



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:57 pm BST

PDB ID : 3TDD
Title : Crystal structure of yeast CP in complex with Belactosin C
Authors : Korotkov, V.S.; Ludwig, A.; Larionov, O.V.; Lygin, A.V.; Groll, M.; de Meijere, A.
Deposited on : 2011-08-10
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

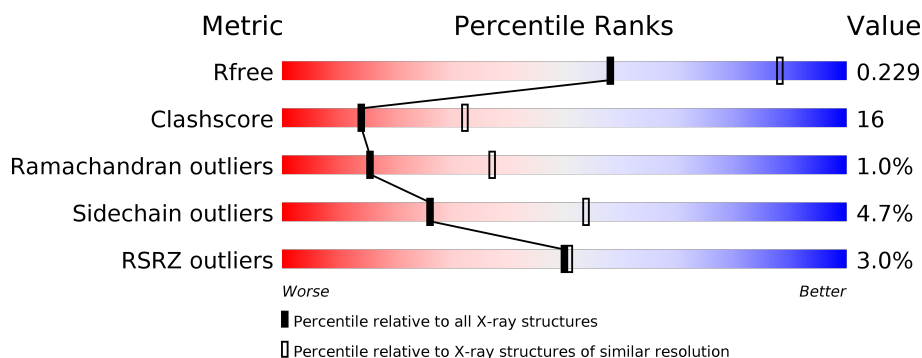
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>78%</div> <div>19%</div> <div>•</div> </div> </div>
1	O	250	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>•</div> </div> </div>
2	B	244	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>33%</div> <div>•</div> </div> </div>
2	P	244	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>33%</div> <div>5%</div> </div> </div>
3	C	241	<div> <div>6%</div> <div> <div></div> <div>60%</div> <div>38%</div> <div>•</div> </div> </div>
3	Q	241	<div> <div>16%</div> <div> <div></div> <div>62%</div> <div>36%</div> <div>•</div> </div> </div>

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

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50979 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

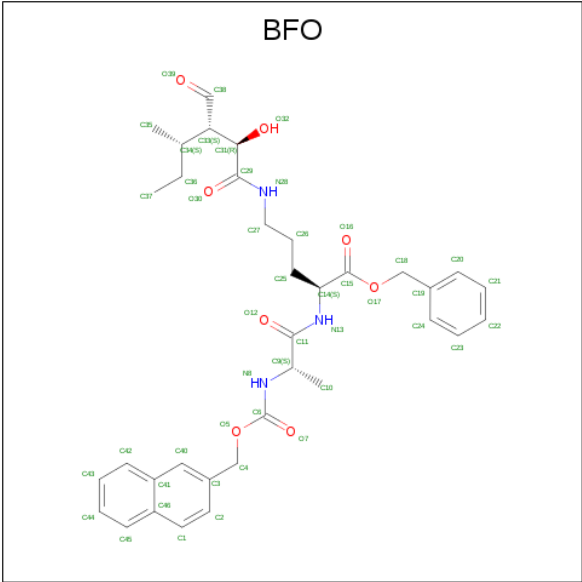
- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is benzyl N-[(naphthalen-2-ylmethoxy)carbonyl]-L-alanyl-N 5 -[(2R,3S,4S)-3-formyl-2-hydroxy-4-methylhexanoyl]-L-ornithinate (three-letter code: BFO) (formula: C₃₅H₄₃N₃O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	K	1	Total	C	N	O	0	0
			46	35	3	8		
15	Y	1	Total	C	N	O	0	0
			46	35	3	8		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	59	Total	O	0	0
			59	59		
16	B	37	Total	O	0	0
			37	37		
16	C	42	Total	O	0	0
			42	42		
16	D	42	Total	O	0	0
			42	42		
16	E	21	Total	O	0	0
			21	21		
16	F	46	Total	O	0	0
			46	46		
16	G	60	Total	O	0	0
			60	60		
16	H	49	Total	O	0	0
			49	49		
16	I	68	Total	O	0	0
			68	68		
16	J	50	Total	O	0	0
			50	50		

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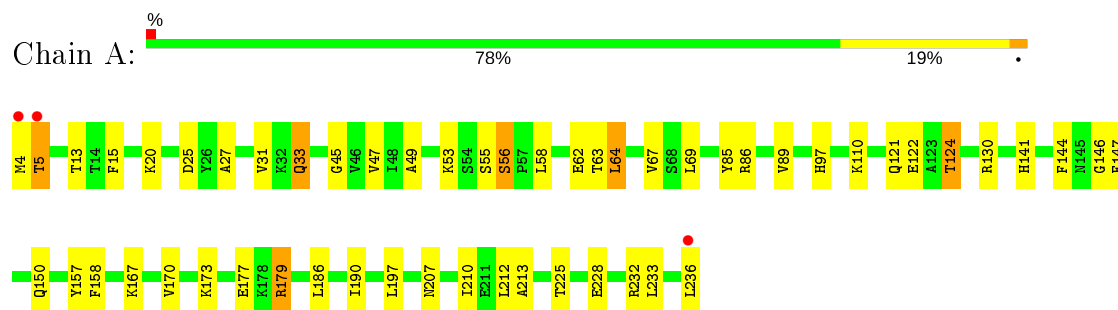
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	K	48	Total 48	O 48	0	0
16	L	56	Total 56	O 56	0	0
16	M	71	Total 71	O 71	0	0
16	N	59	Total 59	O 59	0	0
16	O	34	Total 34	O 34	0	0
16	P	29	Total 29	O 29	0	0
16	Q	29	Total 29	O 29	0	0
16	R	28	Total 28	O 28	0	0
16	S	20	Total 20	O 20	0	0
16	T	34	Total 34	O 34	0	0
16	U	62	Total 62	O 62	0	0
16	V	47	Total 47	O 47	0	0
16	W	61	Total 61	O 61	0	0
16	X	47	Total 47	O 47	0	0
16	Y	48	Total 48	O 48	0	0
16	Z	53	Total 53	O 53	0	0
16	1	80	Total 80	O 80	0	0
16	2	59	Total 59	O 59	0	0

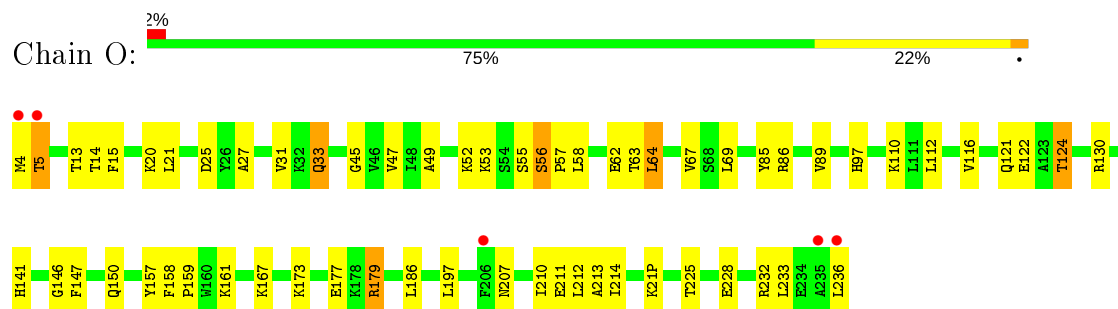
3 Residue-property plots [i](#)

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

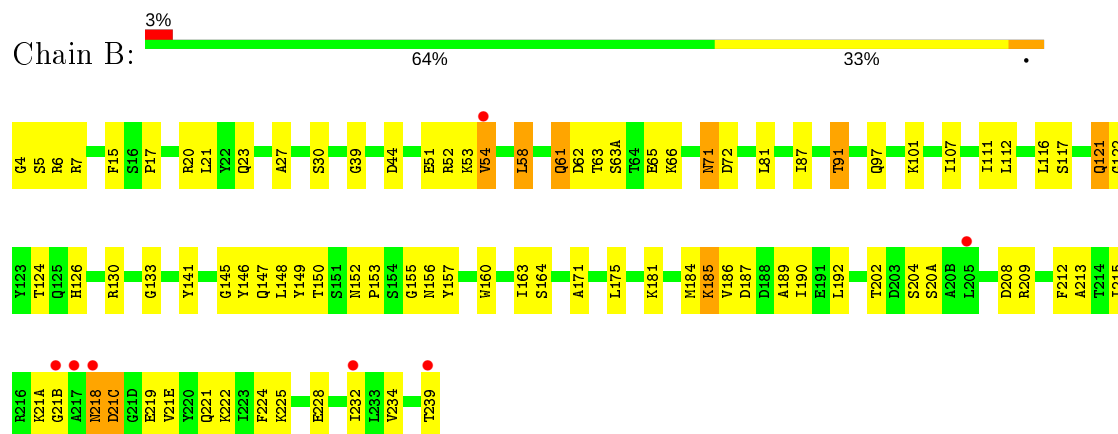
- Molecule 1: Proteasome component Y7



- Molecule 1: Proteasome component Y7

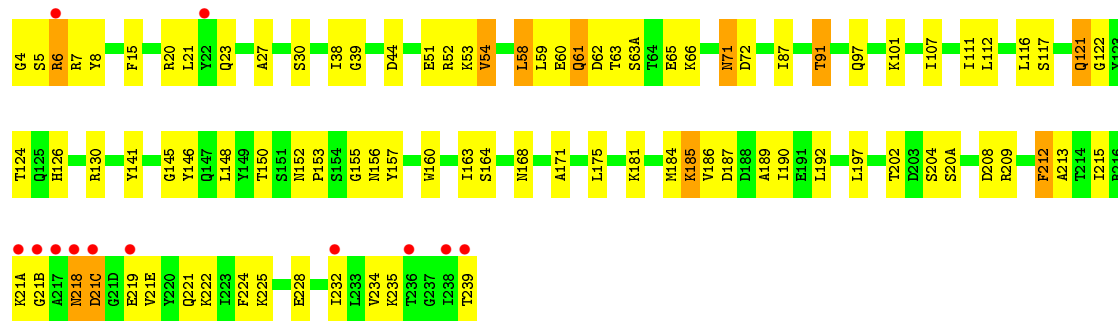


- Molecule 2: Proteasome component Y13



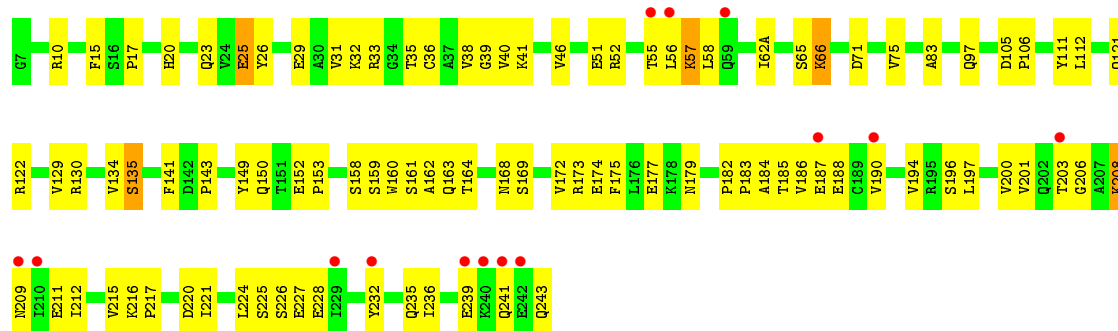
- Molecule 2: Proteasome component Y13

Chain P: 



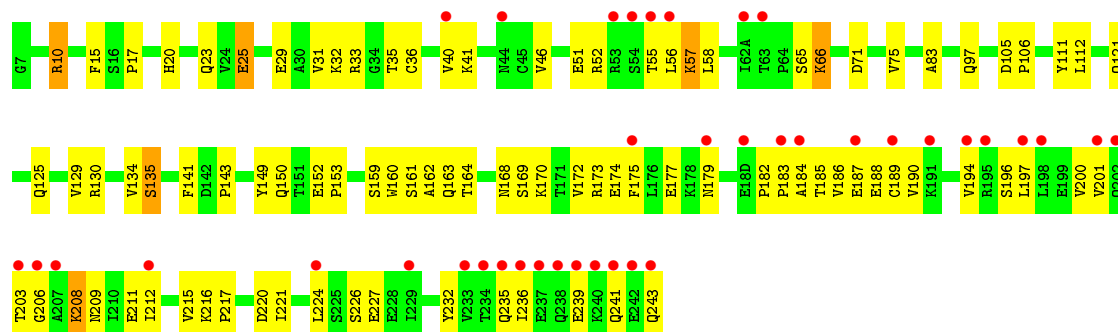
• Molecule 3: Proteasome component PRE6

Chain C: 



• Molecule 3: Proteasome component PRE6

Chain Q: 



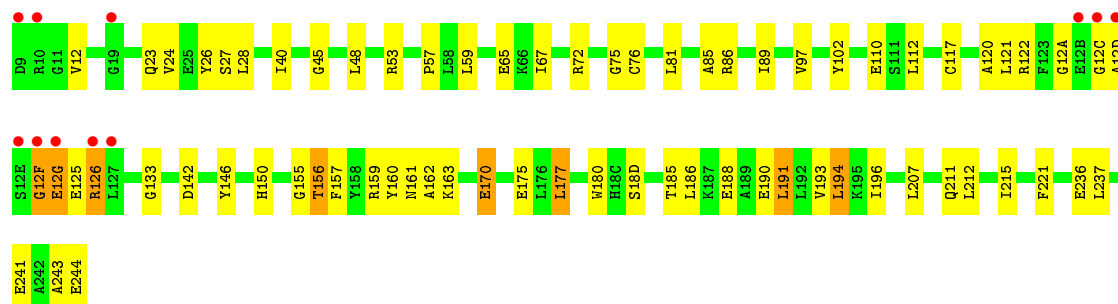
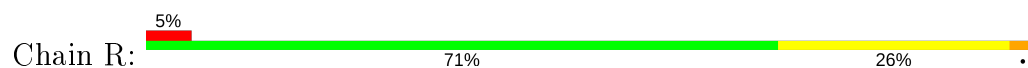
• Molecule 4: Proteasome component PUP2

Chain D: 

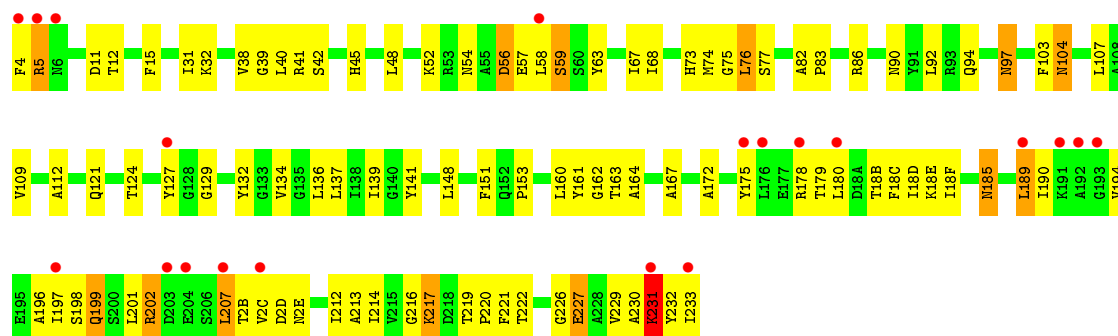




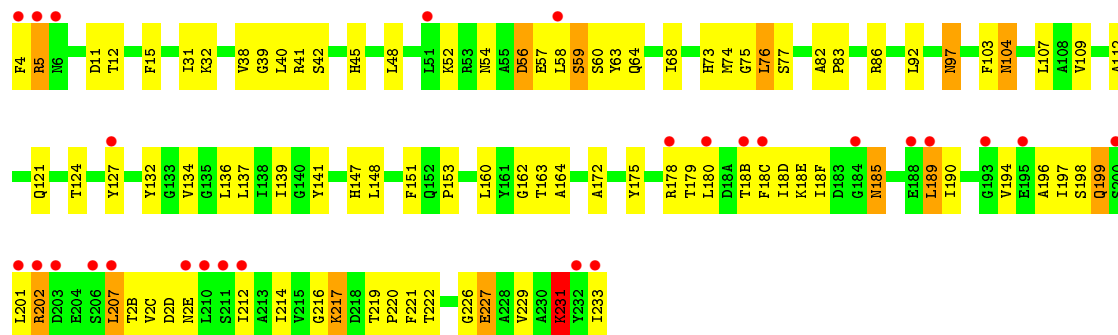
• Molecule 4: Proteasome component PUP2



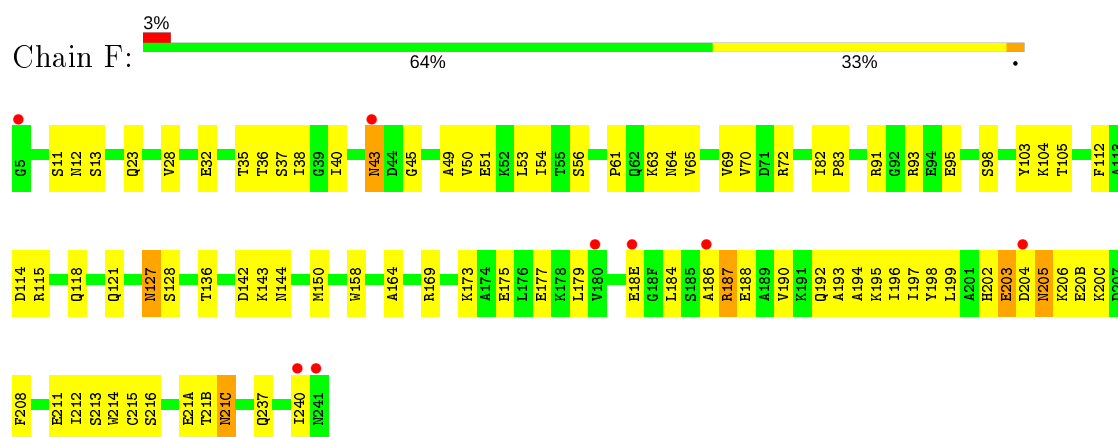
• Molecule 5: Proteasome component PRE5



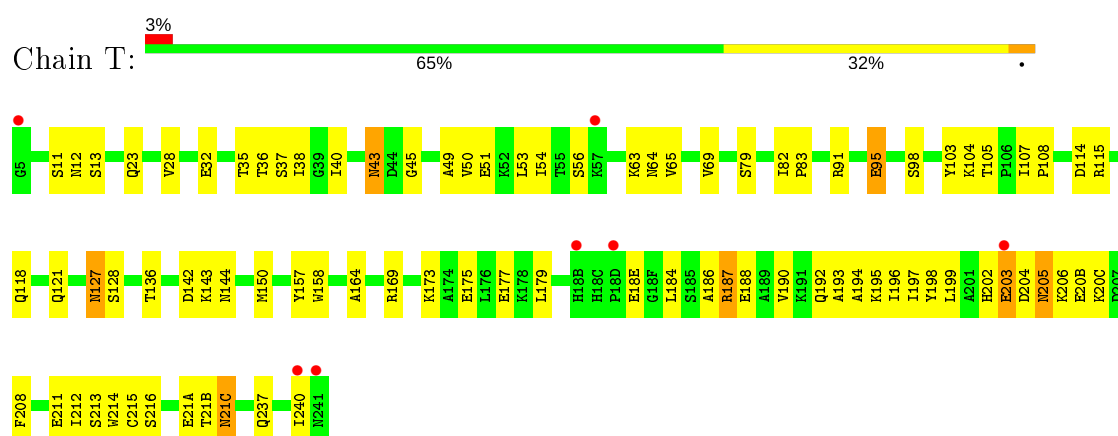
• Molecule 5: Proteasome component PRE5



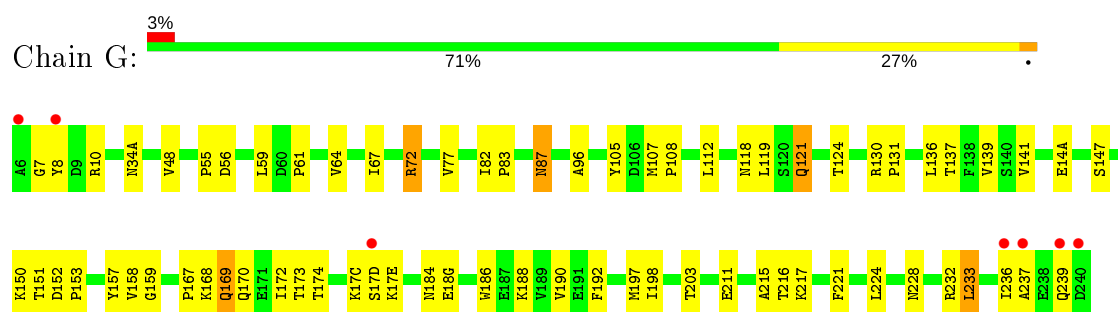
• Molecule 6: Proteasome component C1



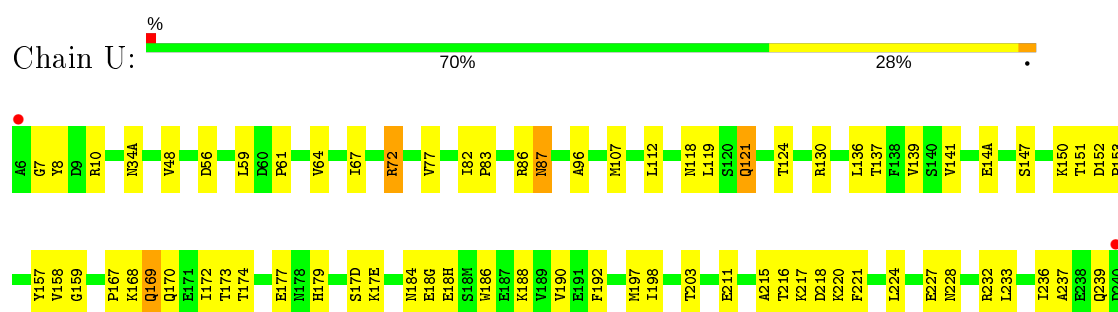
- Molecule 6: Proteasome component C1



- Molecule 7: Proteasome component C7-alpha

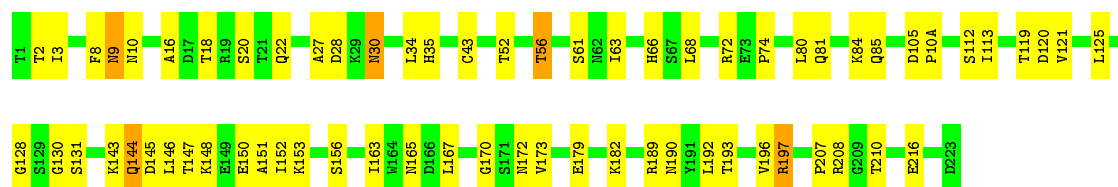


- Molecule 7: Proteasome component C7-alpha



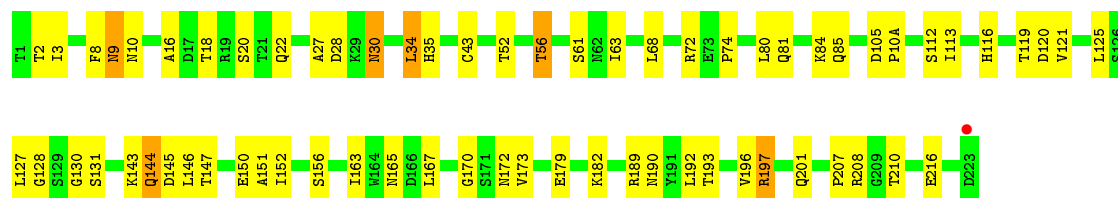
- Molecule 8: Proteasome component PUP1

Chain H: 



