



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 06:33 PM BST

PDB ID : 3MG8  
Title : Structure of yeast 20S open-gate proteasome with Compound 16  
Authors : Sintchak, M.D.  
Deposited on : 2010-04-05  
Resolution : 2.59 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 : 2.13  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

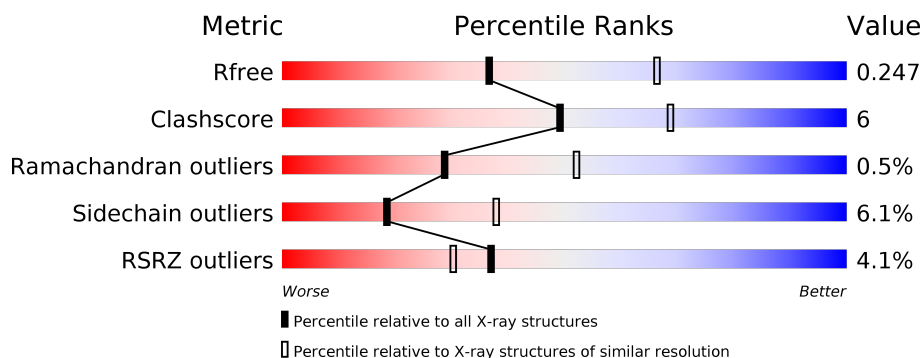
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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>3%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>.</div> </div> </div>
1	O	250	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>.</div> </div> </div>
2	B	245	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>..</div> </div> </div>
2	P	245	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>..</div> </div> </div>
3	C	243	<div> <div>11%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>..</div> </div> </div>
3	Q	243	<div> <div>20%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	250	
4	R	250	
5	E	234	
5	S	234	
6	F	248	
6	T	248	
7	G	252	
7	U	252	
8	H	222	
8	V	222	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	241	
12	Z	241	
13	1	266	
13	M	266	
14	2	196	
14	N	196	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	F	243	-	-	-	X

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49429 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	235	Total	C	N	O	S	0	0	0
			1829	1158	303	365	3			
2	P	235	Total	C	N	O	S	0	0	0
			1829	1158	303	365	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	237	Total	C	N	O	S	0	0	0
			1848	1175	323	346	4			
6	T	237	Total	C	N	O	S	0	0	0
			1848	1175	323	346	4			

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

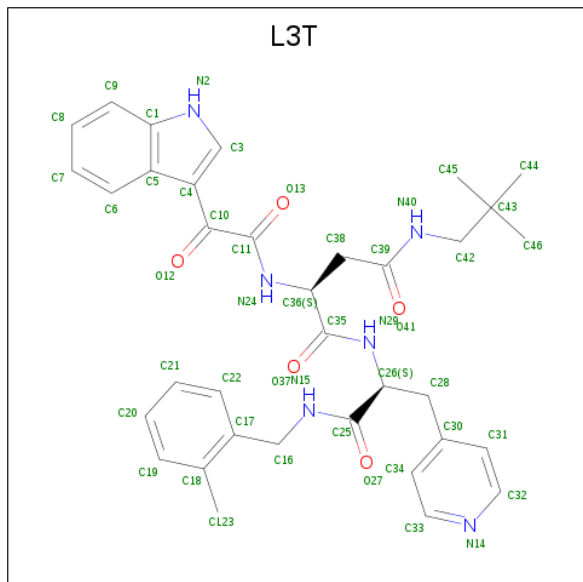
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total	Mg	0	0
			1	1		
15	I	2	Total	Mg	0	0
			2	2		
15	N	1	Total	Mg	0	0
			1	1		
15	L	2	Total	Mg	0	0
			2	2		
15	F	2	Total	Mg	0	0
			2	2		

- Molecule 16 is N-(2,2-dimethylpropyl)-N 2 -[1H-indol-3-yl(oxo)acetyl]-L-asparaginyln-N-(2-methylbenzyl)-3-pyridin-4-yl-L-alaninamide (three-letter code: L3T) (formula:  $C_{35}H_{40}N_6O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			46	35	6	5		
16	Y	1	Total	C	N	O	0	0
			46	35	6	5		

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).





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

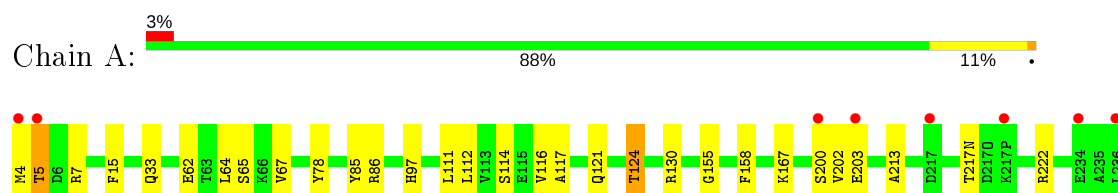
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	K	2	Total	O	0	0
			2	2		
18	L	3	Total	O	0	0
			3	3		

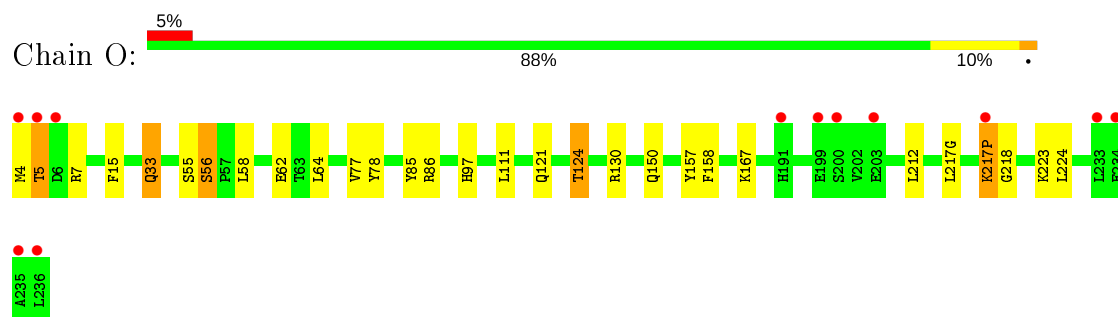
### 3 Residue-property plots [i](#)

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

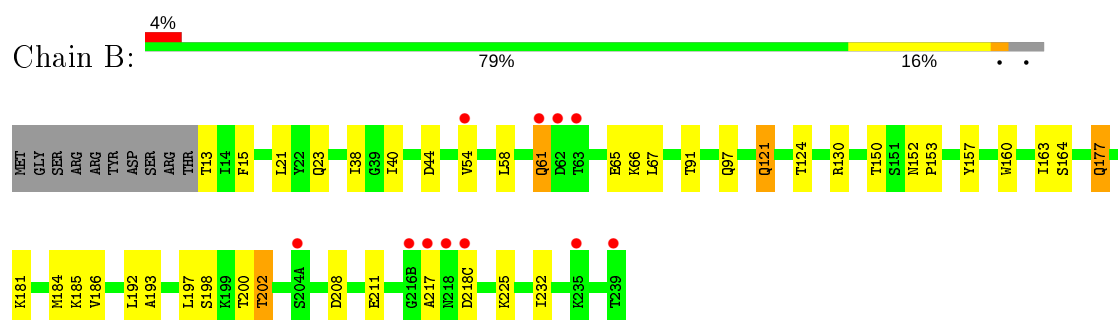
- Molecule 1: Proteasome component Y7



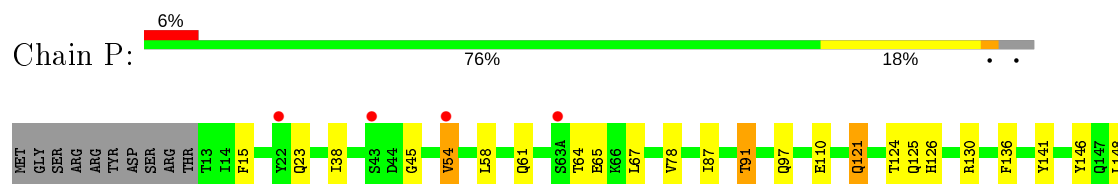
- Molecule 1: Proteasome component Y7

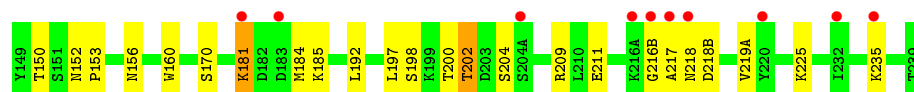


- Molecule 2: Proteasome component Y13

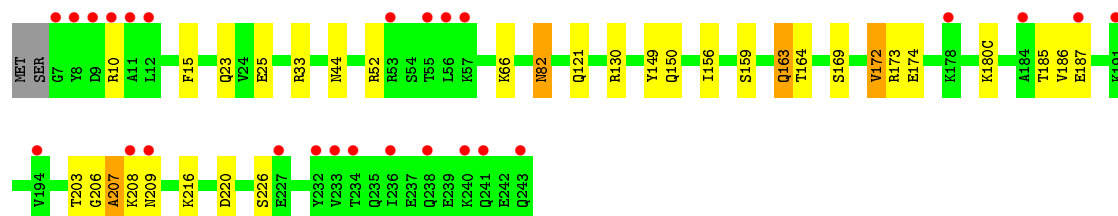
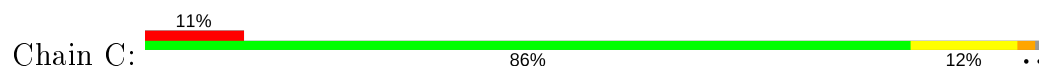


- Molecule 2: Proteasome component Y13

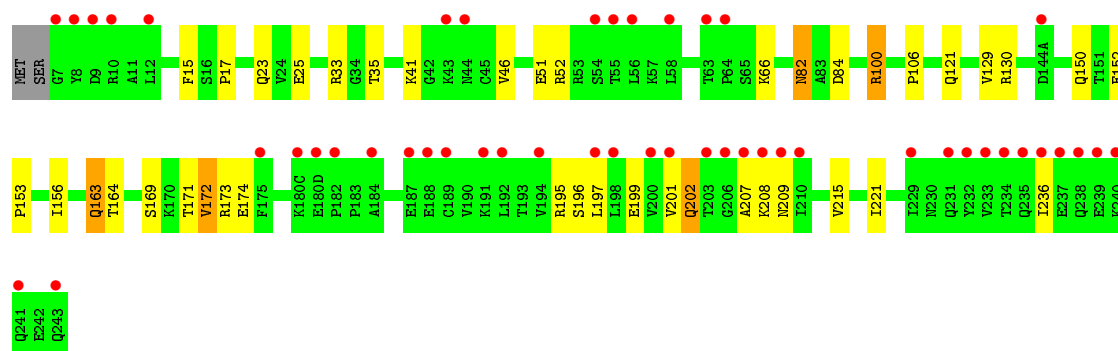
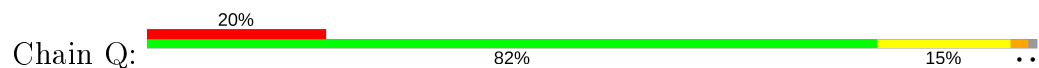




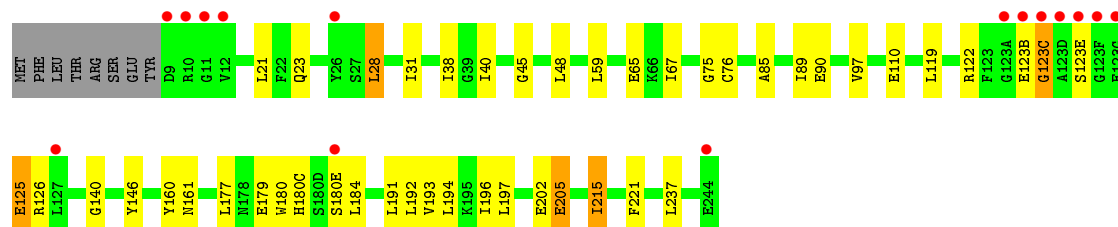
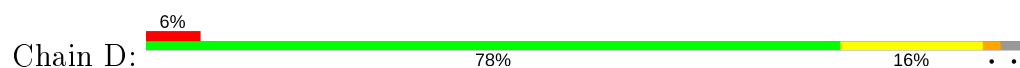
• Molecule 3: Proteasome component PRE6



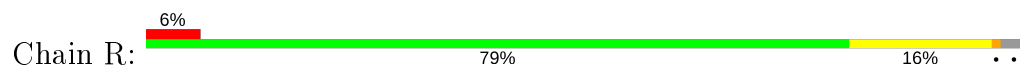
• Molecule 3: Proteasome component PRE6



• Molecule 4: Proteasome component PUP2

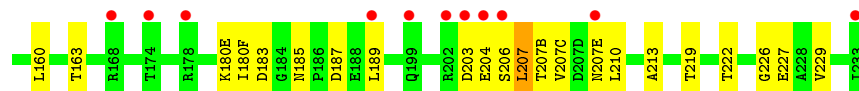
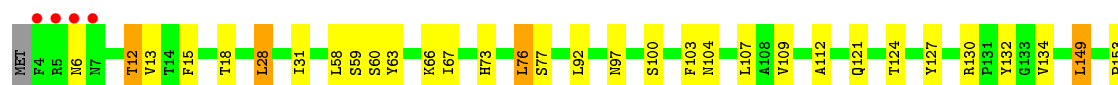
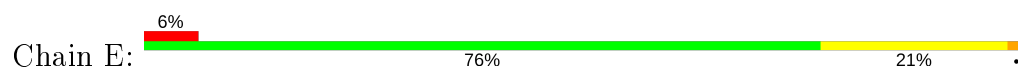


• Molecule 4: Proteasome component PUP2

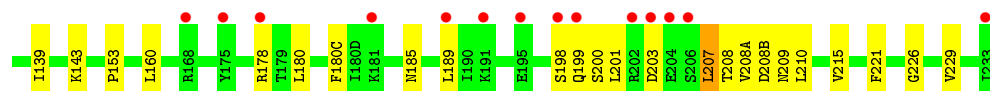
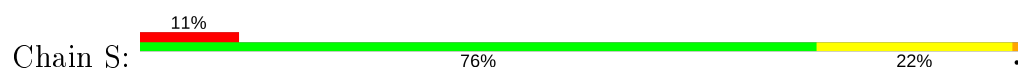




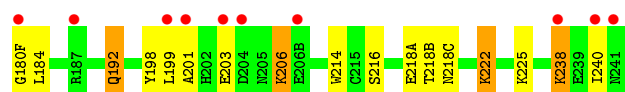
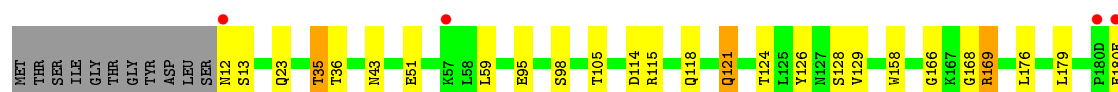
• Molecule 5: Proteasome component PRE5



