



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:48 PM GMT

PDB ID : 4FZC
Title : 20S yeast proteasome in complex with cepafungin I
Authors : Stein, M.; Beck, P.; Kaiser, M.; Dudler, R.; Becker, C.F.W.; Groll, M.
Deposited on : 2012-07-06
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

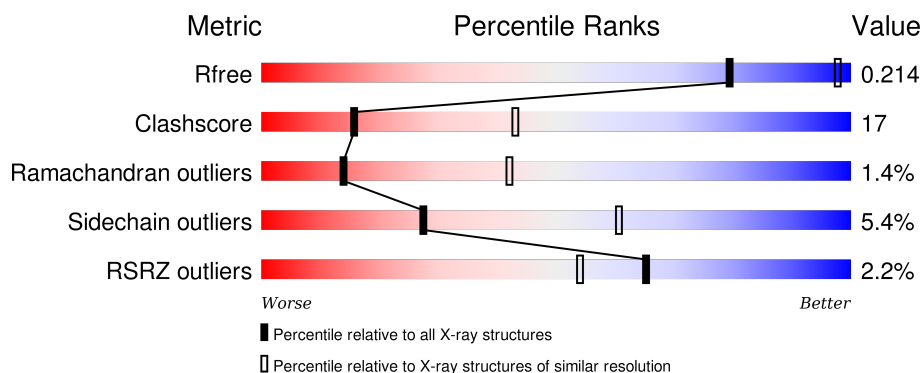
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	<div> <div>2%</div> <div>71% 26% .</div> </div>
1	O	250	<div> <div>3%</div> <div>72% 26% .</div> </div>
2	B	244	<div> <div>3%</div> <div>61% 32% 6%</div> </div>
2	P	244	<div> <div>5%</div> <div>61% 33% 6%</div> </div>
3	C	241	<div> <div>6%</div> <div>62% 34% .</div> </div>

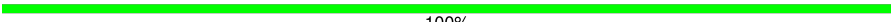
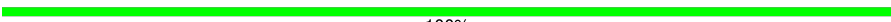
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	241	
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	M	233	
13	a	233	
14	N	196	
14	b	196	
15	c	4	
15	d	4	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	e	4	 100%
15	f	4	 100%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 51020 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			

Continued on next page...

Continued from previous page...

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	a	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	b	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called Cepafungin I.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	c	4	Total	C	N	O	0	0	0
			38	28	4	6			
15	d	4	Total	C	N	O	0	0	0
			38	28	4	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	e	4	Total	C	N	O	0	0	0
			38	28	4	6			
15	f	4	Total	C	N	O	0	0	0
			38	28	4	6			

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	55	Total	O	0	0
			55	55		
16	B	37	Total	O	0	0
			37	37		
16	C	41	Total	O	0	0
			41	41		
16	D	40	Total	O	0	0
			40	40		
16	E	23	Total	O	0	0
			23	23		
16	F	46	Total	O	0	0
			46	46		
16	G	59	Total	O	0	0
			59	59		
16	H	53	Total	O	0	0
			53	53		
16	I	68	Total	O	0	0
			68	68		
16	J	51	Total	O	0	0
			51	51		
16	K	43	Total	O	0	0
			43	43		
16	L	58	Total	O	0	0
			58	58		
16	M	71	Total	O	0	0
			71	71		
16	N	58	Total	O	0	0
			58	58		
16	O	33	Total	O	0	0
			33	33		
16	P	27	Total	O	0	0
			27	27		
16	Q	26	Total	O	0	0
			26	26		

Continued on next page...

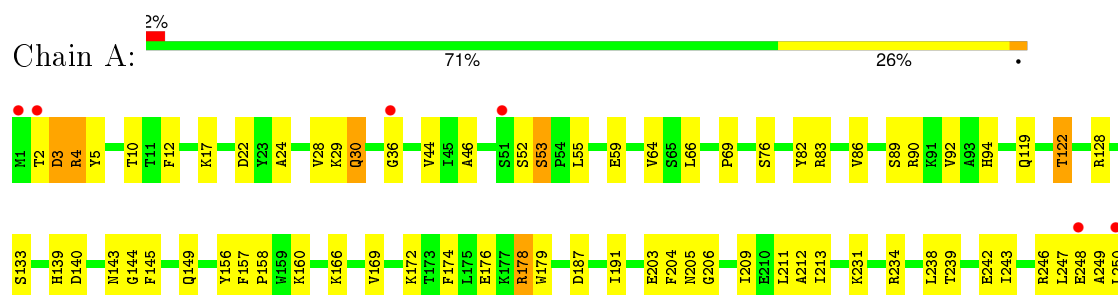
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	R	28	Total 28	O 28	0	0
16	S	21	Total 21	O 21	0	0
16	T	38	Total 38	O 38	0	0
16	U	62	Total 62	O 62	0	0
16	V	47	Total 47	O 47	0	0
16	W	57	Total 57	O 57	0	0
16	X	47	Total 47	O 47	0	0
16	Y	41	Total 41	O 41	0	0
16	Z	55	Total 55	O 55	0	0
16	a	74	Total 74	O 74	0	0
16	b	60	Total 60	O 60	0	0
16	f	1	Total 1	O 1	0	0

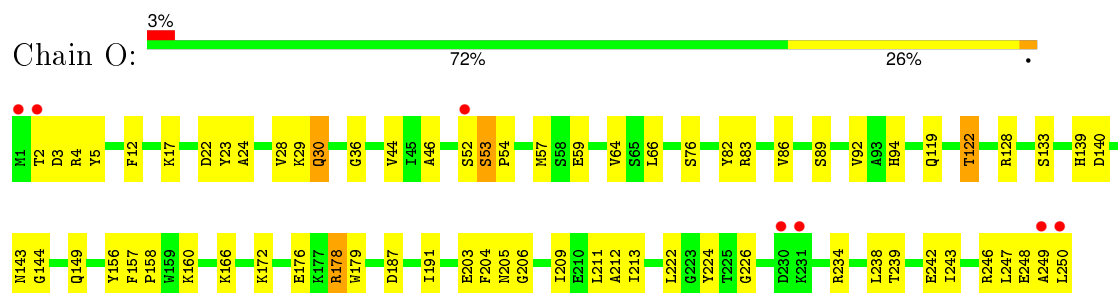
3 Residue-property plots [i](#)