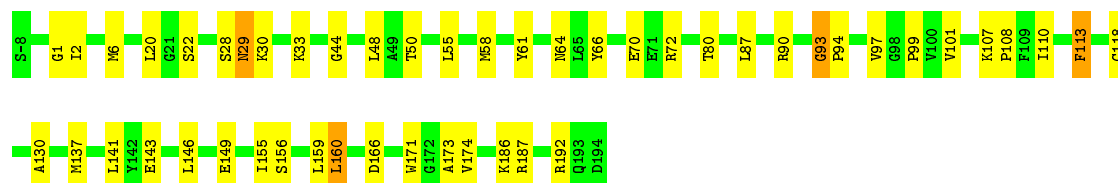
• Molecule 8: Proteasome component PUP1

Chain V: 




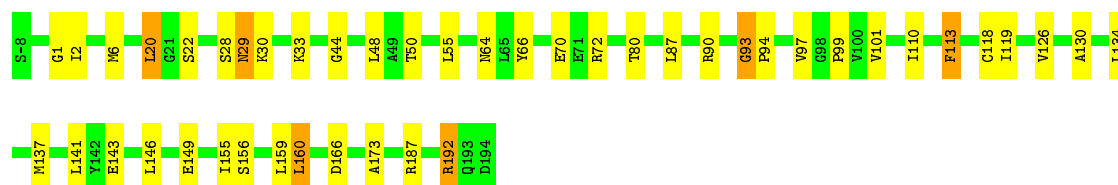
• Molecule 9: Proteasome component PUP3

Chain I: 



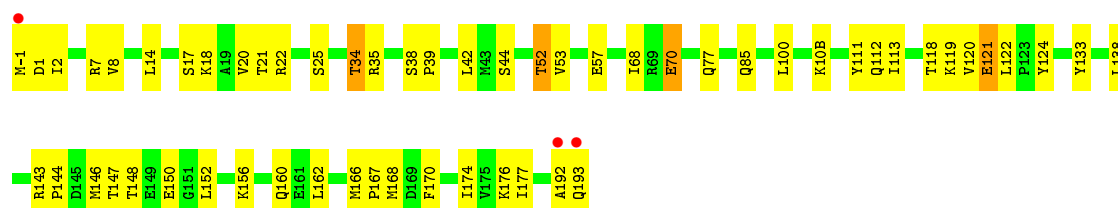
• Molecule 9: Proteasome component PUP3

Chain W: 

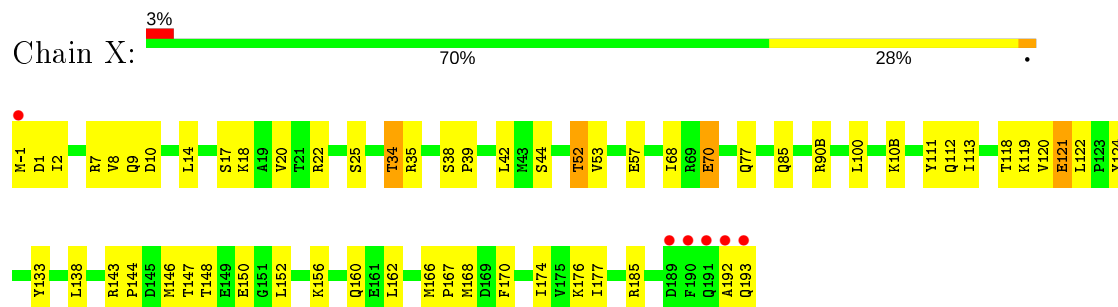


• Molecule 10: Proteasome component C11

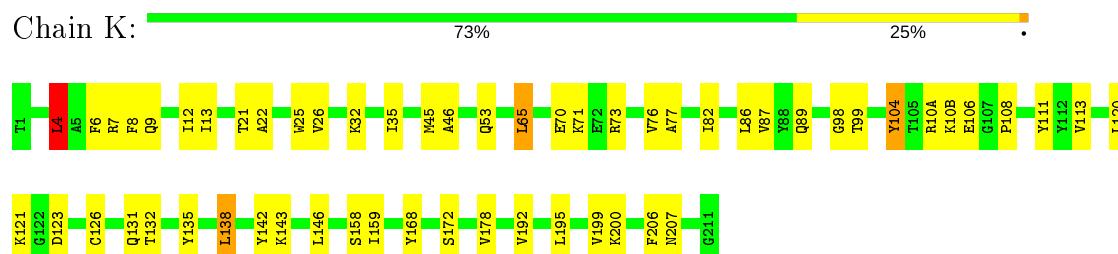
Chain J: 



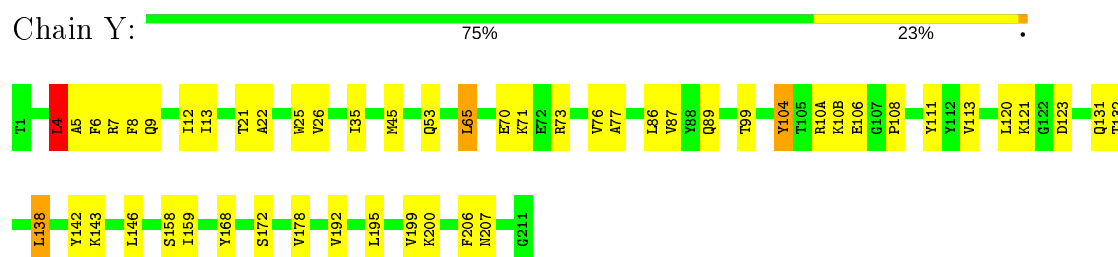
- Molecule 10: Proteasome component C11



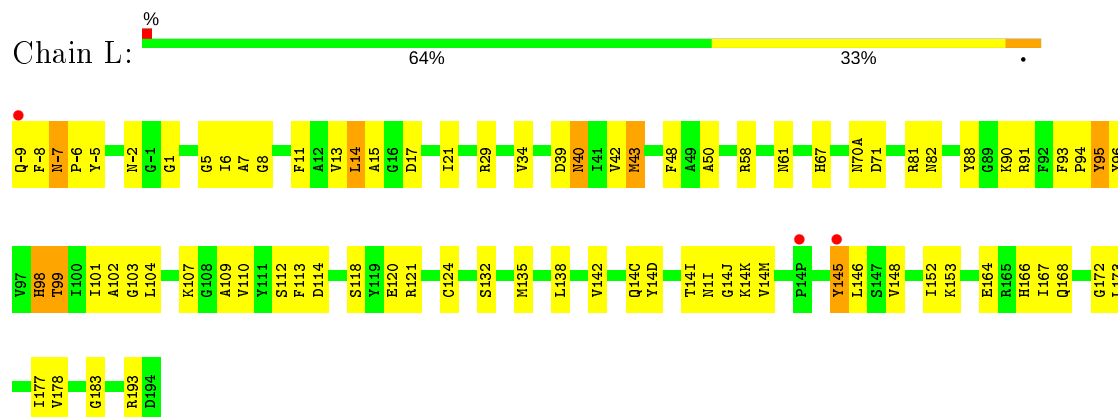
- Molecule 11: Proteasome component PRE2



- Molecule 11: Proteasome component PRE2

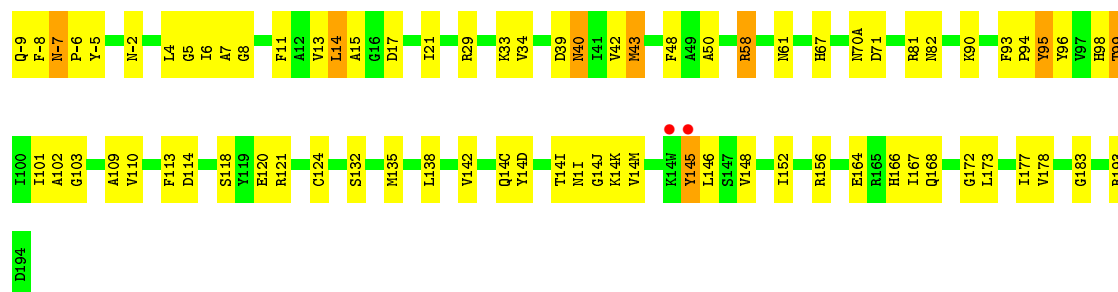


- Molecule 12: Proteasome component C5

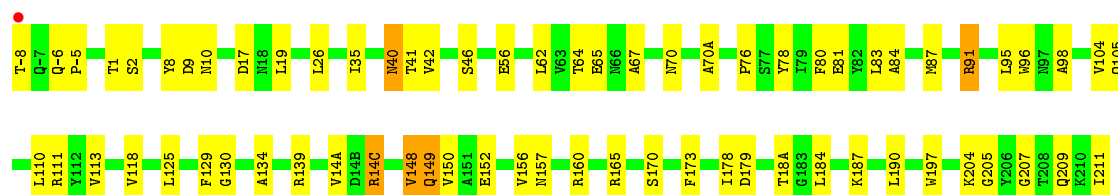


- Molecule 12: Proteasome component C5

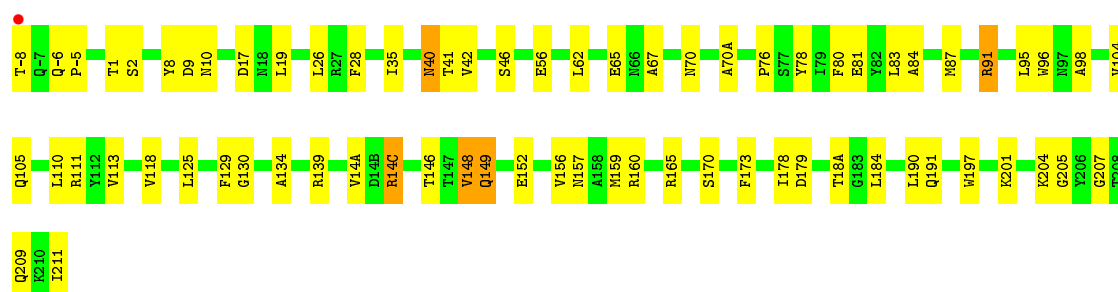




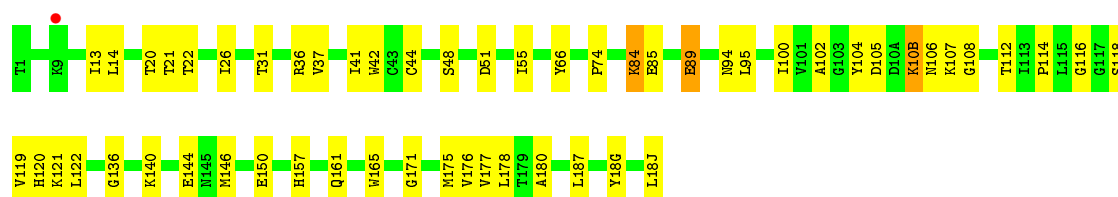
• Molecule 13: Proteasome component PRE4



• Molecule 13: Proteasome component PRE4



• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.93Å 301.60Å 144.20Å 90.00° 112.94° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 49.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (15.00-2.70) 99.6 (49.37-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.236 0.205 , 0.229	Depositor DCC
R_{free} test set	14306 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.892	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50979	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: BFO

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	0.36	0/1952	0.62	0/2642
1	O	0.38	0/1952	0.63	0/2642
2	B	0.36	0/1935	0.62	0/2618
2	P	0.36	0/1935	0.62	0/2618
3	C	0.34	0/1920	0.61	0/2598
3	Q	0.35	0/1920	0.61	0/2598
4	D	0.35	0/1887	0.61	0/2541
4	R	0.36	0/1887	0.62	0/2541
5	E	0.35	0/1823	0.59	0/2463
5	S	0.35	0/1823	0.59	0/2463
6	F	0.35	0/1937	0.60	0/2614
6	T	0.36	0/1937	0.60	0/2614
7	G	0.38	0/1959	0.61	0/2652
7	U	0.39	0/1959	0.61	0/2652
8	H	0.39	0/1716	0.67	0/2326
8	V	0.37	0/1716	0.67	0/2326
9	I	0.39	0/1611	0.66	0/2174
9	W	0.40	0/1611	0.66	0/2174
10	J	0.38	0/1613	0.64	0/2173
10	X	0.39	0/1613	0.64	0/2173
11	K	0.40	0/1681	0.66	1/2274 (0.0%)
11	Y	0.40	0/1681	0.66	1/2274 (0.0%)
12	L	0.38	0/1795	0.67	1/2420 (0.0%)
12	Z	0.39	0/1795	0.66	1/2420 (0.0%)
13	1	0.38	0/1855	0.66	1/2514 (0.0%)
13	M	0.38	0/1855	0.66	1/2514 (0.0%)
14	2	0.37	0/1541	0.63	1/2087 (0.0%)
14	N	0.38	0/1541	0.63	1/2087 (0.0%)
All	All	0.37	0/50450	0.63	8/68192 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	95	LEU	N-CA-C	-5.75	95.47	111.00
11	Y	4	LEU	CA-CB-CG	5.73	128.49	115.30
13	1	95	LEU	N-CA-C	-5.61	95.85	111.00
11	K	4	LEU	CA-CB-CG	5.61	128.19	115.30
12	L	95	TYR	N-CA-C	-5.24	96.85	111.00
14	N	22	THR	N-CA-C	-5.18	97.01	111.00
14	2	22	THR	N-CA-C	-5.13	97.14	111.00
12	Z	95	TYR	N-CA-C	-5.09	97.25	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	49	0
1	O	1915	0	1926	53	0
2	B	1905	0	1901	81	0
2	P	1905	0	1901	85	0
3	C	1891	0	1900	100	0
3	Q	1891	0	1900	91	0
4	D	1862	0	1836	52	0
4	R	1862	0	1836	56	0
5	E	1795	0	1797	90	0
5	S	1795	0	1797	90	0
6	F	1897	0	1886	66	0
6	T	1897	0	1886	62	0
7	G	1921	0	1910	63	0
7	U	1921	0	1910	64	0
8	H	1685	0	1688	48	0
8	V	1685	0	1688	52	0
9	I	1581	0	1574	37	0
9	W	1581	0	1574	40	0
10	J	1585	0	1590	55	0
10	X	1585	0	1590	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1644	0	1594	49	0
11	Y	1644	0	1594	44	0
12	L	1757	0	1711	67	0
12	Z	1757	0	1711	72	0
13	1	1824	0	1832	61	0
13	M	1824	0	1832	58	0
14	2	1512	0	1481	43	0
14	N	1512	0	1481	44	0
15	K	46	0	42	3	0
15	Y	46	0	42	3	0
16	1	80	0	0	5	0
16	2	59	0	0	4	0
16	A	59	0	0	2	0
16	B	37	0	0	1	0
16	C	42	0	0	3	0
16	D	42	0	0	3	0
16	E	21	0	0	1	0
16	F	46	0	0	3	0
16	G	60	0	0	1	0
16	H	49	0	0	2	0
16	I	68	0	0	1	0
16	J	50	0	0	1	0
16	K	48	0	0	2	0
16	L	56	0	0	4	0
16	M	71	0	0	1	0
16	N	59	0	0	4	0
16	O	34	0	0	2	0
16	P	29	0	0	2	0
16	Q	29	0	0	3	0
16	R	28	0	0	4	0
16	S	20	0	0	1	0
16	T	34	0	0	1	0
16	U	62	0	0	3	0
16	V	47	0	0	4	0
16	W	61	0	0	1	0
16	X	47	0	0	4	0
16	Y	48	0	0	1	0
16	Z	53	0	0	5	0
All	All	50979	0	49336	1551	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 16.