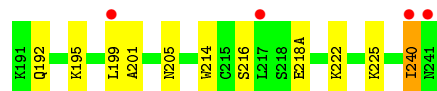
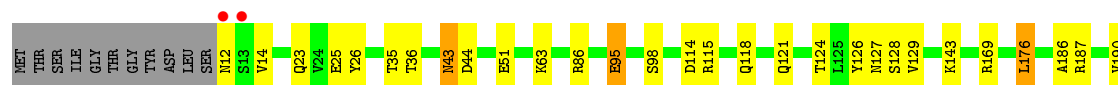
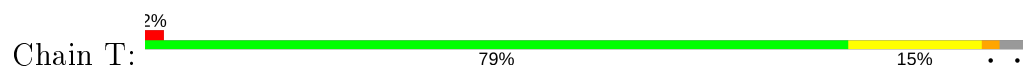
• Molecule 5: Proteasome component PRE5



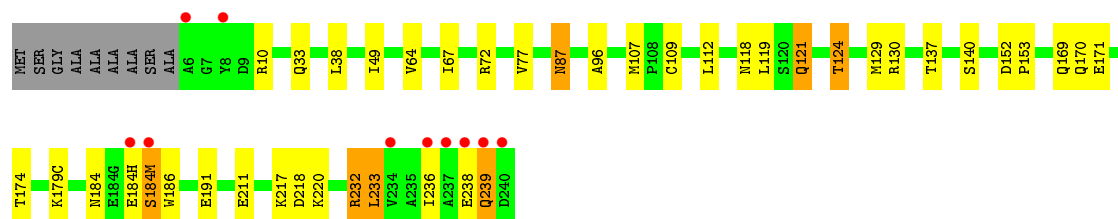
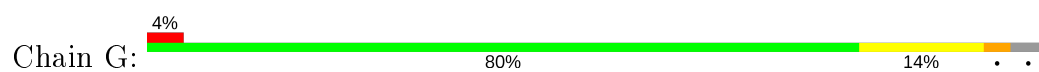
• Molecule 6: Proteasome component C1



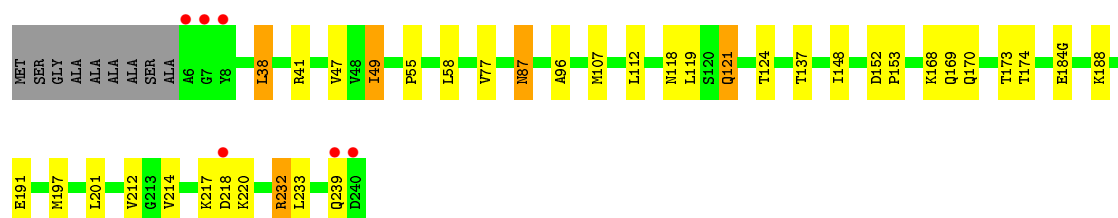
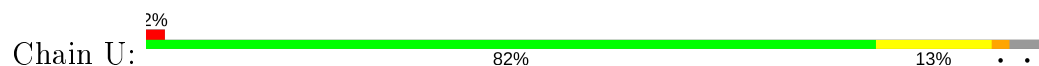
• Molecule 6: Proteasome component C1



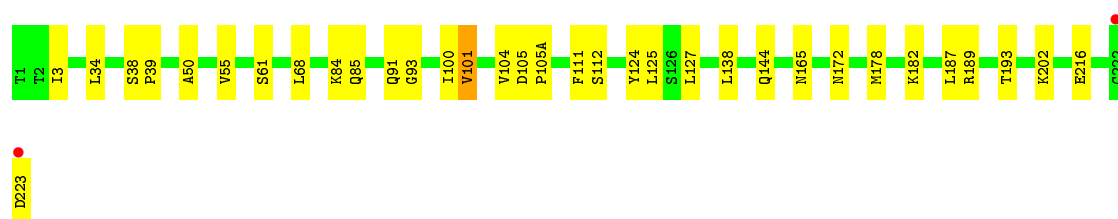
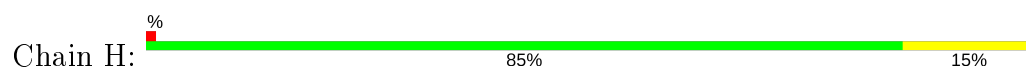
• Molecule 7: Proteasome component C7-alpha



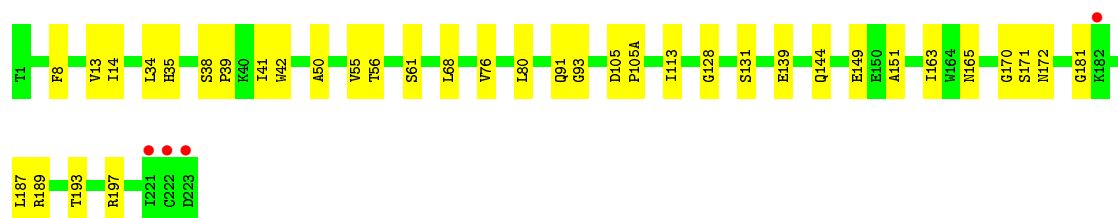
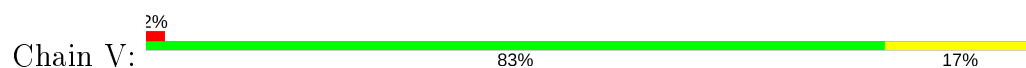
- Molecule 7: Proteasome component C7-alpha



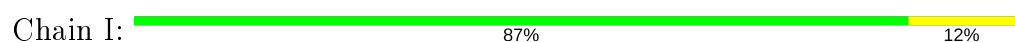
- Molecule 8: Proteasome component PUP1



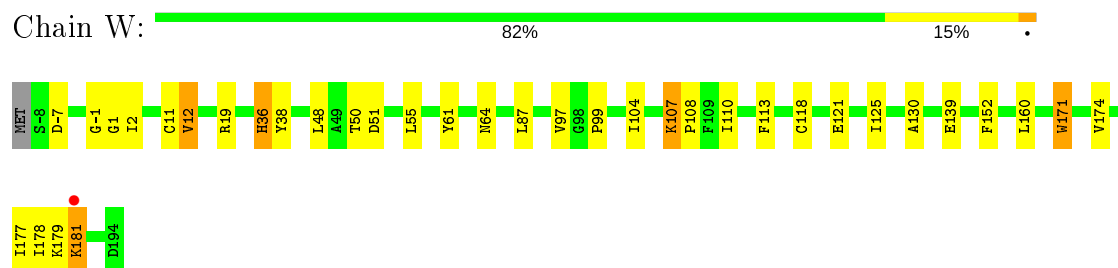
- Molecule 8: Proteasome component PUP1



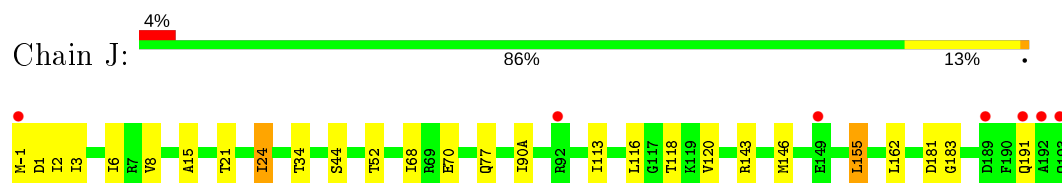
- Molecule 9: Proteasome component PUP3



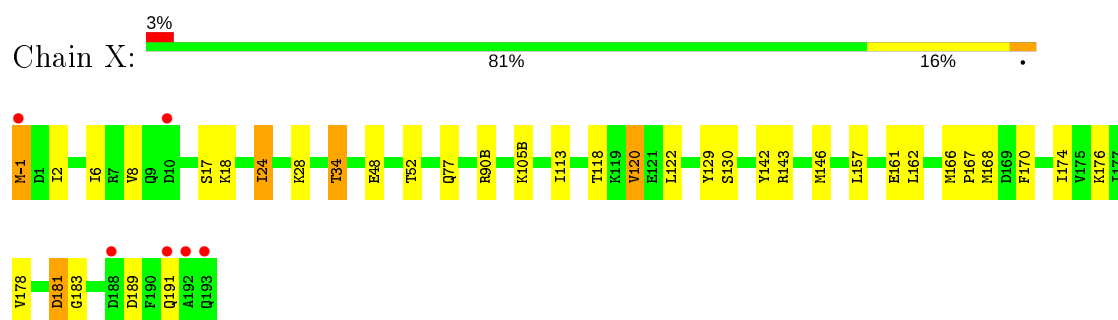
- Molecule 9: Proteasome component PUP3



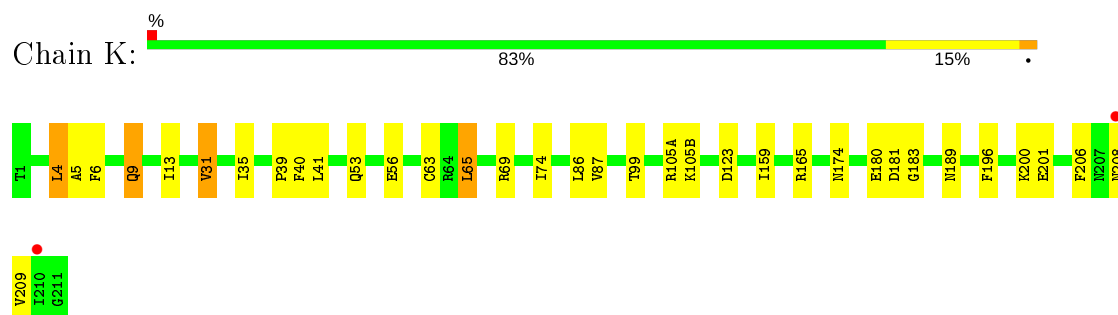
- Molecule 10: Proteasome component C11



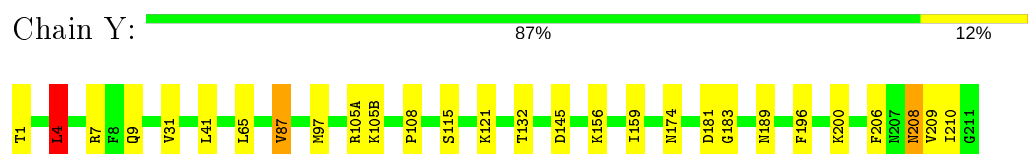
- Molecule 10: Proteasome component C11



- Molecule 11: Proteasome component PRE2

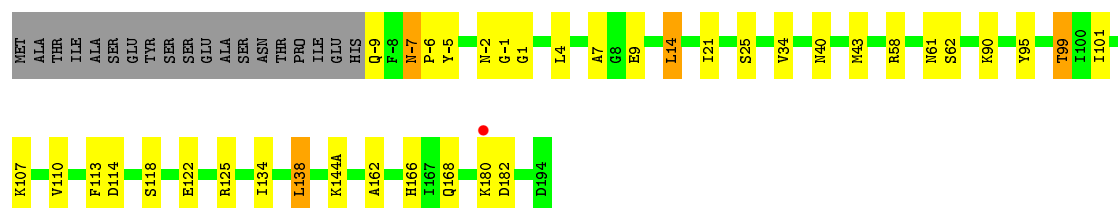


- Molecule 11: Proteasome component PRE2




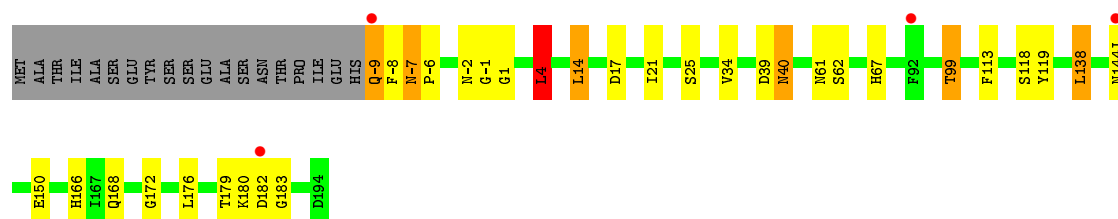
- Molecule 12: Proteasome component C5

Chain L: 




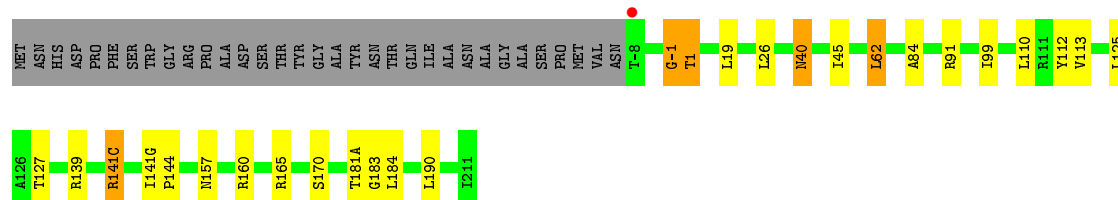
- Molecule 12: Proteasome component C5

Chain Z: 



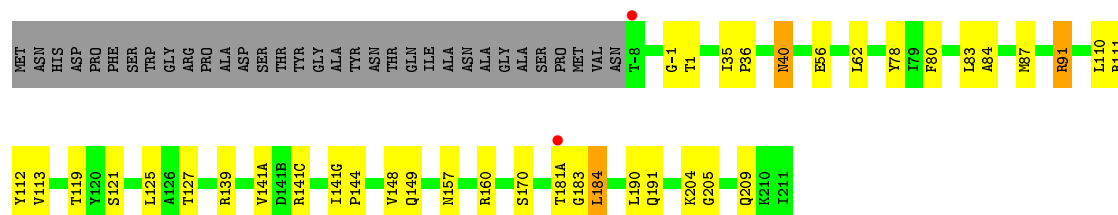
- Molecule 13: Proteasome component PRE4

Chain M: 




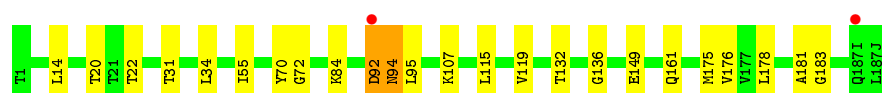
- Molecule 13: Proteasome component PRE4

Chain 1: 

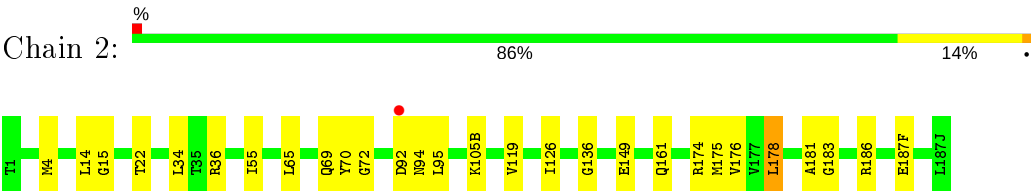


- Molecule 14: Proteasome component PRE3

Chain N: 