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

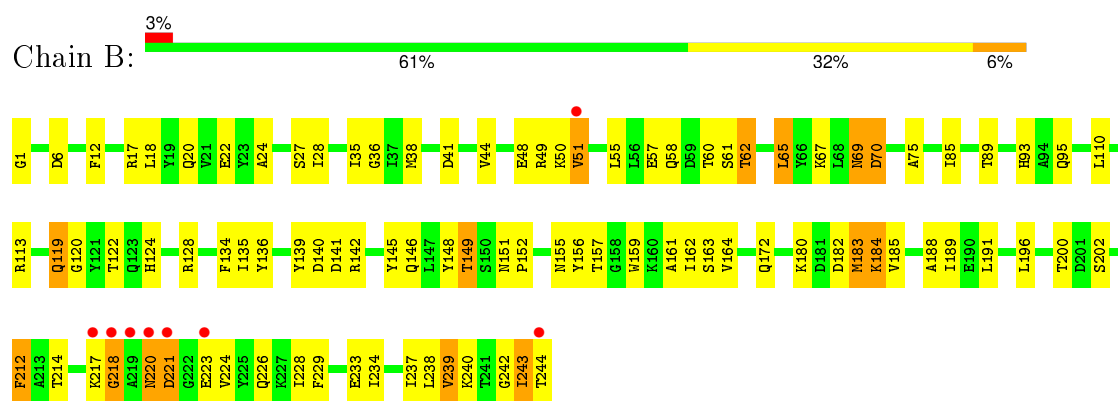
• Molecule 1: Proteasome component Y7



• Molecule 1: Proteasome component Y7

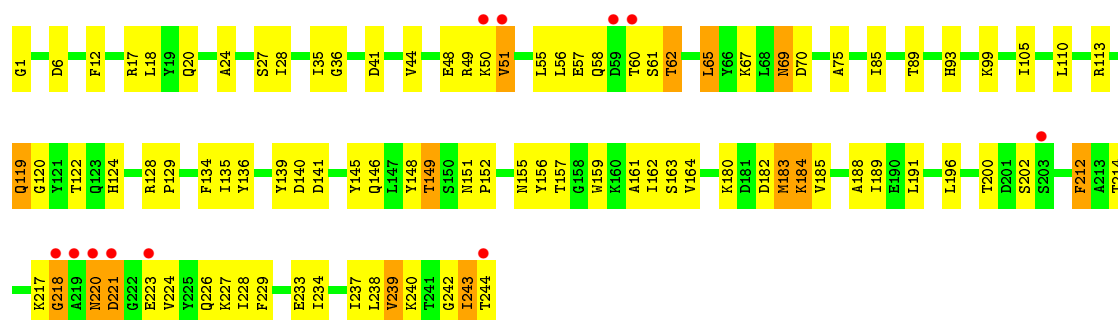


• Molecule 2: Proteasome component Y13

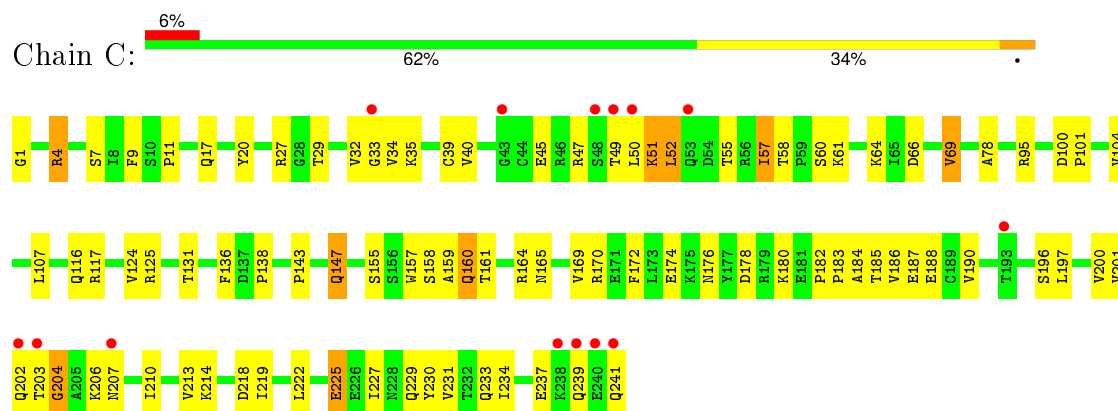


• Molecule 2: Proteasome component Y13

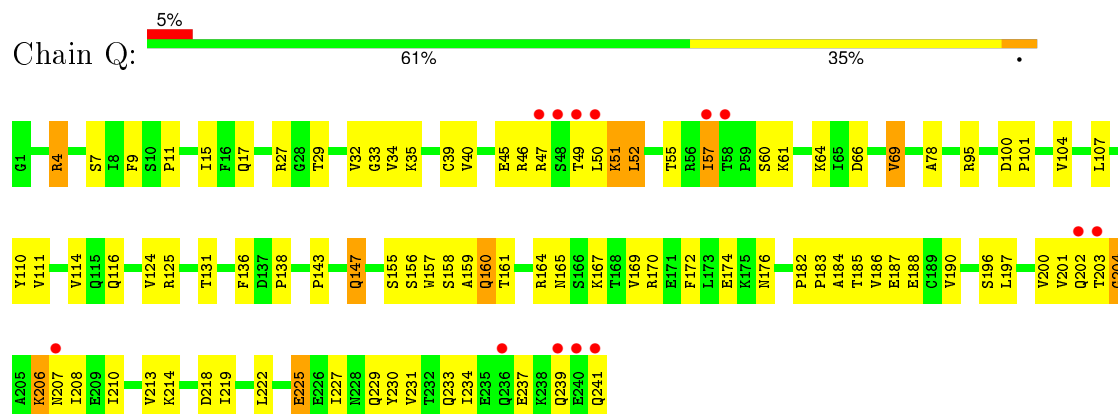




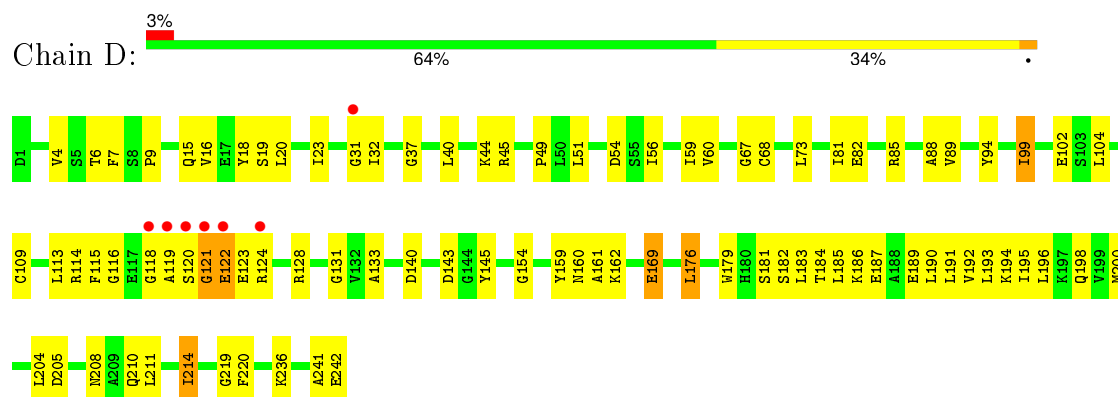
• Molecule 3: Proteasome component PRE6



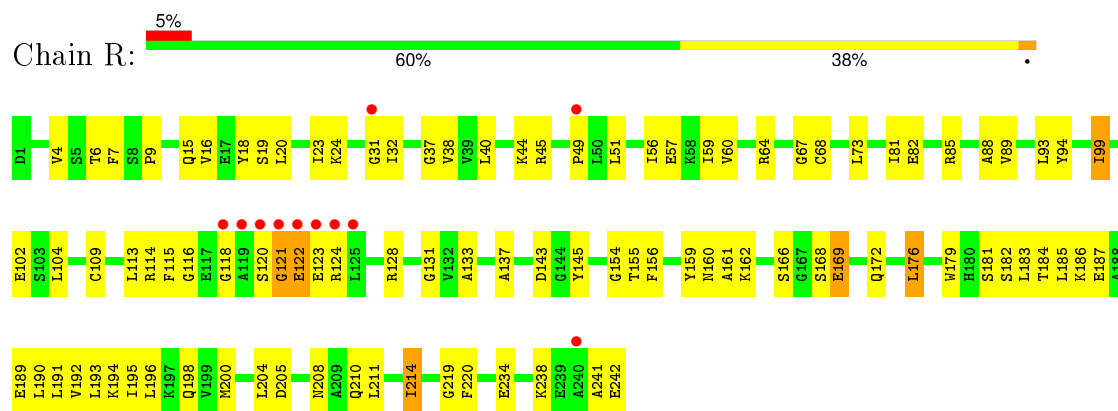
• Molecule 3: Proteasome component PRE6



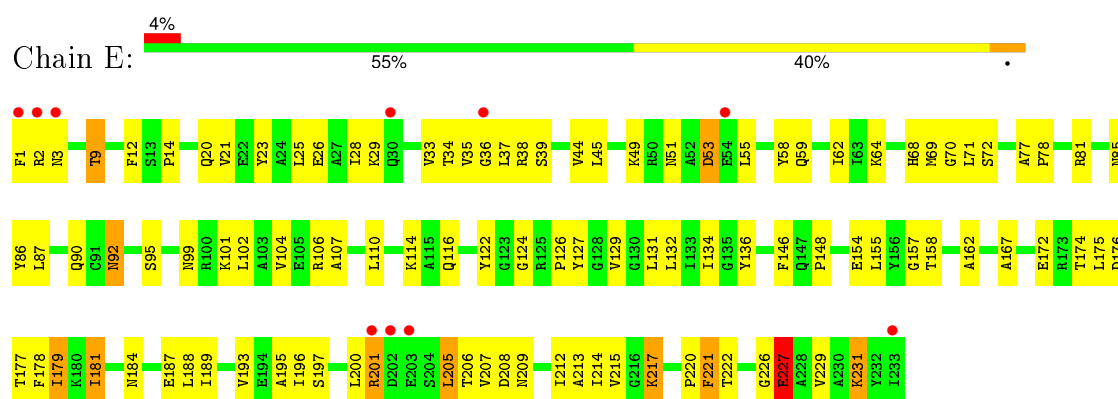
• Molecule 4: Proteasome component PUP2



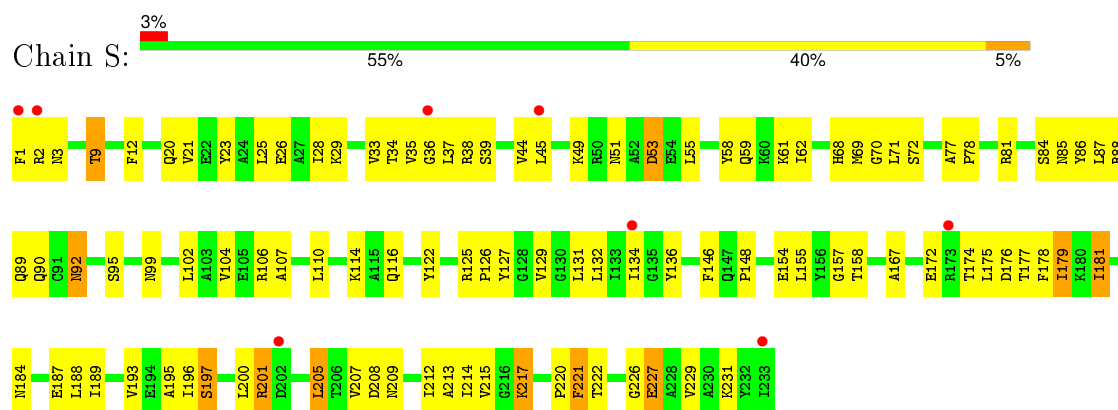
- Molecule 4: Proteasome component PUP2



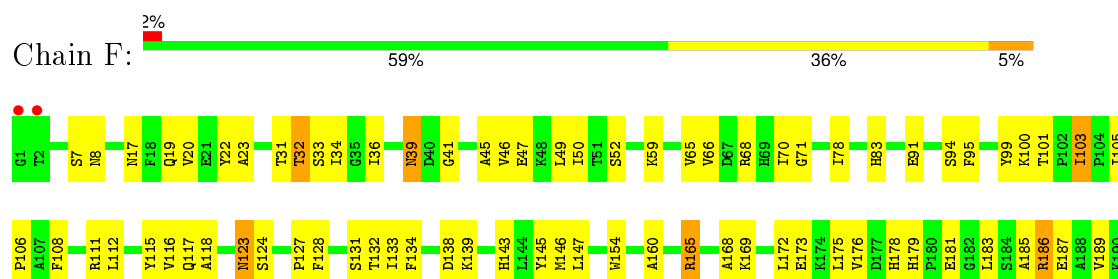
- Molecule 5: Proteasome component PRE5



- Molecule 5: Proteasome component PRE5

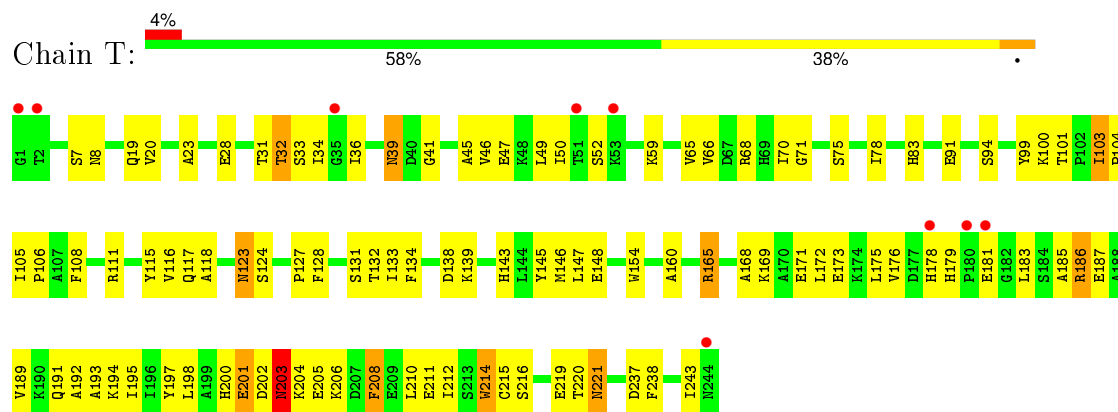


- Molecule 6: Proteasome component C1

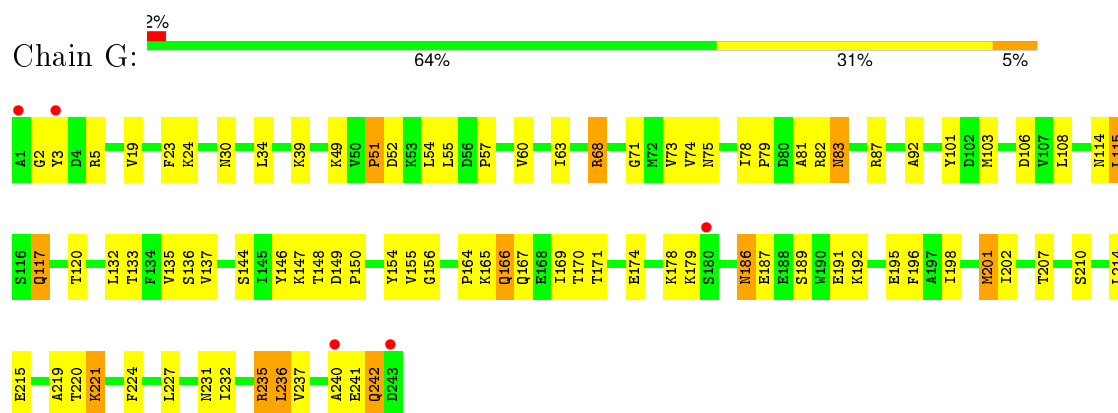




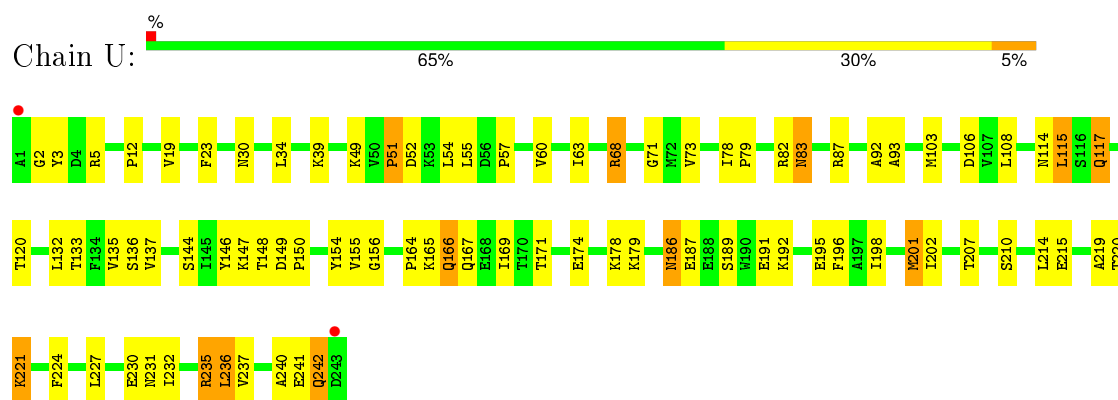
• Molecule 6: Proteasome component C1



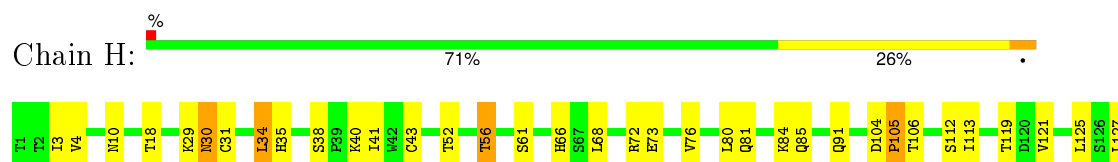
• Molecule 7: Proteasome component C7-alpha



• Molecule 7: Proteasome component C7-alpha



• Molecule 8: Proteasome component PUP1

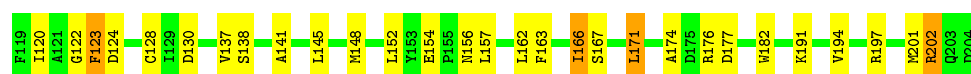
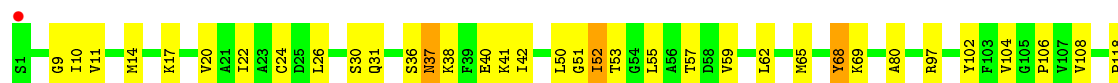




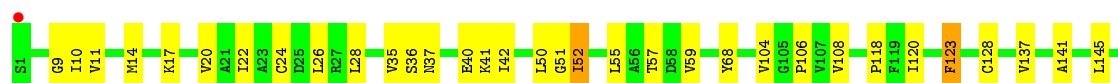
• Molecule 8: Proteasome component PUP1



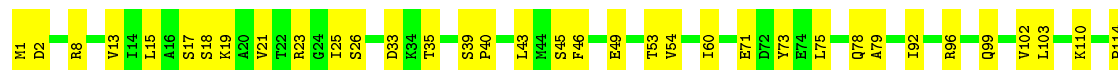
• Molecule 9: Proteasome component PUP3



• Molecule 9: Proteasome component PUP3

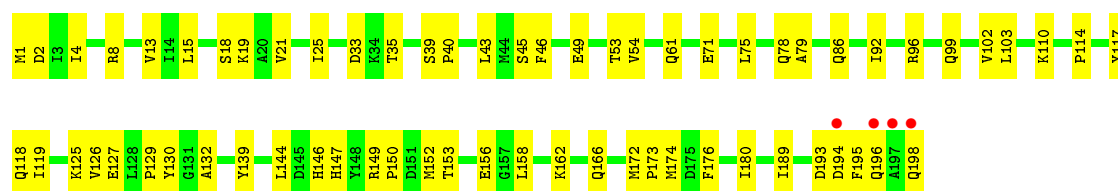


• Molecule 10: Proteasome component C11



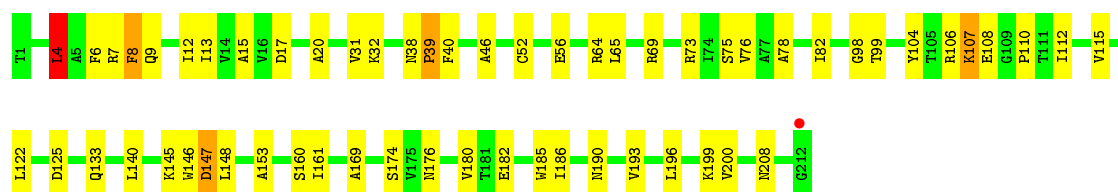
• Molecule 10: Proteasome component C11





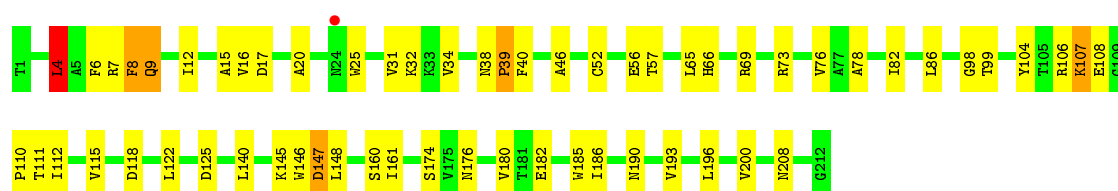
• Molecule 11: Proteasome component PRE2

Chain K:

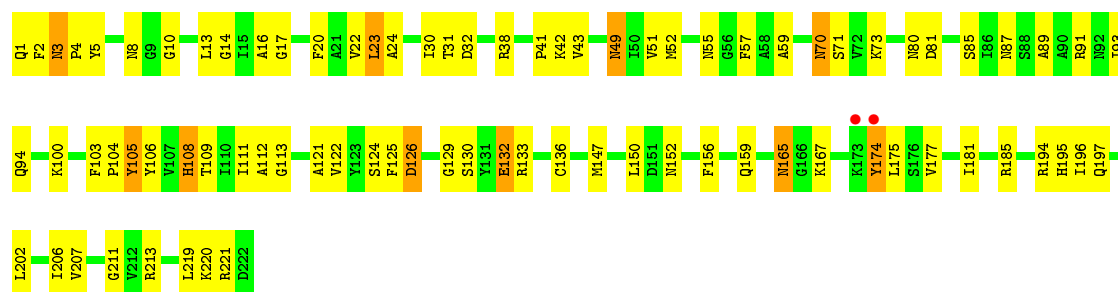


• Molecule 11: Proteasome component PRE2

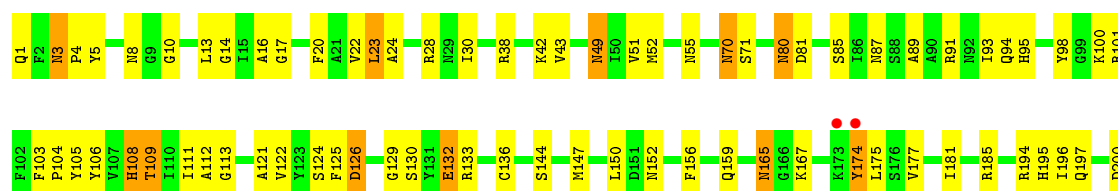
Chain Y:



• Molecule 12: Proteasome component C5



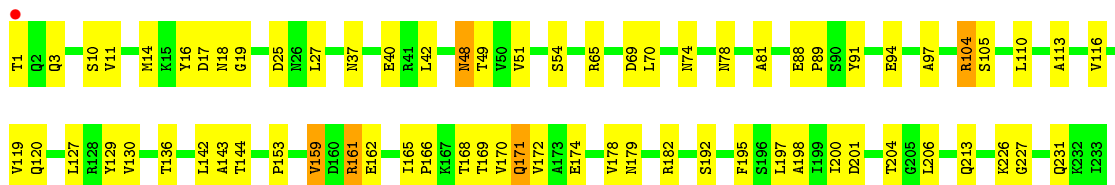
• Molecule 12: Proteasome component C5





- Molecule 13: Proteasome component PRE4

Chain M: 70% 28%



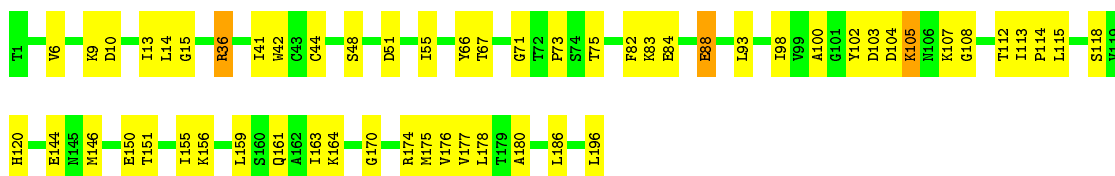
- Molecule 13: Proteasome component PRE4

Chain a: 94% 6%



- Molecule 14: Proteasome component PRE3

Chain N: 71% 27%



- Molecule 14: Proteasome component PRE3

Chain b: 96%



- Molecule 15: Cepafungin I

Chain c: 100%

There are no outlier residues recorded for this chain.

- Molecule 15: Cepafungin I

Chain d: 100%

There are no outlier residues recorded for this chain.

- Molecule 15: Cepafungin I

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 15: Cepafungin I

Chain f:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.68Å 301.02Å 144.83Å 90.00° 112.86° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 24.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-2.80) 98.1 (24.96-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.80Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.214 , 0.244 0.214 , 0.214	Depositor DCC
R_{free} test set	12755 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 256455 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	51020	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 0W6, 0W5, LYO

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	0.37	0/1952	0.63	0/2642
1	O	0.38	0/1952	0.63	0/2642
2	B	0.37	0/1935	0.63	0/2618
2	P	0.38	0/1935	0.63	0/2618
3	C	0.35	0/1920	0.62	0/2598
3	Q	0.36	0/1920	0.62	0/2598
4	D	0.35	0/1887	0.63	0/2541
4	R	0.36	0/1887	0.63	0/2541
5	E	0.35	0/1823	0.60	0/2463
5	S	0.35	0/1823	0.60	0/2463
6	F	0.38	0/1937	0.61	0/2614
6	T	0.37	0/1937	0.62	0/2614
7	G	0.40	0/1959	0.63	0/2652
7	U	0.39	0/1959	0.62	0/2652
8	H	0.38	0/1716	0.66	0/2326
8	V	0.37	0/1716	0.66	0/2326
9	I	0.38	0/1611	0.65	0/2174
9	W	0.39	0/1611	0.66	0/2174
10	J	0.39	0/1613	0.64	0/2173
10	X	0.40	0/1613	0.65	0/2173
11	K	0.40	0/1681	0.67	1/2274 (0.0%)
11	Y	0.40	0/1681	0.67	1/2274 (0.0%)
12	L	0.39	0/1795	0.66	1/2420 (0.0%)
12	Z	0.39	0/1795	0.67	0/2420
13	M	0.39	0/1855	0.65	1/2514 (0.0%)
13	a	0.39	0/1855	0.66	1/2514 (0.0%)
14	N	0.40	0/1541	0.65	0/2087
14	b	0.39	0/1541	0.65	0/2087
15	c	1.45	0/6	1.00	0/7
15	d	1.58	0/6	0.69	0/7
15	e	1.53	0/6	1.01	0/7
15	f	1.38	0/6	0.86	0/7

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.38	0/50474	0.64	5/68220 (0.0%)

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	110	LEU	N-CA-C	-5.40	96.42	111.00
13	a	110	LEU	N-CA-C	-5.39	96.46	111.00
11	K	4	LEU	CA-CB-CG	5.35	127.60	115.30
11	Y	4	LEU	CA-CB-CG	5.25	127.39	115.30
12	L	105	TYR	N-CA-C	-5.16	97.06	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	174	TYR	Sidechain
12	Z	174	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1929	63	0
1	O	1915	0	1929	58	0
2	B	1905	0	1904	91	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1905	0	1904	88	0
3	C	1891	0	1903	81	0
3	Q	1891	0	1903	83	0
4	D	1862	0	1839	68	0
4	R	1862	0	1839	78	0
5	E	1795	0	1800	92	0
5	S	1795	0	1800	94	0
6	F	1897	0	1889	79	0
6	T	1897	0	1889	82	0
7	G	1921	0	1913	72	0
7	U	1921	0	1913	72	0
8	H	1685	0	1687	44	0
8	V	1685	0	1687	47	0
9	I	1581	0	1574	53	0
9	W	1581	0	1574	46	0
10	J	1585	0	1590	62	0
10	X	1585	0	1590	65	0
11	K	1644	0	1594	47	0
11	Y	1644	0	1594	49	0
12	L	1757	0	1711	62	0
12	Z	1757	0	1711	65	0
13	M	1824	0	1832	56	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	37	0
14	b	1512	0	1481	0	0
15	c	38	0	43	0	0
15	d	38	0	43	0	0
15	e	38	0	43	0	0
15	f	38	0	43	0	0
16	A	55	0	0	5	0
16	B	37	0	0	5	0
16	C	41	0	0	3	0
16	D	40	0	0	5	0
16	E	23	0	0	6	0
16	F	46	0	0	3	0
16	G	59	0	0	1	0
16	H	53	0	0	4	0
16	I	68	0	0	5	0
16	J	51	0	0	2	0
16	K	43	0	0	2	0
16	L	58	0	0	2	0
16	M	71	0	0	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	N	58	0	0	2	0
16	O	33	0	0	1	0
16	P	27	0	0	3	0
16	Q	26	0	0	3	0
16	R	28	0	0	5	0
16	S	21	0	0	2	0
16	T	38	0	0	6	0
16	U	62	0	0	3	0
16	V	47	0	0	3	0
16	W	57	0	0	2	0
16	X	47	0	0	3	0
16	Y	41	0	0	4	0
16	Z	55	0	0	2	0
16	a	74	0	0	0	0
16	b	60	0	0	0	0
16	f	1	0	0	0	0
All	All	51020	0	49464	1572	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 17.