All (1551) 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)
2:P:202:THR:HG22	2:P:204:SER:H	1.10	1.16
2:B:202:THR:HG22	2:B:204:SER:H	1.11	1.07
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.23	1.03
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.23	1.00
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.45	0.98
2:B:15:PHE:H	3:C:23:GLN:HE22	1.06	0.98
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.46	0.95
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.66	0.93
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.67	0.92
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.11	0.92
10:J:2:ILE:HD13	10:J:162:LEU:HD13	1.51	0.91
3:Q:65:SER:HB2	16:Q:303:HOH:O	1.69	0.91
3:C:163:GLN:NE2	3:C:164:THR:H	1.67	0.91
2:B:71:ASN:ND2	2:B:72:ASP:H	1.69	0.91
7:U:96:ALA:HA	7:U:107:MET:HE2	1.53	0.90
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.71	0.90
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.72	0.90
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.37	0.89
1:O:15:PHE:H	2:P:23:GLN:HE22	1.15	0.89
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.54	0.89
7:G:96:ALA:HA	7:G:107:MET:HE2	1.52	0.89
5:S:207:LEU:HD23	5:S:207:LEU:H	1.37	0.89
3:C:163:GLN:HE21	3:C:164:THR:N	1.68	0.89
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.35	0.88
10:X:2:ILE:HD13	10:X:162:LEU:HD13	1.54	0.88
5:E:207:LEU:H	5:E:207:LEU:HD23	1.38	0.88
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.36	0.88
2:P:71:ASN:ND2	2:P:72:ASP:H	1.70	0.88
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.12	0.87
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.87	0.87
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.54	0.87
8:H:128:GLY:O	8:H:131:SER:HB2	1.73	0.86
3:C:185:THR:HB	3:C:188:GLU:HG2	1.54	0.86
8:V:128:GLY:O	8:V:131:SER:HB2	1.76	0.86
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.74	0.86
1:A:15:PHE:H	2:B:23:GLN:HE22	1.23	0.85
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.57	0.85
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.41	0.85
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.23	0.85
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.74	0.84
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.27	0.83
5:E:198:SER:HA	5:E:201:LEU:HG	1.61	0.82
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.95	0.82
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.45	0.82
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.60	0.81
5:S:198:SER:HA	5:S:201:LEU:HG	1.61	0.81
3:C:185:THR:HG22	3:C:187:GLU:H	1.46	0.81
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.45	0.81
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.60	0.81
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.93	0.81
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.45	0.81
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.96	0.80
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.45	0.80
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.28	0.80
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.44	0.80
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.61	0.80
3:C:15:PHE:H	4:D:23:GLN:HE22	1.30	0.80
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.48	0.79
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.64	0.79
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.95	0.79
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.95	0.78
1:A:124:THR:CG2	2:B:130:ARG:HH21	1.97	0.78
5:E:12:THR:HG21	5:E:124:THR:HA	1.65	0.78
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.64	0.78
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.31	0.78
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.49	0.77
2:B:202:THR:HG22	2:B:204:SER:N	1.95	0.77
13:M:40:ASN:H	13:M:40:ASN:HD22	1.32	0.77
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.65	0.77
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.67	0.77
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.67	0.76
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.50	0.76
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.68	0.76
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.32	0.76
5:S:12:THR:HG21	5:S:124:THR:HA	1.65	0.76
12:L:166:HIS:HD2	12:L:168:GLN:H	1.34	0.76
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.68	0.76
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.01	0.75
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.65	0.75
2:P:202:THR:HG22	2:P:204:SER:N	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:144:GLU:HG2	16:2:1115:HOH:O	1.86	0.74
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.85	0.74
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.51	0.74
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.36	0.74
7:U:86:ARG:HD2	16:U:248:HOH:O	1.85	0.74
7:G:77:VAL:HG12	7:G:137:THR:HB	1.68	0.74
13:1:40:ASN:HD22	13:1:40:ASN:H	1.32	0.74
10:J:-1:MET:HG2	10:J:1:ASP:H	1.53	0.74
7:U:77:VAL:HG12	7:U:137:THR:HB	1.70	0.74
7:G:121:GLN:O	7:G:124:THR:HB	1.87	0.73
7:U:121:GLN:O	7:U:124:THR:HB	1.88	0.73
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.53	0.73
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.52	0.73
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.54	0.73
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.70	0.73
7:U:198:ILE:HG23	7:U:203:THR:O	1.89	0.73
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.19	0.73
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.02	0.73
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.18	0.73
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.85	0.73
7:G:198:ILE:HG23	7:G:203:THR:O	1.89	0.72
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.19	0.72
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.36	0.72
10:J:143:ARG:O	10:J:146:MET:HG3	1.89	0.72
6:T:35:THR:HG21	6:T:51:GLU:O	1.90	0.72
10:X:156:LYS:O	10:X:160:GLN:HG3	1.88	0.72
10:X:-1:MET:HG2	10:X:1:ASP:H	1.54	0.72
10:J:156:LYS:O	10:J:160:GLN:HG3	1.90	0.72
2:B:71:ASN:HD22	2:B:72:ASP:H	1.38	0.72
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.04	0.71
6:F:35:THR:HG21	6:F:51:GLU:O	1.89	0.71
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.70	0.71
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.70	0.71
2:P:71:ASN:HD22	2:P:72:ASP:H	1.38	0.71
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.54	0.71
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.72	0.71
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.05	0.71
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.72	0.71
2:B:51:GLU:OE2	2:B:202:THR:HG23	1.91	0.70
5:S:207:LEU:H	5:S:207:LEU:CD2	2.04	0.70
2:P:51:GLU:OE2	2:P:202:THR:HG23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:185:THR:HG22	3:C:187:GLU:N	2.05	0.70
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.39	0.70
5:E:207:LEU:H	5:E:207:LEU:CD2	2.05	0.70
8:V:34:LEU:HB2	16:V:578:HOH:O	1.91	0.70
10:X:143:ARG:O	10:X:146:MET:HG3	1.91	0.70
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.71	0.70
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.40	0.69
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.57	0.69
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.06	0.69
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.22	0.69
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.75	0.69
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.74	0.69
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.91	0.69
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.74	0.69
14:2:48:SER:HB3	14:2:51:ASP:HB2	1.75	0.69
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.27	0.69
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.73	0.69
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.93	0.69
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.41	0.69
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.07	0.69
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.74	0.69
5:S:132:TYR:O	5:S:153:PRO:HB3	1.93	0.68
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.41	0.68
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.73	0.68
3:C:163:GLN:HE21	3:C:164:THR:H	0.83	0.68
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.75	0.68
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.09	0.68
14:2:1:THR:OG1	16:2:1033:HOH:O	2.10	0.68
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.59	0.68
3:C:71:ASP:HA	10:J:68:ILE:HD13	1.76	0.68
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.76	0.68
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.41	0.68
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.58	0.68
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.76	0.68
11:K:142:TYR:O	11:K:143:LYS:HD2	1.94	0.68
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.76	0.68
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.76	0.68
2:B:15:PHE:H	3:C:23:GLN:NE2	1.88	0.67
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.77	0.67
7:U:236:ILE:HD12	7:U:237:ALA:N	2.09	0.67
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	2.01	0.67
9:W:6:MET:HE1	9:W:155:ILE:HA	1.76	0.67
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.07	0.67
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.77	0.67
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.60	0.67
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.76	0.66
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.76	0.66
7:G:236:ILE:HD12	7:G:237:ALA:N	2.10	0.66
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.96	0.66
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.77	0.66
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.30	0.66
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.76	0.66
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.42	0.66
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.31	0.66
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.43	0.66
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.10	0.66
6:F:173:LYS:O	6:F:177:GLU:HG3	1.95	0.66
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.60	0.66
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.31	0.65
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.25	0.65
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.95	0.65
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.10	0.65
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.77	0.65
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.78	0.65
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.79	0.65
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.96	0.65
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.61	0.65
7:G:59:LEU:O	7:G:61:PRO:HD3	1.96	0.65
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.78	0.65
2:B:71:ASN:ND2	2:B:72:ASP:N	2.43	0.65
5:E:132:TYR:O	5:E:153:PRO:HB3	1.96	0.65
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.61	0.65
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.97	0.65
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.79	0.65
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.11	0.65
2:P:71:ASN:ND2	2:P:72:ASP:N	2.45	0.65
2:B:181:LYS:O	2:B:184:MET:HG3	1.97	0.65
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.62	0.65
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.94	0.65
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.79	0.65
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.79	0.64
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.79	0.64
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.60	0.64
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.96	0.64
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.80	0.64
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.33	0.64
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.80	0.64
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.79	0.64
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.32	0.64
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.79	0.64
10:X:-1:MET:HG2	10:X:1:ASP:N	2.13	0.64
4:D:81:LEU:HD12	4:D:133:GLY:HA3	1.80	0.64
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.79	0.64
2:P:181:LYS:O	2:P:184:MET:HG3	1.98	0.64
7:U:59:LEU:O	7:U:61:PRO:HD3	1.97	0.64
10:J:-1:MET:HG2	10:J:1:ASP:N	2.12	0.63
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.80	0.63
12:L:13:VAL:HG12	12:L:177:ILE:HG13	1.80	0.63
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.63	0.63
7:U:87:ASN:HD22	7:U:87:ASN:C	2.02	0.63
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.98	0.63
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.29	0.63
3:C:41:LYS:HG2	3:C:161:SER:O	1.99	0.63
16:B:565:HOH:O	3:C:33:ARG:HD2	1.98	0.63
4:R:72:ARG:HG3	16:R:1302:HOH:O	1.99	0.63
4:R:85:ALA:O	4:R:89:ILE:HG12	1.99	0.63
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.80	0.63
5:S:15:PHE:H	6:T:23:GLN:HE22	1.47	0.63
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.80	0.63
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.81	0.63
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.81	0.63
3:Q:52:ARG:HH21	3:Q:211:GLU:HB3	1.63	0.63
6:T:187:ARG:HG3	6:T:187:ARG:HH11	1.62	0.63
3:C:169:SER:HA	3:C:172:VAL:CG1	2.28	0.63
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.80	0.62
3:C:52:ARG:HH21	3:C:211:GLU:HB3	1.63	0.62
11:K:168:TYR:CZ	15:K:999:BFO:H42	2.33	0.62
2:P:121:GLN:O	2:P:124:THR:HB	1.98	0.62
10:X:7:ARG:HG2	10:X:7:ARG:HH11	1.63	0.62
11:Y:168:TYR:CZ	15:Y:999:BFO:H42	2.33	0.62
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:226:GLY:O	5:S:229:VAL:HG22	1.99	0.62
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.13	0.62
3:Q:215:VAL:HG23	3:Q:221:ILE:HG12	1.81	0.62
9:I:6:MET:HE1	9:I:155:ILE:HA	1.82	0.62
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.82	0.62
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.29	0.62
3:C:46:VAL:O	3:C:215:VAL:HG12	2.00	0.62
6:T:173:LYS:O	6:T:177:GLU:HG3	1.99	0.62
5:E:167:ALA:HB3	16:E:1131:HOH:O	1.99	0.62
5:E:226:GLY:O	5:E:229:VAL:HG22	2.00	0.62
7:G:87:ASN:HD22	7:G:87:ASN:C	2.02	0.62
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.30	0.61
8:H:152:ILE:O	8:H:156:SER:HB2	2.00	0.61
10:J:7:ARG:HG2	10:J:7:ARG:HH11	1.65	0.61
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.81	0.61
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	2.02	0.61
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.82	0.61
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.13	0.61
9:I:29:ASN:HD22	9:I:30:LYS:HG3	1.64	0.61
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.01	0.61
2:B:52:ARG:HH22	2:B:63(A):SER:HB3	1.66	0.61
3:C:175:PHE:O	3:C:179:ASN:HB2	2.01	0.61
4:D:85:ALA:O	4:D:89:ILE:HG12	2.01	0.61
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.65	0.61
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.30	0.61
10:X:90(B):ARG:NH1	16:X:266:HOH:O	2.32	0.61
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	1.83	0.61
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.83	0.60
8:V:152:ILE:O	8:V:156:SER:HB2	2.01	0.60
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.83	0.60
7:G:77:VAL:CG1	7:G:137:THR:HB	2.31	0.60
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.30	0.60
2:B:97:GLN:NE2	9:I:64:ASN:HD22	1.99	0.60
2:P:52:ARG:HH22	2:P:63(A):SER:HB3	1.64	0.60
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.32	0.60
12:Z:21:ILE:HD12	12:Z:21:ILE:C	2.22	0.60
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.01	0.60
2:B:121:GLN:O	2:B:124:THR:HB	2.02	0.60
11:K:45:MET:SD	15:K:999:BFO:H37	2.41	0.60
4:D:102:TYR:O	12:L:81:ARG:HG3	2.02	0.60
14:N:157:HIS:HD2	14:2:140:LYS:NZ	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.36	0.60
5:S:190:ILE:O	5:S:194:VAL:HG23	2.01	0.60
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.82	0.60
2:P:228:GLU:O	2:P:232:ILE:HG22	2.02	0.60
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	1.83	0.60
13:1:35:ILE:HG12	13:1:56:GLU:HG3	1.84	0.60
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.84	0.60
3:C:206:GLY:HA2	3:C:209:ASN:HD22	1.67	0.60
3:C:232:TYR:O	3:C:236:ILE:HG13	2.01	0.60
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.84	0.60
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.00	0.60
12:L:21:ILE:HD12	12:L:21:ILE:C	2.22	0.59
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.67	0.59
1:O:159:PRO:O	2:P:59:LEU:HD12	2.03	0.59
2:P:239:THR:OXT	2:P:239:THR:HG22	2.02	0.59
6:T:127:ASN:HD22	6:T:128:SER:N	1.99	0.59
7:U:107:MET:HE3	7:U:112:LEU:HB2	1.84	0.59
13:M:150:VAL:HG21	16:M:1069:HOH:O	2.00	0.59
11:Y:138:LEU:HD13	11:Y:158:SER:OG	2.03	0.59
3:C:169:SER:HA	3:C:172:VAL:HG12	1.83	0.59
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.67	0.59
14:N:140:LYS:NZ	14:2:157:HIS:HD2	1.99	0.59
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.01	0.59
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.18	0.59
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.84	0.59
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.50	0.59
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.38	0.59
3:C:186:VAL:O	3:C:190:VAL:HG23	2.03	0.59
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.38	0.59
12:L:14(C):GLN:HG2	8:V:210:THR:CG2	2.32	0.59
13:M:35:ILE:HG12	13:M:56:GLU:HG3	1.84	0.59
7:U:77:VAL:CG1	7:U:137:THR:HB	2.32	0.59
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.01	0.59
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.18	0.59
12:Z:14(I):THR:O	12:Z:14(K):LYS:HB2	2.03	0.59
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.16	0.59
6:F:127:ASN:HD22	6:F:128:SER:N	2.00	0.59
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.85	0.59
5:S:2(C):VAL:HA	5:S:233:ILE:HD11	1.85	0.59
2:B:15:PHE:N	3:C:23:GLN:HE22	1.89	0.59
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.02	0.59
7:U:96:ALA:CA	7:U:107:MET:HE2	2.31	0.59
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.84	0.59
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.84	0.58
5:E:15:PHE:H	6:F:23:GLN:HE22	1.51	0.58
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.50	0.58
3:Q:206:GLY:HA2	3:Q:209:ASN:HD22	1.67	0.58
4:R:53:ARG:HG2	4:R:53:ARG:O	2.03	0.58
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	1.96	0.58
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.85	0.58
4:R:102:TYR:O	12:Z:81:ARG:HG3	2.02	0.58
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.69	0.58
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.85	0.58
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.86	0.58
3:Q:169:SER:HA	3:Q:172:VAL:HG12	1.85	0.58
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.67	0.58
4:D:67:ILE:HD12	4:D:211:GLN:HE21	1.68	0.58
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.84	0.58
5:E:220:PRO:O	5:E:222:THR:HG23	2.04	0.58
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.85	0.58
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.85	0.58
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.85	0.58
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.84	0.58
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.00	0.58
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.51	0.58
2:B:228:GLU:O	2:B:232:ILE:HG22	2.04	0.58
10:J:25:SER:HB2	11:K:131:GLN:HE22	1.69	0.58
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.39	0.57
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.19	0.57
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.33	0.57
5:E:2(C):VAL:HA	5:E:233:ILE:HD11	1.86	0.57
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	2.07	0.57
4:R:175:GLU:HB3	4:R:196:ILE:HD13	1.86	0.57
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.33	0.57
8:V:20:SER:HB3	8:V:28:ASP:HB3	1.87	0.57
9:W:29:ASN:HD22	9:W:30:LYS:HG3	1.68	0.57
3:Q:71:ASP:HA	10:X:68:ILE:HD13	1.86	0.57
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.69	0.57
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.86	0.57
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.39	0.57
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:194:VAL:O	5:E:197:ILE:HG22	2.05	0.57
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.86	0.57
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.87	0.57
10:X:25:SER:HB2	11:Y:131:GLN:HE22	1.70	0.57
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.34	0.57
7:G:107:MET:HE3	7:G:112:LEU:HB2	1.86	0.57
13:M:14(C):ARG:CG	13:M:14(C):ARG:HH11	2.16	0.57
4:R:24:VAL:O	4:R:27:SER:HB3	2.04	0.57
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.86	0.57
11:Y:45:MET:SD	15:Y:999:BFO:H37	2.45	0.57
7:G:96:ALA:CA	7:G:107:MET:HE2	2.30	0.57
13:M:40:ASN:ND2	13:M:40:ASN:H	2.01	0.57
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.40	0.57
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.86	0.57
6:T:186:ALA:O	6:T:190:VAL:HG23	2.05	0.57
5:E:190:ILE:O	5:E:194:VAL:HG23	2.04	0.57
6:F:186:ALA:O	6:F:190:VAL:HG23	2.05	0.57
12:L:93:PHE:N	12:L:94:PRO:HD3	2.19	0.57
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.34	0.57
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.04	0.57
10:X:34:THR:HG21	10:X:176:LYS:HZ2	1.70	0.57
11:Y:10(B):LYS:N	11:Y:10(B):LYS:HD2	2.07	0.57
11:Y:35:ILE:CD1	11:Y:53:GLN:HA	2.34	0.57
2:B:239:THR:OXT	2:B:239:THR:HG22	2.05	0.57
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.04	0.57
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.40	0.57
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.53	0.57
6:T:38:ILE:HG12	6:T:197:ILE:HD11	1.87	0.57
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.39	0.57
3:C:35:THR:HB	3:C:51:GLU:HG3	1.86	0.56
1:O:173:LYS:O	1:O:177:GLU:HG3	2.05	0.56
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.86	0.56
4:D:53:ARG:HG2	4:D:53:ARG:O	2.05	0.56
8:H:153:LYS:HD2	16:H:712:HOH:O	2.05	0.56
8:H:20:SER:HB3	8:H:28:ASP:HB3	1.87	0.56
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.70	0.56
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.71	0.56
4:D:175:GLU:HB3	4:D:196:ILE:HD13	1.86	0.56
5:E:73:HIS:HE1	5:E:107:LEU:O	1.88	0.56
3:C:65:SER:HB2	16:C:274:HOH:O	2.04	0.56
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.86	0.56
12:L:14(I):THR:O	12:L:14(K):LYS:HB2	2.05	0.56
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.41	0.56
5:S:73:HIS:HE1	5:S:107:LEU:O	1.88	0.56
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.86	0.56
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.36	0.56
14:N:10(B):LYS:HD3	14:N:10(B):LYS:O	2.06	0.56
5:S:207:LEU:N	5:S:207:LEU:HD23	2.14	0.56
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.05	0.56
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.87	0.56
11:K:35:ILE:CD1	11:K:53:GLN:HA	2.35	0.56
3:Q:170:LYS:HB2	16:Q:833:HOH:O	2.05	0.56
1:A:173:LYS:O	1:A:177:GLU:HG3	2.05	0.56
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.40	0.56
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.87	0.56
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.06	0.56
2:B:71:ASN:HD22	2:B:72:ASP:N	2.00	0.56
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.87	0.56
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.41	0.56
14:2:10(B):LYS:C	14:2:10(B):LYS:HD3	2.27	0.56
14:2:10(B):LYS:HD3	14:2:10(B):LYS:O	2.05	0.56
10:J:52:THR:CG2	10:J:53:VAL:N	2.68	0.56
2:P:71:ASN:HD22	2:P:72:ASP:N	2.01	0.56
8:V:196:VAL:HG23	16:V:652:HOH:O	2.04	0.56
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.87	0.56
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.21	0.56
13:M:70:ASN:ND2	13:M:70(A):ALA:HA	2.21	0.56
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	1.88	0.56
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.87	0.55
9:I:90:ARG:HD2	16:I:1159:HOH:O	2.04	0.55
10:J:148:THR:HG21	10:J:177:ILE:HD13	1.88	0.55
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.71	0.55
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.06	0.55
13:1:40:ASN:HD22	13:1:40:ASN:N	1.98	0.55
13:1:46:SER:OG	13:1:98:ALA:HB3	2.06	0.55
5:S:194:VAL:O	5:S:197:ILE:HG22	2.05	0.55
6:T:136:THR:O	6:T:150:MET:HA	2.06	0.55
13:1:14(C):ARG:CG	13:1:14(C):ARG:HH11	2.15	0.55
1:A:4:MET:SD	1:A:5:THR:N	2.72	0.55
6:F:91:ARG:O	6:F:95:GLU:HB2	2.07	0.55
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:70:ASN:ND2	13:1:70(A):ALA:HA	2.21	0.55
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.89	0.55
1:O:33:GLN:HA	1:O:33:GLN:HE21	1.72	0.55
5:S:220:PRO:O	5:S:222:THR:HG23	2.06	0.55
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.89	0.55
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.88	0.55
4:D:112:LEU:C	4:D:112:LEU:HD13	2.27	0.55
2:P:87:ILE:O	2:P:91:THR:HG23	2.06	0.55
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.22	0.55
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.71	0.55
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.03	0.55
13:1:40:ASN:ND2	13:1:40:ASN:H	2.02	0.55
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.42	0.55
14:2:37:VAL:HG22	14:2:41:ILE:O	2.07	0.54
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.71	0.54
11:K:22:ALA:HB3	11:K:25:TRP:HD1	1.72	0.54
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.27	0.54
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.43	0.54
10:X:148:THR:HG21	10:X:177:ILE:HD13	1.89	0.54
1:A:58:LEU:HD12	7:G:173:THR:HG23	1.90	0.54
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.88	0.54
2:P:185:LYS:HD3	2:P:186:VAL:N	2.23	0.54
4:R:177:LEU:HA	5:S:58:LEU:HD11	1.88	0.54
2:B:185:LYS:HD3	2:B:186:VAL:N	2.23	0.54
1:O:161:LYS:HD2	2:P:58:LEU:HA	1.89	0.54
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.73	0.54
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	1.99	0.54
13:1:67:ALA:HB3	16:1:1339:HOH:O	2.06	0.54
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.89	0.54
12:L:14(I):THR:O	12:L:1(I):ASN:HB3	2.07	0.54
12:L:5:GLY:O	12:L:124:CYS:HA	2.07	0.54
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.89	0.54
11:K:12:ILE:HB	11:K:178:VAL:HB	1.88	0.54
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.54	0.54
2:P:160:TRP:CD2	2:P:163:ILE:HD13	2.42	0.54
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.88	0.54
4:R:112:LEU:C	4:R:112:LEU:HD13	2.28	0.54
1:A:69:LEU:HD23	1:A:69:LEU:C	2.28	0.54
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.71	0.54
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.08	0.54
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.71	0.54
