3	C	53	ARG
10	J	49	ALA
13	M	2	SER
3	Q	53	ARG
13	1	2	SER
10	X	49	ALA
10	J	8	VAL
10	X	8	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	203 (97%)	6 (3%)	42	62
1	O	209/209 (100%)	204 (98%)	5 (2%)	49	68
2	B	203/216 (94%)	193 (95%)	10 (5%)	25	40
2	P	203/216 (94%)	193 (95%)	10 (5%)	25	40
3	C	213/226 (94%)	200 (94%)	13 (6%)	18	30
3	Q	213/226 (94%)	200 (94%)	13 (6%)	18	30
4	D	198/215 (92%)	186 (94%)	12 (6%)	18	30
4	R	198/215 (92%)	187 (94%)	11 (6%)	21	34
5	E	192/193 (100%)	173 (90%)	19 (10%)	8	11
5	S	192/193 (100%)	174 (91%)	18 (9%)	8	13
6	F	201/239 (84%)	185 (92%)	16 (8%)	12	18
6	T	201/239 (84%)	184 (92%)	17 (8%)	10	16
7	G	207/210 (99%)	194 (94%)	13 (6%)	18	28
7	U	207/210 (99%)	195 (94%)	12 (6%)	20	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	181/214 (85%)	171 (94%)	10 (6%)	21	35
8	V	181/214 (85%)	172 (95%)	9 (5%)	24	40
9	I	172/173 (99%)	168 (98%)	4 (2%)	50	70
9	W	172/173 (99%)	168 (98%)	4 (2%)	50	70
10	J	175/175 (100%)	167 (95%)	8 (5%)	27	43
10	X	175/175 (100%)	166 (95%)	9 (5%)	24	39
11	K	169/235 (72%)	158 (94%)	11 (6%)	17	27
11	Y	169/235 (72%)	158 (94%)	11 (6%)	17	27
12	L	185/201 (92%)	174 (94%)	11 (6%)	19	32
12	Z	185/201 (92%)	174 (94%)	11 (6%)	19	32
13	1	199/224 (89%)	192 (96%)	7 (4%)	36	55
13	M	199/224 (89%)	192 (96%)	7 (4%)	36	55
14	2	162/178 (91%)	154 (95%)	8 (5%)	25	40
14	N	162/178 (91%)	155 (96%)	7 (4%)	29	46
All	All	5332/5816 (92%)	5040 (94%)	292 (6%)	21	35

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	119	ILE
1	A	135	SER
1	A	158	PHE
1	A	179	ARG
2	B	58	LEU
2	B	71	ASN
2	B	121	GLN
2	B	150	THR
2	B	163	ILE
2	B	185	LYS
2	B	192	LEU
2	B	212	PHE
2	B	215	ILE
2	B	218	ASN
3	C	10	ARG
3	C	25	GLU

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Mol	Chain	Res	Type
3	C	57	LYS
3	C	66	LYS
3	C	121	GLN
3	C	150	GLN
3	C	163	GLN
3	C	172	VAL
3	C	174	GLU
3	C	208	LYS
3	C	210	ILE
3	C	212	ILE
3	C	227	GLU
4	D	28	LEU
4	D	48	LEU
4	D	52	LYS
4	D	76	CYS
4	D	110	GLU
4	D	126	ARG
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	196	ILE
4	D	215	ILE
4	D	237	LEU
5	E	11	ASP
5	E	12	THR
5	E	28	LEU
5	E	32	LYS
5	E	56	ASP
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	185	ASN
5	E	189	LEU
5	E	197	ILE
5	E	207	LEU
5	E	212	ILE
5	E	214	ILE
5	E	227	GLU
5	E	231	LYS

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Mol	Chain	Res	Type
6	F	35	THR
6	F	43	ASN
6	F	54	ILE
6	F	56	SER
6	F	121	GLN
6	F	127	ASN
6	F	135	SER
6	F	144	ASN
6	F	176	LEU
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
7	G	35	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	169	GLN
7	G	172	ILE
7	G	184	ASN
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	30	ASN
8	H	37	ILE
8	H	41	ILE
8	H	55	VAL
8	H	63	ILE
8	H	68	LEU
8	H	121	VAL
8	H	144	GLN
8	H	159	ILE
8	H	223	ASP
9	I	-3	ILE
9	I	29	ASN
9	I	160	LEU