All (1572) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:107:LYS:H	11:Y:107:LYS:HD2	1.04	1.19
11:K:107:LYS:H	11:K:107:LYS:HD2	1.04	1.16
12:L:52:MET:HB2	12:L:111:ILE:HG22	1.34	1.10
1:A:176:GLU:HG2	2:B:55:LEU:HD21	1.15	1.08
12:Z:52:MET:HB2	12:Z:111:ILE:HG22	1.32	1.06
2:P:200:THR:HG22	2:P:202:SER:H	1.17	1.05
2:B:200:THR:HG22	2:B:202:SER:H	1.18	1.04
12:Z:13:LEU:HD11	12:Z:150:LEU:HD21	1.40	1.03
12:L:13:LEU:HD11	12:L:150:LEU:HD21	1.40	1.02
5:E:12:PHE:HB2	6:F:19:GLN:HE22	1.23	1.01
10:J:1:MET:HG2	10:J:2:ASP:H	1.30	0.97
10:X:1:MET:HG2	10:X:2:ASP:H	1.30	0.96
1:O:176:GLU:HG2	2:P:55:LEU:HD21	1.47	0.95
2:P:69:ASN:ND2	2:P:70:ASP:H	1.65	0.95
13:M:179:ASN:HD22	13:M:182:ARG:HH11	0.98	0.95
7:G:92:ALA:HA	7:G:103:MET:HE2	1.48	0.95
1:A:128:ARG:HH21	7:G:120:THR:HG22	1.32	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:128:ARG:HH21	7:U:120:THR:HG22	1.31	0.93
5:S:178:PHE:HA	5:S:181:ILE:HG12	1.51	0.93
2:B:69:ASN:ND2	2:B:70:ASP:H	1.66	0.92
5:S:12:PHE:HB2	6:T:19:GLN:HE22	1.34	0.90
2:P:49:ARG:HH22	2:P:61:SER:HB3	1.36	0.90
3:Q:60:SER:HB2	16:Q:303:HOH:O	1.71	0.89
2:B:49:ARG:HH22	2:B:61:SER:HB3	1.36	0.89
5:E:178:PHE:HA	5:E:181:ILE:HG12	1.52	0.89
11:K:40:PHE:HB3	11:K:73:ARG:HH21	1.38	0.89
9:I:14:MET:HE3	9:I:166:ILE:HG12	1.54	0.88
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.40	0.87
11:Y:107:LYS:N	11:Y:107:LYS:HD2	1.89	0.87
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.39	0.87
11:Y:40:PHE:HB3	11:Y:73:ARG:HH21	1.40	0.86
3:C:160:GLN:HA	3:C:160:GLN:HE21	1.40	0.85
5:E:205:LEU:HA	5:E:209:ASN:HD22	1.41	0.85
1:O:128:ARG:HH21	7:U:120:THR:CG2	1.90	0.85
13:M:119:VAL:HG23	13:M:200:ILE:HG22	1.58	0.84
11:K:107:LYS:N	11:K:107:LYS:HD2	1.90	0.84
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.23	0.84
3:C:185:THR:HG22	3:C:187:GLU:H	1.43	0.84
5:E:205:LEU:HA	5:E:209:ASN:ND2	1.93	0.84
5:S:205:LEU:HA	5:S:209:ASN:HD22	1.40	0.84
5:S:205:LEU:HA	5:S:209:ASN:ND2	1.92	0.83
7:G:55:LEU:O	7:G:57:PRO:HD3	1.79	0.83
1:A:176:GLU:CG	2:B:55:LEU:HD21	2.06	0.82
10:X:162:LYS:O	10:X:166:GLN:HG3	1.79	0.82
13:M:161:ARG:HG3	13:M:161:ARG:HH11	1.45	0.82
6:T:91:GLU:HG2	6:T:111:ARG:HB3	1.61	0.82
13:M:48:ASN:H	13:M:48:ASN:HD22	1.26	0.82
5:E:205:LEU:H	5:E:205:LEU:HD23	1.45	0.81
1:O:12:PHE:H	2:P:20:GLN:HE22	1.24	0.81
5:S:205:LEU:HD23	5:S:205:LEU:H	1.45	0.81
10:J:162:LYS:O	10:J:166:GLN:HG3	1.80	0.81
7:U:55:LEU:O	7:U:57:PRO:HD3	1.81	0.81
1:A:128:ARG:HH21	7:G:120:THR:CG2	1.94	0.81
2:P:122:THR:HG22	3:Q:125:ARG:HH21	1.45	0.81
2:B:223:GLU:HG2	2:B:224:VAL:H	1.44	0.81
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.46	0.80
5:E:162:ALA:HB3	16:E:320:HOH:O	1.80	0.80
7:U:63:ILE:HD12	7:U:215:GLU:HG2	1.61	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:THR:HG22	3:C:125:ARG:HH21	1.46	0.80
3:Q:233:GLN:O	3:Q:237:GLU:HG2	1.82	0.80
2:P:223:GLU:HG2	2:P:224:VAL:H	1.46	0.80
6:F:91:GLU:HG2	6:F:111:ARG:HB3	1.64	0.79
5:S:200:LEU:HD11	5:S:205:LEU:HD22	1.63	0.79
10:X:33:ASP:OD2	10:X:35:THR:HG22	1.83	0.79
3:C:233:GLN:O	3:C:237:GLU:HG2	1.83	0.79
7:G:202:ILE:HG23	7:G:207:THR:O	1.82	0.78
1:A:29:LYS:HA	1:A:29:LYS:HE2	1.65	0.78
3:C:169:VAL:HG23	3:C:196:SER:HB2	1.66	0.78
2:B:12:PHE:H	3:C:17:GLN:HE22	1.28	0.78
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.48	0.78
7:U:221:LYS:HE3	7:U:221:LYS:HA	1.65	0.78
6:T:34:ILE:HG22	6:T:160:ALA:CB	2.14	0.78
11:Y:107:LYS:H	11:Y:107:LYS:CD	1.88	0.78
12:L:195:HIS:HD2	12:L:197:GLN:H	1.31	0.78
7:G:221:LYS:HE3	7:G:221:LYS:HA	1.66	0.78
5:E:200:LEU:HD11	5:E:205:LEU:HD22	1.65	0.78
1:O:122:THR:CG2	2:P:128:ARG:HH21	1.96	0.78
1:A:239:THR:OG1	1:A:242:GLU:HG3	1.85	0.77
1:O:29:LYS:HE2	1:O:29:LYS:HA	1.66	0.77
3:Q:169:VAL:HG23	3:Q:196:SER:HB2	1.65	0.77
7:U:103:MET:HE3	7:U:108:LEU:HD13	1.67	0.77
2:B:200:THR:HG22	2:B:202:SER:N	1.99	0.77
4:R:159:TYR:CE2	4:R:162:LYS:HD3	2.20	0.77
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.68	0.76
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.66	0.76
6:F:31:THR:HG21	6:F:47:GLU:O	1.84	0.76
3:C:204:GLY:HA3	3:C:207:ASN:HB2	1.66	0.76
4:D:159:TYR:CE2	4:D:162:LYS:HD3	2.21	0.76
1:A:122:THR:CG2	2:B:128:ARG:HH21	1.99	0.76
5:E:12:PHE:HB2	6:F:19:GLN:NE2	2.00	0.76
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.30	0.75
2:P:200:THR:HG22	2:P:202:SER:N	1.99	0.75
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.67	0.75
7:U:202:ILE:HG23	7:U:207:THR:O	1.85	0.75
1:A:12:PHE:H	2:B:20:GLN:HE22	1.31	0.75
10:X:149:ARG:O	10:X:152:MET:HG3	1.87	0.75
6:T:31:THR:HG21	6:T:47:GLU:O	1.84	0.75
10:J:33:ASP:OD2	10:J:35:THR:HG22	1.85	0.75
7:G:63:ILE:HD12	7:G:215:GLU:HG2	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:34:ILE:HG22	6:F:160:ALA:CB	2.17	0.75
3:Q:95:ARG:NH1	3:Q:101:PRO:HB3	2.01	0.75
1:O:239:THR:OG1	1:O:242:GLU:HG3	1.86	0.75
10:J:149:ARG:O	10:J:152:MET:HG3	1.87	0.75
11:K:64:ARG:HD2	16:K:330:HOH:O	1.87	0.74
6:F:65:VAL:HG12	16:F:308:HOH:O	1.86	0.74
3:C:95:ARG:NH1	3:C:101:PRO:HB3	2.03	0.74
8:V:52:THR:O	8:V:56:THR:HB	1.87	0.74
5:S:197:SER:HA	5:S:200:LEU:HG	1.69	0.74
9:W:14:MET:HE3	9:W:166:ILE:HG12	1.70	0.74
12:L:17:GLY:HA3	12:L:20:PHE:CE2	2.23	0.74
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.35	0.74
3:Q:204:GLY:HA3	3:Q:207:ASN:HB2	1.67	0.74
12:Z:17:GLY:HA3	12:Z:20:PHE:CE2	2.22	0.74
5:S:136:TYR:CE2	5:S:217:LYS:HA	2.23	0.74
7:G:117:GLN:O	7:G:120:THR:HB	1.88	0.74
4:R:122:GLU:HG2	4:R:123:GLU:H	1.51	0.74
3:Q:161:THR:HG21	3:Q:169:VAL:HG13	1.71	0.73
7:U:117:GLN:O	7:U:120:THR:HB	1.89	0.73
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.33	0.73
13:M:179:ASN:HD22	13:M:182:ARG:NH1	1.81	0.73
2:B:122:THR:CG2	3:C:125:ARG:HH21	2.02	0.73
1:A:178:ARG:HB3	1:A:178:ARG:NH1	2.04	0.73
5:E:136:TYR:CE2	5:E:217:LYS:HA	2.23	0.73
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.71	0.73
1:A:17:LYS:HE3	1:A:22:ASP:OD1	1.89	0.73
1:O:178:ARG:HB3	1:O:178:ARG:NH1	2.03	0.73
13:M:89:PRO:HD2	13:M:120:GLN:OE1	1.88	0.73
3:Q:64:LYS:HE3	3:Q:219:ILE:HD12	1.70	0.73
8:H:52:THR:O	8:H:56:THR:HB	1.87	0.73
3:C:9:PHE:H	4:D:15:GLN:HE22	1.36	0.72
4:D:122:GLU:HG2	4:D:123:GLU:H	1.52	0.72
2:P:69:ASN:ND2	2:P:70:ASP:N	2.37	0.72
2:B:48:GLU:OE2	2:B:200:THR:HG23	1.89	0.72
9:W:35:VAL:HG13	16:X:224:HOH:O	1.89	0.72
6:T:65:VAL:HG12	16:T:324:HOH:O	1.90	0.72
11:Y:12:ILE:HB	11:Y:180:VAL:HB	1.73	0.71
3:C:161:THR:HG21	3:C:169:VAL:HG13	1.72	0.71
1:O:83:ARG:HE	7:U:114:ASN:HD21	1.38	0.71
5:S:81:ARG:HG3	5:S:81:ARG:HH11	1.54	0.71
3:C:64:LYS:HE3	3:C:219:ILE:HD12	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:197:SER:HA	5:E:200:LEU:HG	1.71	0.71
5:E:81:ARG:HG3	5:E:81:ARG:HH11	1.55	0.71
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.53	0.71
6:T:143:HIS:HD2	16:T:301:HOH:O	1.72	0.71
11:K:12:ILE:HB	11:K:180:VAL:HB	1.72	0.71
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.27	0.70
2:P:48:GLU:OE2	2:P:200:THR:HG23	1.89	0.70
4:R:161:ALA:HB3	5:S:55:LEU:HD23	1.73	0.70
1:A:187:ASP:O	1:A:191:ILE:HG12	1.91	0.70
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.27	0.70
5:E:99:ASN:HB2	13:M:94:GLU:HG2	1.74	0.70
1:O:187:ASP:O	1:O:191:ILE:HG12	1.92	0.70
2:B:69:ASN:ND2	2:B:70:ASP:N	2.39	0.70
6:T:75:SER:HA	16:T:334:HOH:O	1.91	0.70
8:V:195:VAL:HG23	16:V:321:HOH:O	1.92	0.69
2:P:141:ASP:OD2	10:X:110:LYS:HE2	1.91	0.69
3:Q:213:VAL:HG23	3:Q:219:ILE:HG12	1.75	0.69
4:D:176:LEU:HD22	5:E:55:LEU:HD11	1.75	0.69
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.74	0.69
4:D:60:VAL:HG21	4:D:81:ILE:HD13	1.74	0.69
4:R:60:VAL:HG21	4:R:81:ILE:HD13	1.74	0.69
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.72	0.69
3:C:213:VAL:HG23	3:C:219:ILE:HG12	1.75	0.69
2:P:69:ASN:HD22	2:P:70:ASP:N	1.90	0.69
4:R:64:ARG:HG3	16:R:328:HOH:O	1.92	0.69
1:O:83:ARG:HE	7:U:114:ASN:ND2	1.90	0.68
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.75	0.68
3:C:157:TRP:CE2	4:D:51:LEU:HD23	2.29	0.68
3:C:160:GLN:CA	3:C:160:GLN:HE21	2.06	0.68
4:R:191:LEU:O	4:R:195:ILE:HG12	1.93	0.68
2:B:69:ASN:HD22	2:B:70:ASP:N	1.92	0.68
7:U:34:LEU:HD23	7:U:201:MET:HE3	1.76	0.68
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.74	0.68
12:L:126:ASP:HB2	12:L:130:SER:H	1.57	0.68
2:B:38:MET:HE3	16:B:301:HOH:O	1.94	0.68
1:O:178:ARG:HB3	1:O:178:ARG:HH11	1.59	0.67
12:Z:126:ASP:HB2	12:Z:130:SER:H	1.59	0.67
2:P:122:THR:CG2	3:Q:125:ARG:HH21	2.07	0.67
1:A:178:ARG:HH11	1:A:178:ARG:HB3	1.60	0.67
1:O:82:TYR:O	1:O:86:VAL:HG23	1.95	0.67
1:O:17:LYS:HE3	1:O:22:ASP:OD1	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:12:PHE:HB2	6:T:19:GLN:NE2	2.07	0.67
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.43	0.67
7:G:30:ASN:HD22	7:G:164:PRO:HG2	1.58	0.67
2:P:85:ILE:O	2:P:89:THR:HG23	1.95	0.67
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.60	0.67
5:S:181:ILE:CG2	5:S:187:GLU:HB2	2.25	0.67
4:R:185:LEU:O	4:R:189:GLU:HG3	1.95	0.67
5:E:172:GLU:OE1	6:F:52:SER:HB2	1.94	0.67
1:A:83:ARG:HE	7:G:114:ASN:HD21	1.43	0.67
4:R:45:ARG:O	4:R:45:ARG:HG2	1.95	0.67
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.05	0.66
11:K:196:LEU:O	11:K:200:VAL:HG23	1.95	0.66
13:M:27:LEU:HB2	13:M:192:SER:HB2	1.76	0.66
2:P:184:LYS:HD3	2:P:185:VAL:N	2.10	0.66
5:E:181:ILE:CG2	5:E:187:GLU:HB2	2.25	0.66
13:M:179:ASN:ND2	13:M:182:ARG:HH11	1.83	0.66
7:G:92:ALA:CA	7:G:103:MET:HE2	2.22	0.66
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.61	0.66
4:D:191:LEU:O	4:D:195:ILE:HG12	1.95	0.66
13:M:16:TYR:CE2	13:M:170:VAL:HG22	2.30	0.66
7:G:34:LEU:HD23	7:G:201:MET:HE3	1.76	0.66
2:B:184:LYS:HD3	2:B:185:VAL:N	2.10	0.66
7:U:30:ASN:HD22	7:U:164:PRO:HG2	1.61	0.66
11:K:107:LYS:H	11:K:107:LYS:CD	1.88	0.66
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.77	0.66