5:S:198:SER:HA	5:S:201:LEU:CG	2.36	0.54
6:T:91:ARG:O	6:T:95:GLU:HB2	2.08	0.54
13:1:146:THR:HA	16:1:323:HOH:O	2.06	0.54
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.08	0.54
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.90	0.54
4:R:186:LEU:O	4:R:190:GLU:HG3	2.07	0.54
10:X:35:ARG:NH1	10:X:57:GLU:HG2	2.23	0.54
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.05	0.54
3:C:163:GLN:HE22	3:C:173:ARG:NE	2.05	0.54
4:D:12(F):GLY:HA3	16:D:965:HOH:O	2.08	0.54
4:D:24:VAL:O	4:D:27:SER:HB3	2.08	0.54
2:P:168:ASN:HA	16:P:943:HOH:O	2.08	0.54
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.37	0.54
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.71	0.54
6:F:136:THR:O	6:F:150:MET:HA	2.08	0.54
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.89	0.54
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.90	0.53
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.89	0.53
8:V:52:THR:O	8:V:56:THR:HB	2.08	0.53
5:E:207:LEU:HD23	5:E:207:LEU:N	2.15	0.53
11:K:138:LEU:HD13	11:K:158:SER:OG	2.07	0.53
12:L:14(C):GLN:HG2	8:V:210:THR:HG21	1.90	0.53
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.22	0.53
3:Q:163:GLN:HE22	3:Q:173:ARG:NE	2.04	0.53
11:Y:22:ALA:HB3	11:Y:25:TRP:HD1	1.71	0.53
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.90	0.53
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.07	0.53
12:Z:29:ARG:NH1	12:Z:193:ARG:HB3	2.23	0.53
2:B:87:ILE:O	2:B:91:THR:HG23	2.08	0.53
11:K:86:LEU:HD13	11:K:86:LEU:C	2.29	0.53
13:M:17:ASP:HA	13:M:173:PHE:CB	2.39	0.53
13:M:46:SER:OG	13:M:98:ALA:HB3	2.08	0.53
6:T:175:GLU:OE1	6:T:199:LEU:HD23	2.09	0.53
6:T:79:SER:HA	16:T:1238:HOH:O	2.08	0.53
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.39	0.53
4:R:81:LEU:HB3	16:R:599:HOH:O	2.07	0.53
9:W:6:MET:CE	9:W:155:ILE:HA	2.37	0.53
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.89	0.53
4:R:156:THR:HG22	5:S:83:PRO:HD3	1.89	0.53
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:29:ASN:C	9:W:29:ASN:HD22	2.11	0.53
13:1:152:GLU:O	13:1:156:VAL:HG23	2.08	0.53
3:C:227:GLU:OE1	3:C:227:GLU:N	2.40	0.53
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.90	0.53
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.72	0.53
9:I:29:ASN:HD22	9:I:29:ASN:C	2.11	0.53
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.08	0.53
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.71	0.53
6:T:63:LYS:O	6:T:65:VAL:N	2.41	0.53
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.22	0.53
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.09	0.53
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.91	0.53
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.04	0.53
11:Y:35:ILE:HD11	11:Y:53:GLN:HA	1.91	0.53
10:J:52:THR:HG22	10:J:53:VAL:H	1.74	0.53
5:S:227:GLU:N	5:S:227:GLU:CD	2.62	0.53
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.39	0.53
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.89	0.53
9:I:29:ASN:HD21	9:I:30:LYS:NZ	2.06	0.53
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.23	0.53
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.39	0.52
5:E:227:GLU:CD	5:E:227:GLU:N	2.62	0.52
8:H:210:THR:CG2	12:Z:14(C):GLN:HG2	2.39	0.52
9:I:113:PHE:HA	9:I:118:CYS:O	2.09	0.52
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.45	0.52
7:U:82:ILE:N	7:U:83:PRO:HD2	2.24	0.52
3:C:190:VAL:O	3:C:194:VAL:HG23	2.09	0.52
5:E:179:THR:O	5:E:18(B):THR:HB	2.09	0.52
7:G:192:PHE:CD1	7:G:192:PHE:C	2.82	0.52
1:O:27:ALA:O	1:O:31:VAL:HG23	2.09	0.52
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.15	0.52
14:2:89:GLU:OE1	14:2:89:GLU:HA	2.07	0.52
8:H:52:THR:O	8:H:56:THR:HB	2.09	0.52
12:L:14(I):THR:HG21	12:L:14(M):VAL:HB	1.91	0.52
6:T:203:GLU:C	6:T:205:ASN:H	2.12	0.52
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.30	0.52
6:F:203:GLU:C	6:F:205:ASN:H	2.12	0.52
4:R:65:GLU:HA	16:R:750:HOH:O	2.08	0.52
9:W:113:PHE:HA	9:W:118:CYS:O	2.09	0.52
12:Z:6:ILE:HG12	12:Z:124:CYS:CB	2.39	0.52
14:N:37:VAL:HG22	14:N:41:ILE:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:207:LEU:C	4:R:207:LEU:HD23	2.30	0.52
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.91	0.52
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.91	0.52
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.43	0.52
9:I:6:MET:CE	9:I:155:ILE:HA	2.39	0.52
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.10	0.52
5:S:52:LYS:O	5:S:63:TYR:HD2	1.93	0.52
10:X:52:THR:CG2	10:X:53:VAL:N	2.72	0.52
13:1:159:MET:HE3	16:1:450:HOH:O	2.09	0.52
4:D:185:THR:OG1	4:D:188:GLU:HG3	2.09	0.52
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.30	0.52
10:J:35:ARG:NH1	10:J:57:GLU:HG2	2.24	0.52
5:S:231:LYS:HD2	5:S:231:LYS:H	1.75	0.52
12:Z:14(I):THR:O	12:Z:1(I):ASN:HB3	2.09	0.52
5:E:74:MET:HE2	5:E:109:VAL:HG22	1.90	0.52
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.39	0.52
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.91	0.52
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.09	0.51
10:X:113:ILE:HA	10:X:118:THR:O	2.09	0.51
14:2:85:GLU:O	14:2:89:GLU:HB2	2.10	0.51
5:E:231:LYS:HD2	5:E:231:LYS:H	1.74	0.51
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.92	0.51
9:W:130:ALA:HB2	9:W:166:ASP:HB2	1.90	0.51
12:Z:6:ILE:HG12	12:Z:124:CYS:HB2	1.92	0.51
1:A:27:ALA:O	1:A:31:VAL:HG23	2.10	0.51
4:D:142:ASP:HA	16:D:1309:HOH:O	2.10	0.51
6:F:28:VAL:O	6:F:32:GLU:HG3	2.10	0.51
14:N:14:LEU:O	14:N:175:MET:HA	2.10	0.51
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.42	0.51
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.35	0.51
16:N:583:HOH:O	13:1:211:ILE:HD11	2.09	0.51
4:D:186:LEU:O	4:D:190:GLU:HG3	2.10	0.51
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.93	0.51
13:M:40:ASN:HD22	13:M:40:ASN:N	1.97	0.51
6:T:237:GLN:O	6:T:240:ILE:HG22	2.10	0.51
7:U:192:PHE:C	7:U:192:PHE:CD1	2.82	0.51
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.41	0.51
2:B:213:ALA:HA	2:B:222:LYS:O	2.11	0.51
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.92	0.51
4:D:237:LEU:O	4:D:241:GLU:HG3	2.11	0.51
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:HIS:HD2	8:H:61:SER:OG	1.94	0.51
14:N:85:GLU:O	14:N:89:GLU:HB2	2.10	0.51
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	1.93	0.51
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.91	0.51
10:J:113:ILE:HA	10:J:118:THR:O	2.11	0.51
13:M:152:GLU:O	13:M:156:VAL:HG23	2.10	0.51
1:O:150:GLN:O	1:O:157:TYR:HA	2.11	0.51
2:P:213:ALA:HA	2:P:222:LYS:O	2.11	0.51
5:S:179:THR:O	5:S:18(B):THR:HB	2.10	0.51
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.91	0.51
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.46	0.51
13:1:17:ASP:HA	13:1:173:PHE:CB	2.41	0.51
2:P:112:LEU:HD23	2:P:112:LEU:C	2.30	0.51
2:P:121:GLN:NE2	16:P:462:HOH:O	2.44	0.51
4:R:185:THR:OG1	4:R:188:GLU:HG3	2.11	0.51
6:T:69:VAL:HG12	16:1:811:HOH:O	2.09	0.51
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.10	0.51
1:A:110:LYS:HG2	16:A:285:HOH:O	2.10	0.51
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.11	0.51
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.92	0.51
14:N:89:GLU:HA	14:N:89:GLU:OE1	2.11	0.51
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.92	0.50
3:C:122:ARG:NH2	16:C:806:HOH:O	2.43	0.50
7:G:8:TYR:C	7:G:10:ARG:H	2.14	0.50
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.93	0.50
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.92	0.50
11:K:99:THR:HG22	11:K:113:VAL:O	2.10	0.50
5:S:54:ASN:ND2	5:S:56:ASP:O	2.44	0.50
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.93	0.50
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.92	0.50
12:L:145:TYR:CD1	12:L:146:LEU:N	2.79	0.50
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.23	0.50
13:M:35:ILE:N	13:M:35:ILE:HD12	2.27	0.50
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.26	0.50
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.76	0.50
3:C:52:ARG:HD2	3:C:208:LYS:O	2.11	0.50
5:E:198:SER:HA	5:E:201:LEU:CG	2.37	0.50
6:F:127:ASN:HD22	6:F:127:ASN:C	2.12	0.50
1:O:47:VAL:HG23	1:O:212:LEU:HD21	1.92	0.50
9:W:156:SER:O	9:W:160:LEU:HB2	2.12	0.50
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.41	0.50
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.93	0.50
1:O:121:GLN:O	1:O:124:THR:HB	2.11	0.50
1:O:47:VAL:CG2	1:O:212:LEU:HD21	2.42	0.50
16:L:200:HOH:O	9:W:192:ARG:HG3	2.11	0.50
10:X:10(B):LYS:NZ	10:X:10(B):LYS:HB2	2.27	0.50
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.94	0.50
6:F:63:LYS:O	6:F:65:VAL:N	2.43	0.50
4:R:121:LEU:N	16:R:853:HOH:O	2.42	0.50
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.12	0.50
3:C:235:GLN:O	3:C:239:GLU:HG2	2.12	0.50
6:F:114:ASP:O	6:F:118:GLN:HG2	2.11	0.50
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.11	0.50
8:H:81:GLN:O	8:H:85:GLN:HG3	2.12	0.50
11:K:195:LEU:O	11:K:199:VAL:HG23	2.11	0.50
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.15	0.50
4:R:243:ALA:O	4:R:244:GLU:HB2	2.10	0.50
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.42	0.50
2:B:224:PHE:N	2:B:224:PHE:CD2	2.80	0.50
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.94	0.50
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	2.12	0.50
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.94	0.50
4:R:237:LEU:O	4:R:241:GLU:HG3	2.12	0.50
5:S:74:MET:HE2	5:S:109:VAL:HG22	1.94	0.50
13:1:149:GLN:H	13:1:149:GLN:NE2	2.10	0.50
10:J:133:TYR:HD1	16:Y:593:HOH:O	1.94	0.50
2:P:224:PHE:N	2:P:224:PHE:HD2	2.10	0.50
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.27	0.50
2:B:20:ARG:HH11	2:B:20:ARG:HG2	1.77	0.50
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.11	0.50
4:D:97:VAL:HG11	11:K:65:LEU:HD22	1.92	0.50
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.92	0.50
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.47	0.50
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.93	0.50
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:NH1	2.27	0.50
1:A:62:GLU:H	1:A:62:GLU:CD	2.15	0.49
16:F:1121:HOH:O	13:M:67:ALA:HB3	2.12	0.49
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.75	0.49
2:P:20:ARG:HH11	2:P:20:ARG:HG2	1.77	0.49
7:U:8:TYR:C	7:U:10:ARG:H	2.15	0.49
7:U:141:VAL:HG21	7:U:216:THR:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:121:LYS:O	14:2:122:LEU:HD23	2.12	0.49
14:2:14:LEU:O	14:2:175:MET:HA	2.12	0.49
2:B:150:THR:O	2:B:157:TYR:HA	2.11	0.49
4:D:243:ALA:O	4:D:244:GLU:HB2	2.11	0.49
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.42	0.49
2:P:150:THR:O	2:P:157:TYR:HA	2.12	0.49
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.13	0.49
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.80	0.49
12:L:166:HIS:CD2	12:L:168:GLN:H	2.23	0.49
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.58	0.49
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.27	0.49
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.41	0.49
8:V:81:GLN:O	8:V:85:GLN:HG3	2.12	0.49
8:V:84:LYS:HG3	8:V:85:GLN:N	2.28	0.49
2:B:224:PHE:HD2	2:B:224:PHE:N	2.09	0.49
5:E:58:LEU:HD12	5:E:58:LEU:N	2.27	0.49
9:I:156:SER:O	9:I:160:LEU:HB2	2.12	0.49
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.33	0.49
2:P:224:PHE:N	2:P:224:PHE:CD2	2.80	0.49
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.33	0.49
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.95	0.49
6:T:114:ASP:O	6:T:118:GLN:HG2	2.12	0.49
10:J:168:MET:HE3	10:X:168:MET:HE3	1.94	0.49
5:E:97:ASN:HD21	12:L:61:ASN:ND2	2.03	0.49
7:G:82:ILE:N	7:G:83:PRO:HD2	2.27	0.49
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.13	0.49
14:2:107:LYS:HG2	14:2:108:GLY:H	1.77	0.49
4:D:207:LEU:HD23	4:D:207:LEU:C	2.31	0.49
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.12	0.49
6:T:127:ASN:HD22	6:T:127:ASN:C	2.15	0.49
5:E:54:ASN:ND2	5:E:56:ASP:O	2.44	0.49
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.94	0.49
1:O:69:LEU:HD23	1:O:69:LEU:C	2.32	0.49
2:P:111:ILE:HD11	10:X:70:GLU:HG2	1.95	0.49
6:T:35:THR:CG2	6:T:36:THR:N	2.76	0.49
1:A:150:GLN:O	1:A:157:TYR:HA	2.13	0.49
5:E:52:LYS:O	5:E:63:TYR:HD2	1.95	0.49
6:F:49:ALA:HA	6:F:211:GLU:O	2.13	0.49
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.94	0.49
9:W:29:ASN:HD21	9:W:30:LYS:NZ	2.10	0.49
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:105:ASP:HB3	14:2:106:ASN:HB2	1.95	0.49
1:A:85:TYR:O	1:A:89:VAL:HG23	2.12	0.49
2:B:234:VAL:HA	2:B:239:THR:HA	1.94	0.49
6:F:237:GLN:O	6:F:240:ILE:HG22	2.12	0.49
3:Q:160:TRP:CZ2	4:R:59:LEU:HD23	2.48	0.49
6:T:28:VAL:O	6:T:32:GLU:HG3	2.13	0.49
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.93	0.49
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	1.95	0.49
7:G:141:VAL:HG21	7:G:216:THR:HA	1.93	0.49
10:J:10(B):LYS:HB2	10:J:10(B):LYS:HZ3	1.77	0.49
10:J:52:THR:HG22	10:J:53:VAL:N	2.28	0.49
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.95	0.49
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.28	0.49
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.95	0.49
2:B:160:TRP:CE3	2:B:163:ILE:HD13	2.48	0.48
14:N:144:GLU:HG2	16:N:798:HOH:O	2.12	0.48
7:U:96:ALA:HA	7:U:107:MET:CE	2.36	0.48
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.95	0.48
7:G:96:ALA:HA	7:G:107:MET:CE	2.34	0.48
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.96	0.48
12:L:177:ILE:HD12	12:L:177:ILE:N	2.27	0.48
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.43	0.48
4:R:175:GLU:OE1	4:R:175:GLU:HA	2.12	0.48
5:S:2(C):VAL:HG13	5:S:2(D):ASP:N	2.27	0.48
5:S:58:LEU:N	5:S:58:LEU:HD12	2.28	0.48
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.78	0.48
10:X:22:ARG:NE	16:X:541:HOH:O	2.31	0.48
3:C:152:GLU:HB2	3:C:153:PRO:HD2	1.94	0.48
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.28	0.48
12:L:6:ILE:HG12	12:L:124:CYS:CB	2.43	0.48
4:D:175:GLU:HA	4:D:175:GLU:OE1	2.13	0.48
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.95	0.48
11:K:35:ILE:HD11	11:K:53:GLN:HA	1.94	0.48
12:L:109:ALA:HB2	12:L:121:ARG:NH2	2.28	0.48
12:L:6:ILE:HG12	12:L:124:CYS:HB2	1.96	0.48
13:M:184:LEU:HD23	13:M:184:LEU:C	2.34	0.48
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.12	0.48
5:S:201:LEU:O	5:S:202:ARG:HB2	2.14	0.48
6:T:142:ASP:O	6:T:144:ASN:N	2.47	0.48
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.95	0.48
11:Y:21:THR:HG22	11:Y:26:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.13	0.48
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.94	0.48
12:L:48:PHE:CZ	12:L:50:ALA:HB3	2.48	0.48
1:O:62:GLU:CD	1:O:62:GLU:H	2.16	0.48
3:Q:112:LEU:HD13	3:Q:112:LEU:O	2.13	0.48
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	1.94	0.48
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.48	0.48
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.29	0.48
13:1:35:ILE:HD12	13:1:35:ILE:N	2.28	0.48
3:C:241:GLN:C	3:C:243:GLN:H	2.17	0.48
4:D:170:GLU:N	4:D:170:GLU:OE1	2.47	0.48
6:F:69:VAL:HG12	16:F:319:HOH:O	2.13	0.48
14:N:107:LYS:HG2	14:N:108:GLY:H	1.79	0.48
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.13	0.48
3:Q:241:GLN:C	3:Q:243:GLN:H	2.17	0.48
3:C:105:ASP:OD2	3:C:106:PRO:HD2	2.13	0.48
13:M:149:GLN:NE2	13:M:149:GLN:H	2.12	0.48
14:N:105:ASP:HB3	14:N:106:ASN:HB2	1.95	0.48
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.42	0.48
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.28	0.48
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.11	0.48
4:D:191:LEU:HD21	4:D:236:GLU:OE2	2.14	0.48
11:K:6:PHE:HA	11:K:123:ASP:O	2.14	0.48
2:P:224:PHE:H	2:P:224:PHE:HD2	1.62	0.48
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.49	0.48
8:V:18:THR:HB	8:V:30:ASN:HD22	1.79	0.48
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.14	0.48
12:Z:58:ARG:NH2	16:Z:1275:HOH:O	2.46	0.48
13:1:14(A):VAL:O	13:1:14(A):VAL:HG23	2.14	0.48
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.96	0.48
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.14	0.48
14:2:20:THR:HG23	14:2:31:THR:OG1	2.14	0.48
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.28	0.48
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.95	0.48
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.29	0.48
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.95	0.48
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.14	0.48
9:I:48:LEU:HG	9:I:50:THR:HG22	1.96	0.48
11:K:10(A):ARG:NH1	11:K:10(A):ARG:HG2	2.28	0.48
13:M:113:VAL:HA	13:M:118:VAL:O	2.13	0.48
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.14	0.48
5:S:18(D):ILE:HG23	5:S:18(E):LYS:HG3	1.96	0.48
10:X:25:SER:HB2	11:Y:131:GLN:NE2	2.28	0.48
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.49	0.48
2:P:160:TRP:CE3	2:P:163:ILE:HD13	2.49	0.48
2:P:20:ARG:NH1	2:P:20:ARG:HG2	2.28	0.48
7:U:168:LYS:O	7:U:172:ILE:HG13	2.14	0.48
1:A:197:LEU:CD2	1:A:210:ILE:HD12	2.44	0.47
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.96	0.47
14:N:20:THR:HG23	14:N:31:THR:OG1	2.13	0.47
2:P:141:TYR:CE2	2:P:145:GLY:HA2	2.49	0.47
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.49	0.47
10:X:193:GLN:HG2	10:X:193:GLN:OXT	2.13	0.47
8:H:210:THR:HG21	12:Z:14(C):GLN:HG2	1.95	0.47
12:Z:48:PHE:CZ	12:Z:50:ALA:HB3	2.49	0.47
12:Z:8:PHE:HB2	13:1:8:THR:HG23	1.97	0.47
1:A:197:LEU:HD23	1:A:210:ILE:HD12	1.95	0.47
7:G:87:ASN:ND2	7:G:87:ASN:C	2.67	0.47
12:L:43:MET:CB	12:L:101:ILE:HG22	2.32	0.47
5:S:45:HIS:HB2	5:S:189:LEU:HD12	1.96	0.47
6:T:45:GLY:HA3	6:T:215:CYS:O	2.14	0.47
7:U:87:ASN:ND2	7:U:87:ASN:C	2.67	0.47
14:2:21:THR:HG22	14:2:26:ILE:HA	1.96	0.47
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.78	0.47
10:J:168:MET:HE2	10:X:168:MET:HE2	1.96	0.47
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.35	0.47
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.12	0.47
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.95	0.47
9:W:130:ALA:HB2	9:W:166:ASP:CB	2.44	0.47
13:1:104:VAL:CG2	13:1:178:ILE:HG22	2.44	0.47
3:C:55:THR:C	3:C:56:LEU:HD22	2.35	0.47
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.28	0.47
10:J:25:SER:HB2	11:K:131:GLN:NE2	2.29	0.47
11:K:21:THR:HG22	11:K:26:VAL:HA	1.94	0.47
14:N:157:HIS:HD2	14:2:140:LYS:HZ1	1.62	0.47
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.14	0.47
13:1:184:LEU:C	13:1:184:LEU:HD23	2.35	0.47
1:A:47:VAL:CG2	1:A:212:LEU:HD21	2.45	0.47
2:B:224:PHE:HD2	2:B:224:PHE:H	1.61	0.47
7:G:188:LYS:HA	7:G:188:LYS:HD3	1.74	0.47
7:U:158:VAL:HG22	7:U:159:GLY:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:186:TRP:O	7:U:190:VAL:HG23	2.14	0.47
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.96	0.47
3:C:71:ASP:HA	10:J:68:ILE:HD11	1.93	0.47
1:O:85:TYR:O	1:O:89:VAL:HG23	2.14	0.47
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.50	0.47
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.15	0.47
6:T:63:LYS:O	6:T:65:VAL:HG23	2.14	0.47
8:V:3:ILE:HG22	8:V:16:ALA:HB2	1.95	0.47
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.97	0.47
1:A:47:VAL:HG23	1:A:212:LEU:HD21	1.95	0.47
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.95	0.47
7:G:158:VAL:HG22	7:G:159:GLY:N	2.30	0.47
6:T:49:ALA:HA	6:T:211:GLU:O	2.14	0.47
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.97	0.47
2:B:112:LEU:C	2:B:112:LEU:HD23	2.35	0.47
3:C:106:PRO:HG2	3:C:143:PRO:HG2	1.96	0.47
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.14	0.47
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.97	0.47
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.14	0.47
13:1:113:VAL:HA	13:1:118:VAL:O	2.15	0.47
1:A:49:ALA:HB2	1:A:212:LEU:HG	1.96	0.47
5:E:18(D):ILE:HG13	5:E:18(D):ILE:O	2.14	0.47
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.97	0.47
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.95	0.47
2:P:234:VAL:HA	2:P:239:THR:HA	1.95	0.47
4:R:170:GLU:OE1	4:R:170:GLU:N	2.48	0.47
7:U:169:GLN:NE2	7:U:170:GLN:N	2.63	0.47
1:O:58:LEU:HD12	7:U:173:THR:HG23	1.97	0.47
10:X:166:MET:HA	10:X:167:PRO:HD3	1.73	0.47
10:X:52:THR:HG22	10:X:53:VAL:H	1.78	0.47
5:E:2(C):VAL:HG13	5:E:2(D):ASP:N	2.29	0.47
6:F:35:THR:CG2	6:F:36:THR:N	2.78	0.47
7:G:151:THR:HG22	7:G:157:TYR:CB	2.45	0.47
9:I:101:VAL:O	9:I:110:ILE:HA	2.14	0.47
2:B:101:LYS:NZ	10:J:85:GLN:NE2	2.63	0.47
1:O:197:LEU:CD2	1:O:210:ILE:HD12	2.45	0.47
3:Q:163:GLN:HE21	3:Q:164:THR:H	0.82	0.47
13:1:40:ASN:ND2	13:1:40:ASN:N	2.61	0.47
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.14	0.47
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.50	0.47
5:E:179:THR:HG22	5:E:179:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:142:ASP:O	6:F:144:ASN:N	2.49	0.47
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.97	0.47
8:H:84:LYS:HG3	8:H:85:GLN:N	2.29	0.47
13:M:80:PHE:CE2	13:M:111:ARG:HB3	2.50	0.47
1:O:197:LEU:HD23	1:O:210:ILE:HD12	1.96	0.47
7:U:67:ILE:CD1	7:U:211:GLU:HG2	2.44	0.47
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.97	0.47
12:Z:114:ASP:CB	12:Z:118:SER:H	2.28	0.47
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.25	0.47
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.96	0.46
1:A:62:GLU:C	1:A:64:LEU:H	2.18	0.46
3:C:52:ARG:NH2	3:C:211:GLU:HB3	2.29	0.46
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.97	0.46
8:H:112:SER:OG	8:H:120:ASP:HB2	2.15	0.46
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.50	0.46
5:E:45:HIS:HB2	5:E:189:LEU:HD12	1.98	0.46
6:F:63:LYS:O	6:F:65:VAL:HG23	2.15	0.46
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.98	0.46
13:M:-6:GLN:O	13:M:-6:GLN:HG3	2.16	0.46
1:O:62:GLU:C	1:O:64:LEU:H	2.17	0.46
2:P:27:ALA:O	2:P:30:SER:HB3	2.15	0.46
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.30	0.46
3:C:33:ARG:HB3	3:C:33:ARG:HH11	1.80	0.46
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.97	0.46
12:L:-2:ASN:HA	12:L:21:ILE:O	2.15	0.46
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.50	0.46
3:Q:125:GLN:NE2	16:Q:872:HOH:O	2.48	0.46
3:Q:182:PRO:O	3:Q:184:ALA:N	2.49	0.46
5:S:41:ARG:NH1	5:S:42:SER:O	2.49	0.46
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.45	0.46
10:X:35:ARG:HH11	10:X:57:GLU:HG2	1.80	0.46
12:Z:109:ALA:HA	16:Z:375:HOH:O	2.15	0.46
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.50	0.46
3:C:160:TRP:CZ2	4:D:59:LEU:HD23	2.51	0.46
8:H:18:THR:HB	8:H:30:ASN:HD22	1.81	0.46
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.98	0.46
2:P:122:GLY:C	2:P:124:THR:H	2.19	0.46
6:T:212:ILE:HG22	6:T:213:SER:N	2.31	0.46
12:Z:1(I):ASN:ND2	16:Z:1057:HOH:O	2.41	0.46
13:1:80:PHE:CE2	13:1:111:ARG:HB3	2.51	0.46
5:S:104:ASN:HB2	13:1:81:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197:LEU:O	3:C:201:VAL:HG23	2.15	0.46
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.97	0.46
3:Q:57:LYS:HD2	3:Q:57:LYS:C	2.36	0.46
5:S:179:THR:O	5:S:179:THR:HG22	2.15	0.46
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.62	0.46
2:B:27:ALA:O	2:B:30:SER:HB3	2.15	0.46
7:G:186:TRP:O	7:G:190:VAL:HG23	2.16	0.46
14:N:13:ILE:HG12	14:N:177:VAL:HG13	1.96	0.46
5:S:190:ILE:CG2	5:S:212:ILE:HD13	2.45	0.46
9:W:48:LEU:HG	9:W:50:THR:HG22	1.97	0.46
10:X:35:ARG:NH1	10:X:57:GLU:CG	2.78	0.46
11:Y:86:LEU:O	11:Y:89:GLN:HB2	2.15	0.46
12:Z:103:GLY:HA2	12:Z:178:VAL:HG11	1.98	0.46
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.13	0.46
3:C:57:LYS:C	3:C:57:LYS:HD2	2.35	0.46
14:N:44:CYS:HB2	14:N:100:ILE:HB	1.96	0.46
3:Q:52:ARG:NH2	3:Q:211:GLU:HB3	2.29	0.46
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.30	0.46
8:V:172:ASN:ND2	8:V:193:THR:HA	2.31	0.46
14:2:107:LYS:HG2	14:2:108:GLY:N	2.31	0.46
7:G:131:PRO:HB3	16:G:243:HOH:O	2.15	0.46
10:J:35:ARG:NH1	10:J:57:GLU:CG	2.79	0.46
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.16	0.46
1:O:159:PRO:HB2	2:P:60:GLU:HB3	1.98	0.46
6:T:43:ASN:HD22	6:T:43:ASN:N	2.14	0.46
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.16	0.46
7:G:136:LEU:O	7:G:150:LYS:HA	2.16	0.46
13:1:83:LEU:O	13:1:87:MET:HG2	2.16	0.46
2:B:141:TYR:CE2	2:B:145:GLY:HA2	2.51	0.46
2:B:225:LYS:HG3	2:B:228:GLU:OE1	2.16	0.46
16:D:1143:HOH:O	5:E:86:ARG:HD3	2.15	0.46
6:F:45:GLY:HA3	6:F:215:CYS:O	2.15	0.46
7:G:168:LYS:O	7:G:172:ILE:HG13	2.16	0.46
10:J:124:TYR:CD2	10:J:138:LEU:HD13	2.51	0.46
10:J:148:THR:CG2	10:J:177:ILE:HD13	2.46	0.46
12:L:148:VAL:O	12:L:152:ILE:HG13	2.15	0.46
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.12	0.46
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.46	0.46
13:M:211:ILE:HD11	16:2:193:HOH:O	2.15	0.46
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.16	0.46
5:S:134:VAL:O	5:S:153:PRO:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:33:LYS:HE2	12:Z:33:LYS:HB3	1.79	0.46
14:2:146:MET:HE3	14:2:150:GLU:HB3	1.98	0.45
2:B:171:ALA:O	2:B:175:LEU:HG	2.16	0.45
5:E:201:LEU:O	5:E:202:ARG:HB2	2.15	0.45
6:F:127:ASN:ND2	6:F:127:ASN:C	2.69	0.45
6:F:13:SER:HB2	7:G:130:ARG:HD3	1.98	0.45
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.51	0.45
2:B:111:ILE:HD11	10:J:70:GLU:HG2	1.98	0.45
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.32	0.45
5:S:38:VAL:HG12	5:S:39:GLY:N	2.30	0.45
9:W:101:VAL:O	9:W:110:ILE:HA	2.16	0.45
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.13	0.45
6:F:212:ILE:HG22	6:F:213:SER:N	2.32	0.45
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.52	0.45
10:J:7:ARG:HG2	10:J:7:ARG:NH1	2.29	0.45
12:L:-8:PHE:HB2	13:M:-8:THR:HG23	1.99	0.45
13:M:14(C):ARG:CG	13:M:14(C):ARG:NH1	2.80	0.45
4:R:243:ALA:O	4:R:244:GLU:CB	2.63	0.45
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.52	0.45
10:X:7:ARG:NH1	10:X:7:ARG:HG2	2.28	0.45
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.47	0.45
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.16	0.45
3:C:224:LEU:N	3:C:224:LEU:HD12	2.31	0.45
7:G:17(C):LYS:HE3	7:G:17(C):LYS:HB2	1.70	0.45
10:J:85:GLN:HB3	16:J:203:HOH:O	2.16	0.45
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.47	0.45
4:R:191:LEU:HD21	4:R:236:GLU:OE2	2.17	0.45
3:C:173:ARG:O	3:C:177:GLU:HG3	2.16	0.45
6:F:43:ASN:HD22	6:F:43:ASN:N	2.14	0.45
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.31	0.45
10:J:35:ARG:HH11	10:J:57:GLU:HG2	1.81	0.45
11:K:76:VAL:N	11:K:106:GLU:OE2	2.42	0.45
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.51	0.45
10:X:7:ARG:NE	16:X:195:HOH:O	2.44	0.45
11:Y:131:GLN:HG3	11:Y:132:THR:N	2.32	0.45
3:C:190:VAL:HG13	3:C:212:ILE:HG21	1.99	0.45
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.81	0.45
6:F:53:LEU:HD11	6:F:205:ASN:OD1	2.16	0.45
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.99	0.45
1:O:21(P):LYS:N	16:O:1029:HOH:O	2.49	0.45