● Molecule 14: Proteasome component PRE3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.33Å 299.19Å 145.67Å 90.00° 113.13° 90.00°	Depositor
Resolution (Å)	49.88 – 2.59 49.77 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.2 (49.88-2.59) 95.2 (49.77-2.59)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.224 , 0.252 0.220 , 0.247	Depositor DCC
$R_{free}$ test set	6368 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 30.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	49429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: L3T, MG, 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	0.41	0/1951	0.56	0/2639
1	O	0.42	0/1951	0.55	0/2639
2	B	0.40	0/1857	0.57	0/2513
2	P	0.40	0/1857	0.55	0/2513
3	C	0.41	0/1918	0.55	0/2591
3	Q	0.40	0/1918	0.55	0/2591
4	D	0.43	0/1883	0.58	0/2529
4	R	0.42	0/1884	0.58	1/2532 (0.0%)
5	E	0.40	0/1819	0.58	1/2451 (0.0%)
5	S	0.39	0/1821	0.55	0/2457
6	F	0.42	0/1885	0.55	0/2540
6	T	0.43	0/1886	0.56	0/2543
7	G	0.44	0/1956	0.54	0/2643
7	U	0.43	0/1958	0.56	0/2649
8	H	0.41	0/1714	0.56	0/2320
8	V	0.41	0/1714	0.56	0/2320
9	I	0.45	0/1608	0.58	0/2165
9	W	0.75	1/1609 (0.1%)	0.63	1/2168 (0.0%)
10	J	0.42	0/1611	0.58	0/2167
10	X	0.41	0/1611	0.57	0/2167
11	K	0.42	0/1680	0.58	0/2271
11	Y	0.40	0/1680	0.58	1/2271 (0.0%)
12	L	0.44	0/1793	0.58	0/2414
12	Z	0.43	0/1793	0.58	1/2414 (0.0%)
13	1	0.44	0/1852	0.63	0/2504
13	M	0.74	1/1853 (0.1%)	0.70	2/2507 (0.1%)
14	2	0.43	0/1538	0.55	0/2078
14	N	0.72	1/1539 (0.1%)	0.62	2/2081 (0.1%)
All	All	0.46	3/50139 (0.0%)	0.58	9/67677 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	-1	GLY	C-N	26.20	1.94	1.34
9	W	36	HIS	C-N	24.30	1.90	1.34
14	N	92	ASP	C-N	22.99	1.86	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	-1	GLY	O-C-N	-14.36	99.72	122.70
14	N	92	ASP	O-C-N	-10.87	105.30	122.70
9	W	36	HIS	CA-C-N	-10.45	94.21	117.20
13	M	-1	GLY	CA-C-N	-7.69	100.29	117.20
14	N	92	ASP	CA-C-N	7.17	132.96	117.20
11	Y	4	LEU	CA-CB-CG	5.85	128.75	115.30
5	E	76	LEU	CA-CB-CG	5.76	128.55	115.30
4	R	59	LEU	CA-CB-CG	5.29	127.47	115.30
12	Z	4	LEU	CA-CB-CG	5.27	127.43	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1925	21	0
1	O	1915	0	1925	23	0
2	B	1829	0	1828	25	0
2	P	1829	0	1828	27	0
3	C	1891	0	1899	19	0
3	Q	1891	0	1899	31	0
4	D	1862	0	1832	25	0
4	R	1862	0	1833	20	0
5	E	1795	0	1793	31	0
5	S	1795	0	1795	32	0
6	F	1848	0	1842	24	0
6	T	1848	0	1843	24	0
7	G	1921	0	1907	29	0
7	U	1921	0	1909	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1685	0	1686	24	0
8	V	1685	0	1686	22	0
9	I	1581	0	1574	22	0
9	W	1581	0	1574	28	0
10	J	1585	0	1591	16	0
10	X	1585	0	1591	23	0
11	K	1644	0	1594	27	0
11	Y	1644	0	1594	19	0
12	L	1757	0	1712	22	0
12	Z	1757	0	1712	27	0
13	1	1824	0	1833	29	0
13	M	1824	0	1833	24	0
14	2	1512	0	1478	15	0
14	N	1512	0	1478	14	0
15	F	2	0	0	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	2	0	0	0	0
15	N	1	0	0	0	0
16	K	46	0	40	4	0
16	Y	46	0	40	2	0
17	K	12	0	13	0	0
17	Y	12	0	13	1	0
18	K	2	0	0	0	0
18	L	3	0	0	0	0
All	All	49429	0	49100	581	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 6.