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.78	0.66
3:Q:157:TRP:CE2	4:R:51:LEU:HD23	2.31	0.66
11:Y:196:LEU:O	11:Y:200:VAL:HG23	1.95	0.66
1:A:82:TYR:O	1:A:86:VAL:HG23	1.96	0.66
2:P:119:GLN:O	2:P:122:THR:HB	1.95	0.65
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.78	0.65
3:C:185:THR:HB	3:C:188:GLU:HG2	1.79	0.65
2:B:119:GLN:O	2:B:122:THR:HB	1.97	0.65
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.78	0.65
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.62	0.65
8:H:81:GLN:O	8:H:85:GLN:HG3	1.95	0.65
2:B:85:ILE:O	2:B:89:THR:HG23	1.97	0.65
3:C:51:LYS:O	3:C:52:LEU:HB2	1.97	0.65
12:L:100:LYS:HE3	12:L:103:PHE:O	1.96	0.65
2:B:141:ASP:OD2	10:J:110:LYS:HE2	1.98	0.64
7:G:73:VAL:CG1	7:G:133:THR:HB	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLN:O	1:A:122:THR:HB	1.97	0.64
1:A:83:ARG:HE	7:G:114:ASN:ND2	1.95	0.64
9:I:14:MET:CE	9:I:166:ILE:HG12	2.27	0.64
12:L:206:ILE:HD12	12:L:206:ILE:N	2.13	0.64
12:Z:206:ILE:HD12	12:Z:206:ILE:N	2.13	0.64
12:Z:52:MET:CB	12:Z:111:ILE:HG22	2.18	0.64
12:Z:100:LYS:HE3	12:Z:103:PHE:O	1.96	0.64
9:W:52:ILE:HB	9:W:59:VAL:HG13	1.78	0.64
8:V:81:GLN:O	8:V:85:GLN:HG3	1.97	0.64
2:B:148:TYR:CZ	3:C:57:ILE:HG13	2.33	0.64
5:E:178:PHE:HA	5:E:181:ILE:CG1	2.27	0.64
4:R:16:VAL:O	4:R:19:SER:HB3	1.98	0.64
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.79	0.64
9:I:97:ARG:HD2	16:I:364:HOH:O	1.98	0.64
5:S:189:ILE:HG23	5:S:212:ILE:HG21	1.80	0.64
10:X:1:MET:HG2	10:X:2:ASP:N	2.08	0.64
8:V:218:VAL:HB	9:W:194:VAL:HB	1.80	0.64
5:S:178:PHE:HA	5:S:181:ILE:CG1	2.27	0.63
9:W:14:MET:HE1	9:W:166:ILE:HA	1.79	0.63
11:Y:99:THR:HG22	11:Y:115:VAL:O	1.98	0.63
7:G:187:GLU:HG2	7:G:192:LYS:CB	2.28	0.63
4:D:185:LEU:O	4:D:189:GLU:HG3	1.99	0.63
2:B:55:LEU:HD22	2:B:55:LEU:N	2.13	0.63
7:U:73:VAL:CG1	7:U:133:THR:HB	2.28	0.63
10:X:1:MET:CG	10:X:2:ASP:H	2.09	0.63
5:S:189:ILE:O	5:S:193:VAL:HG23	1.97	0.63
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.79	0.63
11:Y:145:LYS:HB2	11:Y:148:LEU:CD1	2.28	0.63
1:O:119:GLN:O	1:O:122:THR:HB	1.98	0.63
5:S:172:GLU:OE1	6:T:52:SER:HB2	1.99	0.63
5:S:179:ILE:O	5:S:179:ILE:HD13	1.98	0.63
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.79	0.63
4:D:16:VAL:O	4:D:19:SER:HB3	1.98	0.63
12:L:103:PHE:N	12:L:104:PRO:HD3	2.14	0.63
12:L:22:VAL:HG12	12:L:206:ILE:HG13	1.80	0.63
5:E:189:ILE:O	5:E:193:VAL:HG23	1.99	0.63
10:X:39:SER:HB2	10:X:40:PRO:HD2	1.80	0.63
9:W:171:LEU:HD11	9:W:201:MET:HB3	1.81	0.63
10:J:158:LEU:HD13	10:J:198:GLN:HE22	1.64	0.63
12:Z:103:PHE:N	12:Z:104:PRO:HD3	2.13	0.63
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:179:ILE:O	5:E:179:ILE:HD13	1.99	0.62
8:H:167:LEU:HD22	12:Z:196:ILE:O	1.99	0.62
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.98	0.62
12:L:24:ALA:HB1	12:L:202:LEU:HD11	1.82	0.62
10:J:153:THR:OG1	10:J:156:GLU:HG3	1.99	0.62
4:D:45:ARG:O	4:D:45:ARG:HG2	1.98	0.62
7:G:73:VAL:HG12	7:G:133:THR:HB	1.82	0.62
2:P:99:LYS:NZ	10:X:86:GLN:HE22	1.98	0.62
10:X:119:ILE:HG12	10:X:125:LYS:HG3	1.81	0.62
2:P:119:GLN:HG3	3:Q:78:ALA:HB1	1.82	0.62
4:D:6:THR:HG23	5:E:20:GLN:NE2	2.15	0.62
12:Z:22:VAL:HG12	12:Z:206:ILE:HG13	1.81	0.62
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.81	0.62
9:I:36:SER:HB2	10:J:126:VAL:HG21	1.81	0.62
2:P:55:LEU:N	2:P:55:LEU:HD22	2.15	0.62
10:X:158:LEU:HD13	10:X:198:GLN:HE22	1.63	0.62
4:R:193:LEU:HD22	4:R:211:LEU:HD11	1.80	0.62
9:W:14:MET:CE	9:W:166:ILE:HG12	2.29	0.62
9:I:171:LEU:HD11	9:I:201:MET:HB3	1.82	0.62
1:A:169:VAL:HG23	16:A:317:HOH:O	1.99	0.62
10:X:53:THR:HG23	10:X:54:VAL:N	2.15	0.62
5:S:154:GLU:OE2	6:T:59:LYS:HD2	2.00	0.62
5:E:69:MET:HE2	5:E:104:VAL:HA	1.82	0.62
2:P:93:HIS:HB2	16:P:304:HOH:O	2.00	0.62
6:F:66:VAL:HB	6:F:70:ILE:HB	1.82	0.62
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.81	0.62
5:E:189:ILE:HG23	5:E:212:ILE:HG21	1.81	0.61
10:X:15:LEU:HD12	10:X:43:LEU:HD23	1.82	0.61
11:K:145:LYS:HB2	11:K:148:LEU:CD1	2.30	0.61
5:S:207:VAL:HG13	5:S:208:ASP:N	2.15	0.61
10:J:1:MET:HG2	10:J:2:ASP:N	2.08	0.61
10:J:39:SER:HB2	10:J:40:PRO:HD2	1.82	0.61
4:D:241:ALA:O	4:D:242:GLU:HB2	2.00	0.61
6:F:33:SER:HB3	6:F:46:VAL:HG23	1.81	0.61
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.81	0.61
11:K:99:THR:HG22	11:K:115:VAL:O	2.01	0.61
7:U:83:ASN:C	7:U:83:ASN:HD22	2.02	0.61
5:S:200:LEU:O	5:S:201:ARG:HB2	2.00	0.61
12:L:52:MET:CB	12:L:111:ILE:HG22	2.19	0.61
5:E:205:LEU:H	5:E:205:LEU:CD2	2.14	0.61
5:E:77:ALA:HB3	5:E:78:PRO:HD3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.81	0.61
10:J:117:TYR:CE1	10:J:127:GLU:HG3	2.35	0.61
5:S:77:ALA:HB3	5:S:78:PRO:HD3	1.82	0.61
5:S:205:LEU:H	5:S:205:LEU:CD2	2.14	0.61
10:J:53:THR:HG23	10:J:54:VAL:N	2.13	0.61
4:R:241:ALA:O	4:R:242:GLU:HB2	1.99	0.61
4:R:89:VAL:HG21	11:Y:65:LEU:HD22	1.83	0.61
6:T:66:VAL:HB	6:T:70:ILE:HB	1.82	0.61
2:P:244:THR:OXT	2:P:244:THR:HG22	2.00	0.61
1:O:158:PRO:O	2:P:56:LEU:HD12	2.01	0.61
5:E:207:VAL:HG13	5:E:208:ASP:N	2.16	0.61
1:A:30:GLN:HA	1:A:30:GLN:HE21	1.65	0.61
7:U:73:VAL:HG12	7:U:133:THR:HB	1.81	0.61
6:T:33:SER:HB3	6:T:46:VAL:HG23	1.81	0.61
1:O:30:GLN:HE21	1:O:30:GLN:HA	1.65	0.61
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.31	0.60
10:X:117:TYR:CE1	10:X:127:GLU:HG3	2.36	0.60
4:R:113:LEU:HB2	16:R:317:HOH:O	2.01	0.60
13:M:51:VAL:HG22	13:M:116:VAL:HG22	1.83	0.60
5:E:55:LEU:HD12	5:E:55:LEU:N	2.16	0.60
12:L:30:ILE:HD12	12:L:30:ILE:C	2.22	0.60
12:Z:24:ALA:HB1	12:Z:202:LEU:HD11	1.82	0.60
4:D:89:VAL:HG11	11:K:65:LEU:CD2	2.32	0.60
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.84	0.60
4:R:89:VAL:HG11	11:Y:65:LEU:CD2	2.32	0.60
3:Q:165:ASN:HB2	3:Q:200:VAL:HG11	1.84	0.60
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.83	0.60
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.81	0.60
1:A:172:LYS:O	1:A:176:GLU:HG3	2.02	0.60
5:S:55:LEU:N	5:S:55:LEU:HD12	2.17	0.60
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.30	0.60
9:I:52:ILE:HB	9:I:59:VAL:HG13	1.82	0.60
2:B:220:ASN:O	2:B:221:ASP:HB2	2.01	0.60
5:E:200:LEU:O	5:E:201:ARG:HB2	2.01	0.60
5:S:127:TYR:O	5:S:148:PRO:HB3	2.02	0.60
14:N:114:PRO:HD2	14:N:118:SER:O	2.02	0.60
7:U:241:GLU:O	7:U:242:GLN:HB2	2.02	0.60
2:B:223:GLU:HG2	2:B:224:VAL:N	2.17	0.59
3:C:35:LYS:HD3	3:C:158:SER:HA	1.84	0.59
5:E:205:LEU:N	5:E:205:LEU:HD23	2.17	0.59
11:Y:31:VAL:HA	12:Z:132:GLU:OE2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:193:LEU:HD22	4:D:211:LEU:HD11	1.83	0.59
7:U:169:ILE:HD12	7:U:201:MET:CE	2.32	0.59
8:H:34:LEU:HB2	16:H:326:HOH:O	2.02	0.59
8:H:195:VAL:HA	16:H:348:HOH:O	2.01	0.59
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.32	0.59
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.01	0.59
10:X:153:THR:OG1	10:X:156:GLU:HG3	2.03	0.59
3:Q:35:LYS:HD3	3:Q:158:SER:HA	1.85	0.59
16:B:319:HOH:O	3:C:27:ARG:HD2	2.02	0.59
10:J:15:LEU:HD12	10:J:43:LEU:HD23	1.83	0.59
3:C:155:SER:HB2	4:D:51:LEU:HD21	1.84	0.59
12:Z:14:GLY:O	12:Z:136:CYS:HA	2.02	0.59
13:M:174:GLU:O	13:M:178:VAL:HG23	2.03	0.59
4:D:89:VAL:HG21	11:K:65:LEU:HD22	1.83	0.59
7:G:241:GLU:O	7:G:242:GLN:HB2	2.03	0.59
7:U:167:GLN:NE2	7:U:171:THR:HG23	2.18	0.59
3:C:165:ASN:HB2	3:C:200:VAL:HG11	1.84	0.59
5:E:45:LEU:HG	5:E:134:ILE:HD13	1.85	0.59
2:B:244:THR:HG22	2:B:244:THR:OXT	2.03	0.59
7:G:167:GLN:NE2	7:G:171:THR:HG23	2.17	0.59
2:P:220:ASN:O	2:P:221:ASP:HB2	2.02	0.59
12:Z:30:ILE:HD12	12:Z:30:ILE:C	2.23	0.59
3:C:172:PHE:O	3:C:176:ASN:HB2	2.03	0.58
9:W:36:SER:HB2	10:X:126:VAL:HG21	1.84	0.58
11:K:106:ARG:HD3	11:K:182:GLU:OE1	2.03	0.58
7:U:51:PRO:HG2	7:U:52:ASP:H	1.67	0.58
9:W:17:LYS:HD3	9:W:156:ASN:HD22	1.68	0.58
6:F:105:ILE:HG21	6:F:143:HIS:HB2	1.85	0.58
1:O:172:LYS:O	1:O:176:GLU:HG3	2.03	0.58
12:Z:202:LEU:HB2	12:Z:219:LEU:HD11	1.85	0.58
1:O:66:LEU:C	1:O:66:LEU:HD23	2.24	0.58
11:Y:106:ARG:HD3	11:Y:182:GLU:OE1	2.03	0.58
3:C:34:VAL:HG12	3:C:159:ALA:HB1	1.85	0.58
1:A:66:LEU:HD23	1:A:66:LEU:C	2.23	0.58
7:G:169:ILE:HD12	7:G:201:MET:CE	2.33	0.58
2:P:99:LYS:HZ2	10:X:86:GLN:HE22	1.51	0.58
14:N:66:TYR:CD2	14:N:73:PRO:HB3	2.39	0.58
3:Q:167:LYS:HB2	16:Q:313:HOH:O	2.02	0.58
11:Y:7:ARG:HG2	11:Y:110:PRO:HB2	1.84	0.58
6:T:105:ILE:HG21	6:T:143:HIS:HB2	1.85	0.58
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:123:PHE:N	9:I:123:PHE:CD2	2.72	0.58
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.85	0.58
9:W:50:LEU:CD2	9:W:52:ILE:HD11	2.34	0.58
12:L:2:PHE:HB2	13:M:1:THR:HG23	1.86	0.58
12:L:14:GLY:O	12:L:136:CYS:HA	2.03	0.58
13:M:49:THR:OG1	13:M:89:PRO:HG3	2.04	0.58
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.04	0.58
1:A:204:PHE:CE1	1:A:209:ILE:HD11	2.39	0.58
1:O:128:ARG:NH2	7:U:120:THR:HG22	2.12	0.57
12:L:202:LEU:HB2	12:L:219:LEU:HD11	1.85	0.57
3:Q:34:VAL:HG12	3:Q:159:ALA:HB1	1.86	0.57
7:G:189:SER:HB2	7:G:191:GLU:OE2	2.03	0.57
7:G:39:LYS:HB2	7:G:187:GLU:O	2.03	0.57
14:N:14:LEU:O	14:N:175:MET:HA	2.03	0.57
16:E:319:HOH:O	12:L:73:LYS:HE3	2.04	0.57
1:O:246:ARG:HH11	1:O:246:ARG:HG3	1.69	0.57
7:G:51:PRO:HG2	7:G:52:ASP:H	1.68	0.57
3:Q:51:LYS:HD2	3:Q:52:LEU:N	2.19	0.57
2:B:124:HIS:HB3	3:C:124:VAL:HG12	1.87	0.57
10:J:119:ILE:HG12	10:J:125:LYS:HG3	1.85	0.57
7:U:39:LYS:HB2	7:U:187:GLU:O	2.05	0.57
11:K:31:VAL:HA	12:L:132:GLU:OE2	2.04	0.57
10:J:53:THR:CG2	10:J:54:VAL:N	2.66	0.57
5:E:127:TYR:O	5:E:148:PRO:HB3	2.03	0.57
6:T:185:ALA:O	6:T:189:VAL:HG23	2.04	0.57
7:G:83:ASN:C	7:G:83:ASN:HD22	2.07	0.57
7:U:92:ALA:HA	7:U:103:MET:HE2	1.85	0.57
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.04	0.57
6:F:83:HIS:HD2	6:F:128:PHE:CE2	2.22	0.57
3:C:160:GLN:NE2	3:C:161:THR:H	2.02	0.57
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.04	0.57
2:P:119:GLN:CG	3:Q:78:ALA:HB1	2.35	0.57
6:F:32:THR:HG23	6:F:47:GLU:OE2	2.05	0.57