3:Q:35:THR:OG1	3:Q:66:LYS:NZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:159:LEU:HD21	9:W:173:ALA:HB1	1.98	0.45
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.51	0.45
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.52	0.45
2:B:39:GLY:C	2:B:148:LEU:HD21	2.37	0.45
6:F:40:ILE:HD12	6:F:193:ALA:HB2	1.99	0.45
9:I:130:ALA:HB2	9:I:166:ASP:CB	2.47	0.45
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.98	0.45
6:T:192:GLN:O	6:T:196:ILE:HG13	2.16	0.45
7:U:236:ILE:HD12	7:U:236:ILE:C	2.37	0.45
3:C:75:VAL:HG13	3:C:221:ILE:HD13	1.99	0.45
5:E:227:GLU:CD	5:E:227:GLU:H	2.20	0.45
10:J:166:MET:HA	10:J:167:PRO:HD3	1.74	0.45
1:O:4:MET:SD	1:O:5:THR:N	2.76	0.45
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.16	0.45
1:A:121:GLN:O	1:A:124:THR:HB	2.16	0.45
12:L:114:ASP:CB	12:L:118:SER:H	2.29	0.45
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.47	0.45
4:R:86:ARG:HD3	4:R:86:ARG:HA	1.81	0.45
5:S:56:ASP:H	5:S:59:SER:HB3	1.82	0.45
4:D:243:ALA:O	4:D:244:GLU:CB	2.64	0.45
4:D:59:LEU:C	4:D:59:LEU:HD13	2.37	0.45
5:E:41:ARG:NH1	5:E:42:SER:O	2.50	0.45
11:K:131:GLN:HG3	11:K:132:THR:N	2.32	0.45
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.17	0.45
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.46	0.45
5:S:2(C):VAL:CG1	5:S:2(D):ASP:N	2.80	0.45
5:S:52:LYS:HB2	5:S:63:TYR:HB3	1.98	0.45
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.99	0.45
7:U:151:THR:HG22	7:U:157:TYR:CB	2.47	0.45
8:V:143:LYS:HG2	8:V:146:LEU:HD21	1.99	0.45
8:V:143:LYS:HE2	8:V:146:LEU:HD23	1.98	0.45
2:B:122:GLY:C	2:B:124:THR:H	2.19	0.45
2:B:17:PRO:HA	3:C:26:TYR:CZ	2.51	0.45
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.52	0.45
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.47	0.45
7:G:107:MET:HE3	7:G:112:LEU:HD13	1.99	0.45
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.98	0.45
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.47	0.45
1:O:122:GLU:C	1:O:124:THR:H	2.21	0.45
5:S:216:GLY:O	5:S:217:LYS:C	2.55	0.45
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:208:ARG:HG3	16:V:1135:HOH:O	2.17	0.45
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.99	0.44
5:E:4:PHE:CG	5:E:5:ARG:N	2.85	0.44
5:E:56:ASP:H	5:E:59:SER:HB3	1.82	0.44
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.81	0.44
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.47	0.44
13:M:-5:PRO:HD3	13:M:96:TRP:CE2	2.52	0.44
2:P:171:ALA:O	2:P:175:LEU:HG	2.16	0.44
2:P:215:ILE:HG12	2:P:221:GLN:HG2	1.99	0.44
2:P:5:SER:O	2:P:7:ARG:N	2.50	0.44
5:S:39:GLY:O	5:S:162:GLY:HA2	2.16	0.44
8:V:172:ASN:HD22	8:V:193:THR:HA	1.82	0.44
13:1:190:LEU:HD12	13:1:190:LEU:N	2.32	0.44
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.47	0.44
8:H:172:ASN:HD22	8:H:193:THR:HA	1.82	0.44
9:I:90:ARG:HH11	9:I:90:ARG:HA	1.82	0.44
1:O:33:GLN:CA	1:O:33:GLN:HE21	2.29	0.44
6:T:203:GLU:O	6:T:206:LYS:HD2	2.18	0.44
8:V:189:ARG:O	8:V:190:ASN:HB2	2.17	0.44
10:X:124:TYR:CD2	10:X:138:LEU:HD13	2.52	0.44
10:X:52:THR:HG22	10:X:53:VAL:N	2.32	0.44
13:1:9:ASP:OD1	13:1:10:ASN:N	2.50	0.44
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.53	0.44
6:F:192:GLN:O	6:F:196:ILE:HG13	2.17	0.44
12:L:109:ALA:HA	16:L:975:HOH:O	2.17	0.44
14:N:121:LYS:O	14:N:122:LEU:HD23	2.17	0.44
5:S:4:PHE:CG	5:S:5:ARG:N	2.84	0.44
10:X:44:SER:OG	10:X:100:LEU:HB2	2.16	0.44
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.48	0.44
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.48	0.44
3:C:112:LEU:HD13	3:C:112:LEU:O	2.17	0.44
3:C:182:PRO:O	3:C:184:ALA:N	2.50	0.44
6:T:127:ASN:ND2	6:T:127:ASN:C	2.70	0.44
10:X:100:LEU:CD2	10:X:112:GLN:HG3	2.47	0.44
11:Y:35:ILE:HD13	11:Y:53:GLN:HA	1.99	0.44
13:1:201:LYS:HA	16:1:731:HOH:O	2.16	0.44
11:K:200:LYS:HE2	16:K:1088:HOH:O	2.18	0.44
13:M:83:LEU:O	13:M:87:MET:HG2	2.17	0.44
14:N:14:LEU:HD11	14:N:102:ALA:HB3	2.00	0.44
14:N:107:LYS:HG2	14:N:108:GLY:N	2.32	0.44
5:S:38:VAL:HG22	5:S:164:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:18(D):ILE:HG13	5:S:18(D):ILE:O	2.17	0.44
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.99	0.44
2:B:63:THR:HG22	2:B:63:THR:O	2.17	0.44
3:C:134:VAL:HG12	3:C:135:SER:N	2.33	0.44
4:D:117:CYS:HB3	4:D:155:GLY:O	2.18	0.44
5:E:38:VAL:HG22	5:E:164:ALA:HB2	2.00	0.44
10:J:35:ARG:HA	10:J:35:ARG:HD3	1.76	0.44
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.32	0.44
4:R:59:LEU:HD13	4:R:59:LEU:C	2.38	0.44
7:U:139:VAL:HA	7:U:147:SER:O	2.18	0.44
8:V:112:SER:OG	8:V:120:ASP:HB2	2.17	0.44
3:C:41:LYS:HD3	3:C:160:TRP:O	2.18	0.44
2:B:17:PRO:HA	3:C:26:TYR:CE1	2.52	0.44
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.60	0.44
11:K:86:LEU:O	11:K:89:GLN:HB2	2.17	0.44
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.99	0.44
2:P:39:GLY:C	2:P:148:LEU:HD21	2.38	0.44
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.98	0.44
7:U:224:LEU:HB3	7:U:228:ASN:HB2	1.99	0.44
9:W:33:LYS:O	9:W:44:GLY:HA2	2.17	0.44
10:X:34:THR:CG2	10:X:176:LYS:NZ	2.80	0.44
2:B:184:MET:HE2	2:B:189:ALA:N	2.32	0.44
6:F:51:GLU:OE1	6:F:53:LEU:HD21	2.18	0.44
9:I:93:GLY:N	9:I:94:PRO:CD	2.81	0.44
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.47	0.44
5:S:172:ALA:HB2	5:S:196:ALA:O	2.17	0.44
6:T:194:ALA:O	6:T:198:TYR:HD1	2.01	0.44
10:X:85:GLN:HB3	16:X:463:HOH:O	2.18	0.44
5:E:185:ASN:C	5:E:185:ASN:HD22	2.20	0.44
8:H:172:ASN:ND2	8:H:193:THR:HA	2.33	0.44
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.99	0.44
16:C:1154:HOH:O	11:K:82:ILE:HG13	2.17	0.44
3:Q:31:VAL:HG11	3:Q:135:SER:HB2	1.99	0.44
3:Q:75:VAL:HG13	3:Q:221:ILE:HD13	1.99	0.44
4:R:194:LEU:HA	4:R:194:LEU:HD12	1.86	0.44
5:S:160:LEU:HD13	5:S:163:THR:HB	1.99	0.44
5:S:227:GLU:CD	5:S:227:GLU:H	2.20	0.44
6:T:202:HIS:CG	6:T:202:HIS:O	2.71	0.44
4:R:97:VAL:HG11	11:Y:65:LEU:HD22	1.99	0.44
1:A:13:THR:O	2:B:130:ARG:HD3	2.18	0.43
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:TYR:OH	2:B:21(A):LYS:HB2	2.18	0.43
5:E:175:TYR:HB2	5:E:199:GLN:HG2	2.00	0.43
5:E:2(C):VAL:CG1	5:E:2(D):ASP:N	2.81	0.43
6:F:202:HIS:O	6:F:202:HIS:CG	2.70	0.43
8:H:148:LYS:O	8:H:152:ILE:HG13	2.18	0.43
10:J:120:VAL:HG13	10:J:122:LEU:HG	1.99	0.43
14:N:26:ILE:HB	13:1:165:ARG:HA	2.00	0.43
2:P:52:ARG:HH22	2:P:63(A):SER:CB	2.31	0.43
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.88	0.43
12:Z:99:THR:HG22	16:Z:231:HOH:O	2.17	0.43
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.99	0.43
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.53	0.43
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.99	0.43
3:C:35:THR:OG1	3:C:66:LYS:NZ	2.50	0.43
5:E:39:GLY:O	5:E:162:GLY:HA2	2.18	0.43
7:G:14(A):GLU:OE2	8:H:72:ARG:HD3	2.18	0.43
9:I:159:LEU:HD21	9:I:173:ALA:HB1	2.00	0.43
10:J:100:LEU:CD2	10:J:112:GLN:HG3	2.48	0.43
2:P:63:THR:HG22	2:P:63:THR:O	2.18	0.43
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.52	0.43
12:Z:99:THR:CG2	16:Z:231:HOH:O	2.66	0.43
13:1:62:LEU:HD23	13:1:62:LEU:HA	1.83	0.43
1:A:170:VAL:HB	16:A:402:HOH:O	2.18	0.43
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.17	0.43
14:N:94:ASN:ND2	16:N:946:HOH:O	2.42	0.43
2:P:146:TYR:OH	2:P:21(A):LYS:HB2	2.17	0.43
7:U:107:MET:CE	7:U:112:LEU:HD13	2.49	0.43
1:O:97:HIS:HD2	8:V:61:SER:OG	2.01	0.43
10:X:148:THR:CG2	10:X:177:ILE:HD13	2.46	0.43
14:2:44:CYS:HB2	14:2:100:ILE:HB	1.99	0.43
1:A:144:PHE:CD2	9:I:72:ARG:HD2	2.53	0.43
14:N:21:THR:HG22	14:N:26:ILE:HA	2.00	0.43
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.84	0.43
5:S:147:HIS:HA	16:S:575:HOH:O	2.18	0.43
7:U:136:LEU:O	7:U:150:LYS:HA	2.16	0.43
11:Y:25:TRP:CZ3	12:Z:132:SER:HA	2.54	0.43
12:Z:39:ASP:OD2	12:Z:67:HIS:HE1	2.01	0.43
3:C:20:HIS:HB3	3:C:25:GLU:OE1	2.19	0.43
3:C:31:VAL:HG11	3:C:135:SER:HB2	2.01	0.43
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.48	0.43
6:F:203:GLU:O	6:F:206:LYS:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.99	0.43
11:K:35:ILE:HD13	11:K:53:GLN:HA	1.98	0.43
12:L:98:HIS:HD2	16:L:199:HOH:O	2.00	0.43
2:P:222:LYS:NZ	2:P:228:GLU:OE2	2.48	0.43
3:Q:190:VAL:HG13	3:Q:212:ILE:HG21	2.00	0.43
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.83	0.43
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.53	0.43
7:U:227:GLU:HG2	16:U:1255:HOH:O	2.19	0.43
9:W:2:ILE:HG21	9:W:130:ALA:HB3	2.01	0.43
11:Y:172:SER:HA	11:Y:192:VAL:HG23	2.01	0.43
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.53	0.43
5:E:160:LEU:HD13	5:E:163:THR:HB	1.99	0.43
5:E:38:VAL:HG12	5:E:39:GLY:N	2.32	0.43
10:J:20:VAL:HG11	11:K:120:LEU:HD11	2.01	0.43
11:K:172:SER:HA	11:K:192:VAL:HG23	2.00	0.43
5:S:77:SER:OG	5:S:137:LEU:HB2	2.18	0.43
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.19	0.43
10:X:111:TYR:CE1	10:X:121:GLU:HG3	2.54	0.43
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.26	0.43
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.49	0.43
4:D:86:ARG:HD3	4:D:86:ARG:HA	1.84	0.43
8:H:143:LYS:HE2	8:H:146:LEU:HD23	2.00	0.43
11:K:71:LYS:HG3	16:K:866:HOH:O	2.18	0.43
5:E:103:PHE:HE2	13:M:62:LEU:HD21	1.83	0.43
5:E:103:PHE:O	13:M:78:TYR:HA	2.19	0.43
6:T:38:ILE:HG22	6:T:164:ALA:HB2	2.00	0.43
7:U:215:ALA:HB2	7:U:221:PHE:HD2	1.84	0.43
9:W:29:ASN:H	9:W:29:ASN:ND2	2.17	0.43
12:Z:148:VAL:O	12:Z:152:ILE:HG13	2.19	0.43
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.99	0.43
11:K:70:GLU:O	11:K:71:LYS:C	2.57	0.43
13:M:190:LEU:HD12	13:M:190:LEU:N	2.34	0.43
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.54	0.43
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.49	0.43
2:B:21:LEU:HD13	2:B:124:THR:HG23	2.00	0.43
2:B:186:VAL:O	2:B:190:ILE:HG13	2.19	0.43
3:C:29:GLU:OE2	3:C:32:LYS:HE2	2.19	0.43
5:E:18(C):PHE:CD1	5:E:18(C):PHE:C	2.92	0.43
2:P:225:LYS:HG3	2:P:228:GLU:OE1	2.18	0.43
3:Q:206:GLY:CA	3:Q:209:ASN:HD22	2.30	0.43
3:Q:33:ARG:HH11	3:Q:33:ARG:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:175:TYR:HB2	5:S:199:GLN:HG2	2.00	0.43
8:V:144:GLN:HB2	8:V:144:GLN:HE21	1.60	0.43
5:S:103:PHE:O	13:1:78:TYR:HA	2.18	0.43
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.54	0.43
12:L:138:LEU:O	12:L:142:VAL:HB	2.18	0.43
12:L:103:GLY:HA2	12:L:178:VAL:HG11	2.00	0.43
1:O:112:LEU:O	1:O:116:VAL:HG23	2.19	0.43
5:S:18(C):PHE:C	5:S:18(E):LYS:H	2.21	0.43
12:L:167:ILE:O	8:V:167:LEU:HD22	2.19	0.43
2:B:52:ARG:HH22	2:B:63(A):SER:CB	2.31	0.42
2:B:121:GLN:HG3	3:C:83:ALA:HB1	2.00	0.42
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.82	0.42
9:I:33:LYS:O	9:I:44:GLY:HA2	2.19	0.42
12:L:1:GLY:N	16:L:755:HOH:O	2.51	0.42
1:O:110:LYS:HG2	16:O:376:HOH:O	2.19	0.42
1:O:55:SER:O	1:O:56:SER:HB2	2.19	0.42
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.82	0.42
8:V:18:THR:CB	8:V:30:ASN:HD22	2.32	0.42
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.19	0.42
3:C:206:GLY:CA	3:C:209:ASN:HD22	2.30	0.42
5:E:172:ALA:HB2	5:E:196:ALA:O	2.19	0.42
5:E:216:GLY:O	5:E:217:LYS:C	2.57	0.42
7:G:139:VAL:HA	7:G:147:SER:O	2.19	0.42
8:H:2:THR:OG1	8:H:130:GLY:HA3	2.19	0.42
13:M:165:ARG:HA	14:2:26:ILE:HB	2.00	0.42
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.34	0.42
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.19	0.42
3:Q:57:LYS:O	3:Q:57:LYS:HE3	2.19	0.42
5:S:18(C):PHE:CD1	5:S:18(C):PHE:C	2.93	0.42
5:S:214:ILE:O	5:S:221:PHE:HA	2.19	0.42
5:S:216:GLY:O	5:S:219:THR:N	2.46	0.42
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.49	0.42
6:F:70:VAL:HG11	6:F:112:PHE:CE1	2.54	0.42
6:F:194:ALA:O	6:F:198:TYR:HD1	2.02	0.42
7:G:67:ILE:CD1	7:G:211:GLU:HG2	2.49	0.42
12:L:17:ASP:HA	12:L:172:GLY:O	2.20	0.42
14:N:116:GLY:HA3	16:N:194:HOH:O	2.18	0.42
9:W:80:THR:HG23	9:W:113:PHE:CE1	2.54	0.42
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.53	0.42
14:N:161:GLN:NE2	14:N:165:TRP:HE1	2.17	0.42
1:O:207:ASN:HA	1:O:233:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:44:ASP:OD2	2:P:186:VAL:HG23	2.20	0.42
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.55	0.42
6:T:13:SER:HB2	7:U:130:ARG:HD3	2.01	0.42
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.55	0.42
2:B:5:SER:O	2:B:7:ARG:N	2.52	0.42
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.20	0.42
5:E:214:ILE:O	5:E:221:PHE:HA	2.20	0.42
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.01	0.42
7:G:105:TYR:OH	8:H:66:HIS:HE1	2.02	0.42
11:K:111:TYR:CE1	11:K:121:LYS:HB2	2.54	0.42
13:M:40:ASN:ND2	13:M:40:ASN:N	2.61	0.42
14:N:114:PRO:HD2	14:N:118:SER:O	2.20	0.42
2:P:52:ARG:NH2	2:P:63(A):SER:HB3	2.32	0.42
3:Q:40:VAL:HG23	3:Q:189:CYS:SG	2.59	0.42
3:C:163:GLN:NE2	3:C:173:ARG:HH21	2.18	0.42
3:C:224:LEU:N	3:C:224:LEU:CD1	2.83	0.42
5:E:161:TYR:OH	6:F:61:PRO:HD2	2.20	0.42
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	2.01	0.42
9:I:58:MET:O	9:I:61:TYR:HB3	2.20	0.42
12:Z:114:ASP:HB3	12:Z:118:SER:H	1.83	0.42
12:Z:138:LEU:O	12:Z:142:VAL:HB	2.20	0.42
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.19	0.42
13:1:191:GLN:HB3	13:1:191:GLN:HE21	1.59	0.42
5:E:18(C):PHE:C	5:E:18(E):LYS:H	2.22	0.42
6:F:103:TYR:O	6:F:104:LYS:HB3	2.20	0.42
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.20	0.42
12:L:114:ASP:HB3	12:L:118:SER:H	1.85	0.42
14:N:107:LYS:CG	14:N:108:GLY:H	2.33	0.42
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.55	0.42
2:P:117:SER:HB3	2:P:155:GLY:O	2.19	0.42
2:P:163:ILE:HG13	2:P:164:SER:N	2.33	0.42
3:Q:41:LYS:HD3	3:Q:160:TRP:O	2.20	0.42
3:Q:29:GLU:OE2	3:Q:32:LYS:HE2	2.20	0.42
4:R:117:CYS:HB3	4:R:155:GLY:O	2.19	0.42
5:S:185:ASN:HD22	5:S:185:ASN:C	2.21	0.42
6:T:53:LEU:HD13	6:T:20(C):LYS:HD2	2.02	0.42
7:U:34(A):ASN:HA	7:U:167:PRO:HG2	2.01	0.42
8:V:3:ILE:HD11	8:V:127:LEU:HB2	2.01	0.42
11:Y:76:VAL:N	11:Y:106:GLU:OE2	2.46	0.42
12:Z:43:MET:CB	12:Z:101:ILE:HG22	2.33	0.42
1:A:207:ASN:HA	1:A:233:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ILE:HG13	2:B:164:SER:N	2.34	0.42
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.54	0.42
5:E:52:LYS:CB	5:E:63:TYR:HB3	2.50	0.42
6:F:50:VAL:HG22	6:F:51:GLU:N	2.35	0.42
7:G:169:GLN:NE2	7:G:170:GLN:N	2.67	0.42
12:L:114:ASP:CB	12:L:118:SER:HB3	2.43	0.42
1:O:45:GLY:HA2	1:O:147:PHE:CE2	2.54	0.42
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.55	0.42
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.50	0.42
6:F:93:ARG:HD2	16:F:842:HOH:O	2.19	0.42
7:G:48:VAL:HG23	7:G:48:VAL:O	2.20	0.42
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.83	0.42
1:O:233:LEU:O	1:O:236:LEU:HB2	2.20	0.42
4:R:142:ASP:OD2	4:R:142:ASP:C	2.58	0.42
7:U:218:ASP:O	7:U:220:LYS:HB2	2.20	0.42
8:V:2:THR:OG1	8:V:130:GLY:HA3	2.20	0.42
13:1:130:GLY:O	13:1:134:ALA:HB3	2.20	0.42
2:B:53:LYS:HG2	2:B:54:VAL:HG23	2.01	0.42
3:C:36:CYS:N	3:C:51:GLU:HG2	2.35	0.42
4:D:195:LYS:HE2	4:D:199:GLN:OE1	2.20	0.42
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.55	0.42
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.50	0.42
7:G:136:LEU:O	7:G:150:LYS:HG3	2.20	0.42
7:G:215:ALA:HB2	7:G:221:PHE:HD2	1.85	0.42
8:H:3:ILE:HG22	8:H:16:ALA:HB2	2.02	0.42
9:I:66:TYR:CE1	9:I:70:GLU:HG3	2.55	0.42
9:I:87:LEU:HD11	9:I:99:PRO:HG2	2.02	0.42
2:P:202:THR:HG21	2:P:204:SER:HB2	2.01	0.42
3:Q:152:GLU:HB2	3:Q:153:PRO:CD	2.49	0.42
8:V:116:HIS:HB2	16:V:1297:HOH:O	2.18	0.42
1:A:179:ARG:CB	1:A:179:ARG:HH11	2.26	0.41
1:A:55:SER:O	1:A:56:SER:HB2	2.19	0.41
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.49	0.41
4:D:39:GLY:O	4:D:162:ALA:HA	2.20	0.41
8:H:189:ARG:O	8:H:190:ASN:HB2	2.19	0.41
8:H:208:ARG:CZ	9:I:149:GLU:HB2	2.50	0.41
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.55	0.41
2:P:121:GLN:C	2:P:121:GLN:NE2	2.74	0.41
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.50	0.41
12:L:153:LYS:HG2	8:V:201:GLN:HG3	2.01	0.41
9:W:126:VAL:CG1	9:W:134:LEU:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:120:VAL:HG13	10:X:122:LEU:HG	2.02	0.41
10:X:-1:MET:CG	10:X:1:ASP:H	2.30	0.41
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	2.02	0.41
13:1:14(C):ARG:CG	13:1:14(C):ARG:NH1	2.79	0.41
13:1:1:THR:OG1	13:1:2:SER:N	2.53	0.41
13:1:-6:GLN:HG3	13:1:-6:GLN:O	2.19	0.41
2:B:209:ARG:HH11	2:B:209:ARG:HG2	1.86	0.41
3:C:97:GLN:NE2	3:C:97:GLN:HA	2.35	0.41
5:E:134:VAL:O	5:E:153:PRO:HG3	2.19	0.41
5:E:207:LEU:N	5:E:207:LEU:CD2	2.80	0.41
8:H:9:ASN:OD1	8:H:10:ASN:N	2.53	0.41
10:J:111:TYR:CE1	10:J:121:GLU:HG3	2.54	0.41
10:J:44:SER:OG	10:J:100:LEU:HB2	2.20	0.41
12:L:15:ALA:HB1	12:L:173:LEU:HD11	2.02	0.41
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.34	0.41
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.50	0.41
5:S:64:GLN:NE2	5:S:82:ALA:HB2	2.35	0.41
9:W:93:GLY:N	9:W:94:PRO:CD	2.81	0.41
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.20	0.41
5:S:103:PHE:HE2	13:1:62:LEU:HD21	1.84	0.41
1:A:122:GLU:C	1:A:124:THR:H	2.21	0.41
6:F:21(B):THR:O	6:F:21(C):ASN:HB2	2.19	0.41
11:K:46:ALA:HB3	11:K:98:GLY:O	2.20	0.41
1:O:13:THR:O	2:P:130:ARG:HD3	2.21	0.41
3:Q:97:GLN:NE2	3:Q:97:GLN:HA	2.35	0.41
4:R:159:ARG:HB3	5:S:60:SER:HB3	2.01	0.41
6:T:184:LEU:HD11	6:T:188:GLU:HB3	2.02	0.41
6:T:54:ILE:HG13	6:T:208:PHE:HA	2.01	0.41
10:J:144:PRO:CG	11:Y:207:ASN:HD21	2.33	0.41
14:2:51:ASP:O	14:2:55:ILE:HG13	2.21	0.41
14:2:77:GLU:HB2	16:2:217:HOH:O	2.20	0.41
2:B:81:LEU:HD23	2:B:133:GLY:HA3	2.03	0.41
4:D:137:LEU:HA	4:D:149:PHE:O	2.21	0.41
7:G:236:ILE:HD12	7:G:236:ILE:C	2.40	0.41
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.88	0.41
10:J:14:LEU:HD12	10:J:42:LEU:HD23	2.02	0.41
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.50	0.41
13:M:130:GLY:O	13:M:134:ALA:HB3	2.20	0.41
13:M:62:LEU:HD23	13:M:62:LEU:HA	1.83	0.41
13:M:9:ASP:OD1	13:M:10:ASN:N	2.53	0.41
1:O:186:LEU:HD21	1:O:214:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:215:VAL:O	3:Q:215:VAL:HG13	2.20	0.41
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.83	0.41
4:R:150:HIS:O	4:R:157:PHE:HA	2.20	0.41
6:T:12:ASN:HB3	6:T:127:ASN:HA	2.02	0.41
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.51	0.41
11:Y:168:TYR:CE2	15:Y:999:BFO:H42	2.55	0.41
2:B:202:THR:HG21	2:B:204:SER:HB2	2.01	0.41
3:C:158:SER:HB2	4:D:59:LEU:HD21	2.03	0.41
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.21	0.41
7:G:233:LEU:O	7:G:236:ILE:HG13	2.21	0.41
8:H:18:THR:CB	8:H:30:ASN:HD22	2.33	0.41
12:L:-5:TYR:CE2	12:L:96:TYR:HB2	2.55	0.41
13:M:187:LYS:HB3	13:M:190:LEU:HD11	2.02	0.41
6:T:157:TYR:CD1	6:T:157:TYR:C	2.94	0.41
6:T:21(B):THR:O	6:T:21(C):ASN:HB2	2.21	0.41
7:U:48:VAL:O	7:U:48:VAL:HG23	2.21	0.41
11:K:207:ASN:HD21	10:X:144:PRO:CG	2.33	0.41
10:X:185:ARG:HH11	10:X:185:ARG:HG2	1.86	0.41
11:Y:70:GLU:O	11:Y:71:LYS:C	2.59	0.41
12:Z:-5:TYR:CD2	12:Z:96:TYR:HB2	2.56	0.41
12:Z:-5:TYR:CE2	12:Z:96:TYR:HB2	2.55	0.41
1:A:4:MET:O	1:A:5:THR:O	2.38	0.41
3:C:38:VAL:HG22	3:C:39:GLY:N	2.35	0.41
5:E:77:SER:OG	5:E:137:LEU:HB2	2.20	0.41
5:E:216:GLY:O	5:E:219:THR:N	2.46	0.41
6:F:54:ILE:HG13	6:F:208:PHE:HA	2.01	0.41
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.01	0.41
11:K:25:TRP:HH2	12:L:135:MET:HB2	1.85	0.41
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.74	0.41
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.50	0.41
11:Y:111:TYR:CE1	11:Y:121:LYS:HB2	2.55	0.41
11:Y:8:PHE:CE2	11:Y:13:ILE:HG12	2.55	0.41
1:A:45:GLY:HA2	1:A:147:PHE:CE2	2.56	0.41
2:B:44:ASP:OD2	2:B:186:VAL:HG23	2.21	0.41
2:B:52:ARG:NH2	2:B:63(A):SER:HB3	2.33	0.41
3:C:152:GLU:HB2	3:C:153:PRO:CD	2.50	0.41
5:E:194:VAL:CG1	5:E:207:LEU:HD11	2.51	0.41
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.55	0.41
6:F:12:ASN:HB3	6:F:127:ASN:HA	2.02	0.41
6:F:184:LEU:HD11	6:F:188:GLU:HB3	2.03	0.41
6:F:35:THR:CG2	6:F:51:GLU:O	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:8:TYR:C	7:G:10:ARG:N	2.74	0.41
8:H:144:GLN:HE21	8:H:144:GLN:HB2	1.59	0.41
12:L:39:ASP:OD2	12:L:67:HIS:HE1	2.04	0.41
12:L:88:TYR:CE2	12:L:91:ARG:HD3	2.56	0.41
1:O:4:MET:O	1:O:5:THR:O	2.38	0.41
2:P:235:LYS:N	2:P:235:LYS:HD3	2.35	0.41
5:S:18(C):PHE:CD1	5:S:18(D):ILE:N	2.89	0.41
6:T:103:TYR:O	6:T:104:LYS:HB3	2.20	0.41
12:Z:14(D):TYR:CG	12:Z:14(J):GLY:HA2	2.56	0.41
8:H:167:LEU:HD22	12:Z:167:ILE:O	2.20	0.41
3:C:225:SER:OG	3:C:228:GLU:HG3	2.21	0.41
6:F:20(B):GLU:CD	6:F:20(C):LYS:HE3	2.41	0.41
8:H:144:GLN:O	8:H:145:ASP:HB2	2.21	0.41
11:K:73:ARG:NH2	11:K:104:TYR:O	2.54	0.41
1:O:141:HIS:HA	1:O:146:GLY:O	2.21	0.41
2:P:38:ILE:HD12	2:P:197:LEU:HG	2.03	0.41
3:Q:111:TYR:C	3:Q:111:TYR:CD2	2.94	0.41
5:S:194:VAL:CG1	5:S:207:LEU:HD11	2.51	0.41
7:U:179:HIS:ND1	7:U:179:HIS:C	2.74	0.41
10:X:9:GLN:HG3	10:X:10:ASP:OD2	2.21	0.41
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.84	0.41
12:Z:8:GLY:HA3	12:Z:11:PHE:CZ	2.56	0.41
13:1:190:LEU:CD1	13:1:190:LEU:N	2.83	0.41
13:1:19:LEU:HD12	13:1:28:PHE:O	2.21	0.41
1:A:233:LEU:O	1:A:236:LEU:HB2	2.21	0.41
3:C:111:TYR:CD2	3:C:111:TYR:C	2.94	0.41
6:F:43:ASN:N	6:F:43:ASN:ND2	2.69	0.41
11:K:200:LYS:HG3	11:K:206:PHE:HB2	2.02	0.41
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.21	0.41
14:N:14:LEU:N	14:N:14:LEU:HD12	2.36	0.41
2:P:186:VAL:O	2:P:190:ILE:HG13	2.20	0.41
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.49	0.41
7:U:14(A):GLU:OE2	8:V:72:ARG:HD3	2.20	0.41
9:W:90:ARG:HH11	9:W:90:ARG:HA	1.84	0.41
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	2.02	0.41
12:Z:93:PHE:N	12:Z:94:PRO:CD	2.83	0.41
14:2:107:LYS:CG	14:2:108:GLY:H	2.32	0.41
1:A:232:ARG:NH1	1:A:232:ARG:HG3	2.35	0.41
4:D:150:HIS:O	4:D:157:PHE:HA	2.20	0.41
5:E:18(C):PHE:CD1	5:E:18(D):ILE:N	2.89	0.41
5:E:52:LYS:HB2	5:E:63:TYR:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:107:MET:HA	7:G:108:PRO:HD3	1.94	0.41
12:L:14(D):TYR:CG	12:L:14(J):GLY:HA2	2.56	0.41
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.35	0.41
5:S:18(C):PHE:C	5:S:18(E):LYS:N	2.74	0.41
7:U:83:PRO:HG2	16:U:557:HOH:O	2.20	0.41
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.02	0.41
9:W:20:LEU:C	9:W:20:LEU:HD13	2.42	0.41
10:J:168:MET:CE	10:X:168:MET:CE	2.99	0.41
12:Z:152:ILE:O	12:Z:156:ARG:HG3	2.21	0.41
5:E:40:LEU:HD23	5:E:40:LEU:N	2.36	0.41
8:H:196:VAL:HG23	16:H:520:HOH:O	2.20	0.41
11:K:32:LYS:N	11:K:32:LYS:HD2	2.36	0.41
5:S:40:LEU:N	5:S:40:LEU:HD23	2.36	0.41
7:U:152:ASP:HB2	7:U:153:PRO:HD2	2.02	0.41
8:V:144:GLN:O	8:V:145:ASP:HB2	2.21	0.41
3:C:57:LYS:C	3:C:57:LYS:CD	2.90	0.40
3:C:57:LYS:HE3	3:C:57:LYS:O	2.20	0.40
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.50	0.40
5:E:90:ASN:O	5:E:94:GLN:HG3	2.20	0.40
7:G:107:MET:CE	7:G:112:LEU:HD13	2.50	0.40
9:I:80:THR:HG23	9:I:113:PHE:CE1	2.56	0.40
10:J:21:THR:HG22	10:J:22:ARG:N	2.35	0.40
13:M:190:LEU:CD1	13:M:190:LEU:N	2.84	0.40
1:O:52:LYS:HG3	1:O:211:GLU:HB2	2.02	0.40
3:Q:20:HIS:HB3	3:Q:25:GLU:OE1	2.21	0.40
4:R:177:LEU:HD13	5:S:58:LEU:HD11	2.04	0.40
9:W:87:LEU:HD11	9:W:99:PRO:HG2	2.02	0.40
12:Z:114:ASP:HB2	12:Z:118:SER:CB	2.47	0.40
12:Z:-8:PHE:HB3	13:1:-8:THR:HG23	2.03	0.40
5:E:67:ILE:HG21	5:E:213:ALA:HB2	2.03	0.40
7:G:55:PRO:HG2	7:G:56:ASP:H	1.86	0.40
12:L:104:LEU:HA	12:L:107:LYS:O	2.22	0.40
13:M:1:THR:OG1	13:M:2:SER:N	2.53	0.40
1:O:14:THR:O	1:O:21:LEU:HD23	2.21	0.40
2:P:184:MET:HE2	2:P:189:ALA:N	2.37	0.40
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.56	0.40
2:P:53:LYS:HG2	2:P:54:VAL:HG23	2.03	0.40
2:P:7:ARG:HD2	2:P:8:TYR:CZ	2.56	0.40
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.51	0.40
8:V:22:GLN:CG	8:V:27:ALA:HB2	2.51	0.40
8:V:9:ASN:OD1	8:V:10:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:126:VAL:HG11	9:W:134:LEU:HB3	2.03	0.40
11:Y:25:TRP:HH2	12:Z:135:MET:HB2	1.86	0.40
3:C:215:VAL:O	3:C:215:VAL:HG13	2.21	0.40
5:E:230:ALA:C	5:E:232:TYR:H	2.24	0.40
11:K:8:PHE:CE2	11:K:13:ILE:HG12	2.56	0.40
12:L:113:PHE:N	12:L:113:PHE:CD1	2.88	0.40
12:L:98:HIS:HE1	12:L:112:SER:HB2	1.87	0.40
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.55	0.40
9:W:72:ARG:NH2	16:W:1026:HOH:O	2.47	0.40
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.57	0.40
12:Z:11:PHE:CE1	12:Z:148:VAL:HA	2.56	0.40
1:A:186:LEU:O	1:A:190:ILE:HG13	2.22	0.40
4:D:115:SER:O	4:D:118:ASP:HB2	2.22	0.40
8:H:22:GLN:CG	8:H:27:ALA:HB2	2.52	0.40
11:K:168:TYR:CE2	15:K:999:BFO:H42	2.57	0.40
11:K:25:TRP:CZ3	12:L:132:SER:HA	2.56	0.40
5:S:68:ILE:HB	5:S:76:LEU:HD21	2.03	0.40
7:U:18(H):GLU:N	7:U:18(H):GLU:CD	2.75	0.40
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.54	0.40
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.74	0.40
1:A:141:HIS:HA	1:A:146:GLY:O	2.21	0.40
2:B:141:TYR:C	2:B:141:TYR:CD1	2.95	0.40
2:B:117:SER:HB3	2:B:155:GLY:O	2.22	0.40
9:I:174:VAL:HG21	9:I:186:LYS:HE3	2.04	0.40
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.18	0.40
2:P:209:ARG:HH11	2:P:209:ARG:HG2	1.85	0.40
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	2.00	0.40
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	2.19	0.40
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.22	0.40
7:U:82:ILE:HG22	7:U:83:PRO:HD3	2.04	0.40
8:V:208:ARG:CZ	9:W:149:GLU:HB2	2.51	0.40
9:W:80:THR:HG22	9:W:119:ILE:HD13	2.03	0.40
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	2.04	0.40
10:X:14:LEU:HD12	10:X:42:LEU:HD23	2.04	0.40
12:Z:15:ALA:HB1	12:Z:173:LEU:HD11	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%)	232 (94%)	11 (4%)	5 (2%)	7	19
1	O	248/250 (99%)	230 (93%)	13 (5%)	5 (2%)	7	19
2	B	242/244 (99%)	222 (92%)	15 (6%)	5 (2%)	7	18
2	P	242/244 (99%)	223 (92%)	14 (6%)	5 (2%)	7	18
3	C	239/241 (99%)	218 (91%)	18 (8%)	3 (1%)	12	30
3	Q	239/241 (99%)	216 (90%)	20 (8%)	3 (1%)	12	30
4	D	240/242 (99%)	228 (95%)	8 (3%)	4 (2%)	9	23
4	R	240/242 (99%)	228 (95%)	7 (3%)	5 (2%)	7	18
5	E	231/233 (99%)	208 (90%)	18 (8%)	5 (2%)	6	17
5	S	231/233 (99%)	208 (90%)	18 (8%)	5 (2%)	6	17
6	F	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	19	43
6	T	242/244 (99%)	222 (92%)	18 (7%)	2 (1%)	19	43
7	G	241/243 (99%)	227 (94%)	12 (5%)	2 (1%)	19	43
7	U	241/243 (99%)	225 (93%)	14 (6%)	2 (1%)	19	43
8	H	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	29	54
8	V	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	29	54
9	I	202/204 (99%)	195 (96%)	6 (3%)	1 (0%)	29	54
9	W	202/204 (99%)	196 (97%)	5 (2%)	1 (0%)	29	54
10	J	196/198 (99%)	187 (95%)	7 (4%)	2 (1%)	15	37
10	X	196/198 (99%)	187 (95%)	7 (4%)	2 (1%)	15	37
11	K	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
11	Y	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
12	L	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	29	54
12	Z	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	29	54
13	1	231/233 (99%)	213 (92%)	17 (7%)	1 (0%)	34	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/233 (99%)	213 (92%)	17 (7%)	1 (0%)	34	60
14	2	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6312/6368 (99%)	5915 (94%)	332 (5%)	65 (1%)	15	37