All (581) 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)
13:M:-1:GLY:C	13:M:1:THR:H1	1.31	1.31
14:N:92:ASP:C	14:N:94:ASN:N	1.86	1.26
9:W:36:HIS:C	9:W:38:TYR:N	1.89	1.24
13:1:-1:GLY:C	13:1:1:THR:H1	1.37	1.23
2:P:200:THR:O	2:P:202:THR:N	1.71	1.22
13:M:-1:GLY:C	13:M:1:THR:N	1.94	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:-1:GLY:C	13:1:1:THR:N	2.02	1.12
9:I:-1:GLY:C	9:I:1:GLY:N	2.04	1.11
9:W:-1:GLY:C	9:W:1:GLY:N	2.04	1.10
14:2:70:TYR:C	14:2:72:GLY:N	2.06	1.08
14:N:70:TYR:C	14:N:72:GLY:N	2.09	1.06
13:M:141(G):ILE:C	13:M:144:PRO:N	2.09	1.06
13:1:141(G):ILE:C	13:1:144:PRO:N	2.10	1.05
8:H:91:GLN:C	8:H:93:GLY:N	2.14	1.01
7:U:96:ALA:HA	7:U:107:MET:HE2	1.44	0.99
9:I:36:HIS:C	9:I:38:TYR:N	2.21	0.94
7:G:96:ALA:HA	7:G:107:MET:HE2	1.50	0.94
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.33	0.94
9:W:-1:GLY:C	9:W:1:GLY:H1	1.72	0.93
9:I:-1:GLY:C	9:I:1:GLY:H1	1.71	0.92
12:Z:-1:GLY:C	12:Z:1:GLY:N	2.23	0.91
7:G:218:ASP:C	7:G:220:LYS:N	2.24	0.91
2:B:200:THR:C	2:B:202:THR:N	2.22	0.90
8:V:187:LEU:C	8:V:189:ARG:N	2.24	0.90
8:H:187:LEU:C	8:H:189:ARG:N	2.24	0.90
9:W:-1:GLY:C	9:W:1:GLY:H3	1.71	0.88
9:I:-1:GLY:C	9:I:1:GLY:H3	1.73	0.87
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.37	0.87
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.58	0.85
6:F:35:THR:HG21	6:F:51:GLU:O	1.79	0.83
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.40	0.83
6:T:192:GLN:NE2	6:T:195:LYS:HE3	1.94	0.82
5:E:207:LEU:HA	5:E:207(E):ASN:HD22	1.45	0.82
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.24	0.82
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.44	0.82
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.44	0.80
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.94	0.80
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.30	0.79
9:W:179:LYS:C	9:W:181:LYS:N	2.35	0.79
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.30	0.79
3:C:15:PHE:H	4:D:23:GLN:HE22	1.29	0.79
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.95	0.79
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.32	0.78
11:K:31:VAL:HG11	16:K:213:L3T:C21	2.14	0.78
5:E:15:PHE:H	6:F:23:GLN:HE22	1.31	0.78
3:C:163:GLN:NE2	3:C:164:THR:H	1.82	0.77
13:M:141(C):ARG:HH11	13:M:141(C):ARG:HG3	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:15:PHE:H	2:P:23:GLN:HE22	1.33	0.77
6:T:192:GLN:HE22	6:T:195:LYS:HE3	1.49	0.77
12:L:180:LYS:C	12:L:182:ASP:N	2.38	0.77
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.99	0.76
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.48	0.76
7:G:184(M):SER:HA	7:G:186:TRP:N	2.01	0.76
11:K:31:VAL:HG11	16:K:213:L3T:H21	1.68	0.75
11:K:40:PHE:HA	11:K:183:GLY:N	2.00	0.75
12:Z:-1:GLY:C	12:Z:1:GLY:H1	1.88	0.74
2:B:13:THR:O	3:C:130:ARG:HD3	1.87	0.74
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.68	0.74
14:2:92:ASP:O	14:2:94:ASN:N	2.20	0.74
7:U:96:ALA:CA	7:U:107:MET:HE2	2.17	0.74
13:M:40:ASN:H	13:M:40:ASN:HD22	1.35	0.73
2:P:121:GLN:O	2:P:124:THR:HB	1.87	0.73
3:C:163:GLN:HE21	3:C:164:THR:H	1.33	0.73
12:Z:-1:GLY:C	12:Z:1:GLY:CA	2.56	0.73
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.37	0.72
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	1.87	0.72
4:D:202:GLU:C	4:D:205:GLU:N	2.43	0.72
7:U:121:GLN:O	7:U:124:THR:HB	1.90	0.72
9:W:36:HIS:CA	9:W:38:TYR:N	2.52	0.72
10:J:181:ASP:C	10:J:183:GLY:N	2.43	0.71
13:M:-1:GLY:C	13:M:1:THR:H2	1.91	0.71
8:V:91:GLN:C	8:V:93:GLY:N	2.43	0.71
12:Z:180:LYS:C	12:Z:182:ASP:N	2.43	0.71
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.72	0.71
2:B:181:LYS:O	2:B:184:MET:HG3	1.91	0.71
14:2:92:ASP:C	14:2:94:ASN:N	2.44	0.71
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.73	0.71
12:Z:-1:GLY:O	12:Z:1:GLY:HA3	1.91	0.71
6:F:168:GLY:HA3	6:F:201:ALA:HB1	1.73	0.70
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.36	0.70
10:J:24:ILE:HD11	10:X:129:TYR:HB3	1.73	0.70
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.74	0.70
12:L:-1:GLY:C	12:L:1:GLY:N	2.45	0.70
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.55	0.70
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.74	0.70
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.40	0.70
8:H:202:LYS:HE3	12:Z:150:GLU:OE2	1.91	0.70
11:K:181:ASP:C	11:K:183:GLY:CA	2.60	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:196:PHE:HZ	11:Y:209:VAL:HG21	1.57	0.70
5:S:52:LYS:HB2	5:S:63:TYR:HB3	1.73	0.69
6:T:35:THR:HG21	6:T:51:GLU:O	1.91	0.69
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.40	0.69
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.75	0.68
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.42	0.68
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.42	0.68
10:X:-1:MET:HA	10:X:-1:MET:HE2	1.75	0.68
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.93	0.67
13:1:181(A):THR:O	13:1:183:GLY:N	2.28	0.66
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.41	0.66
11:K:181:ASP:C	11:K:183:GLY:HA2	2.16	0.66
12:Z:-1:GLY:C	12:Z:1:GLY:HA3	2.15	0.66
8:H:91:GLN:O	8:H:93:GLY:N	2.26	0.66
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.26	0.66
5:E:12:THR:HG21	5:E:124:THR:HA	1.77	0.66
7:U:218:ASP:C	7:U:220:LYS:N	2.49	0.66
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.76	0.66
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.78	0.66
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.78	0.66
11:K:181:ASP:O	11:K:183:GLY:HA2	1.96	0.65
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.77	0.65
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.44	0.65
3:Q:171:THR:O	3:Q:174:GLU:HB3	1.97	0.65
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.44	0.65
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.79	0.65
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.62	0.65
11:K:181:ASP:C	11:K:183:GLY:HA3	2.17	0.65
6:T:199:LEU:C	6:T:201:ALA:N	2.51	0.65
4:D:122:ARG:HA	4:D:126:ARG:HD3	1.78	0.64
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.62	0.64
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.62	0.64
4:R:12:VAL:HG23	4:R:13:SER:H	1.63	0.64
11:Y:31:VAL:HG21	16:Y:212:L3T:H21	1.78	0.64
9:I:36:HIS:CA	9:I:38:TYR:N	2.61	0.63
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.13	0.63
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.44	0.63
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.78	0.63
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.96	0.62
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.29	0.62
2:P:97:GLN:HE21	9:W:61:TYR:HA	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:180(E):LYS:O	5:E:183:ASP:N	2.33	0.62
6:F:35:THR:CG2	6:F:51:GLU:O	2.46	0.62
3:Q:100:ARG:HH11	3:Q:106:PRO:HG3	1.65	0.62
13:1:-1:GLY:CA	13:1:1:THR:H1	2.11	0.62
10:X:28:LYS:HE3	11:Y:121:LYS:O	1.98	0.62
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.64	0.61
13:1:-1:GLY:C	13:1:1:THR:H2	1.99	0.61
13:1:-1:GLY:CA	13:1:1:THR:N	2.62	0.61
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.13	0.61
12:Z:179:THR:HG1	12:Z:182:ASP:N	1.98	0.61
4:D:179:GLU:HB3	4:D:192:LEU:HD21	1.81	0.61
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.82	0.61
1:A:200:SER:O	1:A:202:VAL:HA	2.00	0.61
11:Y:181:ASP:C	11:Y:183:GLY:N	2.54	0.61
12:L:-1:GLY:C	12:L:1:GLY:H3	2.04	0.61
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.49	0.61
7:U:87:ASN:C	7:U:87:ASN:HD22	2.03	0.60
3:C:163:GLN:HE21	3:C:164:THR:N	1.99	0.60
1:A:7:ARG:CG	6:F:128:SER:HB3	2.30	0.60
12:L:166:HIS:HD2	12:L:168:GLN:H	1.47	0.60
5:S:60:SER:C	5:S:63:TYR:N	2.55	0.60
3:Q:163:GLN:HA	3:Q:163:GLN:HE21	1.65	0.60
10:X:2:ILE:HG12	10:X:130:SER:HB3	1.84	0.60
7:G:121:GLN:O	7:G:124:THR:HB	2.02	0.60
7:G:96:ALA:CA	7:G:107:MET:HE2	2.29	0.60
2:B:121:GLN:O	2:B:124:THR:HB	2.02	0.59
5:S:73:HIS:HE1	5:S:107:LEU:O	1.84	0.59
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	1.99	0.59
5:E:207:LEU:HA	5:E:207(E):ASN:ND2	2.14	0.59
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.34	0.59
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.99	0.59
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.84	0.59
5:S:132:TYR:O	5:S:153:PRO:HB3	2.02	0.59
7:G:96:ALA:HA	7:G:107:MET:CE	2.29	0.59
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.68	0.59
9:I:179:LYS:C	9:I:181:LYS:N	2.56	0.59
7:U:107:MET:HE1	7:U:112:LEU:HD13	1.84	0.59
10:J:-1:MET:HA	10:J:1:ASP:N	2.18	0.59
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	1.99	0.59
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.33	0.58
9:I:179:LYS:O	9:I:181:LYS:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:233:ILE:C	4:R:235:LYS:N	2.57	0.58
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.85	0.58
10:J:-1:MET:HA	10:J:1:ASP:H3	1.68	0.58
13:M:-1:GLY:CA	13:M:1:THR:H1	2.13	0.58
13:M:-1:GLY:CA	13:M:1:THR:N	2.66	0.58
14:N:181:ALA:O	14:N:183:GLY:N	2.37	0.58
1:O:55:SER:O	1:O:56:SER:HB3	2.03	0.58
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.69	0.58
4:R:123(D):ALA:HB3	4:R:126:ARG:HG3	1.86	0.58
1:A:7:ARG:HG2	6:F:128:SER:HB3	1.86	0.58
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.86	0.58
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.84	0.58
5:S:180:LEU:HA	5:S:180(C):PHE:CE2	2.39	0.58
1:A:121:GLN:O	1:A:124:THR:HB	2.04	0.57
10:X:181:ASP:C	10:X:183:GLY:N	2.58	0.57
6:T:35:THR:CG2	6:T:51:GLU:O	2.52	0.57
1:A:15:PHE:H	2:B:23:GLN:HE22	1.51	0.57
4:D:123(C):GLY:HA2	4:D:126:ARG:H	1.70	0.57
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.69	0.57
13:M:40:ASN:N	13:M:40:ASN:HD22	1.99	0.57
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.05	0.57
2:B:15:PHE:H	3:C:23:GLN:HE22	1.53	0.57
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.87	0.56
9:I:36:HIS:HA	9:I:38:TYR:N	2.20	0.56
4:R:186:LEU:O	4:R:190:GLU:HG3	2.06	0.56
5:S:134:VAL:O	5:S:153:PRO:HG3	2.06	0.56
8:V:187:LEU:O	8:V:189:ARG:N	2.38	0.56
5:S:15:PHE:H	6:T:23:GLN:HE22	1.54	0.56
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.14	0.56
10:J:15:ALA:HB2	10:J:155:LEU:HD11	1.87	0.56
7:U:107:MET:CE	7:U:112:LEU:HD13	2.36	0.56
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.71	0.55
1:O:7:ARG:HG2	6:T:128:SER:HB3	1.88	0.55
2:P:54:VAL:HA	2:P:209:ARG:HH12	1.70	0.55
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.06	0.55
8:V:128:GLY:O	8:V:131:SER:HB3	2.07	0.55
5:E:207(B):THR:H	5:E:207(E):ASN:HD22	1.54	0.55
10:J:2:ILE:HD13	10:J:162:LEU:HD13	1.88	0.55
14:2:181:ALA:C	14:2:183:GLY:N	2.60	0.55
11:K:31:VAL:CG1	16:K:213:L3T:H21	2.35	0.55
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.02	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:181(A):THR:O	13:M:183:GLY:N	2.40	0.55
1:O:121:GLN:O	1:O:124:THR:HB	2.06	0.55
11:Y:196:PHE:CZ	11:Y:209:VAL:HG21	2.38	0.55
11:Y:208:ASN:HD22	11:Y:208:ASN:H	1.53	0.55
6:F:199:LEU:C	6:F:201:ALA:N	2.61	0.54
6:T:186:ALA:O	6:T:190:VAL:HG23	2.07	0.54
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.04	0.54
10:J:181:ASP:O	10:J:183:GLY:HA3	2.07	0.54
14:N:181:ALA:HB3	14:N:183:GLY:HA3	1.89	0.54
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.55	0.54
4:D:180(E):SER:C	4:D:184:LEU:N	2.60	0.54
5:E:73:HIS:HE1	5:E:107:LEU:O	1.90	0.54
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.90	0.54
9:W:12:VAL:HG23	9:W:178:ILE:HB	1.88	0.54
6:F:13:SER:HB2	7:G:130:ARG:HB3	1.90	0.54
6:F:179:LEU:HD11	6:F:192:GLN:HG2	1.90	0.54
9:I:10:ASP:HB3	9:I:181:LYS:HE2	1.89	0.54
5:S:17:PRO:HA	6:T:26:TYR:CD1	2.43	0.54
5:S:86:ARG:O	5:S:90:ASN:HB2	2.08	0.53
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.03	0.53
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.56	0.53
6:T:12:ASN:C	6:T:14:VAL:H	2.11	0.53
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.90	0.53
13:1:112:TYR:CE1	13:1:127:THR:HG22	2.42	0.53
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.72	0.53
5:E:60:SER:C	5:E:63:TYR:N	2.62	0.53
6:T:43:ASN:HD22	6:T:44:ASP:N	2.07	0.53
6:F:218(B):THR:HB	6:F:222:LYS:HE3	1.91	0.53
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.39	0.53
13:M:165:ARG:HD3	8:V:139:GLU:OE1	2.09	0.53
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.74	0.52
13:1:35:ILE:HG12	13:1:56:GLU:HG2	1.90	0.52
11:Y:31:VAL:CG2	16:Y:212:L3T:H21	2.39	0.52
12:L:9:GLU:O	12:L:107:LYS:HA	2.09	0.52
10:X:-1:MET:CE	10:X:-1:MET:HA	2.40	0.52
1:A:7:ARG:HD2	5:E:127:TYR:CD2	2.45	0.52
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.19	0.52
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.92	0.52
4:D:21:LEU:HD21	5:E:130:ARG:HD3	1.92	0.52
5:E:180(F):ILE:C	5:E:183:ASP:N	2.63	0.52
12:L:43:MET:HG3	12:L:101:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:157:ASN:ND2	13:M:160:ARG:HH11	2.01	0.52
2:P:97:GLN:NE2	9:W:61:TYR:HA	2.24	0.52
5:E:207(E):ASN:O	5:E:210:LEU:N	2.43	0.52
3:Q:163:GLN:NE2	3:Q:164:THR:H	2.07	0.52
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.89	0.52
3:C:203:THR:HA	3:C:206:GLY:N	2.24	0.52
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.23	0.52
5:E:207:LEU:HD23	5:E:207:LEU:H	1.74	0.52
8:H:172:ASN:HD22	8:H:193:THR:HA	1.74	0.52
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.40	0.52
11:K:39:PRO:O	11:K:183:GLY:N	2.43	0.52
11:K:165:ARG:HH22	11:K:208:ASN:HD22	1.56	0.52
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.91	0.52
1:O:217(G):LEU:HD13	1:O:218:GLY:HA2	1.91	0.52
5:S:12:THR:HG21	5:S:124:THR:HA	1.93	0.51
5:S:207:LEU:HD12	5:S:210:LEU:HD22	1.92	0.51
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.92	0.51
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.92	0.51
13:1:-1:GLY:O	13:1:1:THR:N	2.23	0.51
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.20	0.51
12:L:-1:GLY:O	12:L:1:GLY:HA3	2.10	0.51
10:X:24:ILE:O	10:X:24:ILE:HG12	2.08	0.51
4:D:123(C):GLY:HA2	4:D:125:GLU:HA	1.92	0.51
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.93	0.51
1:O:97:HIS:HD2	8:V:61:SER:OG	1.93	0.51
6:F:198:TYR:HB3	6:F:240:ILE:HD12	1.92	0.51
7:U:168:LYS:HD3	7:U:201:LEU:HD22	1.93	0.51
6:F:203:GLU:O	6:F:206:LYS:HG3	2.11	0.51
7:G:184(M):SER:CA	7:G:186:TRP:N	2.73	0.51
9:I:12:VAL:HG23	9:I:178:ILE:HB	1.92	0.51
6:T:114:ASP:O	6:T:118:GLN:HG2	2.10	0.51
2:P:87:ILE:O	2:P:91:THR:HG23	2.11	0.51
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.38	0.51
13:1:111:ARG:HH11	13:1:121:SER:HB2	1.74	0.51
8:V:91:GLN:O	8:V:93:GLY:N	2.44	0.51
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.93	0.51
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.46	0.51
1:O:5:THR:HB	1:O:7:ARG:HH21	1.76	0.50
6:T:216:SER:HB3	6:T:218(A):GLU:HB2	1.91	0.50
5:E:31:ILE:HD11	5:E:153:PRO:HD3	1.91	0.50
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:60:SER:HA	5:S:63:TYR:N	2.26	0.50
11:K:200:LYS:HG3	11:K:206:PHE:HB2	1.93	0.50
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	1.92	0.50
9:W:36:HIS:HA	9:W:38:TYR:N	2.26	0.50
14:2:34:LEU:HD13	14:2:176:VAL:HG23	1.94	0.50
7:G:109:CYS:HB2	7:G:140:SER:OG	2.11	0.50
7:G:218:ASP:C	7:G:220:LYS:CA	2.80	0.50
14:2:181:ALA:O	14:2:183:GLY:N	2.45	0.50