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Mol	Chain	Res	Type
9	I	171	TRP
10	J	52	THR
10	J	63	ILE
10	J	70	GLU
10	J	77	GLN
10	J	90(A)	ILE
10	J	121	GLU
10	J	166	MET
10	J	177	ILE
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	39	PRO
11	K	65	LEU
11	K	73	ARG
11	K	82	ILE
11	K	87	VAL
11	K	100	MET
11	K	104	TYR
11	K	10(B)	LYS
12	L	-7	ASN
12	L	3	ILE
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	58	ARG
12	L	82	ASN
12	L	98	HIS
12	L	99	THR
12	L	138	LEU
12	L	145	TYR
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	129	PHE
13	M	14(C)	ARG
13	M	149	GLN
13	M	204	LYS
14	N	89	GLU
14	N	10(B)	LYS
14	N	119	VAL
14	N	126	ILE

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Mol	Chain	Res	Type
14	N	149	GLU
14	N	18(A)	ILE
14	N	18(I)	GLN
1	O	33	GLN
1	O	64	LEU
1	O	135	SER
1	O	158	PHE
1	O	179	ARG
2	P	58	LEU
2	P	71	ASN
2	P	121	GLN
2	P	150	THR
2	P	163	ILE
2	P	185	LYS
2	P	192	LEU
2	P	212	PHE
2	P	215	ILE
2	P	218	ASN
3	Q	10	ARG
3	Q	14	ILE
3	Q	25	GLU
3	Q	57	LYS
3	Q	66	LYS
3	Q	121	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	172	VAL
3	Q	174	GLU
3	Q	208	LYS
3	Q	212	ILE
3	Q	227	GLU
4	R	28	LEU
4	R	48	LEU
4	R	76	CYS
4	R	110	GLU
4	R	126	ARG
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	196	ILE
4	R	215	ILE
4	R	237	LEU

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Mol	Chain	Res	Type
5	S	11	ASP
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	111	ARG
5	S	121	GLN
5	S	18(D)	ILE
5	S	185	ASN
5	S	189	LEU
5	S	197	ILE
5	S	207	LEU
5	S	212	ILE
5	S	214	ILE
5	S	227	GLU
5	S	231	LYS
6	T	35	THR
6	T	43	ASN
6	T	54	ILE
6	T	56	SER
6	T	121	GLN
6	T	127	ASN
6	T	135	SER
6	T	144	ASN
6	T	169	ARG
6	T	176	LEU
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
6	T	21(C)	ASN
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	172	ILE

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Mol	Chain	Res	Type
7	U	184	ASN
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	30	ASN
8	V	37	ILE
8	V	41	ILE
8	V	55	VAL
8	V	68	LEU
8	V	121	VAL
8	V	144	GLN
8	V	159	ILE
8	V	223	ASP
9	W	-3	ILE
9	W	29	ASN
9	W	160	LEU
9	W	171	TRP
10	X	52	THR
10	X	63	ILE
10	X	70	GLU
10	X	77	GLN
10	X	90(A)	ILE
10	X	121	GLU
10	X	166	MET
10	X	177	ILE
10	X	184	ILE
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	39	PRO
11	Y	65	LEU
11	Y	73	ARG
11	Y	82	ILE
11	Y	87	VAL
11	Y	100	MET
11	Y	104	TYR
11	Y	10(B)	LYS
12	Z	-7	ASN
12	Z	3	ILE
12	Z	14	LEU
12	Z	25	SER

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Mol	Chain	Res	Type
12	Z	40	ASN
12	Z	58	ARG
12	Z	82	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	138	LEU
12	Z	145	TYR
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	129	PHE
13	1	14(C)	ARG
13	1	149	GLN
13	1	204	LYS
14	2	89	GLU
14	2	10(B)	LYS
14	2	119	VAL
14	2	126	ILE
14	2	144	GLU
14	2	149	GLU
14	2	18(A)	ILE
14	2	18(I)	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (185) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN

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Mol	Chain	Res	Type
3	C	163	GLN
3	C	238	GLN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	199	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	170	GLN
5	E	185	ASN
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	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	184	ASN
7	G	228	ASN
8	H	30	ASN
8	H	66	HIS
8	H	114	HIS
8	H	144	GLN
8	H	165	ASN

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Mol	Chain	Res	Type
8	H	172	ASN
8	H	190	ASN
9	I	81	GLN
10	J	36	GLN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	141	HIS
10	J	186	GLN
11	K	85	ASN
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	HIS
12	L	70(A)	ASN
12	L	82	ASN
12	L	14(B)	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	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	97	GLN
2	P	121	GLN