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
3	C	58	LEU
4	D	12(G)	GLU
5	E	217	LYS
10	J	192	ALA
1	O	5	THR
3	Q	58	LEU
4	R	12(G)	GLU
5	S	217	LYS
10	X	192	ALA
1	A	53	LYS
2	B	6	ARG
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	203	THR
4	D	18(D)	SER
5	E	5	ARG
5	E	202	ARG
6	F	64	ASN
6	F	143	LYS
7	G	239	GLN
8	H	9	ASN
12	L	71	ASP
1	O	53	LYS
2	P	6	ARG
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	203	THR
4	R	18(D)	SER
5	S	5	ARG

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Mol	Chain	Res	Type
5	S	202	ARG
6	T	64	ASN
6	T	143	LYS
7	U	239	GLN
8	V	9	ASN
12	Z	71	ASP
1	A	167	LYS
2	B	20(A)	SER
3	C	183	PRO
4	D	12(F)	GLY
5	E	180	LEU
5	E	231	LYS
1	O	167	LYS
2	P	20(A)	SER
4	R	12(F)	GLY
5	S	180	LEU
5	S	231	LYS
1	O	56	SER
1	A	56	SER
1	A	63	THR
7	G	7	GLY
1	O	63	THR
4	R	120	ALA
7	U	7	GLY
9	I	93	GLY
10	J	8	VAL
10	X	8	VAL
9	W	93	GLY
4	D	12(C)	GLY
13	M	207	GLY
4	R	12(C)	GLY
13	1	207	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%)	204 (98%)	5 (2%)	49	77
1	O	209/209 (100%)	204 (98%)	5 (2%)	49	77
2	B	203/203 (100%)	190 (94%)	13 (6%)	17	39
2	P	203/203 (100%)	190 (94%)	13 (6%)	17	39
3	C	213/213 (100%)	204 (96%)	9 (4%)	30	58
3	Q	213/213 (100%)	204 (96%)	9 (4%)	30	58
4	D	198/198 (100%)	187 (94%)	11 (6%)	21	45
4	R	198/198 (100%)	187 (94%)	11 (6%)	21	45
5	E	192/192 (100%)	176 (92%)	16 (8%)	11	25
5	S	192/192 (100%)	176 (92%)	16 (8%)	11	25
6	F	201/201 (100%)	187 (93%)	14 (7%)	15	35
6	T	201/201 (100%)	186 (92%)	15 (8%)	13	31
7	G	207/207 (100%)	198 (96%)	9 (4%)	29	57
7	U	207/207 (100%)	198 (96%)	9 (4%)	29	57
8	H	181/181 (100%)	173 (96%)	8 (4%)	28	56
8	V	181/181 (100%)	173 (96%)	8 (4%)	28	56
9	I	172/172 (100%)	165 (96%)	7 (4%)	30	59
9	W	172/172 (100%)	166 (96%)	6 (4%)	36	65
10	J	175/175 (100%)	170 (97%)	5 (3%)	42	71
10	X	175/175 (100%)	170 (97%)	5 (3%)	42	71
11	K	169/169 (100%)	163 (96%)	6 (4%)	35	64
11	Y	169/169 (100%)	163 (96%)	6 (4%)	35	64
12	L	185/185 (100%)	174 (94%)	11 (6%)	19	43
12	Z	185/185 (100%)	174 (94%)	11 (6%)	19	43
13	1	199/199 (100%)	191 (96%)	8 (4%)	31	60
13	M	199/199 (100%)	191 (96%)	8 (4%)	31	60
14	2	162/162 (100%)	159 (98%)	3 (2%)	57	82
14	N	162/162 (100%)	159 (98%)	3 (2%)	57	82
All	All	5332/5332 (100%)	5082 (95%)	250 (5%)	26	54