1:O:58:LEU:HD12	7:U:173:THR:HG23	1.92	0.50
5:E:204:GLU:HG3	5:E:206:SER:O	2.12	0.49
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	1.93	0.49
6:T:176:LEU:HB3	7:U:58:LEU:HD21	1.94	0.49
9:W:110:ILE:HD12	9:W:125:ILE:HG12	1.93	0.49
2:P:45:GLY:HA2	2:P:146:TYR:CE1	2.46	0.49
3:Q:84:ASP:CG	3:Q:130:ARG:HH22	2.15	0.49
12:L:180:LYS:O	12:L:182:ASP:N	2.44	0.49
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.42	0.49
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.17	0.49
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.94	0.49
4:D:97:VAL:HG11	11:K:65:LEU:HD22	1.94	0.49
8:V:35:HIS:HB2	8:V:56:THR:HG21	1.94	0.49
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.95	0.49
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.94	0.49
14:N:70:TYR:C	14:N:72:GLY:CA	2.79	0.49
4:R:162:ALA:HB1	4:R:176:LEU:HD22	1.95	0.49
4:D:85:ALA:O	4:D:89:ILE:HG12	2.13	0.49
14:N:181:ALA:O	14:N:183:GLY:CA	2.61	0.49
3:C:163:GLN:CA	3:C:163:GLN:HE21	2.26	0.49
4:D:38:ILE:HD12	4:D:197:LEU:HG	1.95	0.48
13:1:141(A):VAL:HG23	13:1:141(A):VAL:O	2.12	0.48
2:B:150:THR:HG22	2:B:160:TRP:HE1	1.77	0.48
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.95	0.48
12:Z:180:LYS:O	12:Z:182:ASP:N	2.45	0.48
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.28	0.48
4:R:123:PHE:HA	4:R:128:MET:HB3	1.94	0.48
4:R:85:ALA:O	4:R:89:ILE:HG12	2.14	0.48
5:E:207:LEU:HD12	5:E:210:LEU:HD13	1.96	0.48
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.96	0.48
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.62	0.48
8:H:105:ASP:HB2	8:H:105(A):PRO:CD	2.43	0.48
6:T:12:ASN:OD1	6:T:124:THR:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:192:LEU:O	4:D:196:ILE:HG13	2.14	0.48
2:P:181:LYS:O	2:P:184:MET:HG3	2.14	0.48
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.95	0.48
11:K:31:VAL:CG1	16:K:213:L3T:C21	2.89	0.48
10:X:120:VAL:HG13	10:X:122:LEU:HG	1.94	0.48
13:1:36:PRO:HB3	13:1:184:LEU:HD11	1.94	0.48
4:D:180(C):HIS:CE1	4:D:180(E):SER:HB2	2.49	0.48
7:G:233:LEU:O	7:G:236:ILE:HG13	2.14	0.48
2:P:156:ASN:OD1	3:Q:82:ASN:HB2	2.14	0.48
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.96	0.48
13:1:157:ASN:HD22	13:1:160:ARG:NH1	2.09	0.47
4:D:123(C):GLY:HA2	4:D:126:ARG:N	2.28	0.47
3:Q:215:VAL:HG12	3:Q:221:ILE:HG12	1.95	0.47
5:S:60:SER:CA	5:S:63:TYR:N	2.77	0.47
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.14	0.47
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.95	0.47
11:K:196:PHE:HZ	11:K:209:VAL:HG21	1.79	0.47
12:Z:-1:GLY:C	12:Z:1:GLY:H3	2.14	0.47
1:A:67:VAL:HG11	1:A:213:ALA:HB2	1.95	0.47
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.96	0.47
9:W:-1:GLY:O	9:W:1:GLY:N	2.43	0.47
10:X:2:ILE:HD13	10:X:162:LEU:HD13	1.96	0.47
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.96	0.47
14:2:14:LEU:O	14:2:175:MET:HA	2.15	0.47
1:A:78:TYR:HB3	1:A:85:TYR:CD1	2.50	0.47
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.49	0.47
10:J:143:ARG:O	10:J:146:MET:HG3	2.15	0.47
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.95	0.47
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.95	0.47
9:W:55:LEU:HD11	9:W:97:VAL:HG21	1.95	0.47
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.80	0.47
6:F:114:ASP:O	6:F:118:GLN:HG2	2.15	0.47
8:H:105:ASP:HB2	8:H:105(A):PRO:HD2	1.96	0.47
1:A:112:LEU:O	1:A:116:VAL:HG23	2.15	0.47
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.44	0.47
8:V:172:ASN:HD22	8:V:193:THR:HA	1.80	0.47
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.44	0.47
3:C:164:THR:HG21	3:C:172:VAL:HG22	1.98	0.47
12:L:-2:ASN:HA	12:L:21:ILE:O	2.15	0.47
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.45	0.46
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:181:ASP:O	11:Y:183:GLY:HA3	2.15	0.46
7:G:191:GLU:HG3	7:G:232:ARG:HG3	1.97	0.46
9:W:11:CYS:HA	9:W:104:ILE:HD11	1.97	0.46
6:F:166:GLY:O	6:F:169:ARG:HB3	2.15	0.46
6:F:216:SER:HB3	6:F:218(A):GLU:HB2	1.97	0.46
9:I:48:LEU:HG	9:I:50:THR:HG22	1.96	0.46
4:R:121:LEU:HD21	5:S:83:PRO:HB3	1.97	0.46
8:H:187:LEU:O	8:H:189:ARG:N	2.47	0.46
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.85	0.46
4:D:21:LEU:HD21	5:E:130:ARG:CD	2.45	0.46
13:1:83:LEU:O	13:1:87:MET:HG2	2.15	0.46
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.81	0.46
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.51	0.46
8:H:3:ILE:HG13	8:H:100:ILE:HD12	1.98	0.46
9:I:36:HIS:O	9:I:38:TYR:N	2.49	0.46
14:N:149:GLU:H	14:N:149:GLU:CD	2.19	0.46
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.51	0.46
5:S:207:LEU:HA	5:S:209:ASN:HD22	1.81	0.46
7:U:87:ASN:C	7:U:87:ASN:ND2	2.67	0.46
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.51	0.46
1:A:111:LEU:O	1:A:114:SER:HB3	2.16	0.46
11:Y:1:THR:HB	17:Y:213:MES:O1S	2.16	0.46
10:J:113:ILE:HA	10:J:118:THR:O	2.15	0.45
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.99	0.45
2:P:67:LEU:HD22	2:P:211:GLU:HB3	1.98	0.45
10:J:24:ILE:CD1	10:X:129:TYR:HB3	2.44	0.45
1:A:97:HIS:HD2	8:H:61:SER:OG	1.98	0.45
2:B:163:ILE:HG13	2:B:164:SER:N	2.31	0.45
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.98	0.45
5:E:67:ILE:HG21	5:E:213:ALA:HB2	1.98	0.45
2:P:202:THR:HG22	2:P:204:SER:H	1.80	0.45
8:H:84:LYS:HG3	8:H:85:GLN:N	2.31	0.45
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.47	0.45
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.52	0.45
5:S:143:LYS:HE3	13:1:78:TYR:OH	2.17	0.45
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.51	0.45
10:X:161:GLU:HA	10:X:161:GLU:OE2	2.17	0.45
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.99	0.45
3:Q:82:ASN:HD22	3:Q:82:ASN:N	2.15	0.45
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.99	0.45
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:181:ASP:O	10:X:183:GLY:HA3	2.16	0.44
13:1:-1:GLY:HA2	13:1:1:THR:N	2.32	0.44
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.99	0.44
5:S:208:THR:OG1	5:S:209:ASN:HB2	2.17	0.44
9:W:99:PRO:HD2	9:W:113:PHE:HB2	1.99	0.44
13:M:45:ILE:HG12	13:M:99:ILE:HG12	2.00	0.44
5:E:132:TYR:O	5:E:153:PRO:HB3	2.18	0.44
7:U:77:VAL:HG12	7:U:137:THR:HB	1.98	0.44
7:U:191:GLU:HG3	7:U:232:ARG:HG3	1.99	0.44
9:W:107:LYS:HB3	9:W:107:LYS:HE2	1.46	0.44
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.82	0.44
5:E:103:PHE:HE2	13:M:62:LEU:HD21	1.82	0.44
13:1:112:TYR:O	13:1:119:THR:HA	2.18	0.44
2:B:44:ASP:N	2:B:44:ASP:OD2	2.51	0.44
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.98	0.44
1:O:7:ARG:CG	6:T:128:SER:HB3	2.47	0.44
8:V:35:HIS:CB	8:V:56:THR:HG21	2.48	0.44
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.00	0.44
7:G:107:MET:CE	7:G:112:LEU:HD13	2.48	0.44
11:K:6:PHE:HA	11:K:123:ASP:O	2.18	0.44
2:P:216(B):GLY:O	2:P:218:ASN:N	2.51	0.44
3:Q:35:THR:HB	3:Q:51:GLU:HG3	2.00	0.44
14:2:15:GLY:HA2	14:2:174:ARG:O	2.18	0.44
8:H:172:ASN:ND2	8:H:193:THR:HA	2.33	0.44
10:J:90(A):ILE:HG12	10:J:116:LEU:HD23	1.99	0.44
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.99	0.44
12:L:114:ASP:OD1	12:L:118:SER:HB3	2.18	0.44
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.32	0.44
8:H:165:ASN:HD22	13:1:139:ARG:NH1	2.10	0.43
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.99	0.43
10:X:6:ILE:HD11	10:X:142:TYR:CD1	2.53	0.43
13:1:84:ALA:HA	13:1:113:VAL:HG21	2.00	0.43
5:E:160:LEU:HD13	5:E:163:THR:HB	2.00	0.43
11:K:5:ALA:HA	11:K:13:ILE:O	2.18	0.43
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.82	0.43
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.30	0.43
7:U:41:ARG:HG3	7:U:148:ILE:HD12	2.01	0.43
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.18	0.43
3:C:207:ALA:C	3:C:209:ASN:H	2.22	0.43
12:L:122:GLU:OE1	12:L:125:ARG:NH2	2.45	0.43
10:X:113:ILE:HA	10:X:118:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:205:GLY:HA3	13:1:209:GLN:HB3	2.00	0.43
6:F:192:GLN:HE21	6:F:192:GLN:HA	1.83	0.43
7:G:87:ASN:C	7:G:87:ASN:HD22	2.22	0.43
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.67	0.43
5:E:109:VAL:HG12	5:E:149:LEU:HD22	2.01	0.43
5:S:198:SER:HA	5:S:201:LEU:HD12	2.00	0.43
6:T:12:ASN:ND2	6:T:126:TYR:O	2.52	0.43
9:W:152:PHE:HD1	9:W:177:ILE:HD11	1.82	0.43
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.18	0.43
3:Q:169:SER:HA	3:Q:172:VAL:HG13	2.00	0.43
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.83	0.43
10:X:143:ARG:O	10:X:146:MET:HG3	2.18	0.43
2:B:150:THR:O	2:B:157:TYR:HA	2.19	0.43
12:L:134:ILE:HD11	12:L:162:ALA:HB2	2.01	0.43
1:O:33:GLN:HG2	1:O:33:GLN:H	1.69	0.43
9:W:19:ARG:HB2	9:W:171:TRP:HB2	2.00	0.43
10:X:24:ILE:HD13	11:Y:132:THR:HG21	2.00	0.43
12:Z:-9:GLN:HE21	12:Z:-8:PHE:H	1.67	0.43
3:C:216:LYS:HB2	3:C:220:ASP:HB3	2.01	0.43
10:J:-1:MET:HG3	10:J:1:ASP:HB2	2.01	0.43
2:P:141:TYR:CD1	2:P:219(A):VAL:HG21	2.54	0.43
8:H:223:ASP:OD2	8:H:223:ASP:N	2.52	0.42
13:M:40:ASN:ND2	13:M:40:ASN:N	2.67	0.42
5:S:226:GLY:O	5:S:229:VAL:HG22	2.19	0.42
6:T:95:GLU:HG2	6:T:115:ARG:CG	2.49	0.42
8:V:105:ASP:HB2	8:V:105(A):PRO:HD2	2.01	0.42
9:W:48:LEU:HG	9:W:50:THR:HG22	2.01	0.42
1:A:117:ALA:HB1	1:A:155:GLY:O	2.19	0.42
8:H:124:TYR:HB2	8:H:138:LEU:HD13	2.00	0.42
6:T:43:ASN:HD22	6:T:44:ASP:H	1.67	0.42
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.50	0.42
4:R:202:GLU:O	4:R:205:GLU:N	2.52	0.42
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.55	0.42
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.16	0.42
5:E:66:LYS:O	5:E:77:SER:HA	2.19	0.42
6:F:180(F):GLY:O	6:F:184:LEU:N	2.51	0.42
10:J:3:ILE:HD12	10:J:44:SER:HB2	2.01	0.42
4:R:209:GLU:HG3	4:R:226:ASN:HB3	2.01	0.42
6:T:126:TYR:HB2	6:T:129:VAL:HG22	2.01	0.42
11:Y:208:ASN:ND2	11:Y:208:ASN:H	2.17	0.42
12:Z:-9:GLN:HE21	12:Z:-8:PHE:N	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.84	0.42
10:X:178:VAL:HA	10:X:183:GLY:O	2.19	0.42
11:Y:87:VAL:CG1	11:Y:115:SER:HA	2.50	0.42
2:B:40:ILE:HD12	2:B:193:ALA:HB2	2.02	0.42
2:B:61:GLN:OE1	2:B:208:ASP:HA	2.20	0.42
3:C:169:SER:HA	3:C:172:VAL:HG13	2.01	0.42
6:F:121:GLN:HE21	6:F:121:GLN:HB3	1.70	0.42
8:H:100:ILE:HG13	8:H:127:LEU:HD12	2.01	0.42
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	2.02	0.42
3:Q:152:GLU:HB2	3:Q:153:PRO:CD	2.50	0.42
4:R:70:ILE:HD11	4:R:76:CYS:HB2	2.01	0.42
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.85	0.42
8:V:41:ILE:HG12	8:V:76:VAL:HG22	2.01	0.42
10:X:18:LYS:HD3	10:X:174:ILE:HG13	2.02	0.42
7:G:152:ASP:HB2	7:G:153:PRO:HD2	2.01	0.42
8:H:38:SER:HB2	8:H:39:PRO:HD2	2.01	0.42
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.83	0.42
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.55	0.42
5:E:226:GLY:O	5:E:229:VAL:HG22	2.20	0.42
7:G:107:MET:HE1	7:G:112:LEU:HD13	2.01	0.42
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.19	0.42
9:W:51:ASP:OD2	10:X:90(B):ARG:NH2	2.53	0.42
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	2.00	0.42
5:E:134:VAL:O	5:E:153:PRO:HG3	2.20	0.42
13:1:40:ASN:HD22	13:1:40:ASN:H	1.68	0.41
3:C:82:ASN:HD22	3:C:82:ASN:N	2.17	0.41
1:O:78:TYR:HB3	1:O:85:TYR:CD1	2.55	0.41
2:P:148:LEU:HB3	2:P:160:TRP:O	2.19	0.41
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.86	0.41
12:L:99:THR:HG23	12:L:113:PHE:HB2	2.02	0.41
6:F:126:TYR:HE1	7:G:129:MET:SD	2.44	0.41
13:M:141(C):ARG:HH11	13:M:141(C):ARG:CG	2.25	0.41
1:O:217(P):LYS:HE3	1:O:217(P):LYS:N	2.36	0.41
12:Z:39:ASP:OD2	12:Z:67:HIS:HE1	2.03	0.41
7:G:77:VAL:CG1	7:G:137:THR:HB	2.50	0.41
8:H:104:VAL:HG13	8:H:178:MET:HB3	2.03	0.41
2:P:125:GLN:HG3	3:Q:130:ARG:HG3	2.01	0.41
4:R:10:ARG:HD2	5:S:10:GLY:HA2	2.01	0.41
13:1:80:PHE:CZ	13:1:111:ARG:HG2	2.55	0.41
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.55	0.41
7:G:238:GLU:O	7:G:239:GLN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:140:GLY:HA2	4:R:215:ILE:HG12	2.02	0.41
9:I:101:VAL:O	9:I:110:ILE:HA	2.20	0.41
9:I:28:SER:CB	10:J:120:VAL:HG21	2.49	0.41
1:O:77:VAL:HG22	1:O:78:TYR:H	1.85	0.41
5:S:114:HIS:HB3	6:T:86:ARG:NH2	2.36	0.41
7:U:47:VAL:HG22	7:U:214:VAL:HG22	2.01	0.41
4:D:90:GLU:OE2	11:K:69:ARG:NH1	2.53	0.41
5:E:28:LEU:HD12	5:E:153:PRO:HD2	2.03	0.41
3:Q:41:LYS:HA	3:Q:46:VAL:HA	2.02	0.41
7:U:49:ILE:HG13	7:U:212:VAL:HG22	2.02	0.41
9:W:181:LYS:N	9:W:181:LYS:HD2	2.36	0.41
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	2.02	0.41
6:F:238:LYS:HE3	6:F:238:LYS:HB2	1.89	0.41
8:H:101:VAL:HG13	8:H:111:PHE:HB2	2.03	0.41
11:K:86:LEU:C	11:K:86:LEU:HD13	2.41	0.41
14:N:14:LEU:O	14:N:175:MET:HA	2.21	0.41
7:U:38:LEU:HD12	7:U:38:LEU:C	2.40	0.41
5:E:100:SER:O	5:E:104:ASN:HA	2.21	0.41
9:I:-7:ASP:HA	9:I:-6:PRO:HD3	1.94	0.41
1:O:150:GLN:O	1:O:157:TYR:HA	2.21	0.41
5:S:65:LYS:HB3	5:S:65:LYS:HE2	1.83	0.41
4:D:28:LEU:HA	4:D:31:ILE:HD12	2.02	0.41
11:K:63:CYS:SG	11:K:74:ILE:HG21	2.61	0.41
12:L:7:ALA:HB2	12:L:110:VAL:HG23	2.02	0.41
11:Y:97:MET:HG2	11:Y:115:SER:HB3	2.02	0.41
11:K:35:ILE:HG21	11:K:56:GLU:HB3	2.03	0.40
2:P:78:VAL:HG22	2:P:136:PHE:CE2	2.56	0.40
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	2.03	0.40
3:Q:163:GLN:NE2	3:Q:173:ARG:HE	2.13	0.40
2:B:177:GLN:HE21	2:B:177:GLN:HB2	1.64	0.40
12:L:-1:GLY:C	12:L:1:GLY:CA	2.89	0.40
6:T:199:LEU:HD12	6:T:240:ILE:HD12	2.02	0.40
8:V:38:SER:HB2	8:V:39:PRO:HD2	2.03	0.40
10:J:21:THR:HG21	10:X:167:PRO:HB3	2.03	0.40
10:X:166:MET:HA	10:X:167:PRO:HD3	1.88	0.40
6:F:12:ASN:OD1	6:F:124:THR:HA	2.22	0.40
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.56	0.40
5:S:82:ALA:N	5:S:83:PRO:CD	2.85	0.40
8:V:14:ILE:HD11	8:V:42:TRP:HB3	2.03	0.40
9:W:87:LEU:HD11	9:W:99:PRO:HG2	2.02	0.40
5:S:198:SER:C	5:S:200:SER:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/250 (98%)	239 (97%)	5 (2%)	2 (1%)	19	39
1	O	246/250 (98%)	234 (95%)	11 (4%)	1 (0%)	34	57
2	B	231/245 (94%)	222 (96%)	6 (3%)	3 (1%)	12	24
2	P	231/245 (94%)	219 (95%)	9 (4%)	3 (1%)	12	24
3	C	235/243 (97%)	229 (97%)	5 (2%)	1 (0%)	34	57
3	Q	235/243 (97%)	226 (96%)	7 (3%)	2 (1%)	17	35
4	D	232/250 (93%)	219 (94%)	11 (5%)	2 (1%)	17	35
4	R	234/250 (94%)	220 (94%)	13 (6%)	1 (0%)	34	57
5	E	223/234 (95%)	214 (96%)	7 (3%)	2 (1%)	17	35
5	S	227/234 (97%)	215 (95%)	10 (4%)	2 (1%)	17	35
6	F	231/248 (93%)	223 (96%)	8 (4%)	0	100	100
6	T	233/248 (94%)	225 (97%)	7 (3%)	1 (0%)	34	57
7	G	235/252 (93%)	227 (97%)	7 (3%)	1 (0%)	34	57
7	U	239/252 (95%)	233 (98%)	4 (2%)	2 (1%)	19	39
8	H	216/222 (97%)	209 (97%)	7 (3%)	0	100	100
8	V	216/222 (97%)	209 (97%)	5 (2%)	2 (1%)	17	35
9	I	196/205 (96%)	192 (98%)	4 (2%)	0	100	100
9	W	198/205 (97%)	191 (96%)	7 (4%)	0	100	100
10	J	193/198 (98%)	186 (96%)	6 (3%)	1 (0%)	29	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	X	193/198 (98%)	184 (95%)	8 (4%)	1 (0%)	29	52
11	K	208/212 (98%)	201 (97%)	5 (2%)	2 (1%)	15	32
11	Y	208/212 (98%)	201 (97%)	7 (3%)	0	100	100
12	L	216/241 (90%)	210 (97%)	6 (3%)	0	100	100
12	Z	216/241 (90%)	209 (97%)	7 (3%)	0	100	100
13	1	225/266 (85%)	219 (97%)	6 (3%)	0	100	100
13	M	227/266 (85%)	217 (96%)	9 (4%)	1 (0%)	34	57
14	2	188/196 (96%)	184 (98%)	4 (2%)	0	100	100
14	N	190/196 (97%)	184 (97%)	6 (3%)	0	100	100
All	All	6168/6524 (94%)	5941 (96%)	197 (3%)	30 (0%)	29	52