6:F:83:HIS:HD2	6:F:128:PHE:HE2	1.52	0.57
13:M:129:TYR:HE1	13:M:144:THR:HG22	1.69	0.57
5:S:51:ASN:ND2	5:S:53:ASP:O	2.38	0.57
10:J:19:LYS:HD3	10:J:180:ILE:HG13	1.87	0.57
5:E:181:ILE:HG21	5:E:187:GLU:HB2	1.87	0.57
2:B:44:VAL:HG22	2:B:214:THR:HG22	1.86	0.57
6:F:185:ALA:O	6:F:189:VAL:HG23	2.05	0.57
2:P:44:VAL:HG22	2:P:214:THR:HG22	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:196:ILE:O	8:V:167:LEU:HD22	2.05	0.57
3:Q:172:PHE:O	3:Q:176:ASN:HB2	2.05	0.57
3:Q:155:SER:HB2	4:R:51:LEU:HD21	1.87	0.57
6:T:83:HIS:HD2	6:T:128:PHE:HE2	1.52	0.57
11:K:7:ARG:HG2	11:K:110:PRO:HB2	1.86	0.57
2:B:49:ARG:HH22	2:B:61:SER:CB	2.14	0.56
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.40	0.56
3:C:214:LYS:HB2	3:C:218:ASP:HB3	1.87	0.56
4:D:67:GLY:HA3	4:D:220:PHE:CD2	2.40	0.56
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.87	0.56
3:Q:156:SER:HB2	16:Q:320:HOH:O	2.04	0.56
4:D:184:THR:OG1	4:D:187:GLU:HG3	2.05	0.56
9:W:50:LEU:HG	9:W:52:ILE:HD11	1.87	0.56
9:I:50:LEU:CD2	9:I:52:ILE:HD11	2.35	0.56
14:N:114:PRO:HG2	16:N:206:HOH:O	2.05	0.56
9:I:202:ARG:HD3	16:I:365:HOH:O	2.05	0.56
5:S:45:LEU:HG	5:S:134:ILE:HD13	1.86	0.56
1:O:3:ASP:OD2	1:O:5:TYR:HB2	2.05	0.56
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.87	0.56
6:T:83:HIS:HD2	6:T:128:PHE:CE2	2.23	0.56
4:R:186:LYS:O	4:R:190:LEU:HD23	2.05	0.56
2:P:239:VAL:HG12	2:P:240:LYS:HD3	1.87	0.56
5:E:154:GLU:OE2	6:F:59:LYS:HD2	2.05	0.56
6:T:148:GLU:HB3	16:T:338:HOH:O	2.03	0.56
4:D:186:LYS:O	4:D:190:LEU:HD23	2.05	0.56
13:M:19:GLY:HA3	13:M:200:ILE:O	2.04	0.56
3:C:101:PRO:HG2	3:C:138:PRO:CG	2.36	0.56
5:E:226:GLY:O	5:E:229:VAL:HG22	2.05	0.56
3:C:186:VAL:O	3:C:190:VAL:HG23	2.04	0.56
4:R:57:GLU:HA	16:R:311:HOH:O	2.04	0.56
6:F:186:ARG:HG3	6:F:186:ARG:HH11	1.71	0.56
3:C:51:LYS:HD2	3:C:52:LEU:N	2.21	0.56
13:M:119:VAL:CG2	13:M:200:ILE:HG22	2.32	0.56
3:Q:101:PRO:HG2	3:Q:138:PRO:CG	2.35	0.56
6:F:169:LYS:O	6:F:173:GLU:HG3	2.06	0.56
1:O:211:LEU:HD22	1:O:238:LEU:HD12	1.88	0.56
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.41	0.56
3:Q:214:LYS:HB2	3:Q:218:ASP:HB3	1.87	0.56
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.41	0.56
3:Q:160:GLN:NE2	3:Q:161:THR:H	2.03	0.56
2:P:119:GLN:NE2	16:P:311:HOH:O	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:189:SER:HB2	7:U:191:GLU:OE2	2.05	0.56
5:S:226:GLY:O	5:S:229:VAL:HG22	2.06	0.56
6:T:50:ILE:HG13	6:T:208:PHE:HA	1.88	0.56
6:F:220:THR:O	6:F:221:ASN:HB2	2.06	0.56
2:P:223:GLU:HG2	2:P:224:VAL:N	2.19	0.56
12:L:3:ASN:HD22	12:L:4:PRO:CD	2.18	0.56
1:O:248:GLU:C	1:O:250:LEU:H	2.09	0.56
6:T:186:ARG:HH11	6:T:186:ARG:HG3	1.70	0.56
6:T:172:LEU:O	6:T:176:VAL:HG23	2.06	0.55
10:X:53:THR:CG2	10:X:54:VAL:N	2.69	0.55
5:E:207:VAL:CG1	5:E:208:ASP:N	2.70	0.55
2:P:233:GLU:O	2:P:237:ILE:HG22	2.06	0.55
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.87	0.55
1:A:246:ARG:HG3	1:A:246:ARG:HH11	1.70	0.55
14:N:105:LYS:HD3	14:N:105:LYS:O	2.06	0.55
10:X:149:ARG:HH11	10:X:149:ARG:HG2	1.71	0.55
9:I:50:LEU:HG	9:I:52:ILE:HD11	1.89	0.55
4:R:94:TYR:O	12:Z:91:ARG:HG3	2.05	0.55
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.89	0.55
8:H:218:VAL:HB	9:I:194:VAL:HB	1.89	0.55
10:X:19:LYS:HD3	10:X:180:ILE:HG13	1.87	0.55
1:A:248:GLU:C	1:A:250:LEU:H	2.09	0.55
9:W:154:GLU:HG3	9:W:157:LEU:HD21	1.89	0.55
1:A:90:ARG:NH1	16:A:309:HOH:O	2.32	0.55
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.42	0.55
2:B:233:GLU:O	2:B:237:ILE:HG22	2.06	0.55
7:G:75:ASN:HA	16:G:344:HOH:O	2.05	0.55
2:B:119:GLN:HG3	3:C:78:ALA:HB1	1.88	0.55
4:D:176:LEU:HD22	5:E:55:LEU:CD1	2.37	0.55
3:C:197:LEU:O	3:C:201:VAL:HG23	2.06	0.55
2:P:180:LYS:HE2	2:P:182:ASP:OD1	2.07	0.55
10:J:17:SER:HB2	16:J:210:HOH:O	2.06	0.55
5:S:205:LEU:HD23	5:S:205:LEU:N	2.17	0.55
5:S:207:VAL:CG1	5:S:208:ASP:N	2.69	0.55
5:E:62:ILE:HG21	5:E:213:ALA:HB2	1.88	0.55
11:Y:78:ALA:O	11:Y:82:ILE:HG12	2.06	0.55
10:X:194:ASP:HA	10:X:196:GLN:OE1	2.06	0.55
6:T:169:LYS:O	6:T:173:GLU:HG3	2.06	0.55
10:J:174:MET:HE1	10:X:173:PRO:HB2	1.88	0.55
4:R:6:THR:HG23	5:S:20:GLN:NE2	2.22	0.55
13:M:171:GLN:NE2	13:M:171:GLN:H	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:193:VAL:O	5:E:196:ILE:HG22	2.07	0.55
9:I:17:LYS:HD3	9:I:156:ASN:HD22	1.72	0.55
2:B:180:LYS:HE2	2:B:182:ASP:OD1	2.07	0.55
1:O:28:VAL:HG13	1:O:76:SER:O	2.07	0.55
3:Q:230:TYR:O	3:Q:234:ILE:HG13	2.07	0.55
12:L:159:GLN:HG2	8:V:209:THR:HG21	1.89	0.54
2:B:239:VAL:HG12	2:B:240:LYS:HD3	1.87	0.54
3:Q:160:GLN:NE2	3:Q:160:GLN:HA	2.17	0.54
6:T:32:THR:HG23	6:T:47:GLU:OE2	2.07	0.54
12:Z:113:GLY:HA2	12:Z:207:VAL:HG11	1.90	0.54
9:W:123:PHE:N	9:W:123:PHE:CD2	2.75	0.54
14:N:6:VAL:HG23	14:N:155:ILE:HD11	1.89	0.54
4:D:104:LEU:C	4:D:104:LEU:HD13	2.27	0.54
2:P:93:HIS:CE1	2:P:113:ARG:HD3	2.42	0.54
10:J:173:PRO:HB2	10:X:174:MET:HE1	1.88	0.54
10:X:139:TYR:CE2	10:X:172:MET:HG3	2.41	0.54
12:L:121:ALA:HB2	12:L:133:ARG:NH2	2.23	0.54
4:R:32:ILE:CD1	4:R:192:VAL:HG23	2.36	0.54
12:Z:3:ASN:HD22	12:Z:4:PRO:CD	2.20	0.54
10:J:194:ASP:HA	10:J:196:GLN:OE1	2.07	0.54
7:G:155:VAL:HG22	7:G:156:GLY:N	2.23	0.54
11:Y:4:LEU:CD1	11:Y:161:ILE:HG13	2.38	0.54
4:R:67:GLY:HA3	4:R:220:PHE:CD2	2.42	0.54
1:A:211:LEU:HD22	1:A:238:LEU:HD12	1.89	0.54
16:F:305:HOH:O	7:G:82:ARG:HD2	2.08	0.54
6:F:172:LEU:O	6:F:176:VAL:HG23	2.07	0.54
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.73	0.54
1:A:46:ALA:HB2	1:A:211:LEU:HG	1.90	0.54
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.42	0.54
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.43	0.54
7:U:165:LYS:O	7:U:169:ILE:HG12	2.08	0.54
9:I:124:ASP:HB2	16:I:351:HOH:O	2.08	0.54
5:S:207:VAL:HG22	5:S:226:GLY:HA2	1.90	0.54
11:Y:111:THR:HA	16:Y:318:HOH:O	2.08	0.54
13:M:119:VAL:HG23	13:M:200:ILE:CG2	2.34	0.54
8:V:41:ILE:HG13	8:V:76:VAL:HG22	1.89	0.54
5:S:181:ILE:HG21	5:S:187:GLU:HB2	1.89	0.53
1:O:46:ALA:HB2	1:O:211:LEU:HG	1.90	0.53
3:C:35:LYS:HG2	3:C:158:SER:O	2.08	0.53
1:A:3:ASP:OD2	1:A:5:TYR:HB2	2.08	0.53
5:E:95:SER:O	5:E:99:ASN:HA	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.09	0.53
1:O:204:PHE:CE1	1:O:209:ILE:HD11	2.42	0.53
5:E:51:ASN:ND2	5:E:53:ASP:O	2.40	0.53
3:C:222:LEU:N	3:C:222:LEU:HD12	2.24	0.53
11:K:4:LEU:CD1	11:K:161:ILE:HG13	2.38	0.53
4:D:119:ALA:HA	5:E:124:GLY:HA2	1.88	0.53
10:J:139:TYR:CE2	10:J:172:MET:HG3	2.44	0.53
11:Y:111:THR:HG23	16:Y:318:HOH:O	2.09	0.53
8:H:41:ILE:HG13	8:H:76:VAL:HG22	1.90	0.53
9:W:154:GLU:CG	9:W:157:LEU:HD21	2.38	0.53
6:T:123:ASN:HD22	6:T:124:SER:N	2.06	0.53
1:O:160:LYS:HD3	1:O:179:TRP:CH2	2.44	0.53
2:B:62:THR:HG22	2:B:65:LEU:O	2.09	0.53
12:Z:3:ASN:ND2	12:Z:5:TYR:H	2.05	0.53
13:M:227:GLY:HA3	13:M:231:GLN:HB3	1.91	0.53
12:Z:121:ALA:HB2	12:Z:133:ARG:NH2	2.22	0.53
4:R:184:THR:OG1	4:R:187:GLU:HG3	2.07	0.53
2:P:162:ILE:HG13	2:P:163:SER:N	2.22	0.53
1:A:29:LYS:CE	1:A:29:LYS:HA	2.37	0.53
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.90	0.53
11:K:78:ALA:O	11:K:82:ILE:HG12	2.08	0.53
12:L:113:GLY:HA2	12:L:207:VAL:HG11	1.90	0.53
6:F:50:ILE:HG13	6:F:208:PHE:HA	1.90	0.53
2:P:49:ARG:HH22	2:P:61:SER:CB	2.14	0.53
1:O:29:LYS:CE	1:O:29:LYS:HA	2.38	0.53
1:A:94:HIS:HD2	8:H:61:SER:OG	1.91	0.53
7:G:136:SER:HA	7:G:219:ALA:HB1	1.91	0.53
1:A:234:ARG:HG2	1:A:234:ARG:HH11	1.73	0.53
2:B:93:HIS:CE1	2:B:113:ARG:HD3	2.44	0.53
5:S:193:VAL:O	5:S:196:ILE:HG22	2.09	0.53
12:L:147:MET:HE3	9:W:176:ARG:NH2	2.23	0.53
5:S:44:VAL:HG21	5:S:188:LEU:HB3	1.91	0.53
3:C:230:TYR:O	3:C:234:ILE:HG13	2.09	0.53
11:Y:66:HIS:HA	16:Y:335:HOH:O	2.09	0.53
5:E:178:PHE:CA	5:E:181:ILE:HG12	2.34	0.53
5:S:81:ARG:HG3	5:S:81:ARG:NH1	2.23	0.53
9:W:163:PHE:CE1	9:W:197:ARG:HD2	2.43	0.53
5:E:155:LEU:HD13	5:E:158:THR:HB	1.91	0.53
8:H:220:ILE:HD11	9:I:194:VAL:HG21	1.92	0.52
5:E:64:LYS:HB3	16:E:308:HOH:O	2.09	0.52
11:K:76:VAL:N	11:K:108:GLU:OE2	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:234:ARG:HH11	1:O:234:ARG:HG2	1.74	0.52
13:M:48:ASN:HD22	13:M:48:ASN:N	1.93	0.52
16:D:328:HOH:O	5:E:81:ARG:HD3	2.08	0.52
14:N:51:ASP:O	14:N:55:ILE:HG13	2.09	0.52
8:H:104:ASP:O	8:H:106:THR:N	2.42	0.52
8:H:29:LYS:HE2	12:Z:194:ARG:CZ	2.40	0.52
9:I:163:PHE:CE1	9:I:197:ARG:HD2	2.44	0.52
9:I:176:ARG:NH2	12:Z:147:MET:CE	2.72	0.52
1:A:160:LYS:HD3	1:A:179:TRP:CH2	2.43	0.52
10:J:149:ARG:HH11	10:J:149:ARG:HG2	1.73	0.52
4:R:51:LEU:HD11	4:R:56:ILE:HD11	1.91	0.52
3:Q:174:GLU:OE2	4:R:49:PRO:HD2	2.09	0.52
8:H:209:THR:HG21	12:Z:159:GLN:HG2	1.91	0.52
2:B:24:ALA:O	2:B:28:ILE:HG12	2.09	0.52
2:P:24:ALA:O	2:P:28:ILE:HG12	2.08	0.52
10:X:146:HIS:HD2	10:X:147:HIS:CE1	2.28	0.52
14:N:105:LYS:HD3	14:N:105:LYS:C	2.29	0.52
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.91	0.52
4:R:161:ALA:HB3	5:S:55:LEU:CD2	2.38	0.52
4:D:32:ILE:CD1	4:D:192:VAL:HG23	2.37	0.52
10:X:45:SER:OG	10:X:103:LEU:HB2	2.10	0.52
1:O:59:GLU:CD	1:O:59:GLU:H	2.13	0.52
14:N:161:GLN:O	14:N:164:LYS:HB3	2.10	0.52
5:S:178:PHE:CA	5:S:181:ILE:HG12	2.33	0.52
4:D:114:ARG:HG2	4:D:114:ARG:HH11	1.75	0.52
2:P:228:ILE:HD12	2:P:228:ILE:N	2.25	0.52
5:S:95:SER:O	5:S:99:ASN:HA	2.08	0.52
4:D:67:GLY:HA3	4:D:220:PHE:CE2	2.44	0.52
3:C:174:GLU:OE2	4:D:49:PRO:HD2	2.10	0.52
6:T:220:THR:O	6:T:221:ASN:HB2	2.09	0.52
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.74	0.52
10:J:1:MET:CG	10:J:2:ASP:H	2.09	0.52
2:B:119:GLN:CG	3:C:78:ALA:HB1	2.40	0.52
5:S:189:ILE:CG2	5:S:212:ILE:HD13	2.39	0.52
4:D:94:TYR:O	12:L:91:ARG:HG3	2.10	0.52
4:R:204:LEU:HD23	4:R:205:ASP:N	2.25	0.52
12:L:16:ALA:HB2	12:L:122:VAL:HG23	1.91	0.52
3:Q:172:PHE:CD2	3:Q:196:SER:HB3	2.45	0.52
5:E:214:ILE:HG12	5:E:215:VAL:N	2.25	0.52
4:D:51:LEU:HD11	4:D:56:ILE:HD11	1.91	0.52
12:Z:181:ILE:O	12:Z:185:ARG:HG3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:9:LYS:HG2	14:N:10:ASP:OD2	2.09	0.52