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	124	THR
1	A	158	PHE
1	A	179	ARG
2	B	58	LEU
2	B	61	GLN
2	B	62	ASP
2	B	71	ASN
2	B	91	THR
2	B	116	LEU
2	B	121	GLN
2	B	156	ASN
2	B	185	LYS
2	B	187	ASP
2	B	192	LEU
2	B	212	PHE
2	B	218	ASN
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	66	LYS
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	174	GLU
3	C	208	LYS
4	D	28	LEU
4	D	48	LEU
4	D	76	CYS
4	D	110	GLU
4	D	126	ARG
4	D	156	THR
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
5	E	11	ASP
5	E	32	LYS
5	E	56	ASP
5	E	57	GLU
5	E	59	SER

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Mol	Chain	Res	Type
5	E	76	LEU
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	178	ARG
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	43	ASN
6	F	56	SER
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
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	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	169	GLN
7	G	184	ASN
7	G	197	MET
7	G	232	ARG
7	G	233	LEU
8	H	30	ASN
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	121	VAL
8	H	144	GLN
8	H	197	ARG

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Mol	Chain	Res	Type
9	I	20	LEU
9	I	22	SER
9	I	29	ASN
9	I	113	PHE
9	I	160	LEU
9	I	171	TRP
9	I	192	ARG
10	J	34	THR
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	121	GLU
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	87	VAL
11	K	104	TYR
11	K	138	LEU
12	L	-7	ASN
12	L	14	LEU
12	L	40	ASN
12	L	43	MET
12	L	58	ARG
12	L	70(A)	ASN
12	L	82	ASN
12	L	98	HIS
12	L	99	THR
12	L	120	GLU
12	L	145	TYR
13	M	40	ASN
13	M	65	GLU
13	M	91	ARG
13	M	129	PHE
13	M	14(C)	ARG
13	M	148	VAL
13	M	149	GLN
13	M	204	LYS
14	N	84	LYS
14	N	89	GLU
14	N	10(B)	LYS
1	O	33	GLN
1	O	64	LEU

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Mol	Chain	Res	Type
1	O	124	THR
1	O	158	PHE
1	O	179	ARG
2	P	58	LEU
2	P	61	GLN
2	P	62	ASP
2	P	71	ASN
2	P	91	THR
2	P	116	LEU
2	P	121	GLN
2	P	156	ASN
2	P	185	LYS
2	P	187	ASP
2	P	192	LEU
2	P	212	PHE
2	P	218	ASN
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	66	LYS
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	174	GLU
3	Q	208	LYS
4	R	28	LEU
4	R	48	LEU
4	R	76	CYS
4	R	110	GLU
4	R	126	ARG
4	R	156	THR
4	R	170	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
5	S	11	ASP
5	S	32	LYS
5	S	56	ASP
5	S	57	GLU
5	S	59	SER
5	S	76	LEU

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Mol	Chain	Res	Type
5	S	97	ASN
5	S	104	ASN
5	S	121	GLN
5	S	178	ARG
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	43	ASN
6	T	56	SER
6	T	95	GLU
6	T	98	SER
6	T	105	THR
6	T	121	GLN
6	T	127	ASN
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
6	T	21(C)	ASN
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	169	GLN
7	U	184	ASN
7	U	197	MET
7	U	232	ARG
7	U	233	LEU
8	V	30	ASN
8	V	34	LEU
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	121	VAL
8	V	144	GLN
8	V	197	ARG

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Mol	Chain	Res	Type
9	W	20	LEU
9	W	22	SER
9	W	29	ASN
9	W	113	PHE
9	W	160	LEU
9	W	192	ARG
10	X	34	THR
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	121	GLU
11	Y	4	LEU
11	Y	9	GLN
11	Y	65	LEU
11	Y	87	VAL
11	Y	104	TYR
11	Y	138	LEU
12	Z	-7	ASN
12	Z	14	LEU
12	Z	40	ASN
12	Z	43	MET
12	Z	58	ARG
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	120	GLU
12	Z	145	TYR
13	1	40	ASN
13	1	65	GLU
13	1	91	ARG
13	1	129	PHE
13	1	14(C)	ARG
13	1	148	VAL
13	1	149	GLN
13	1	204	LYS
14	2	84	LYS
14	2	89	GLU
14	2	10(B)	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (194) 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
3	C	163	GLN
3	C	209	ASN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	114	GLN
4	D	161	ASN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	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	156	ASN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN

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Mol	Chain	Res	Type
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	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
9	I	81	GLN
9	I	161	ASN
10	J	36	GLN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	141	HIS
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	61	ASN
12	L	70(A)	ASN
12	L	82	ASN
12	L	123	GLN
12	L	1(I)	ASN

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Mol	Chain	Res	Type
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	191	GLN
14	N	69	GLN
14	N	145	ASN
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
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	114	GLN
4	R	161	ASN
4	R	211	GLN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS

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Mol	Chain	Res	Type
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	156	ASN
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
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	29	ASN
9	W	81	GLN
9	W	161	ASN
10	X	36	GLN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	141	HIS
10	X	186	GLN
10	X	193	GLN

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Mol	Chain	Res	Type
11	Y	9	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	70(A)	ASN
12	Z	85	HIS
12	Z	123	GLN
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	191	GLN
14	2	69	GLN
14	2	145	ASN
14	2	157	HIS
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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
15	BFO	Y	999	11	48,48,48	1.96	15 (31%)	59,63,63	1.57	8 (13%)
15	BFO	K	999	11	48,48,48	1.98	16 (33%)	59,63,63	1.57	8 (13%)

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	BFO	Y	999	11	-	15/49/49/49	0/3/3/3
15	BFO	K	999	11	-	15/49/49/49	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	999	BFO	C33-C31	4.31	1.58	1.54
15	K	999	BFO	C33-C31	4.15	1.58	1.54
15	K	999	BFO	C43-C42	3.72	1.45	1.36
15	K	999	BFO	C29-N28	3.68	1.41	1.33
15	Y	999	BFO	C43-C42	3.66	1.45	1.36
15	Y	999	BFO	C29-N28	3.41	1.41	1.33
15	K	999	BFO	C40-C3	3.33	1.45	1.37
15	Y	999	BFO	C4-C3	3.28	1.58	1.50
15	Y	999	BFO	C44-C45	3.25	1.44	1.36
15	Y	999	BFO	C40-C3	3.18	1.44	1.37
15	K	999	BFO	C44-C45	3.16	1.43	1.36
15	K	999	BFO	C4-C3	3.09	1.57	1.50
15	Y	999	BFO	C1-C2	3.02	1.43	1.36
15	Y	999	BFO	C2-C3	2.96	1.45	1.38
15	K	999	BFO	C1-C2	2.94	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	K	999	BFO	C2-C3	2.78	1.44	1.38
15	Y	999	BFO	C14-N13	2.29	1.50	1.45
15	K	999	BFO	C21-C20	2.20	1.43	1.38
15	Y	999	BFO	C6-N8	2.20	1.40	1.34
15	K	999	BFO	C24-C19	2.20	1.43	1.38
15	Y	999	BFO	C10-C9	2.17	1.58	1.52
15	K	999	BFO	C14-N13	2.15	1.50	1.45
15	Y	999	BFO	C23-C24	2.12	1.43	1.38
15	K	999	BFO	C11-N13	2.11	1.38	1.34
15	K	999	BFO	O7-C6	2.10	1.25	1.21
15	K	999	BFO	C25-C14	2.09	1.58	1.53
15	Y	999	BFO	C40-C41	2.08	1.46	1.42
15	Y	999	BFO	O7-C6	2.06	1.25	1.21
15	Y	999	BFO	C26-C27	2.06	1.59	1.51
15	K	999	BFO	C23-C24	2.05	1.43	1.38
15	K	999	BFO	C10-C9	2.00	1.58	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	K	999	BFO	C9-N8-C6	7.05	133.72	120.49
15	Y	999	BFO	C9-N8-C6	7.02	133.65	120.49
15	Y	999	BFO	C4-O5-C6	4.93	126.94	115.93
15	K	999	BFO	C4-O5-C6	4.77	126.59	115.93
15	Y	999	BFO	O17-C18-C19	3.16	116.98	109.39
15	K	999	BFO	O17-C18-C19	3.10	116.84	109.39
15	K	999	BFO	O17-C15-C14	3.07	119.06	111.59
15	Y	999	BFO	O17-C15-C14	2.99	118.86	111.59
15	Y	999	BFO	O5-C4-C3	-2.76	102.76	109.39
15	K	999	BFO	C14-N13-C11	2.72	127.51	121.67
15	K	999	BFO	O5-C4-C3	-2.71	102.89	109.39
15	Y	999	BFO	C14-N13-C11	2.65	127.35	121.67
15	K	999	BFO	O5-C6-N8	-2.37	105.67	110.50
15	Y	999	BFO	O5-C6-N8	-2.29	105.85	110.50
15	K	999	BFO	O16-C15-C14	-2.05	117.80	123.92
15	Y	999	BFO	O16-C15-C14	-2.02	117.90	123.92