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL
3	C	207	ALA
5	E	6	ASN
7	G	239	GLN
2	P	54	VAL
2	P	217	ALA
3	Q	202	GLN
5	S	203	ASP
1	A	5	THR
2	B	217	ALA
11	K	9	GLN
13	M	1	THR
2	P	218(B)	ASP
3	Q	207	ALA
5	S	6	ASN
1	A	167	LYS
2	B	218(C)	ASP
5	E	203	ASP
11	K	180	GLU
4	D	123(E)	SER
8	V	171	SER
6	T	240	ILE
4	D	123(C)	GLY
4	R	123(E)	SER
7	U	239	GLN

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Mol	Chain	Res	Type
1	O	56	SER
10	X	8	VAL
10	J	8	VAL
7	U	55	PRO
8	V	181	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	198 (95%)	11 (5%)	22	45
1	O	209/209 (100%)	198 (95%)	11 (5%)	22	45
2	B	195/204 (96%)	183 (94%)	12 (6%)	18	37
2	P	195/204 (96%)	179 (92%)	16 (8%)	11	22
3	C	213/215 (99%)	195 (92%)	18 (8%)	10	21
3	Q	213/215 (99%)	202 (95%)	11 (5%)	23	46
4	D	198/206 (96%)	183 (92%)	15 (8%)	13	26
4	R	198/206 (96%)	188 (95%)	10 (5%)	24	46
5	E	192/193 (100%)	176 (92%)	16 (8%)	11	22
5	S	192/193 (100%)	175 (91%)	17 (9%)	9	19
6	F	196/205 (96%)	178 (91%)	18 (9%)	9	17
6	T	196/205 (96%)	180 (92%)	16 (8%)	11	22
7	G	207/210 (99%)	189 (91%)	18 (9%)	10	20
7	U	207/210 (99%)	197 (95%)	10 (5%)	25	49
8	H	181/181 (100%)	175 (97%)	6 (3%)	38	64
8	V	181/181 (100%)	175 (97%)	6 (3%)	38	64
9	I	172/173 (99%)	167 (97%)	5 (3%)	42	68
9	W	172/173 (99%)	164 (95%)	8 (5%)	26	50
10	J	175/175 (100%)	166 (95%)	9 (5%)	24	46
10	X	175/175 (100%)	162 (93%)	13 (7%)	13	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	169/169 (100%)	158 (94%)	11 (6%)	17	34
11	Y	169/169 (100%)	158 (94%)	11 (6%)	17	34
12	L	185/201 (92%)	175 (95%)	10 (5%)	22	44
12	Z	185/201 (92%)	174 (94%)	11 (6%)	19	39
13	1	199/224 (89%)	188 (94%)	11 (6%)	21	43
13	M	199/224 (89%)	193 (97%)	6 (3%)	41	67
14	2	162/162 (100%)	154 (95%)	8 (5%)	25	48
14	N	162/162 (100%)	153 (94%)	9 (6%)	21	42
All	All	5306/5454 (97%)	4983 (94%)	323 (6%)	18	38

All (323) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	5	THR
1	A	33	GLN
1	A	62	GLU
1	A	64	LEU
1	A	65	SER
1	A	124	THR
1	A	158	PHE
1	A	203	GLU
1	A	217(N)	THR
1	A	222	ARG
2	B	58	LEU
2	B	61	GLN
2	B	91	THR
2	B	121	GLN
2	B	177	GLN
2	B	185	LYS
2	B	186	VAL
2	B	192	LEU
2	B	198	SER
2	B	202	THR
2	B	225	LYS
2	B	232	ILE
3	C	10	ARG
3	C	25	GLU
3	C	33	ARG

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Mol	Chain	Res	Type
3	C	44	ASN
3	C	52	ARG
3	C	66	LYS
3	C	82	ASN
3	C	121	GLN
3	C	150	GLN
3	C	156	ILE
3	C	163	GLN
3	C	172	VAL
3	C	174	GLU
3	C	180(C)	LYS
3	C	185	THR
3	C	187	GLU
3	C	208	LYS
3	C	226	SER
4	D	28	LEU
4	D	48	LEU
4	D	59	LEU
4	D	65	GLU
4	D	76	CYS
4	D	110	GLU
4	D	119	LEU
4	D	123(B)	GLU
4	D	125	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	205	GLU
4	D	215	ILE
4	D	237	LEU
5	E	12	THR
5	E	13	VAL
5	E	18	THR
5	E	28	LEU
5	E	58	LEU
5	E	76	LEU
5	E	121	GLN
5	E	149	LEU
5	E	185	ASN
5	E	187	ASP
5	E	189	LEU
5	E	207	LEU

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Mol	Chain	Res	Type
5	E	207(C)	VAL
5	E	219	THR
5	E	222	THR
5	E	227	GLU
6	F	35	THR
6	F	36	THR
6	F	43	ASN
6	F	59	LEU
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	129	VAL
6	F	169	ARG
6	F	176	LEU
6	F	180(E)	GLU
6	F	192	GLN
6	F	206	LYS
6	F	214	TRP
6	F	218(C)	ASN
6	F	222	LYS
6	F	225	LYS
6	F	238	LYS
7	G	10	ARG
7	G	33	GLN
7	G	38	LEU
7	G	49	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	171	GLU
7	G	179(C)	LYS
7	G	184	ASN
7	G	184(H)	GLU
7	G	184(M)	SER
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	34	LEU
8	H	55	VAL

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Mol	Chain	Res	Type
8	H	68	LEU
8	H	101	VAL
8	H	144	GLN
8	H	182	LYS
9	I	107	LYS
9	I	160	LEU
9	I	171	TRP
9	I	174	VAL
9	I	181	LYS
10	J	6	ILE
10	J	24	ILE
10	J	34	THR
10	J	52	THR
10	J	68	ILE
10	J	70	GLU
10	J	77	GLN
10	J	155	LEU
10	J	191	GLN
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	41	LEU
11	K	53	GLN
11	K	65	LEU
11	K	87	VAL
11	K	99	THR
11	K	105(A)	ARG
11	K	105(B)	LYS
11	K	201	GLU
12	L	-9	GLN
12	L	-7	ASN
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	58	ARG
12	L	62	SER
12	L	99	THR
12	L	138	LEU
12	L	144(A)	LYS
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG

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Mol	Chain	Res	Type
13	M	141(C)	ARG
13	M	184	LEU
13	M	190	LEU
14	N	20	THR
14	N	22	THR
14	N	31	THR
14	N	84	LYS
14	N	94	ASN
14	N	107	LYS
14	N	115	LEU
14	N	119	VAL
14	N	132	THR
1	O	4	MET
1	O	5	THR
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	111	LEU
1	O	124	THR
1	O	158	PHE
1	O	167	LYS
1	O	217(P)	LYS
1	O	223	LYS
2	P	58	LEU
2	P	61	GLN
2	P	64	THR
2	P	65	GLU
2	P	91	THR
2	P	110	GLU
2	P	121	GLN
2	P	150	THR
2	P	170	SER
2	P	181	LYS
2	P	185	LYS
2	P	192	LEU
2	P	198	SER
2	P	202	THR
2	P	225	LYS
2	P	235	LYS
3	Q	25	GLU
3	Q	66	LYS
3	Q	82	ASN

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Mol	Chain	Res	Type
3	Q	100	ARG
3	Q	121	GLN
3	Q	150	GLN
3	Q	156	ILE
3	Q	163	GLN
3	Q	172	VAL
3	Q	199	GLU
3	Q	208	LYS
4	R	48	LEU
4	R	59	LEU
4	R	65	GLU
4	R	86	ARG
4	R	119	LEU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
5	S	4	PHE
5	S	12	THR
5	S	13	VAL
5	S	33	GLN
5	S	58	LEU
5	S	65	LYS
5	S	76	LEU
5	S	104	ASN
5	S	121	GLN
5	S	160	LEU
5	S	178	ARG
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	208(A)	VAL
5	S	208(B)	ASP
6	T	25	GLU
6	T	36	THR
6	T	43	ASN
6	T	63	LYS
6	T	95	GLU
6	T	98	SER
6	T	121	GLN

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Mol	Chain	Res	Type
6	T	127	ASN
6	T	143	LYS
6	T	169	ARG
6	T	176	LEU
6	T	187	ARG
6	T	205	ASN
6	T	214	TRP
6	T	222	LYS
6	T	225	LYS
7	U	38	LEU
7	U	49	ILE
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	169	GLN
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	13	VAL
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	144	GLN
8	V	149	GLU
9	W	-7	ASP
9	W	12	VAL
9	W	107	LYS
9	W	121	GLU
9	W	160	LEU
9	W	171	TRP
9	W	174	VAL
9	W	181	LYS
10	X	-1	MET
10	X	24	ILE
10	X	34	THR
10	X	48	GLU
10	X	52	THR
10	X	77	GLN
10	X	105(B)	LYS
10	X	120	VAL
10	X	157	LEU

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Mol	Chain	Res	Type
10	X	168	MET
10	X	181	ASP
10	X	189	ASP
10	X	191	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	41	LEU
11	Y	65	LEU
11	Y	87	VAL
11	Y	105(A)	ARG
11	Y	105(B)	LYS
11	Y	145	ASP
11	Y	156	LYS
11	Y	208	ASN
11	Y	210	ILE
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	4	LEU
12	Z	14	LEU
12	Z	25	SER
12	Z	40	ASN
12	Z	62	SER
12	Z	99	THR
12	Z	118	SER
12	Z	138	LEU
12	Z	144(J)	ASN
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	141(C)	ARG
13	1	148	VAL
13	1	149	GLN
13	1	170	SER
13	1	184	LEU
13	1	190	LEU
13	1	191	GLN
13	1	204	LYS
14	2	22	THR
14	2	36	ARG
14	2	105(B)	LYS
14	2	119	VAL
14	2	149	GLU

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Mol	Chain	Res	Type
14	2	178	LEU
14	2	186	ARG
14	2	187(F)	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
2	B	23	GLN
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	150	GLN
3	C	163	GLN
4	D	23	GLN
4	D	108	ASN
4	D	150	HIS
4	D	180(C)	HIS
4	D	226	ASN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	125	GLN
5	E	185	ASN
5	E	207(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	192	GLN
6	F	205	ASN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN

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Mol	Chain	Res	Type
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
10	J	54	GLN
10	J	85	GLN
10	J	112	GLN
10	J	186	GLN
11	K	9	GLN
11	K	85	ASN
11	K	174	ASN
11	K	208	ASN
12	L	-7	ASN
12	L	40	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	123	GLN
12	L	166	HIS
13	M	-7	GLN
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	177	GLN

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Mol	Chain	Res	Type
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	199	GLN
4	R	211	GLN
4	R	226	ASN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	185	ASN
5	S	209	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	147	HIS
6	T	192	GLN
6	T	205	ASN
6	T	241	ASN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	170	GLN
7	U	178	ASN
7	U	182	HIS
7	U	184	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN

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Mol	Chain	Res	Type
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	64	ASN
9	W	81	GLN
10	X	54	GLN
10	X	85	GLN
10	X	96	GLN
10	X	112	GLN
10	X	140	HIS
10	X	141	HIS
10	X	186	GLN
11	Y	85	ASN
11	Y	174	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70	HIS
12	Z	70(A)	ASN
12	Z	144(B)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	ASN
13	1	18	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	38	HIS
14	2	62	HIS
14	2	69	GLN
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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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	L3T	K	213	-	48,49,49	1.95	3 (6%)	63,68,68	1.19	9 (14%)
16	L3T	Y	212	-	48,49,49	1.92	3 (6%)	63,68,68	1.32	8 (12%)
17	MES	Y	213	-	12,12,12	2.35	1 (8%)	14,16,16	1.43	2 (14%)
17	MES	K	214	-	12,12,12	2.25	1 (8%)	14,16,16	1.37	1 (7%)

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	L3T	K	213	-	-	0/39/43/43	0/4/4/4
16	L3T	Y	212	-	-	0/39/43/43	0/4/4/4
17	MES	Y	213	-	-	0/6/14/14	0/1/1/1
17	MES	K	214	-	-	3/6/14/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	213	L3T	CL23-C18	11.94	1.74	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	212	L3T	CL23-C18	11.52	1.74	1.51
17	Y	213	MES	C8-S	-7.94	1.66	1.77
17	K	214	MES	C8-S	-7.58	1.66	1.77
16	Y	212	L3T	C4-C5	-4.37	1.38	1.42
16	K	213	L3T	C4-C5	-3.90	1.39	1.42
16	Y	212	L3T	C4-C10	2.40	1.53	1.49
16	K	213	L3T	C4-C10	2.27	1.53	1.49

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	212	L3T	C4-C10-C11	4.97	125.31	118.60
17	K	214	MES	O3S-S-C8	3.72	111.79	105.77
16	K	213	L3T	C4-C10-C11	3.10	122.79	118.60
16	K	213	L3T	C33-N14-C32	2.74	123.29	116.85
16	Y	212	L3T	C25-C26-N29	-2.67	103.89	111.16
16	Y	212	L3T	C6-C5-C1	2.65	121.68	118.17
16	Y	212	L3T	C33-N14-C32	2.62	123.01	116.85
17	Y	213	MES	O3S-S-C8	2.34	109.55	105.77
16	Y	212	L3T	C34-C33-N14	-2.33	119.56	123.62
16	Y	212	L3T	C36-C35-N29	-2.30	111.65	116.70
16	K	213	L3T	C6-C5-C1	2.29	121.20	118.17
16	K	213	L3T	C36-C35-N29	-2.28	111.69	116.70
16	K	213	L3T	C34-C33-N14	-2.19	119.80	123.62
16	K	213	L3T	C16-C17-C22	-2.18	116.05	121.00
17	Y	213	MES	O2S-S-C8	2.16	109.52	106.92
16	K	213	L3T	C31-C32-N14	-2.08	119.99	123.62
16	K	213	L3T	C30-C28-C26	-2.08	107.66	113.39
16	K	213	L3T	C25-C26-N29	-2.02	105.65	111.16
16	Y	212	L3T	C17-C16-N15	-2.02	108.78	113.03
16	Y	212	L3T	CL23-C18-C17	-2.01	119.57	121.99

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	214	MES	C7-C8-S-O2S
17	K	214	MES	C7-C8-S-O3S
17	K	214	MES	C7-C8-S-O1S

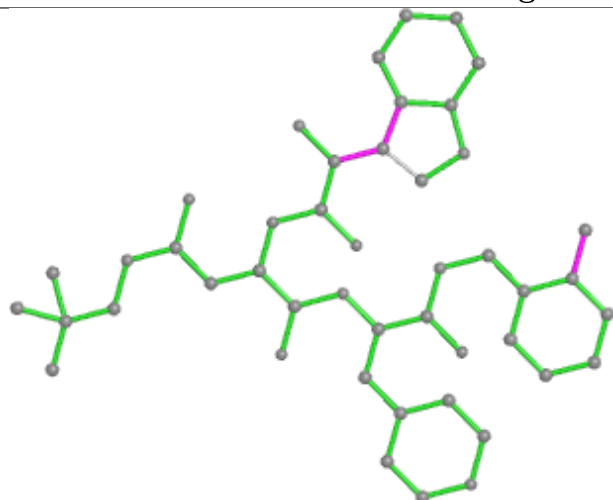
There are no ring outliers.