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Mol	Chain	Res	Type
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	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	114	GLN
4	R	147	GLN
4	R	161	ASN
4	R	199	GLN
4	R	226	ASN
5	S	7	ASN
5	S	64	GLN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	170	GLN
5	S	185	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	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

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Mol	Chain	Res	Type
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	81	GLN
10	X	36	GLN
10	X	54	GLN
10	X	85	GLN
10	X	112	GLN
10	X	141	HIS
10	X	186	GLN
11	Y	85	ASN
11	Y	174	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70	HIS
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	85	HIS
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	157	HIS

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Mol	Chain	Res	Type
14	2	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	TRO	3	4	15	12,16,17	2.37	4 (33%)	11,22,24	2.40	1 (9%)
15	TY5	3	2	15	19,20,21	1.64	3 (15%)	22,25,27	1.19	2 (9%)
15	TY5	4	2	15	19,20,21	1.64	2 (10%)	22,25,27	1.16	2 (9%)
15	TRO	4	4	15	12,16,17	2.45	3 (25%)	11,22,24	2.37	2 (18%)

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	TRO	3	4	15	-	0/3/6/8	0/2/2/2
15	TY5	3	2	15	-	0/10/11/13	0/2/2/2
15	TY5	4	2	15	-	0/10/11/13	0/2/2/2
15	TRO	4	4	15	-	0/3/6/8	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	4	TRO	CB-CG	6.72	1.59	1.51
15	3	4	TRO	CB-CG	6.25	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	4	TRO	CZ3-CE3	3.17	1.43	1.36
15	3	4	TRO	CZ3-CE3	2.94	1.43	1.36
15	3	4	TRO	CH2-CZ2	2.88	1.43	1.36
15	4	4	TRO	CH2-CZ2	2.55	1.42	1.36
15	4	2	TY5	CE2-CZ	2.51	1.43	1.38
15	3	2	TY5	CE2-CZ	2.48	1.43	1.38
15	3	4	TRO	CZ3-CH2	2.30	1.44	1.38
15	4	2	TY5	CE2-CD2	2.11	1.42	1.38
15	3	2	TY5	CE2-CD2	2.08	1.42	1.38
15	3	2	TY5	CD1-CG	2.07	1.43	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3	4	TRO	CB-CG-CD1	-6.84	112.84	126.53
15	4	4	TRO	CB-CG-CD1	-6.79	112.94	126.53
15	3	2	TY5	C49-OH-CZ	3.80	127.04	117.65
15	4	2	TY5	C49-OH-CZ	3.61	126.56	117.65
15	3	2	TY5	OH-C49-C50	2.21	115.79	109.16
15	4	2	TY5	OH-C49-C50	2.10	115.46	109.16
15	4	4	TRO	CD2-CE2-NE1	2.04	112.57	107.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	2	TY5	2	0
15	4	2	TY5	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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$
16	MES	Y	212	-	12,12,12	1.95	3 (25%)	14,16,16	2.28	5 (35%)
16	MES	K	212	-	12,12,12	1.87	3 (25%)	14,16,16	2.30	5 (35%)