11:Y:147:ASP:O	11:Y:148:LEU:C	2.48	0.52
11:K:15:ALA:O	11:K:161:ILE:HD11	2.10	0.52
6:T:116:VAL:HG21	6:T:147:LEU:HD21	1.91	0.52
3:C:172:PHE:CD2	3:C:196:SER:HB3	2.46	0.51
12:L:8:ASN:HA	12:L:30:ILE:O	2.10	0.51
5:S:155:LEU:HD13	5:S:158:THR:HB	1.92	0.51
5:S:38:ARG:NH1	5:S:39:SER:O	2.42	0.51
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.75	0.51
8:H:73:GLU:OE1	8:H:73:GLU:HA	2.10	0.51
1:A:29:LYS:CA	1:A:29:LYS:HE2	2.40	0.51
8:V:18:THR:HB	8:V:30:ASN:HD22	1.76	0.51
9:I:154:GLU:CG	9:I:157:LEU:HD21	2.40	0.51
10:J:146:HIS:HD2	10:J:147:HIS:CE1	2.29	0.51
6:T:47:GLU:OE1	6:T:49:LEU:HD21	2.11	0.51
10:J:139:TYR:HE1	16:X:233:HOH:O	1.92	0.51
12:Z:152:ASN:O	12:Z:156:PHE:HA	2.10	0.51
5:S:1:PHE:O	5:S:3:ASN:N	2.44	0.51
5:E:81:ARG:HG3	5:E:81:ARG:NH1	2.24	0.51
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.91	0.51
13:M:153:PRO:HA	8:V:165:ASN:OD1	2.11	0.51
6:F:31:THR:HG23	6:F:47:GLU:HB3	1.93	0.51
14:N:175:MET:HB2	14:N:186:LEU:HB2	1.92	0.51
6:T:191:GLN:HE21	6:T:194:LYS:HE3	1.76	0.51
4:R:67:GLY:HA3	4:R:220:PHE:CE2	2.45	0.51
4:R:204:LEU:HD23	4:R:204:LEU:C	2.30	0.51
6:F:123:ASN:HD22	6:F:124:SER:N	2.08	0.51
7:U:198:ILE:HG23	7:U:214:LEU:HD11	1.92	0.51
6:T:105:ILE:N	6:T:105:ILE:HD12	2.25	0.51
5:S:214:ILE:HG12	5:S:215:VAL:N	2.25	0.51
1:O:30:GLN:CA	1:O:30:GLN:HE21	2.24	0.51
2:B:162:ILE:HG13	2:B:163:SER:N	2.25	0.51
2:B:217:LYS:O	2:B:218:GLY:C	2.48	0.51
12:L:147:MET:CE	9:W:176:ARG:NH2	2.74	0.51
4:R:196:LEU:O	4:R:200:MET:HG3	2.10	0.51
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.02	0.51
5:S:87:LEU:HD11	5:S:107:ALA:HB1	1.93	0.51
11:Y:32:LYS:HD2	11:Y:32:LYS:N	2.26	0.51
10:X:195:PHE:HA	10:X:198:GLN:HB2	1.93	0.51
2:P:62:THR:HG22	2:P:65:LEU:O	2.11	0.51
13:M:197:LEU:HD23	13:M:198:ALA:N	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.91	0.51
6:F:47:GLU:OE1	6:F:49:LEU:HD21	2.11	0.51
7:G:165:LYS:O	7:G:169:ILE:HG12	2.11	0.51
6:F:116:VAL:HG21	6:F:147:LEU:HD21	1.91	0.51
11:K:32:LYS:N	11:K:32:LYS:HD2	2.26	0.51
10:X:8:ARG:HH11	10:X:8:ARG:HG2	1.76	0.51
3:C:155:SER:CB	4:D:51:LEU:HD21	2.41	0.50
5:E:189:ILE:CG2	5:E:212:ILE:HD13	2.42	0.50
4:D:210:GLN:HA	16:D:319:HOH:O	2.10	0.50
5:E:90:GLN:HG3	5:E:110:LEU:HD13	1.93	0.50
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.46	0.50
6:T:39:ASN:N	6:T:39:ASN:HD22	2.09	0.50
9:W:26:LEU:HD22	9:W:40:GLU:HG2	1.93	0.50
5:E:207:VAL:HG22	5:E:226:GLY:HA2	1.92	0.50
5:E:44:VAL:HG21	5:E:188:LEU:HB3	1.94	0.50
11:Y:76:VAL:N	11:Y:108:GLU:OE2	2.44	0.50
12:L:3:ASN:ND2	12:L:5:TYR:H	2.09	0.50
2:P:217:LYS:O	2:P:218:GLY:C	2.49	0.50
9:I:154:GLU:HG3	9:I:157:LEU:HD21	1.92	0.50
3:C:7:SER:O	4:D:128:ARG:HD3	2.12	0.50
4:D:204:LEU:HD23	4:D:205:ASP:N	2.26	0.50
7:U:155:VAL:HG22	7:U:156:GLY:N	2.26	0.50
4:R:104:LEU:C	4:R:104:LEU:HD13	2.32	0.50
6:T:31:THR:HG23	6:T:47:GLU:HB3	1.94	0.50
14:N:146:MET:CE	14:N:150:GLU:HB3	2.41	0.50
10:J:173:PRO:CB	10:X:174:MET:HE1	2.41	0.50
14:N:9:LYS:O	14:N:107:LYS:HD3	2.10	0.50
5:S:36:GLY:O	5:S:157:GLY:HA2	2.10	0.50
3:Q:222:LEU:N	3:Q:222:LEU:HD12	2.27	0.50
9:I:14:MET:HE1	9:I:166:ILE:HA	1.93	0.50
6:F:49:LEU:HD13	6:F:206:LYS:HD2	1.94	0.50
5:S:189:ILE:HG23	5:S:212:ILE:HD13	1.94	0.50
6:F:105:ILE:N	6:F:105:ILE:HD12	2.26	0.50
4:D:204:LEU:HD23	4:D:204:LEU:C	2.32	0.50
5:E:174:THR:HG22	5:E:177:THR:HB	1.93	0.50
9:W:22:ILE:HG12	9:W:42:ILE:HD12	1.94	0.50
4:R:23:ILE:HD13	4:R:133:ALA:HB2	1.94	0.50
1:A:128:ARG:NH2	7:G:120:THR:HG22	2.15	0.50
7:G:198:ILE:HG23	7:G:214:LEU:HD11	1.92	0.50
10:J:174:MET:HE1	10:X:173:PRO:CB	2.41	0.50
5:E:1:PHE:O	5:E:3:ASN:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:49:LEU:HD13	6:T:206:LYS:HD2	1.92	0.50
2:B:185:VAL:O	2:B:189:ILE:HG13	2.11	0.50
5:E:38:ARG:NH1	5:E:39:SER:O	2.44	0.50
1:O:94:HIS:HD2	8:V:61:SER:OG	1.94	0.50
7:U:136:SER:HA	7:U:219:ALA:HB1	1.93	0.50
2:P:67:LYS:HG3	2:P:226:GLN:OE1	2.11	0.50
2:P:55:LEU:H	2:P:55:LEU:HD22	1.76	0.50
7:G:103:MET:HE3	7:G:108:LEU:HB2	1.93	0.50
13:M:48:ASN:ND2	13:M:48:ASN:N	2.60	0.50
9:W:50:LEU:HD21	9:W:52:ILE:HD11	1.94	0.50
16:R:316:HOH:O	12:Z:95:HIS:HD2	1.94	0.50
4:D:23:ILE:HD13	4:D:133:ALA:HB2	1.94	0.50
8:V:34:LEU:HB2	16:V:317:HOH:O	2.11	0.50
4:R:114:ARG:HH11	4:R:114:ARG:HG2	1.76	0.50
2:B:18:LEU:HD13	2:B:122:THR:HG23	1.93	0.50
6:F:66:VAL:HG11	6:F:108:PHE:CE1	2.47	0.50
12:L:42:LYS:HD2	12:L:55:ASN:ND2	2.27	0.50
9:I:22:ILE:HG12	9:I:42:ILE:HD12	1.93	0.50
8:H:152:ILE:O	8:H:156:SER:HB2	2.12	0.50
13:M:3:GLN:HG3	13:M:3:GLN:O	2.12	0.50
4:R:6:THR:HG22	4:R:7:PHE:N	2.26	0.49
12:L:152:ASN:O	12:L:156:PHE:HA	2.12	0.49
2:B:149:THR:O	2:B:156:TYR:HA	2.12	0.49
9:W:179:LEU:HD22	16:W:313:HOH:O	2.12	0.49
10:J:195:PHE:HA	10:J:198:GLN:HB2	1.94	0.49
8:V:128:GLY:O	8:V:131:SER:HB2	2.10	0.49
7:G:3:TYR:C	7:G:5:ARG:H	2.15	0.49
5:S:90:GLN:HG3	5:S:110:LEU:HD13	1.94	0.49
12:L:194:ARG:CZ	8:V:29:LYS:HE2	2.41	0.49
14:N:103:ASP:HB2	16:N:234:HOH:O	2.12	0.49
6:T:105:ILE:HD13	6:T:138:ASP:HB3	1.93	0.49
4:D:6:THR:HG22	4:D:7:PHE:N	2.26	0.49
11:Y:15:ALA:O	11:Y:161:ILE:HD11	2.12	0.49
1:O:160:LYS:HD3	1:O:179:TRP:CZ3	2.47	0.49
1:O:205:ASN:HB2	16:O:329:HOH:O	2.12	0.49
8:V:104:ASP:O	8:V:106:THR:N	2.45	0.49
5:S:174:THR:HG22	5:S:177:THR:HB	1.92	0.49
12:Z:16:ALA:HB2	12:Z:122:VAL:HG23	1.93	0.49
6:T:205:GLU:HG3	6:T:206:LYS:HG3	1.94	0.49
12:L:100:LYS:HD3	12:L:105:TYR:CE1	2.47	0.49
11:Y:145:LYS:O	11:Y:148:LEU:HD13	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:181:ILE:O	12:L:185:ARG:HG3	2.12	0.49
1:A:24:ALA:O	1:A:28:VAL:HG23	2.13	0.49
5:S:68:HIS:HE1	5:S:102:LEU:O	1.95	0.49
13:M:18:ASN:HB3	13:M:201:ASP:OD2	2.12	0.49
3:Q:27:ARG:HB2	3:Q:27:ARG:NH1	2.27	0.49
8:V:73:GLU:HA	8:V:73:GLU:OE1	2.12	0.49
5:S:220:PRO:O	5:S:221:PHE:C	2.51	0.49
10:J:174:MET:HG2	10:X:174:MET:CE	2.43	0.49
6:F:175:LEU:HD11	6:F:191:GLN:HG3	1.94	0.49
12:L:94:GLN:HG3	12:L:129:GLY:O	2.11	0.49
1:A:160:LYS:HD3	1:A:179:TRP:CZ3	2.47	0.49
1:O:24:ALA:O	1:O:28:VAL:HG23	2.12	0.49
7:G:174:GLU:O	7:G:178:LYS:HG3	2.12	0.49
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.94	0.49
4:R:155:THR:HG23	5:S:78:PRO:HD3	1.94	0.49
10:J:53:THR:CG2	10:J:54:VAL:H	2.25	0.49
10:J:25:ILE:HG12	10:X:139:TYR:OH	2.12	0.49
6:T:8:ASN:O	6:T:8:ASN:CG	2.51	0.49
12:Z:94:GLN:HG3	12:Z:129:GLY:O	2.12	0.49
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.94	0.49
6:T:193:ALA:O	6:T:197:TYR:HD1	1.95	0.49
4:D:121:GLY:HA3	16:E:315:HOH:O	2.13	0.49
11:K:12:ILE:HG23	11:K:112:ILE:HD11	1.94	0.49
5:S:214:ILE:O	5:S:221:PHE:HA	2.13	0.49
5:E:189:ILE:HG23	5:E:212:ILE:HD13	1.95	0.49
6:T:191:GLN:NE2	6:T:194:LYS:CE	2.76	0.49
5:E:68:HIS:HE1	5:E:102:LEU:O	1.96	0.49
11:K:12:ILE:CG2	11:K:112:ILE:HD11	2.43	0.49
3:Q:190:VAL:HG13	3:Q:210:ILE:HG21	1.94	0.49
5:S:174:THR:HG22	5:S:174:THR:O	2.13	0.49
8:H:173:VAL:HB	8:H:191:LEU:HB2	1.95	0.49
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.93	0.49
13:M:48:ASN:ND2	13:M:48:ASN:H	2.02	0.49
5:E:214:ILE:O	5:E:221:PHE:HA	2.13	0.49
10:J:198:GLN:HG2	10:J:198:GLN:OXT	2.12	0.49
9:I:176:ARG:NH2	12:Z:147:MET:HE3	2.26	0.49
6:F:193:ALA:O	6:F:197:TYR:HD1	1.96	0.49
1:A:59:GLU:CD	1:A:59:GLU:H	2.16	0.49
7:U:92:ALA:HA	7:U:103:MET:CE	2.42	0.48
9:W:17:LYS:CD	9:W:156:ASN:HD22	2.26	0.48
10:J:139:TYR:OH	10:X:25:ILE:HG12	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:174:MET:HE2	10:X:174:MET:HE2	1.94	0.48
10:J:45:SER:OG	10:J:103:LEU:HB2	2.13	0.48
16:T:303:HOH:O	7:U:82:ARG:HD2	2.12	0.48
14:N:67:THR:HA	14:N:71:GLY:O	2.13	0.48
2:P:148:TYR:CZ	3:Q:57:ILE:HG13	2.47	0.48
10:X:198:GLN:OXT	10:X:198:GLN:HG2	2.13	0.48
1:O:246:ARG:NH1	1:O:246:ARG:HG3	2.28	0.48
6:F:191:GLN:HE21	6:F:194:LYS:HE3	1.78	0.48
1:O:139:HIS:HA	1:O:144:GLY:O	2.13	0.48
6:F:45:ALA:HA	6:F:211:GLU:O	2.12	0.48
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.48	0.48
9:W:28:LEU:HA	16:W:316:HOH:O	2.12	0.48
11:Y:12:ILE:HG23	11:Y:112:ILE:HD11	1.95	0.48
12:Z:100:LYS:HD3	12:Z:105:TYR:CE1	2.47	0.48
10:X:53:THR:CG2	10:X:54:VAL:H	2.26	0.48
5:E:174:THR:O	5:E:174:THR:HG22	2.12	0.48
9:I:26:LEU:HD22	9:I:40:GLU:HG2	1.94	0.48
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.43	0.48
2:P:6:ASP:OD1	3:Q:4:ARG:HG3	2.12	0.48
6:F:8:ASN:O	6:F:8:ASN:CG	2.51	0.48
4:R:82:GLU:OE1	11:Y:69:ARG:HD2	2.13	0.48
5:E:14:PRO:HA	6:F:22:TYR:CD2	2.48	0.48
2:B:228:ILE:N	2:B:228:ILE:HD12	2.28	0.48
2:B:55:LEU:H	2:B:55:LEU:HD22	1.75	0.48
6:F:205:GLU:HG3	6:F:206:LYS:HG3	1.94	0.48
2:P:185:VAL:O	2:P:189:ILE:HG13	2.13	0.48
8:V:84:LYS:HG3	8:V:85:GLN:N	2.28	0.48
10:J:53:THR:HG23	10:J:54:VAL:HG23	1.95	0.48
2:P:162:ILE:HG13	2:P:163:SER:H	1.79	0.48
3:Q:29:THR:HB	3:Q:45:GLU:HG3	1.96	0.48
3:Q:182:PRO:O	3:Q:184:ALA:N	2.46	0.48
2:B:67:LYS:HG3	2:B:226:GLN:OE1	2.14	0.48
4:R:4:VAL:CG2	4:R:116:GLY:HA2	2.44	0.48
2:P:149:THR:O	2:P:156:TYR:HA	2.13	0.48
1:O:54:PRO:HG2	7:U:174:GLU:HG2	1.95	0.48
5:E:220:PRO:O	5:E:221:PHE:C	2.52	0.48
2:P:184:LYS:HD3	2:P:185:VAL:H	1.75	0.48
9:W:106:PRO:HB2	9:W:123:PHE:CD2	2.48	0.48
8:H:128:GLY:O	8:H:131:SER:HB2	2.13	0.48
5:E:36:GLY:O	5:E:157:GLY:HA2	2.12	0.48
6:F:20:VAL:O	6:F:23:ALA:HB3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:69:MET:HE2	5:S:104:VAL:HA	1.94	0.48
4:R:93:LEU:CD1	11:Y:57:THR:HG22	2.43	0.48
9:I:10:ILE:HD11	9:I:174:ALA:HB2	1.96	0.48
4:D:4:VAL:CG2	4:D:116:GLY:HA2	2.43	0.48
7:U:235:ARG:NE	7:U:235:ARG:HA	2.29	0.48
6:T:45:ALA:HA	6:T:211:GLU:O	2.13	0.48
8:V:173:VAL:HB	8:V:191:LEU:HB2	1.94	0.48
11:Y:12:ILE:CG2	11:Y:112:ILE:HD11	2.43	0.48
11:K:145:LYS:O	11:K:148:LEU:HD13	2.13	0.48
6:T:175:LEU:HD11	6:T:191:GLN:HG3	1.95	0.48
3:Q:49:THR:HG22	3:Q:50:LEU:HD22	1.95	0.48
10:X:49:GLU:HB2	10:X:99:GLN:HB2	1.96	0.48
7:G:101:TYR:OH	8:H:66:HIS:HE1	1.97	0.48
8:H:18:THR:HB	8:H:30:ASN:HD22	1.79	0.48