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	Y	999	BFO	C10-C9-N8-C6

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Mol	Chain	Res	Type	Atoms
15	Y	999	BFO	C9-C11-N13-C14
15	Y	999	BFO	O12-C11-N13-C14
15	Y	999	BFO	N28-C29-C31-O32
15	Y	999	BFO	O30-C29-C31-O32
15	K	999	BFO	C10-C9-N8-C6
15	K	999	BFO	C9-C11-N13-C14
15	K	999	BFO	N28-C29-C31-O32
15	K	999	BFO	O30-C29-C31-O32
15	K	999	BFO	O12-C11-N13-C14
15	Y	999	BFO	N13-C14-C25-C26
15	K	999	BFO	N13-C14-C25-C26
15	Y	999	BFO	C25-C26-C27-N28
15	K	999	BFO	C25-C26-C27-N28
15	K	999	BFO	C25-C14-C15-O17
15	Y	999	BFO	C25-C14-C15-O17
15	Y	999	BFO	C25-C14-C15-O16
15	K	999	BFO	C25-C14-C15-O16
15	Y	999	BFO	C25-C14-N13-C11
15	Y	999	BFO	C11-C9-N8-C6
15	K	999	BFO	C11-C9-N8-C6
15	K	999	BFO	C25-C14-N13-C11
15	Y	999	BFO	C15-C14-C25-C26
15	K	999	BFO	C15-C14-C25-C26
15	Y	999	BFO	O30-C29-C31-C33
15	K	999	BFO	O30-C29-C31-C33
15	Y	999	BFO	N28-C29-C31-C33
15	K	999	BFO	N28-C29-C31-C33
15	Y	999	BFO	N13-C14-C15-O17
15	K	999	BFO	N13-C14-C15-O17

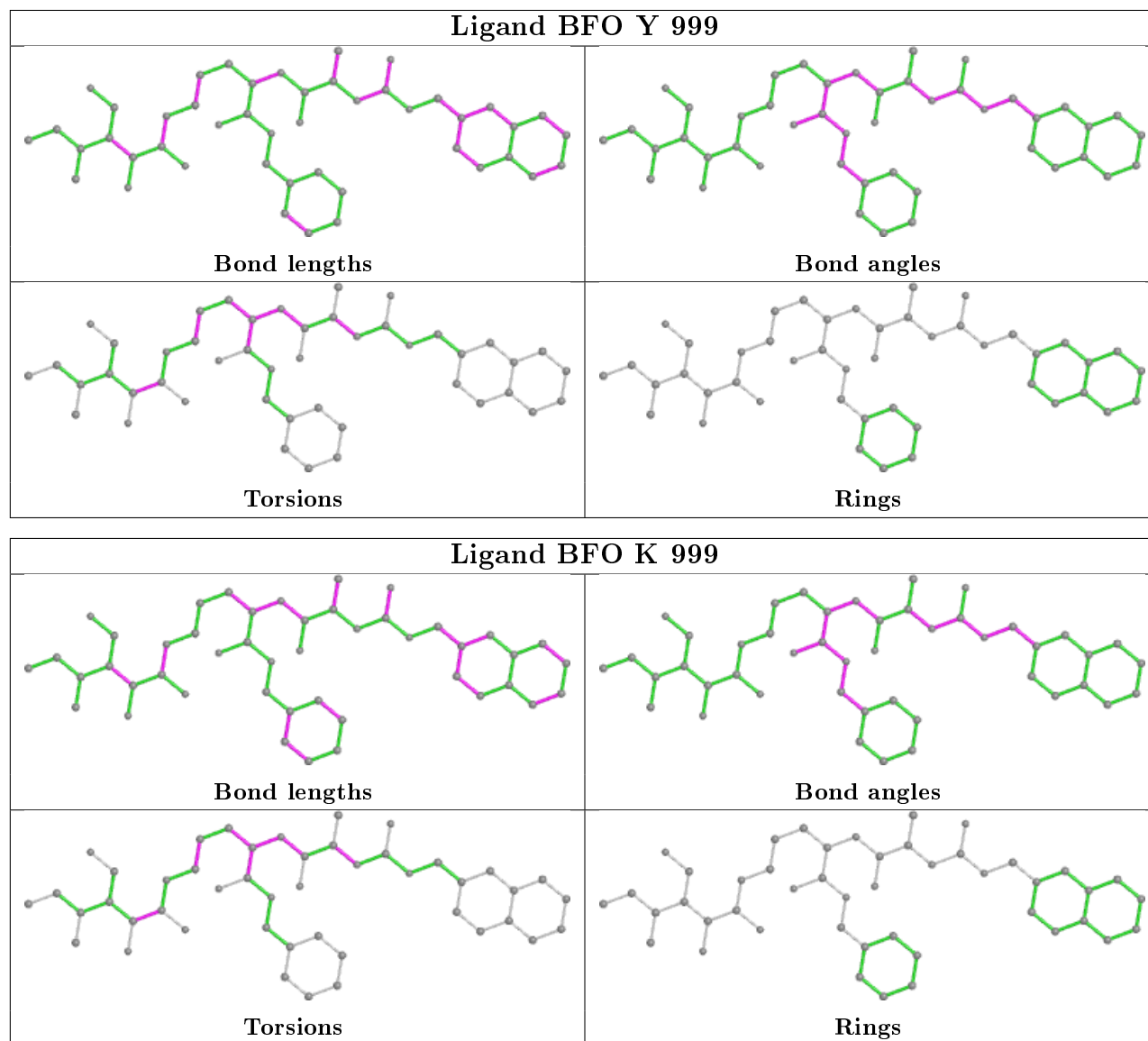
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Y	999	BFO	3	0
15	K	999	BFO	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	250/250 (100%)	-0.19	3 (1%) 79 80	39, 54, 84, 112	0
1	O	250/250 (100%)	-0.09	5 (2%) 65 67	39, 55, 86, 112	0
2	B	244/244 (100%)	0.07	7 (2%) 51 52	39, 57, 97, 121	0
2	P	244/244 (100%)	0.10	12 (4%) 29 28	40, 58, 98, 121	0
3	C	241/241 (100%)	0.19	14 (5%) 23 22	40, 61, 114, 131	0
3	Q	241/241 (100%)	0.50	39 (16%) 1 1	42, 62, 114, 132	0
4	D	242/242 (100%)	0.13	8 (3%) 46 46	39, 62, 95, 128	0
4	R	242/242 (100%)	0.16	11 (4%) 33 31	40, 62, 96, 128	0
5	E	233/233 (100%)	0.30	20 (8%) 10 8	43, 66, 93, 115	0
5	S	233/233 (100%)	0.48	27 (11%) 4 3	44, 67, 94, 115	0
6	F	244/244 (100%)	0.03	8 (3%) 46 46	40, 60, 93, 116	0
6	T	244/244 (100%)	0.06	7 (2%) 51 52	42, 60, 93, 116	0
7	G	243/243 (100%)	-0.16	7 (2%) 51 52	37, 53, 80, 122	0
7	U	243/243 (100%)	-0.15	2 (0%) 86 87	37, 54, 80, 122	0
8	H	222/222 (100%)	-0.32	0 100 100	34, 47, 68, 106	0
8	V	222/222 (100%)	-0.38	1 (0%) 91 92	34, 48, 69, 107	0
9	I	204/204 (100%)	-0.32	0 100 100	36, 47, 64, 81	0
9	W	204/204 (100%)	-0.21	0 100 100	36, 47, 64, 81	0
10	J	198/198 (100%)	-0.17	3 (1%) 73 76	38, 49, 72, 129	0
10	X	198/198 (100%)	-0.17	6 (3%) 50 51	38, 49, 71, 130	0
11	K	212/212 (100%)	-0.28	0 100 100	34, 48, 66, 77	0
11	Y	212/212 (100%)	-0.34	0 100 100	35, 48, 67, 77	0
12	L	222/222 (100%)	-0.24	3 (1%) 75 77	37, 50, 70, 91	0
12	Z	222/222 (100%)	-0.20	2 (0%) 84 85	36, 50, 71, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.30	1 (0%)	92	93	35, 51, 68, 77	0
13	M	233/233 (100%)	-0.30	1 (0%)	92	93	35, 52, 69, 77	0
14	2	196/196 (100%)	-0.22	2 (1%)	82	83	33, 47, 71, 85	0
14	N	196/196 (100%)	-0.30	1 (0%)	91	92	34, 47, 71, 84	0
All	All	6368/6368 (100%)	-0.07	190 (2%)	50	51	33, 53, 88, 132	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(C)	GLY	14.4
4	R	12(D)	ALA	13.8
4	D	12(D)	ALA	10.6
4	D	12(E)	SER	9.2
7	U	240	ASP	8.2
4	R	12(F)	GLY	7.9
3	C	55	THR	7.8
2	B	217	ALA	7.0
3	C	56	LEU	6.6
2	P	217	ALA	6.5
3	Q	236	ILE	6.4
4	R	12(E)	SER	6.4
5	S	5	ARG	6.3
10	X	192	ALA	6.3
2	B	218	ASN	6.2
7	U	6	ALA	5.9
10	X	193	GLN	5.9
4	D	12(F)	GLY	5.8
4	R	126	ARG	5.8
5	E	4	PHE	5.7
1	O	236	LEU	5.6
4	R	12(C)	GLY	5.5
10	J	193	GLN	5.3
3	Q	242	GLU	5.2
5	S	233	ILE	5.1
2	P	218	ASN	4.9
3	Q	56	LEU	4.9
5	S	178	ARG	4.6
10	J	192	ALA	4.6
3	Q	55	THR	4.6
4	D	126	ARG	4.5
3	Q	54	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	O	235	ALA	4.4
7	G	6	ALA	4.4
13	M	-8	THR	4.4
7	G	240	ASP	4.2
2	P	21(B)	GLY	4.1
5	E	180	LEU	4.0
5	E	203	ASP	4.0
5	E	5	ARG	4.0
3	Q	235	GLN	4.0
4	D	12(G)	GLU	4.0
5	S	203	ASP	4.0
1	A	236	LEU	4.0
5	E	233	ILE	4.0
3	Q	189	CYS	3.9
8	V	223	ASP	3.7
2	B	54	VAL	3.7
5	S	4	PHE	3.7
3	Q	194	VAL	3.7
2	P	21(C)	ASP	3.7
3	Q	233	VAL	3.6
3	Q	234	THR	3.6
3	Q	203	THR	3.6
7	G	236	ILE	3.5
1	A	4	MET	3.5
5	S	127	TYR	3.5
13	1	-8	THR	3.5
5	S	201	LEU	3.4
5	S	51	LEU	3.4
1	O	4	MET	3.4
5	S	58	LEU	3.4
3	Q	238	GLN	3.4
3	Q	201	VAL	3.3
6	F	5	GLY	3.3
6	F	240	ILE	3.2
3	Q	241	GLN	3.2
3	Q	243	GLN	3.2
2	B	21(B)	GLY	3.2
3	Q	184	ALA	3.2
3	Q	212	ILE	3.1
2	P	239	THR	3.1
3	C	240	LYS	3.1
3	C	187	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
5	S	206	SER	3.0
3	Q	229	ILE	3.0
14	2	107	LYS	3.0
5	S	210	LEU	3.0
3	Q	63	THR	2.9
2	B	232	ILE	2.9
5	E	191	LYS	2.9
6	T	240	ILE	2.9
5	S	195	GLU	2.8
3	Q	191	LYS	2.8
5	S	18(B)	THR	2.8
6	F	204	ASP	2.8
3	Q	239	GLU	2.8
5	E	178	ARG	2.7
4	R	12(G)	GLU	2.7
5	E	204	GLU	2.7
1	O	5	THR	2.7
3	C	59	GLN	2.7
6	F	180	VAL	2.7
3	C	232	TYR	2.7
2	P	21(A)	LYS	2.7
3	Q	40	VAL	2.6
5	S	18(C)	PHE	2.6
5	S	193	GLY	2.6
12	Z	14(W)	LYS	2.6
4	R	9	ASP	2.6
5	S	180	LEU	2.6
10	X	191	GLN	2.6
3	Q	179	ASN	2.6
5	S	211	SER	2.6
3	Q	202	GLN	2.5
5	S	232	TYR	2.5
5	E	127	TYR	2.5
12	L	-9	GLN	2.5
5	E	175	TYR	2.5
3	Q	187	GLU	2.5
5	S	6	ASN	2.5
3	C	203	THR	2.5
3	Q	44	ASN	2.5
10	X	189	ASP	2.5
3	Q	207	ALA	2.5
3	Q	197	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
5	E	189	LEU	2.4
10	J	-1	MET	2.4
2	B	239	THR	2.4
5	S	207	LEU	2.4
3	Q	53	ARG	2.4
2	P	219	GLU	2.4
2	P	232	ILE	2.4
5	S	189	LEU	2.4
4	R	12(B)	GLU	2.4
3	Q	240	LYS	2.4
5	E	193	GLY	2.4
7	G	239	GLN	2.4
6	T	5	GLY	2.4
2	P	22	TYR	2.3
12	Z	145	TYR	2.3
5	E	2(C)	VAL	2.3
2	P	238	ILE	2.3
5	E	197	ILE	2.3
3	Q	18(D)	GLU	2.3
3	Q	237	GLU	2.3
6	T	241	ASN	2.3
4	D	127	LEU	2.3
6	T	18(B)	HIS	2.3
2	P	236	THR	2.3
3	Q	206	GLY	2.2
6	F	18(E)	GLU	2.2
5	E	176	LEU	2.2
10	X	190	PHE	2.2
5	S	212	ILE	2.2
6	T	18(D)	PRO	2.2
3	C	229	ILE	2.2
5	S	188	GLU	2.2
4	R	127	LEU	2.2
12	L	145	TYR	2.2
5	S	2(E)	ASN	2.2
12	L	14(P)	PRO	2.2
14	N	9	LYS	2.2
3	C	242	GLU	2.2
1	A	5	THR	2.2
3	Q	198	LEU	2.1
5	S	200	SER	2.1
6	F	241	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
7	G	17(D)	SER	2.1
14	2	11	GLY	2.1
2	P	6	ARG	2.1
5	E	192	ALA	2.1
6	F	186	ALA	2.1
3	C	190	VAL	2.1
4	R	19	GLY	2.1
5	E	207	LEU	2.1
6	T	57	LYS	2.1
3	C	209	ASN	2.1
4	R	10	ARG	2.1
6	F	43	ASN	2.1
5	E	231	LYS	2.1
3	Q	62(A)	ILE	2.1
3	Q	183	PRO	2.1
7	G	237	ALA	2.1
3	Q	224	LEU	2.1
1	O	206	PHE	2.1
4	D	10	ARG	2.1
10	X	-1	MET	2.1
3	Q	175	PHE	2.1
5	S	184	GLY	2.1
5	E	58	LEU	2.0
5	S	202	ARG	2.0
6	T	203	GLU	2.0
3	C	210	ILE	2.0
3	C	239	GLU	2.0
7	G	8	TYR	2.0
5	E	6	ASN	2.0
3	C	241	GLN	2.0
3	Q	195	ARG	2.0
2	B	205	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

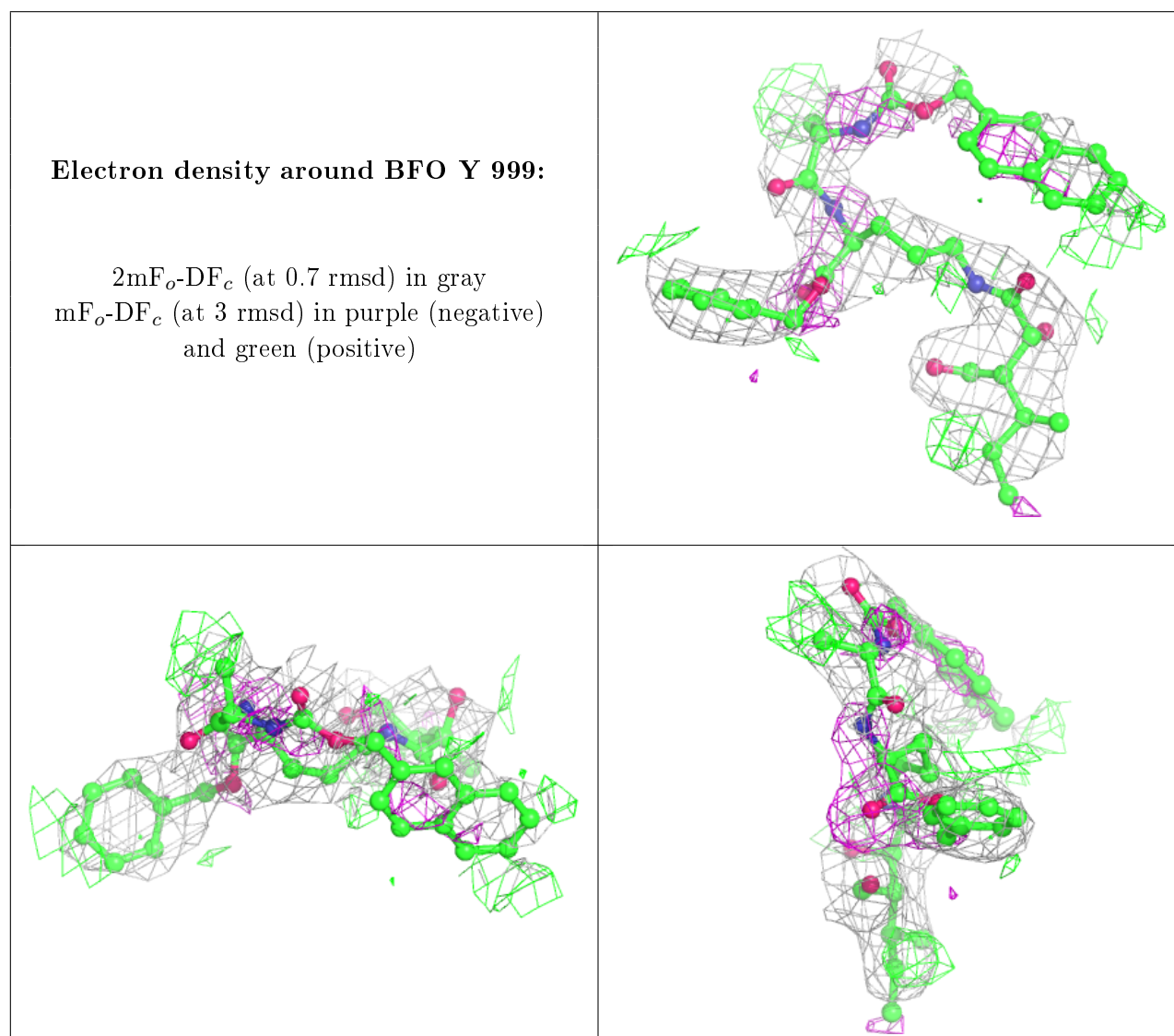
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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.

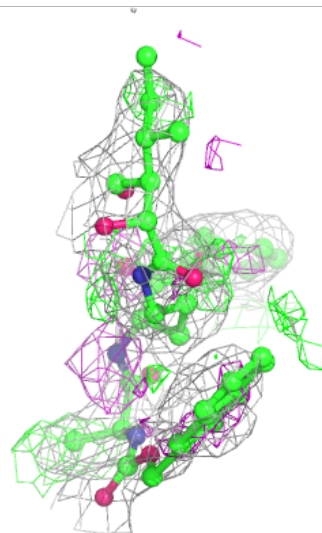
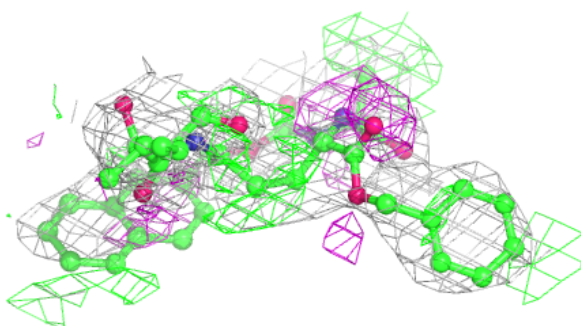
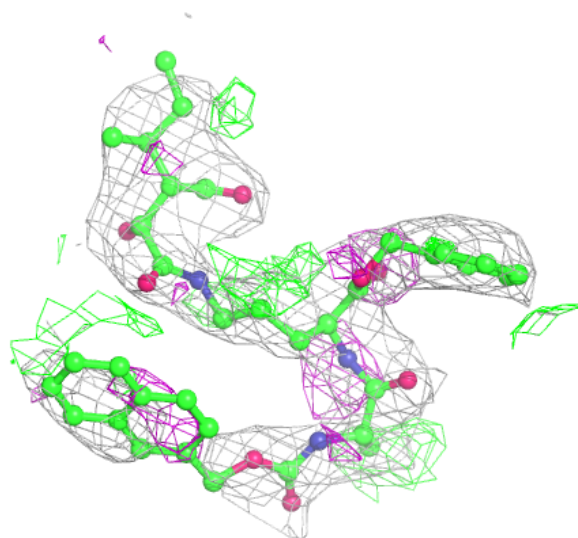
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	BFO	Y	999	46/46	0.79	0.32	50,76,97,98	0
15	BFO	K	999	46/46	0.79	0.32	50,76,97,97	0

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 BFO K 999:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.