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
16	MES	Y	212	-	-	0/6/14/14	0/1/1/1
16	MES	K	212	-	-	0/6/14/14	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	212	MES	O1-C6	-4.41	1.24	1.42
16	Y	212	MES	O1-C6	-4.39	1.24	1.42
16	Y	212	MES	C8-S	2.90	1.81	1.77
16	K	212	MES	C8-S	2.29	1.80	1.77
16	K	212	MES	O2S-S	2.26	1.51	1.45
16	Y	212	MES	O2S-S	2.05	1.51	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	212	MES	O1-C6-C5	4.72	122.19	111.80
16	K	212	MES	O1-C6-C5	4.61	121.94	111.80
16	Y	212	MES	O2S-S-C8	-4.59	101.39	106.92
16	K	212	MES	O2S-S-C8	-4.07	102.01	106.92
16	K	212	MES	C7-N4-C3	3.60	120.44	111.23
16	Y	212	MES	O3S-S-O1S	3.27	119.27	111.27
16	K	212	MES	O3S-S-O1S	3.19	119.07	111.27
16	Y	212	MES	C7-N4-C3	3.17	119.34	111.23
16	K	212	MES	O3S-S-C8	2.54	109.87	105.77
16	Y	212	MES	O3S-S-C8	2.02	109.03	105.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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%)	-0.34	3 (1%) 79 77	35, 49, 79, 105	0
1	O	250/250 (100%)	-0.25	6 (2%) 59 57	37, 51, 81, 104	0
2	B	244/258 (94%)	-0.18	4 (1%) 72 70	36, 53, 91, 117	0
2	P	244/258 (94%)	-0.08	9 (3%) 41 41	37, 54, 93, 117	0
3	C	241/254 (94%)	-0.08	10 (4%) 37 36	39, 56, 110, 125	0
3	Q	241/254 (94%)	0.23	26 (10%) 5 5	39, 59, 111, 125	0
4	D	242/260 (93%)	-0.12	8 (3%) 46 45	39, 57, 92, 123	0
4	R	242/260 (93%)	-0.12	9 (3%) 41 41	40, 58, 91, 123	0
5	E	233/234 (99%)	-0.09	7 (3%) 50 49	42, 59, 86, 111	0
5	S	233/234 (99%)	-0.08	9 (3%) 39 38	42, 60, 87, 111	0
6	F	244/288 (84%)	-0.26	5 (2%) 65 63	36, 52, 90, 106	0
6	T	244/288 (84%)	-0.23	5 (2%) 65 63	36, 53, 91, 107	0
7	G	243/252 (96%)	-0.36	3 (1%) 79 77	34, 48, 76, 115	0
7	U	243/252 (96%)	-0.39	2 (0%) 86 84	35, 48, 75, 115	0
8	H	222/261 (85%)	-0.37	2 (0%) 84 82	35, 47, 69, 97	0
8	V	222/261 (85%)	-0.40	2 (0%) 84 82	35, 48, 69, 97	0
9	I	204/205 (99%)	-0.34	1 (0%) 91 89	34, 47, 67, 82	0
9	W	204/205 (99%)	-0.24	3 (1%) 73 72	36, 48, 68, 82	0
10	J	198/198 (100%)	-0.31	5 (2%) 57 55	34, 48, 66, 124	0
10	X	198/198 (100%)	-0.40	8 (4%) 38 37	36, 49, 66, 125	0
11	K	212/287 (73%)	-0.24	8 (3%) 40 39	33, 48, 75, 85	0
11	Y	212/287 (73%)	-0.22	6 (2%) 53 51	35, 49, 76, 86	0
12	L	222/241 (92%)	-0.40	2 (0%) 84 82	34, 47, 70, 96	0
12	Z	222/241 (92%)	-0.39	2 (0%) 84 82	35, 47, 69, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1	233/266 (87%)	-0.57	0 100 100	34, 46, 61, 68	0
13	M	233/266 (87%)	-0.48	1 (0%) 92 91	32, 46, 62, 66	0
14	2	196/215 (91%)	-0.42	1 (0%) 91 89	33, 44, 67, 80	0
14	N	196/215 (91%)	-0.52	0 100 100	34, 44, 67, 80	0
15	3	1/5 (20%)	-0.19	0 100 100	52, 52, 52, 52	0
15	4	1/5 (20%)	-0.24	0 100 100	55, 55, 55, 55	0
All	All	6370/6948 (91%)	-0.27	147 (2%) 60 58	32, 50, 83, 125	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(D)	ALA	13.5
4	D	12(E)	SER	10.8
4	R	12(F)	GLY	10.6
10	J	192	ALA	8.8
3	Q	56	LEU	8.7
7	U	6	ALA	8.5
3	C	55	THR	8.5
4	R	12(D)	ALA	7.9
10	X	193	GLN	7.8