8:V:220:ILE:HD11	9:W:194:VAL:HG21	1.96	0.48
11:K:147:ASP:O	11:K:148:LEU:C	2.50	0.48
10:J:174:MET:CE	10:X:174:MET:HG2	2.43	0.48
10:X:13:VAL:HG23	10:X:114:PRO:HB2	1.95	0.48
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.95	0.48
7:G:71:GLY:HA3	7:G:224:PHE:CE2	2.49	0.48
2:P:18:LEU:HD13	2:P:122:THR:HG23	1.95	0.48
7:U:166:GLN:NE2	7:U:167:GLN:N	2.62	0.48
2:B:184:LYS:HD3	2:B:185:VAL:H	1.77	0.48
7:U:83:ASN:C	7:U:83:ASN:ND2	2.65	0.48
9:I:50:LEU:HD21	9:I:52:ILE:HD11	1.95	0.48
10:J:172:MET:CE	10:J:174:MET:HB2	2.44	0.48
9:W:148:MET:HE3	9:W:152:LEU:HD11	1.96	0.48
3:C:29:THR:HB	3:C:45:GLU:HG3	1.95	0.48
1:A:139:HIS:HA	1:A:144:GLY:O	2.13	0.48
14:N:41:ILE:HD12	14:N:75:THR:HA	1.96	0.48
7:U:3:TYR:C	7:U:5:ARG:H	2.17	0.48
4:R:176:LEU:HD22	5:S:55:LEU:HD11	1.95	0.47
8:H:175:VAL:HG12	8:H:176:CYS:N	2.29	0.47
10:X:118:GLN:NE2	10:X:132:ALA:H	2.11	0.47
1:A:206:GLY:HA2	1:A:243:ILE:HG21	1.96	0.47
6:F:39:ASN:HD22	6:F:39:ASN:N	2.10	0.47
9:W:14:MET:HB3	9:W:162:LEU:HD11	1.96	0.47
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.14	0.47
14:N:107:LYS:HG2	14:N:108:GLY:H	1.79	0.47
6:T:20:VAL:O	6:T:23:ALA:HB3	2.14	0.47
3:C:182:PRO:O	3:C:184:ALA:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:14:MET:HB3	9:I:162:LEU:HD11	1.96	0.47
3:C:160:GLN:HA	3:C:160:GLN:NE2	2.18	0.47
7:U:39:LYS:NZ	7:U:186:ASN:ND2	2.62	0.47
4:R:241:ALA:O	4:R:242:GLU:CB	2.62	0.47
6:T:168:ALA:O	6:T:172:LEU:HD23	2.15	0.47
6:F:191:GLN:O	6:F:195:ILE:HG13	2.14	0.47
9:I:108:VAL:O	9:I:120:ILE:HA	2.14	0.47
3:Q:32:VAL:HG22	3:Q:33:GLY:N	2.29	0.47
1:O:206:GLY:HA2	1:O:243:ILE:HG21	1.96	0.47
1:A:140:ASP:OD1	1:A:143:ASN:HB2	2.15	0.47
9:W:108:VAL:O	9:W:120:ILE:HA	2.14	0.47
7:U:148:THR:HG22	7:U:154:TYR:HB2	1.96	0.47
5:E:86:TYR:CD1	5:E:114:LYS:HD2	2.50	0.47
7:U:19:VAL:O	7:U:23:PHE:HD2	1.97	0.47
10:J:8:ARG:HH11	10:J:8:ARG:HG2	1.79	0.47
4:R:113:LEU:HD13	5:S:125:ARG:NH2	2.29	0.47
9:W:55:LEU:HG	9:W:57:THR:HG22	1.96	0.47
13:M:40:GLU:OE1	13:M:42:LEU:HB2	2.14	0.47
6:T:183:LEU:HD11	6:T:187:GLU:HB3	1.97	0.47
5:S:200:LEU:HD11	5:S:205:LEU:CD2	2.40	0.47
4:R:121:GLY:O	4:R:122:GLU:HB2	2.13	0.47
2:P:99:LYS:NZ	10:X:86:GLN:NE2	2.61	0.47
13:M:129:TYR:CE1	13:M:144:THR:HG22	2.50	0.47
3:Q:170:ARG:O	3:Q:174:GLU:HG3	2.15	0.47
7:G:148:THR:HG22	7:G:154:TYR:HB2	1.97	0.47
13:M:172:VAL:HG21	16:M:359:HOH:O	2.14	0.47
10:X:61:GLN:HB3	16:X:236:HOH:O	2.13	0.47
7:U:196:PHE:C	7:U:196:PHE:CD1	2.87	0.47
4:D:121:GLY:O	4:D:122:GLU:HB2	2.14	0.47
6:T:191:GLN:O	6:T:195:ILE:HG13	2.15	0.47
10:J:172:MET:HA	10:J:173:PRO:HD3	1.79	0.47
3:C:117:ARG:NH2	16:C:327:HOH:O	2.45	0.47
6:F:183:LEU:HD11	6:F:187:GLU:HB3	1.97	0.47
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.80	0.47
12:Z:109:THR:CG2	16:Z:311:HOH:O	2.63	0.47
14:N:102:TYR:OH	14:N:180:ALA:HB2	2.14	0.47
11:K:208:ASN:HD21	10:X:150:PRO:CG	2.28	0.47
3:Q:51:LYS:NZ	3:Q:52:LEU:HA	2.30	0.47
10:X:172:MET:HA	10:X:173:PRO:HD3	1.79	0.47
16:F:305:HOH:O	7:G:79:PRO:HA	2.14	0.47
4:D:196:LEU:O	4:D:200:MET:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:ARG:NH1	10:J:73:TYR:HB2	2.29	0.47
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.43	0.47
2:P:229:PHE:CD2	2:P:229:PHE:N	2.83	0.47
9:I:55:LEU:HG	9:I:57:THR:HG22	1.95	0.47
1:A:149:GLN:O	1:A:156:TYR:HA	2.14	0.47
3:Q:39:CYS:HA	3:Q:136:PHE:HZ	1.80	0.47
1:O:57:MET:HE1	16:U:317:HOH:O	2.15	0.47
9:I:166:ILE:HG22	9:I:167:SER:N	2.30	0.47
3:Q:160:GLN:NE2	3:Q:160:GLN:CA	2.77	0.47
5:E:69:MET:CE	5:E:104:VAL:HA	2.44	0.47
3:C:190:VAL:HG13	3:C:210:ILE:HG21	1.96	0.47
6:T:191:GLN:NE2	6:T:194:LYS:HE2	2.29	0.47
1:A:231:LYS:HE3	16:A:347:HOH:O	2.13	0.47
3:Q:49:THR:HG22	3:Q:50:LEU:CD2	2.44	0.47
7:G:227:LEU:HB3	7:G:231:ASN:HB2	1.96	0.47
1:O:149:GLN:O	1:O:156:TYR:HA	2.15	0.47
3:C:49:THR:HG22	3:C:50:LEU:HD22	1.97	0.47
11:K:208:ASN:HD21	10:X:150:PRO:HG2	1.79	0.47
3:C:27:ARG:HB2	3:C:27:ARG:NH1	2.29	0.47
6:F:105:ILE:HD13	6:F:138:ASP:HB3	1.97	0.47
12:L:2:PHE:CB	13:M:1:THR:HG23	2.45	0.47
6:F:8:ASN:OD1	6:F:127:PRO:HG3	2.15	0.47
6:T:210:LEU:HD21	6:T:212:ILE:HD11	1.97	0.47
9:W:137:VAL:CG1	9:W:145:LEU:HB3	2.45	0.47
2:B:243:ILE:O	2:B:243:ILE:HG22	2.15	0.47
7:G:191:GLU:O	7:G:195:GLU:HG3	2.15	0.47
4:D:241:ALA:O	4:D:242:GLU:CB	2.63	0.47
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.97	0.47
3:C:32:VAL:HG22	3:C:33:GLY:N	2.28	0.47
6:F:132:THR:O	6:F:146:MET:HA	2.15	0.47
8:H:84:LYS:HG3	8:H:85:GLN:N	2.30	0.46
1:A:246:ARG:HG3	1:A:246:ARG:NH1	2.28	0.46
6:F:191:GLN:NE2	6:F:194:LYS:CE	2.78	0.46
2:P:110:LEU:C	2:P:110:LEU:HD23	2.35	0.46
5:E:227:GLU:CD	5:E:227:GLU:N	2.69	0.46
5:S:181:ILE:O	5:S:181:ILE:HG22	2.15	0.46
2:P:49:ARG:NH2	2:P:58:GLN:HE21	2.12	0.46
5:E:200:LEU:HD11	5:E:205:LEU:CD2	2.42	0.46
3:C:51:LYS:NZ	3:C:52:LEU:HA	2.29	0.46
16:E:305:HOH:O	6:F:8:ASN:HB2	2.16	0.46
4:D:140:ASP:HA	16:D:338:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:50:LEU:CG	9:W:52:ILE:HD11	2.46	0.46
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.46	0.46
10:X:172:MET:CE	10:X:174:MET:HB2	2.45	0.46
1:A:28:VAL:HG13	1:A:76:SER:O	2.15	0.46
5:E:21:VAL:O	5:E:25:LEU:HD13	2.15	0.46
2:B:229:PHE:CD2	2:B:229:PHE:N	2.83	0.46
2:B:49:ARG:CZ	2:B:58:GLN:HE21	2.28	0.46
1:A:238:LEU:HA	1:A:242:GLU:OE1	2.16	0.46
7:G:135:VAL:HA	7:G:144:SER:O	2.15	0.46
5:E:23:TYR:O	5:E:26:GLU:HB3	2.16	0.46
7:U:135:VAL:HA	7:U:144:SER:O	2.15	0.46
7:U:227:LEU:HB3	7:U:231:ASN:HB2	1.96	0.46
11:Y:176:ASN:HD21	11:Y:190:ASN:HB2	1.80	0.46
12:L:89:ALA:O	12:L:93:ILE:HG12	2.16	0.46
1:A:69:PRO:HD3	16:H:352:HOH:O	2.14	0.46
1:O:52:SER:O	1:O:53:SER:HB2	2.15	0.46
8:V:175:VAL:HG12	8:V:176:CYS:N	2.30	0.46
12:L:125:PHE:CD1	12:L:125:PHE:N	2.82	0.46
2:B:139:TYR:CG	2:B:224:VAL:HG21	2.51	0.46
2:B:49:ARG:NH2	2:B:58:GLN:HE21	2.13	0.46
1:O:238:LEU:HA	1:O:242:GLU:OE1	2.15	0.46
6:F:105:ILE:N	6:F:106:PRO:CD	2.79	0.46
9:I:106:PRO:HB2	9:I:123:PHE:CD2	2.50	0.46
7:G:83:ASN:ND2	7:G:83:ASN:C	2.69	0.46
10:J:49:GLU:HB2	10:J:99:GLN:HB2	1.97	0.46
12:L:108:HIS:HE1	12:L:124:SER:HB2	1.81	0.46
11:Y:12:ILE:HD13	11:Y:112:ILE:HD13	1.97	0.46
7:U:186:ASN:HD22	7:U:186:ASN:C	2.18	0.46
6:T:66:VAL:HG11	6:T:108:PHE:CE1	2.51	0.46
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.97	0.46
2:P:240:LYS:C	2:P:242:GLY:H	2.18	0.46
7:G:235:ARG:NE	7:G:235:ARG:HA	2.30	0.46
7:U:71:GLY:HA3	7:U:224:PHE:CE2	2.50	0.46
7:U:137:VAL:HG21	7:U:220:THR:HA	1.97	0.46
5:S:23:TYR:O	5:S:26:GLU:HB3	2.14	0.46
10:J:75:LEU:HD22	10:J:79:ALA:HB1	1.97	0.46
11:K:140:LEU:HD13	11:K:160:SER:OG	2.16	0.46
8:V:152:ILE:O	8:V:156:SER:HB2	2.14	0.46
7:U:192:LYS:HD3	7:U:195:GLU:OE2	2.16	0.46
6:F:168:ALA:O	6:F:172:LEU:HD23	2.15	0.46
6:F:191:GLN:NE2	6:F:194:LYS:HE2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:165:ILE:N	13:M:166:PRO:HD2	2.31	0.46
3:C:225:GLU:N	3:C:225:GLU:OE1	2.48	0.46
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.46	0.46
1:A:52:SER:O	1:A:53:SER:HB2	2.14	0.46
10:X:130:TYR:CD2	10:X:144:LEU:HD13	2.51	0.46
2:B:17:ARG:NH1	2:B:17:ARG:HG2	2.31	0.46
3:C:100:ASP:OD2	3:C:101:PRO:HD2	2.16	0.46
7:G:186:ASN:C	7:G:186:ASN:HD22	2.19	0.46
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.45	0.46
5:E:35:VAL:HG12	5:E:36:GLY:N	2.31	0.46
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.98	0.46
10:J:129:PRO:HB2	10:J:130:TYR:CD1	2.50	0.46
12:Z:10:GLY:HA3	12:Z:42:LYS:NZ	2.30	0.46
8:V:137:VAL:HG21	8:V:161:ALA:HB2	1.97	0.46
2:P:49:ARG:CZ	2:P:58:GLN:HE21	2.29	0.46
4:D:214:ILE:O	4:D:214:ILE:HG23	2.15	0.46
5:E:87:LEU:HD11	5:E:107:ALA:HB1	1.97	0.46
5:E:131:LEU:HD12	5:E:146:PHE:CD2	2.51	0.46
3:Q:100:ASP:OD2	3:Q:101:PRO:HD2	2.16	0.46
10:J:194:ASP:O	10:J:198:GLN:HB2	2.16	0.46
6:T:103:ILE:HG12	6:T:108:PHE:HB2	1.98	0.46
1:A:205:ASN:HA	1:A:247:LEU:CD1	2.45	0.46
11:K:176:ASN:HD21	11:K:190:ASN:HB2	1.80	0.46
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.16	0.46
12:Z:13:LEU:CD1	12:Z:150:LEU:HD21	2.29	0.45
14:N:146:MET:HE2	14:N:150:GLU:C	2.36	0.45
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.46	0.45
6:T:41:GLY:HA3	6:T:215:CYS:O	2.15	0.45
6:T:99:TYR:O	6:T:100:LYS:HB3	2.15	0.45
6:T:201:GLU:O	6:T:204:LYS:HD2	2.16	0.45
1:A:10:THR:O	2:B:128:ARG:HD3	2.16	0.45
7:G:192:LYS:HD3	7:G:195:GLU:OE2	2.15	0.45
12:L:103:PHE:N	12:L:104:PRO:CD	2.80	0.45
2:B:234:ILE:HD11	16:B:316:HOH:O	2.16	0.45
3:C:227:ILE:O	3:C:231:VAL:HG23	2.16	0.45
2:P:183:MET:HE2	2:P:188:ALA:N	2.31	0.45
8:V:148:LYS:O	8:V:152:ILE:HG13	2.16	0.45
14:N:13:ILE:HG12	14:N:177:VAL:HG13	1.98	0.45
9:I:20:VAL:CG1	9:I:118:PRO:HB3	2.47	0.45
13:M:14:MET:HE3	13:M:159:VAL:HG22	1.99	0.45
3:C:39:CYS:HA	3:C:136:PHE:HZ	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:132:LEU:O	7:G:147:LYS:HA	2.15	0.45
4:R:6:THR:CG2	4:R:7:PHE:N	2.80	0.45
5:E:72:SER:OG	5:E:132:LEU:HB2	2.16	0.45
1:O:203:GLU:OE2	1:O:203:GLU:HA	2.17	0.45
5:S:37:LEU:N	5:S:37:LEU:HD23	2.31	0.45
2:B:240:LYS:C	2:B:242:GLY:H	2.19	0.45
2:P:135:ILE:HD11	2:P:164:VAL:HG22	1.99	0.45
6:T:123:ASN:HD22	6:T:123:ASN:C	2.20	0.45
16:S:309:HOH:O	6:T:8:ASN:HB2	2.16	0.45
11:Y:140:LEU:HD13	11:Y:160:SER:OG	2.16	0.45
5:S:167:ALA:HB2	5:S:195:ALA:O	2.15	0.45
7:U:132:LEU:O	7:U:147:LYS:HA	2.15	0.45
10:J:118:GLN:NE2	10:J:132:ALA:H	2.15	0.45
7:G:137:VAL:HG21	7:G:220:THR:HA	1.97	0.45
7:G:196:PHE:CD1	7:G:196:PHE:C	2.88	0.45
13:M:161:ARG:CG	13:M:161:ARG:HH11	2.20	0.45
2:P:120:GLY:C	2:P:122:THR:H	2.20	0.45
11:K:208:ASN:ND2	10:X:150:PRO:CG	2.80	0.45
6:T:39:ASN:N	6:T:39:ASN:ND2	2.64	0.45
7:G:231:ASN:HD22	7:G:231:ASN:N	2.14	0.45
5:E:227:GLU:CD	5:E:227:GLU:H	2.20	0.45
9:I:80:ALA:HB1	16:I:326:HOH:O	2.17	0.45
1:O:140:ASP:OD1	1:O:143:ASN:HB2	2.16	0.45
6:F:36:ILE:HD12	6:F:192:ALA:HB2	1.98	0.45
5:S:9:THR:HG21	5:S:126:PRO:HG3	1.99	0.45
4:R:73:LEU:HB3	16:R:308:HOH:O	2.16	0.45