3 monomers are involved in 7 short contacts:

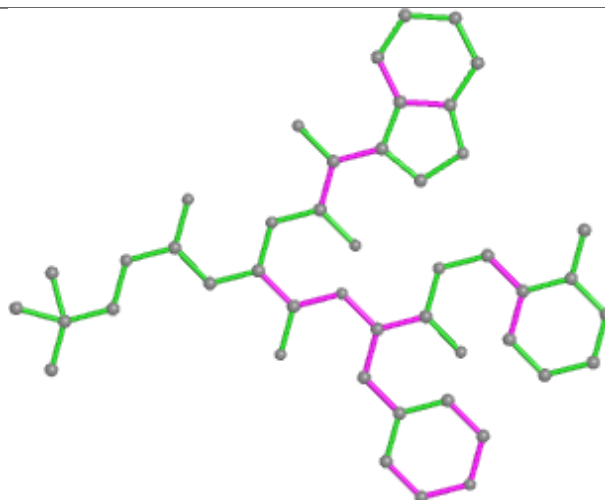
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	213	L3T	4	0
16	Y	212	L3T	2	0
17	Y	213	MES	1	0

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

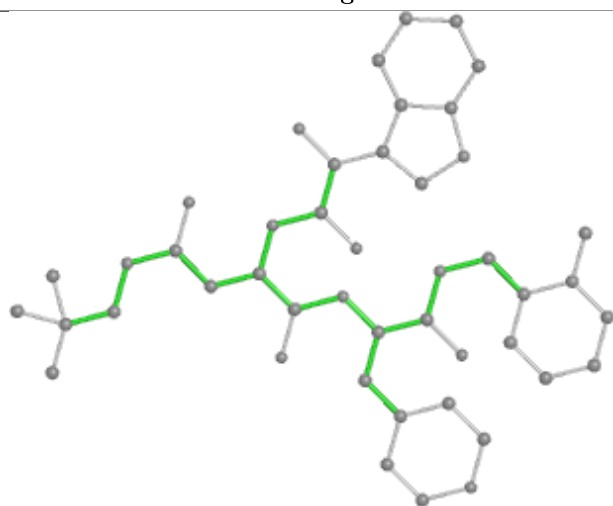
## Ligand L3T K 213



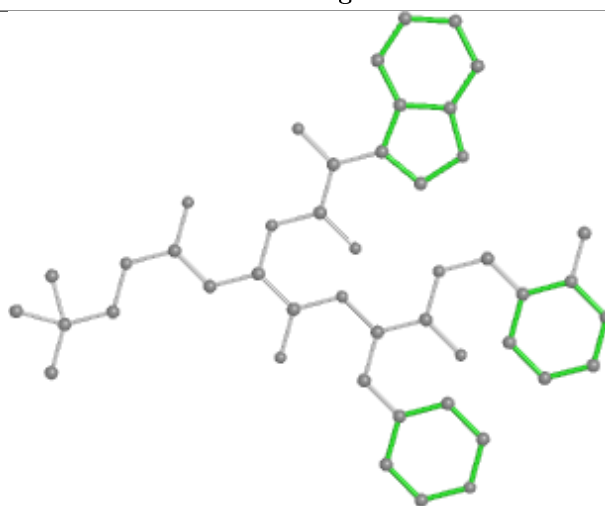
Bond lengths



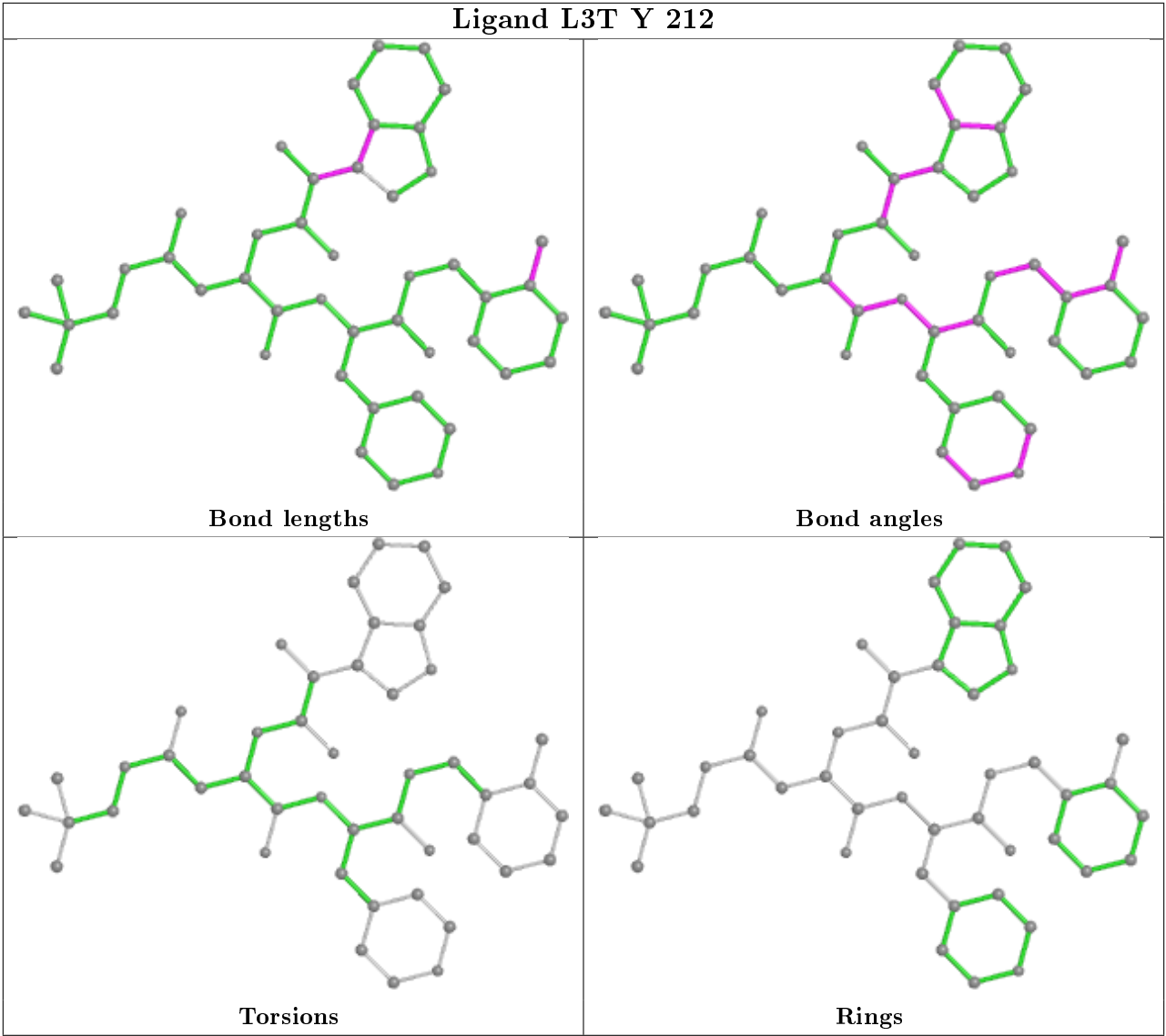
Bond angles



Torsions



Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	E	4
4	D	4
9	W	3
14	N	3
14	2	3

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Mol	Chain	Number of breaks
4	R	3
13	M	3
13	1	3
9	I	3
7	G	3
10	X	2
5	S	2
10	J	2
8	V	2
12	Z	2
12	L	2
3	Q	2
8	H	2
3	C	2
6	F	2
2	P	1
11	K	1
2	B	1
1	A	1
7	U	1
6	T	1
1	O	1
11	Y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	123(G):GLU	C	125:GLU	N	4.17
1	R	123(G):GLU	C	125:GLU	N	4.03
1	C	203:THR	C	206:GLY	N	3.88
1	J	-1:MET	C	1:ASP	N	3.79
1	K	181:ASP	C	183:GLY	N	3.66
1	X	-1:MET	C	1:ASP	N	3.62
1	Q	180(D):GLU	C	182:PRO	N	3.35
1	F	180(F):GLY	C	184:LEU	N	3.23
1	S	204:GLU	C	206:SER	N	3.20
1	E	204:GLU	C	206:SER	N	3.18
1	Q	203:THR	C	206:GLY	N	3.16
1	D	233:ILE	C	235:LYS	N	3.10
1	C	180(D):GLU	C	182:PRO	N	3.07
1	N	181:ALA	C	183:GLY	N	3.04
1	1	181(A):THR	C	183:GLY	N	2.93
1	P	200:THR	C	202:THR	N	2.87

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	202:GLU	C	205:GLU	N	2.86
1	M	181(A):THR	C	183:GLY	N	2.85
1	E	207(E):ASN	C	210:LEU	N	2.84
1	G	180(D):ILE	C	184:ASN	N	2.83
1	O	200:SER	C	202:VAL	N	2.83
1	G	184(M):SER	C	186:TRP	N	2.81
1	A	200:SER	C	202:VAL	N	2.76
1	E	180(F):ILE	C	183:ASP	N	2.63
1	E	60:SER	C	63:TYR	N	2.62
1	F	199:LEU	C	201:ALA	N	2.61
1	D	180(E):SER	C	184:LEU	N	2.60
1	2	181:ALA	C	183:GLY	N	2.60
1	X	181:ASP	C	183:GLY	N	2.58
1	R	233:ILE	C	235:LYS	N	2.57
1	I	179:LYS	C	181:LYS	N	2.56
1	S	60:SER	C	63:TYR	N	2.55
1	Y	181:ASP	C	183:GLY	N	2.54
1	T	199:LEU	C	201:ALA	N	2.51
1	U	218:ASP	C	220:LYS	N	2.49
1	L	-1:GLY	C	1:GLY	N	2.45
1	2	92:ASP	C	94:ASN	N	2.44
1	D	202:GLU	C	205:GLU	N	2.43
1	J	181:ASP	C	183:GLY	N	2.43
1	V	91:GLN	C	93:GLY	N	2.43
1	Z	180:LYS	C	182:ASP	N	2.43
1	L	180:LYS	C	182:ASP	N	2.38
1	W	179:LYS	C	181:LYS	N	2.35
1	G	218:ASP	C	220:LYS	N	2.24
1	H	187:LEU	C	189:ARG	N	2.24
1	V	187:LEU	C	189:ARG	N	2.24
1	Z	-1:GLY	C	1:GLY	N	2.23
1	B	200:THR	C	202:THR	N	2.22
1	I	36:HIS	C	38:TYR	N	2.21
1	H	91:GLN	C	93:GLY	N	2.14
1	1	141(G):ILE	C	144:PRO	N	2.10
1	M	141(G):ILE	C	144:PRO	N	2.09
1	N	70:TYR	C	72:GLY	N	2.09
1	2	70:TYR	C	72:GLY	N	2.06
1	I	-1:GLY	C	1:GLY	N	2.04
1	W	-1:GLY	C	1:GLY	N	2.04
1	1	-1:GLY	C	1:THR	N	2.02
1	M	-1:GLY	C	1:THR	N	1.94

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	36:HIS	C	38:TYR	N	1.89
1	N	92:ASP	C	94:ASN	N	1.86