4	D	12(F)	GLY	7.6
2	B	218	ASN	7.0
12	L	145	TYR	6.9
2	P	217	ALA	6.9
7	G	6	ALA	6.9
4	R	12(E)	SER	6.8
3	C	56	LEU	6.4
3	Q	203	THR	6.4
1	A	4	MET	6.3
10	J	193	GLN	6.0
2	P	218	ASN	5.9
7	U	240	ASP	5.8
5	S	4	PHE	5.7
10	X	192	ALA	5.6
4	R	12(C)	GLY	5.3
4	D	12(G)	GLU	5.2
5	E	4	PHE	5.1
5	S	233	ILE	5.1
4	D	12(C)	GLY	5.0
3	Q	236	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
5	S	203	ASP	4.9
3	Q	240	LYS	4.8
1	O	4	MET	4.8
6	T	240	ILE	4.6
9	W	-8	SER	4.5
3	Q	55	THR	4.5
12	Z	145	TYR	4.5
3	Q	242	GLU	4.4
5	E	203	ASP	4.3
1	O	236	LEU	4.3
4	R	126	ARG	4.3
1	O	235	ALA	4.2
2	B	217	ALA	4.2
12	Z	14(W)	LYS	4.1
10	X	189	ASP	4.1
3	C	240	LYS	4.1
2	P	54	VAL	4.0
5	S	5	ARG	4.0
1	O	55	SER	4.0
5	E	233	ILE	3.9
4	D	126	ARG	3.9
12	L	14(W)	LYS	3.9
7	G	240	ASP	3.9
13	M	-8	THR	3.9
6	F	240	ILE	3.8
3	Q	239	GLU	3.8
4	R	121	LEU	3.7
4	D	127	LEU	3.7
3	Q	243	GLN	3.7
11	Y	208	ASN	3.6
10	X	191	GLN	3.6
2	P	21(B)	GLY	3.6
3	Q	202	GLN	3.4
6	F	204	ASP	3.3
2	B	54	VAL	3.3
3	Q	233	VAL	3.3
3	Q	241	GLN	3.3
11	Y	181	ASP	3.2
9	I	-8	SER	3.2
11	K	211	GLY	3.2
3	Q	207	ALA	3.2
11	K	208	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
6	T	241	ASN	3.1
11	K	40	PHE	3.1
5	E	5	ARG	3.1
1	O	53	LYS	3.0
5	S	204	GLU	3.0
3	Q	208	LYS	2.9
4	R	12(G)	GLU	2.9
10	J	189	ASP	2.9
10	X	188	ASP	2.9
8	V	222	CYS	2.8
7	G	7	GLY	2.8
3	Q	175	PHE	2.8
2	P	239	THR	2.8
3	Q	235	GLN	2.8
4	R	12(A)	GLY	2.7
11	Y	211	GLY	2.7
10	J	191	GLN	2.7
11	K	181	ASP	2.7
3	C	203	THR	2.6
3	Q	53	ARG	2.6
3	C	208	LYS	2.6
10	J	-1	MET	2.6
6	F	5	GLY	2.6
2	P	21(C)	ASP	2.6
8	V	223	ASP	2.5
1	A	236	LEU	2.5
11	Y	180	GLU	2.5
3	C	54	SER	2.5
3	C	202	GLN	2.5
10	X	133	TYR	2.5
5	S	2(C)	VAL	2.5
6	T	238	LYS	2.5
2	B	21(B)	GLY	2.5
5	S	178	ARG	2.5
11	K	180	GLU	2.5
3	Q	18(C)	LYS	2.5
1	O	56	SER	2.4
2	P	219	GLU	2.4
2	P	21(A)	LYS	2.4
3	C	237	GLU	2.4
3	Q	206	GLY	2.4
9	W	182	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
8	H	222	CYS	2.4
3	Q	18(D)	GLU	2.3
3	Q	201	VAL	2.3
3	Q	178	LYS	2.3
11	K	104	TYR	2.3
3	Q	238	GLN	2.3
9	W	181	LYS	2.3
1	A	203	GLU	2.3
3	C	241	GLN	2.3
5	S	6	ASN	2.3
3	Q	54	SER	2.3
11	K	210	ILE	2.2
3	C	209	ASN	2.2
8	H	199	GLU	2.2
10	X	-1	MET	2.2
11	Y	104	TYR	2.2
3	Q	187	GLU	2.2
5	E	204	GLU	2.2
14	2	18(I)	GLN	2.2
6	T	5	GLY	2.1
3	Q	237	GLU	2.1
6	F	18(A)	ASP	2.1
10	X	168	MET	2.1
11	K	207	ASN	2.1
2	P	220	TYR	2.1
5	S	33	GLN	2.1
3	Q	58	LEU	2.1
6	F	20(B)	GLU	2.1
11	Y	209	VAL	2.0
4	R	127	LEU	2.0
5	E	195	GLU	2.0
6	T	6	THR	2.0
5	E	202	ARG	2.0
4	D	125	GLU	2.0

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

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	TRO	4	4	15/16	0.89	0.19	56,63,64,65	0
15	TY5	4	2	19/20	0.92	0.17	58,60,70,70	0
15	TRO	3	4	15/16	0.93	0.16	53,62,64,65	0
15	TY5	3	2	19/20	0.94	0.22	57,61,70,70	0

### 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
16	MES	Y	212	12/12	0.93	0.15	74,77,79,79	0
16	MES	K	212	12/12	0.95	0.18	71,75,78,78	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.