## 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%)	0.07	8 (3%) 47 40	27, 40, 61, 79	0
1	O	250/250 (100%)	0.21	12 (4%) 30 24	30, 45, 71, 82	0
2	B	235/245 (95%)	0.31	11 (4%) 31 25	27, 45, 72, 79	0
2	P	235/245 (95%)	0.30	14 (5%) 21 16	27, 47, 77, 81	0
3	C	241/243 (99%)	0.57	26 (10%) 5 3	29, 53, 92, 111	0
3	Q	241/243 (99%)	0.90	48 (19%) 1 0	33, 58, 102, 121	0
4	D	242/250 (96%)	0.35	15 (6%) 20 15	27, 47, 83, 90	0
4	R	242/250 (96%)	0.41	15 (6%) 20 15	27, 49, 81, 93	0
5	E	233/234 (99%)	0.35	15 (6%) 19 14	33, 47, 77, 86	0
5	S	233/234 (99%)	0.53	26 (11%) 5 3	32, 50, 78, 93	0
6	F	237/248 (95%)	0.14	14 (5%) 22 17	26, 43, 76, 86	0
6	T	237/248 (95%)	0.05	6 (2%) 57 51	26, 43, 67, 84	0
7	G	243/252 (96%)	0.04	10 (4%) 37 30	24, 39, 65, 86	0
7	U	243/252 (96%)	-0.06	6 (2%) 57 51	24, 38, 58, 77	0
8	H	222/222 (100%)	-0.10	2 (0%) 84 82	25, 34, 49, 74	0
8	V	222/222 (100%)	-0.06	4 (1%) 68 64	28, 37, 52, 78	0
9	I	204/205 (99%)	-0.13	0 100 100	23, 33, 45, 60	0
9	W	204/205 (99%)	-0.00	1 (0%) 91 89	25, 35, 48, 64	0
10	J	198/198 (100%)	0.06	7 (3%) 44 36	28, 36, 52, 111	0
10	X	198/198 (100%)	0.08	6 (3%) 50 43	28, 38, 52, 120	0
11	K	212/212 (100%)	-0.10	2 (0%) 84 82	23, 33, 49, 62	0
11	Y	212/212 (100%)	-0.07	0 100 100	25, 35, 51, 58	0
12	L	222/241 (92%)	-0.10	1 (0%) 91 89	24, 35, 53, 60	0
12	Z	222/241 (92%)	-0.07	4 (1%) 68 64	24, 34, 51, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1	233/266 (87%)	-0.18	2 (0%) 84 82	22, 33, 47, 50	0
13	M	233/266 (87%)	-0.10	1 (0%) 92 91	24, 35, 48, 52	0
14	2	196/196 (100%)	-0.07	1 (0%) 91 89	25, 32, 47, 63	0
14	N	196/196 (100%)	-0.15	2 (1%) 82 80	25, 32, 48, 59	0
All	All	6336/6524 (97%)	0.12	259 (4%) 37 30	22, 39, 74, 121	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	7	GLY	10.6
4	R	123(E)	SER	9.6
10	J	192	ALA	9.2
4	D	123(B)	GLU	9.0
7	G	240	ASP	8.4
13	M	-8	THR	8.3
7	G	6	ALA	7.9
5	S	4	PHE	7.9
5	S	206	SER	7.9
4	D	123(E)	SER	7.8
4	R	123(C)	GLY	7.8
2	B	217	ALA	7.8
2	P	217	ALA	7.5
4	R	123(F)	GLY	7.5
4	R	123(D)	ALA	7.4
6	F	12	ASN	7.4
4	R	123(A)	GLY	7.4
4	D	123(C)	GLY	7.3
7	U	240	ASP	7.1
3	C	8	TYR	6.9
10	X	192	ALA	6.8
2	B	218	ASN	6.8
3	Q	236	ILE	6.5
4	D	123(D)	ALA	6.4
10	J	193	GLN	6.3
1	O	4	MET	6.2
10	X	193	GLN	6.2
13	1	-8	THR	6.2
2	P	218	ASN	6.2
4	D	11	GLY	6.0
7	U	6	ALA	6.0
3	C	9	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
4	D	10	ARG	5.8
1	A	5	THR	5.7
4	R	9	ASP	5.7
3	Q	55	THR	5.7
3	C	11	ALA	5.7
3	Q	54	SER	5.7
4	R	123(B)	GLU	5.7
4	R	10	ARG	5.6
5	S	5	ARG	5.6
3	Q	238	GLN	5.5
10	J	-1	MET	5.5
1	O	236	LEU	5.4
3	Q	56	LEU	5.3
4	D	123(F)	GLY	5.3
3	C	243	GLN	5.3
5	E	4	PHE	5.3
2	B	216(B)	GLY	5.1
10	X	191	GLN	5.1
5	E	203	ASP	4.9
3	C	234	THR	4.9
3	C	208	LYS	4.7
5	E	206	SER	4.7
5	S	203	ASP	4.7
5	S	6	ASN	4.7
3	Q	209	ASN	4.5
3	Q	243	GLN	4.4
3	Q	8	TYR	4.3
1	A	236	LEU	4.2
3	C	55	THR	4.2
4	D	9	ASP	4.1
1	O	5	THR	4.1
5	S	63	TYR	4.0
3	Q	241	GLN	4.0
10	X	-1	MET	4.0
4	D	123(A)	GLY	4.0
3	Q	233	VAL	4.0
3	Q	7	GLY	4.0
3	Q	198	LEU	3.9
3	C	56	LEU	3.9
6	F	240	ILE	3.9
6	T	12	ASN	3.9
3	Q	207	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
12	Z	144(J)	ASN	3.8
4	D	127	LEU	3.8
7	G	239	GLN	3.7
13	1	181(A)	THR	3.7
4	R	127	LEU	3.6
3	Q	184	ALA	3.6
8	V	223	ASP	3.6
3	Q	237	GLU	3.6
3	C	191	LYS	3.6
3	Q	229	ILE	3.5
4	R	11	GLY	3.5
5	S	51	LEU	3.5
2	B	63	THR	3.5
6	T	199	LEU	3.5
3	Q	187	GLU	3.4
10	J	191	GLN	3.4
2	B	54	VAL	3.4
7	G	237	ALA	3.4
3	Q	234	THR	3.3
3	C	240	LYS	3.3
5	S	191	LYS	3.3
8	V	222	CYS	3.3
2	P	216(B)	GLY	3.2
4	R	123(G)	GLU	3.2
3	Q	206	GLY	3.2
3	Q	208	LYS	3.2
2	P	54	VAL	3.2
1	A	200	SER	3.2
5	E	202	ARG	3.2
5	E	5	ARG	3.2
1	O	235	ALA	3.1
5	S	233	ILE	3.1
1	O	6	ASP	3.1
5	E	189	LEU	3.1
9	W	181	LYS	3.1
1	A	4	MET	3.1
3	C	236	ILE	3.1
5	E	233	ILE	3.1
1	O	217(P)	LYS	3.1
3	Q	9	ASP	3.0
3	Q	189	CYS	3.0
5	S	8	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	218(C)	ASP	3.0
6	F	201	ALA	3.0
3	Q	239	GLU	3.0
5	E	6	ASN	3.0
4	D	12	VAL	3.0
7	G	236	ILE	3.0
3	Q	64	PRO	3.0
1	O	234	GLU	2.9
10	X	188	ASP	2.9
3	C	10	ARG	2.9
1	A	234	GLU	2.9
3	C	184	ALA	2.9
3	C	53	ARG	2.9
7	G	8	TYR	2.9
5	S	10	GLY	2.9
6	F	199	LEU	2.9
5	E	7	ASN	2.9
3	C	187	GLU	2.8
3	Q	182	PRO	2.8
1	O	203	GLU	2.8
3	Q	180(D)	GLU	2.8
3	Q	43	LYS	2.8
1	O	233	LEU	2.8
3	Q	191	LYS	2.8
3	Q	10	ARG	2.8
3	Q	197	LEU	2.8
5	E	178	ARG	2.8
5	S	57	GLU	2.7
2	P	216(A)	LYS	2.7
7	U	7	GLY	2.7
4	D	180(E)	SER	2.7
5	E	204	GLU	2.7
5	S	204	GLU	2.7
3	C	241	GLN	2.7
14	2	92	ASP	2.7
4	R	186	LEU	2.7
14	N	187(I)	GLN	2.7
5	E	168	ARG	2.7
3	Q	240	LYS	2.7
7	U	218	ASP	2.7
2	P	235	LYS	2.6
2	P	43	SER	2.6

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Mol	Chain	Res	Type	RSRZ
12	Z	-9	GLN	2.6
6	T	241	ASN	2.6
6	T	240	ILE	2.6
3	Q	235	GLN	2.6
5	S	33	GLN	2.6
3	C	209	ASN	2.6
1	O	191	HIS	2.6
5	S	189	LEU	2.5
11	K	208	ASN	2.5
8	V	182	LYS	2.5
7	U	239	GLN	2.5
3	Q	192	LEU	2.5
5	S	195	GLU	2.5
2	P	22	TYR	2.5
3	C	57	LYS	2.5
3	Q	180(C)	LYS	2.5
3	Q	194	VAL	2.5
6	F	180(F)	GLY	2.5
6	T	13	SER	2.5
2	B	62	ASP	2.5
6	F	241	ASN	2.5
3	Q	200	VAL	2.5
7	G	234	VAL	2.5
2	P	204(A)	SER	2.5
3	Q	175	PHE	2.5
5	S	178	ARG	2.4
3	C	233	VAL	2.4
10	X	10	ASP	2.4
3	Q	201	VAL	2.4
3	Q	210	ILE	2.4
2	P	183	ASP	2.4
5	S	168	ARG	2.4
7	U	8	TYR	2.4
3	Q	44	ASN	2.4
3	Q	232	TYR	2.4
6	F	180(D)	PRO	2.4
3	Q	203	THR	2.4
10	J	189	ASP	2.4
6	F	57	LYS	2.4
4	R	22	PHE	2.3
2	B	204(A)	SER	2.3
3	C	232	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	239	THR	2.3
3	Q	63	THR	2.3
7	G	238	GLU	2.3
5	E	199	GLN	2.3
1	O	200	SER	2.3
3	C	194	VAL	2.3
4	D	123(G)	GLU	2.3
6	F	180(E)	GLU	2.3
10	J	92	ARG	2.3
6	T	217	LEU	2.3
6	F	238	LYS	2.3
5	S	11	ASP	2.3
3	C	227	GLU	2.3
3	Q	188	GLU	2.3
4	R	126	ARG	2.2
12	Z	182	ASP	2.2
2	P	232	ILE	2.2
12	Z	92	PHE	2.2
5	S	58	LEU	2.2
2	B	235	LYS	2.2
5	S	202	ARG	2.2
4	D	244	GLU	2.2
6	F	204	ASP	2.2
2	P	181	LYS	2.2
14	N	92	ASP	2.2
3	Q	12	LEU	2.2
3	Q	144(A)	ASP	2.2
5	S	9	ASP	2.2
1	A	203	GLU	2.1
1	A	217(P)	LYS	2.1
3	C	238	GLN	2.1
2	B	61	GLN	2.1
1	A	217	ASP	2.1
8	H	222	CYS	2.1
6	F	203	GLU	2.1
5	S	181	LYS	2.1
4	R	12	VAL	2.1
11	K	210	ILE	2.1
6	F	206(B)	GLU	2.1
8	H	223	ASP	2.1
3	C	12	LEU	2.1
5	S	198	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	178	LYS	2.1
2	P	220	TYR	2.1
5	S	175	TYR	2.1
7	G	184(H)	GLU	2.1
12	L	180	LYS	2.1
5	E	174	THR	2.0
5	E	207(E)	ASN	2.0
7	G	184(M)	SER	2.0
5	S	199	GLN	2.0
8	V	221	ILE	2.0
3	Q	58	LEU	2.0
10	J	149	GLU	2.0
4	D	26	TYR	2.0
1	O	199	GLU	2.0
3	Q	231	GLN	2.0
2	P	63(A)	SER	2.0
6	F	187	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	MG	F	243	1/1	0.63	1.45	121,121,121,121	0
15	MG	I	195	1/1	0.69	0.24	54,54,54,54	0
15	MG	I	196	1/1	0.83	0.26	43,43,43,43	0
15	MG	L	195	1/1	0.86	0.14	48,48,48,48	0
16	L3T	Y	212	46/46	0.89	0.21	33,37,51,52	0
16	L3T	K	213	46/46	0.90	0.20	33,36,51,52	0

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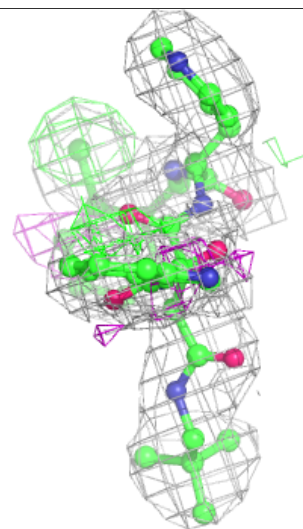
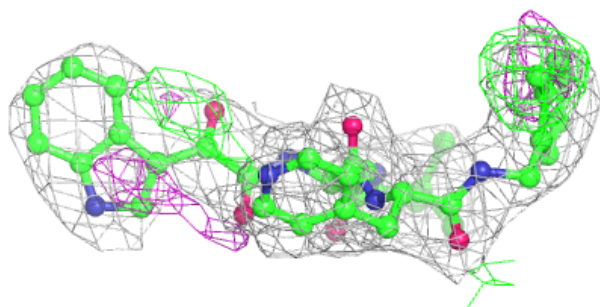
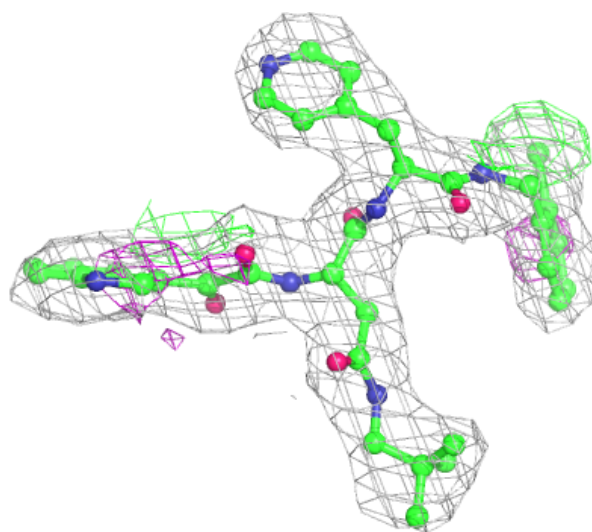
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	MG	L	196	1/1	0.91	0.21	50,50,50,50	0
15	MG	G	241	1/1	0.95	0.07	39,39,39,39	0
15	MG	F	242	1/1	0.95	0.14	67,67,67,67	0
15	MG	H	224	1/1	0.96	0.08	44,44,44,44	0
15	MG	K	212	1/1	0.96	0.20	39,39,39,39	0
15	MG	N	188	1/1	0.96	0.17	36,36,36,36	0
17	MES	Y	213	12/12	0.97	0.20	58,59,60,60	0
17	MES	K	214	12/12	0.98	0.20	55,56,57,57	0

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

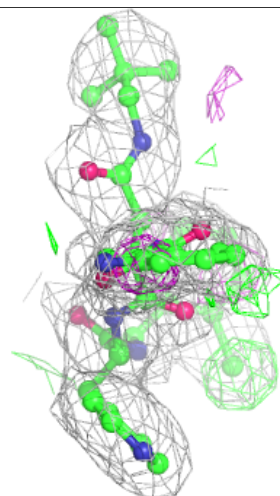
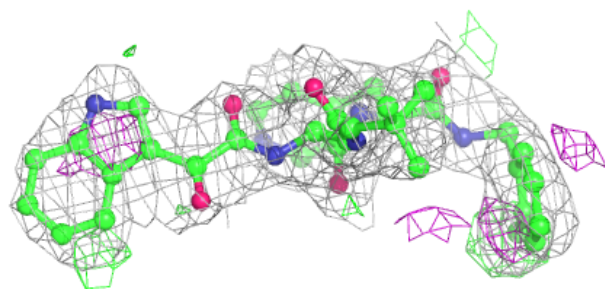
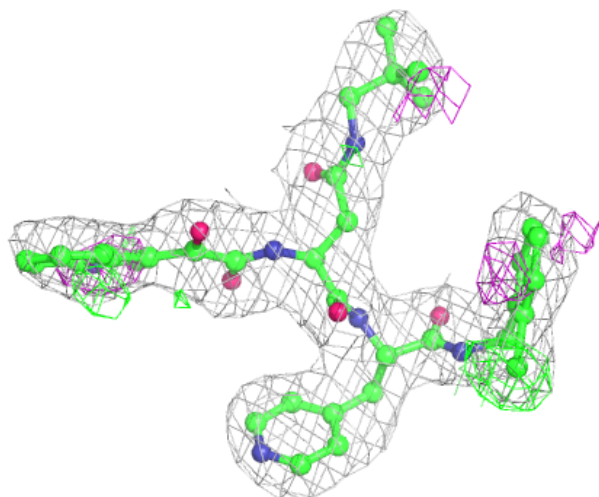
**Electron density around L3T Y 212:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around L3T K 213:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.