4:R:214:ILE:HG23	4:R:214:ILE:O	2.15	0.45
1:A:64:VAL:HG11	1:A:212:ALA:HB3	1.99	0.45
1:O:29:LYS:HE2	1:O:29:LYS:CA	2.41	0.45
11:K:12:ILE:HD13	11:K:112:ILE:HD13	1.98	0.45
9:W:10:ILE:HD11	9:W:174:ALA:HB2	1.99	0.45
9:I:50:LEU:CG	9:I:52:ILE:HD11	2.47	0.45
5:E:129:VAL:O	5:E:148:PRO:HG3	2.16	0.45
6:T:172:LEU:HB3	7:U:54:LEU:HD21	1.98	0.45
12:L:10:GLY:HA3	12:L:42:LYS:NZ	2.31	0.45
12:Z:51:VAL:HG23	12:Z:112:ALA:HB3	1.99	0.45
4:D:113:LEU:HD23	4:D:115:PHE:HE1	1.81	0.45
5:E:37:LEU:HD23	5:E:37:LEU:N	2.32	0.45
7:G:39:LYS:NZ	7:G:186:ASN:ND2	2.65	0.45
3:Q:165:ASN:CB	3:Q:200:VAL:HG11	2.45	0.45
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:SER:HB2	16:C:311:HOH:O	2.17	0.45
5:E:167:ALA:HB2	5:E:195:ALA:O	2.17	0.45
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.99	0.45
10:X:75:LEU:HD22	10:X:79:ALA:HB1	1.97	0.45
2:P:243:ILE:O	2:P:243:ILE:HG22	2.17	0.45
4:R:113:LEU:HD13	5:S:125:ARG:HH21	1.82	0.45
10:J:174:MET:CE	10:X:174:MET:CE	2.95	0.45
10:X:139:TYR:CZ	10:X:172:MET:HG3	2.51	0.45
8:V:38:SER:OG	8:V:41:ILE:HD13	2.17	0.45
2:B:162:ILE:HG13	2:B:163:SER:H	1.81	0.45
12:Z:109:THR:HG23	16:Z:311:HOH:O	2.16	0.45
3:C:49:THR:HG22	3:C:50:LEU:CD2	2.46	0.45
7:G:232:ILE:O	7:G:235:ARG:N	2.50	0.45
10:J:13:VAL:HG23	10:J:114:PRO:HB2	1.98	0.45
11:Y:174:SER:HA	11:Y:193:VAL:HG23	1.99	0.45
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.16	0.45
4:R:176:LEU:HD22	5:S:55:LEU:CD1	2.47	0.44
4:D:31:GLY:O	4:D:161:ALA:HA	2.18	0.44
9:W:50:LEU:HG	9:W:52:ILE:CD1	2.47	0.44
3:Q:27:ARG:HB2	3:Q:27:ARG:CZ	2.46	0.44
6:T:8:ASN:OD1	6:T:127:PRO:HG3	2.17	0.44
3:C:1:GLY:N	16:C:330:HOH:O	2.50	0.44
9:I:137:VAL:CG1	9:I:145:LEU:HB3	2.47	0.44
12:L:41:PRO:HA	16:L:345:HOH:O	2.17	0.44
5:S:72:SER:OG	5:S:132:LEU:HB2	2.17	0.44
2:B:110:LEU:HD23	2:B:110:LEU:C	2.36	0.44
4:R:9:PRO:HA	5:S:23:TYR:CD2	2.51	0.44
4:D:9:PRO:HD2	16:D:331:HOH:O	2.16	0.44
6:F:99:TYR:O	6:F:100:LYS:HB3	2.17	0.44
3:Q:227:ILE:O	3:Q:231:VAL:HG23	2.17	0.44
1:A:55:LEU:HD12	7:G:170:THR:HG23	1.99	0.44
14:N:156:LYS:HG2	14:N:196:LEU:HD11	1.99	0.44
6:F:103:ILE:HG12	6:F:108:PHE:HB2	1.99	0.44
3:C:165:ASN:CB	3:C:200:VAL:HG11	2.46	0.44
12:Z:42:LYS:HD2	12:Z:55:ASN:ND2	2.32	0.44
11:K:174:SER:HA	11:K:193:VAL:HG23	1.99	0.44
3:Q:107:LEU:HD13	3:Q:107:LEU:O	2.17	0.44
5:E:101:LYS:HA	16:E:302:HOH:O	2.17	0.44
8:H:148:LYS:O	8:H:152:ILE:HG13	2.17	0.44
6:F:39:ASN:N	6:F:39:ASN:ND2	2.66	0.44
10:J:190:ARG:HA	16:J:247:HOH:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:50:LYS:HG2	2:P:51:VAL:HG23	1.99	0.44
5:S:21:VAL:O	5:S:25:LEU:HD13	2.17	0.44
7:U:237:VAL:O	7:U:240:ALA:HB3	2.18	0.44
13:M:25:ASP:HA	13:M:195:PHE:HA	2.00	0.44
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.99	0.44
5:S:227:GLU:N	5:S:227:GLU:CD	2.69	0.44
2:B:60:THR:O	2:B:60:THR:HG22	2.18	0.44
12:Z:125:PHE:CD1	12:Z:125:PHE:N	2.85	0.44
2:B:50:LYS:HG2	2:B:51:VAL:HG23	1.98	0.44
7:U:191:GLU:O	7:U:195:GLU:HG3	2.17	0.44
4:D:6:THR:CG2	4:D:7:PHE:N	2.80	0.44
10:J:139:TYR:HD1	16:Y:317:HOH:O	2.00	0.44
2:B:24:ALA:O	2:B:27:SER:HB3	2.18	0.44
5:S:102:LEU:HA	16:S:321:HOH:O	2.18	0.44
13:M:17:ASP:HB3	13:M:166:PRO:HA	1.98	0.44
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.99	0.44
12:Z:38:ARG:NH1	12:Z:221:ARG:HB3	2.33	0.44
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.18	0.44
5:E:181:ILE:HG22	5:E:181:ILE:O	2.17	0.44
13:M:161:ARG:NH1	13:M:161:ARG:HG3	2.20	0.44
3:C:95:ARG:HH11	3:C:101:PRO:HB3	1.82	0.44
9:W:166:ILE:HG22	9:W:167:SER:N	2.31	0.44
5:S:129:VAL:O	5:S:148:PRO:HG3	2.18	0.44
9:I:17:LYS:CD	9:I:156:ASN:HD22	2.29	0.44
3:Q:40:VAL:HG22	3:Q:143:PRO:HB2	2.00	0.44
11:K:40:PHE:CB	11:K:73:ARG:HH21	2.21	0.44
5:E:99:ASN:HB2	13:M:94:GLU:CG	2.46	0.44
6:T:191:GLN:HE21	6:T:194:LYS:CE	2.30	0.44
6:T:165:ARG:O	6:T:169:LYS:HG3	2.17	0.44
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.99	0.44
5:S:227:GLU:CD	5:S:227:GLU:H	2.19	0.44
13:M:88:GLU:HB2	13:M:91:TYR:CD2	2.53	0.44
6:T:132:THR:O	6:T:146:MET:HA	2.17	0.44
7:U:115:LEU:HA	7:U:115:LEU:HD12	1.83	0.44
11:K:46:ALA:HB3	11:K:98:GLY:O	2.18	0.44
10:J:139:TYR:CZ	10:J:172:MET:HG3	2.53	0.44
4:R:7:PHE:HB2	5:S:20:GLN:OE1	2.18	0.44
14:N:84:GLU:O	14:N:88:GLU:HB2	2.17	0.44
1:O:64:VAL:HG11	1:O:212:ALA:HB3	1.99	0.44
4:D:109:CYS:HB3	4:D:154:GLY:O	2.18	0.44
6:F:133:ILE:HA	6:F:145:TYR:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:74:VAL:HG11	7:G:81:ALA:CB	2.48	0.44
2:B:120:GLY:C	2:B:122:THR:H	2.21	0.44
2:P:139:TYR:CG	2:P:224:VAL:HG21	2.52	0.44
10:X:53:THR:HG23	10:X:54:VAL:HG23	2.00	0.44
9:I:50:LEU:HG	9:I:52:ILE:CD1	2.47	0.44
5:S:69:MET:CE	5:S:104:VAL:HA	2.47	0.44
12:L:174:TYR:CD1	12:L:175:LEU:N	2.86	0.44
9:W:20:VAL:CG1	9:W:118:PRO:HB3	2.48	0.44
3:C:27:ARG:CZ	3:C:27:ARG:HB2	2.48	0.43
9:I:104:VAL:HG23	9:I:106:PRO:HD3	2.00	0.43
14:N:107:LYS:HG2	14:N:108:GLY:N	2.33	0.43
5:S:35:VAL:HG12	5:S:36:GLY:N	2.32	0.43
1:O:205:ASN:HA	1:O:247:LEU:CD1	2.48	0.43
2:B:229:PHE:N	2:B:229:PHE:HD2	2.16	0.43
5:S:86:TYR:CD1	5:S:114:LYS:HD2	2.53	0.43
3:C:131:THR:O	3:C:147:GLN:HA	2.18	0.43
6:F:41:GLY:HA3	6:F:215:CYS:O	2.17	0.43
3:Q:239:GLN:C	3:Q:241:GLN:H	2.22	0.43
6:T:105:ILE:N	6:T:106:PRO:CD	2.82	0.43
12:Z:126:ASP:HB2	12:Z:130:SER:HB3	2.01	0.43
2:P:65:LEU:HD12	2:P:75:ALA:HA	2.00	0.43
12:Z:51:VAL:CG2	12:Z:112:ALA:HB3	2.48	0.43
7:U:78:ILE:N	7:U:79:PRO:HD2	2.33	0.43
6:F:32:THR:CG2	6:F:47:GLU:OE2	2.66	0.43
2:P:99:LYS:HZ3	10:X:86:GLN:NE2	2.15	0.43
1:A:234:ARG:NH1	1:A:234:ARG:HG2	2.33	0.43
3:C:170:ARG:O	3:C:174:GLU:HG3	2.18	0.43
7:U:174:GLU:O	7:U:178:LYS:HG3	2.17	0.43
12:Z:28:ARG:NE	12:Z:200:ASP:OD2	2.36	0.43
11:Y:25:TRP:CH2	12:Z:144:SER:HA	2.53	0.43
6:T:178:HIS:O	6:T:179:HIS:CG	2.72	0.43
6:T:36:ILE:HD12	6:T:192:ALA:HB2	2.00	0.43
2:P:60:THR:O	2:P:60:THR:HG22	2.19	0.43
2:P:17:ARG:NH1	2:P:17:ARG:HG2	2.33	0.43
2:B:119:GLN:NE2	16:B:310:HOH:O	2.50	0.43
6:T:31:THR:CG2	6:T:32:THR:N	2.82	0.43
4:D:161:ALA:HB3	5:E:55:LEU:HD23	2.00	0.43
12:Z:126:ASP:HB2	12:Z:130:SER:N	2.31	0.43
1:A:94:HIS:CD2	8:H:61:SER:OG	2.70	0.43
12:Z:103:PHE:N	12:Z:104:PRO:CD	2.80	0.43
3:C:164:ARG:O	3:C:165:ASN:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:159:TRP:CD2	2:P:162:ILE:HD13	2.54	0.43
10:X:118:GLN:NE2	10:X:132:ALA:O	2.52	0.43
12:Z:85:SER:HB2	12:Z:87:ASN:OD1	2.19	0.43
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.53	0.43
3:C:40:VAL:HG22	3:C:143:PRO:HB2	2.01	0.43
3:Q:225:GLU:N	3:Q:225:GLU:OE1	2.50	0.43
13:M:161:ARG:CG	13:M:161:ARG:NH1	2.81	0.43
3:Q:155:SER:CB	4:R:51:LEU:HD21	2.47	0.43
7:U:241:GLU:O	7:U:242:GLN:CB	2.65	0.43
3:Q:214:LYS:HD2	3:Q:218:ASP:OD1	2.19	0.43
2:B:35:ILE:HG12	2:B:196:LEU:HD21	2.00	0.43
5:S:174:THR:O	5:S:177:THR:HB	2.18	0.43
5:E:131:LEU:HB2	5:E:146:PHE:HB3	2.00	0.43
5:S:167:ALA:CB	5:S:195:ALA:O	2.67	0.43
4:R:214:ILE:HA	4:R:219:GLY:O	2.19	0.43
7:G:237:VAL:O	7:G:240:ALA:HB3	2.19	0.43
3:Q:69:VAL:HG13	3:Q:104:VAL:HG22	2.00	0.43
3:C:239:GLN:C	3:C:241:GLN:H	2.22	0.43
6:F:201:GLU:O	6:F:204:LYS:HD2	2.18	0.43
2:P:189:ILE:HG23	2:P:212:PHE:CE2	2.54	0.43
3:C:214:LYS:HD2	3:C:218:ASP:OD1	2.19	0.43
9:W:123:PHE:HA	9:W:128:CYS:O	2.19	0.43
5:E:174:THR:O	5:E:177:THR:HB	2.18	0.43
4:R:73:LEU:HD12	4:R:131:GLY:HA3	2.00	0.43
9:I:69:LYS:NZ	16:I:324:HOH:O	2.51	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.43
10:X:4:ILE:HD13	10:X:4:ILE:HA	1.91	0.43
12:Z:13:LEU:O	12:Z:23:LEU:HD23	2.18	0.43
3:C:160:GLN:CA	3:C:160:GLN:NE2	2.78	0.43
10:X:149:ARG:NH1	10:X:149:ARG:HG2	2.34	0.43
1:O:28:VAL:HG11	1:O:133:SER:HB2	2.01	0.43
8:H:156:SER:O	8:H:160:GLN:HG3	2.19	0.43
9:W:41:LYS:O	9:W:51:GLY:HA2	2.19	0.43
6:T:133:ILE:HA	6:T:145:TYR:O	2.19	0.43
1:O:222:LEU:HD23	1:O:224:TYR:O	2.19	0.43
7:U:12:PRO:HD3	16:U:328:HOH:O	2.19	0.43
4:R:234:GLU:O	4:R:238:LYS:HG3	2.19	0.43
4:R:159:TYR:CD2	4:R:162:LYS:HD3	2.54	0.43
6:F:95:PHE:CD2	6:F:103:ILE:HD12	2.54	0.43
2:P:140:ASP:OD2	2:P:146:GLN:NE2	2.47	0.43
13:M:104:ARG:HG3	13:M:105:SER:N	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:86:LEU:HD13	11:Y:86:LEU:C	2.39	0.43
7:U:68:ARG:NH1	7:U:68:ARG:HB2	2.33	0.43
11:Y:106:ARG:NH1	11:Y:106:ARG:HG2	2.34	0.43
11:K:75:SER:HB2	11:K:108:GLU:OE2	2.18	0.43
13:M:201:ASP:HB3	13:M:204:THR:OG1	2.18	0.43
4:D:214:ILE:HA	4:D:219:GLY:O	2.19	0.43
1:A:145:PHE:HD1	16:A:306:HOH:O	2.01	0.43
8:V:40:LYS:HE2	8:V:183:ASP:HA	2.00	0.43
3:Q:7:SER:O	4:R:128:ARG:HD3	2.18	0.43
11:K:169:ALA:HB1	9:W:178:ALA:O	2.18	0.43
14:N:44:CYS:HB2	14:N:98:ILE:HB	2.00	0.43
4:D:236:LYS:HE2	4:D:236:LYS:HB3	1.77	0.43
3:C:101:PRO:HG2	3:C:138:PRO:HG3	2.01	0.43
4:R:113:LEU:HD23	4:R:115:PHE:HE1	1.83	0.43
2:B:183:MET:HE2	2:B:188:ALA:N	2.33	0.43
8:H:38:SER:OG	8:H:41:ILE:HD13	2.19	0.43
1:A:231:LYS:HB2	16:A:347:HOH:O	2.19	0.43
1:O:234:ARG:NH1	1:O:234:ARG:HG2	2.33	0.43
10:X:8:ARG:NH1	10:X:8:ARG:HG2	2.34	0.43
9:I:26:LEU:CD2	9:I:40:GLU:HG2	2.49	0.43
10:J:130:TYR:CD2	10:J:144:LEU:HD13	2.54	0.43
8:V:10:ASN:O	8:V:179:GLU:HG3	2.19	0.43
12:L:57:PHE:CZ	12:L:59:ALA:HB3	2.54	0.43
6:T:71:GLY:O	6:T:134:PHE:HA	2.19	0.43
4:R:31:GLY:O	4:R:161:ALA:HA	2.19	0.42
6:F:165:ARG:HB3	6:F:165:ARG:HE	1.50	0.42
6:T:172:LEU:HD22	6:T:195:ILE:HD13	2.01	0.42
2:P:24:ALA:O	2:P:27:SER:HB3	2.19	0.42
4:D:59:ILE:HD12	4:D:210:GLN:HE21	1.84	0.42
7:U:232:ILE:O	7:U:235:ARG:N	2.51	0.42
2:P:229:PHE:HD2	2:P:229:PHE:N	2.17	0.42
10:J:118:GLN:NE2	10:J:132:ALA:O	2.52	0.42
11:Y:16:VAL:HG21	11:Y:34:VAL:HG23	2.00	0.42
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.19	0.42
2:P:41:ASP:N	2:P:41:ASP:OD2	2.49	0.42
12:L:213:ARG:CB	12:L:213:ARG:HH11	2.32	0.42
2:B:135:ILE:HD11	2:B:164:VAL:HG22	2.01	0.42
4:D:60:VAL:HG21	4:D:81:ILE:CD1	2.47	0.42
8:H:80:LEU:HD12	8:H:113:ILE:HD11	2.00	0.42
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.54	0.42
13:M:11:VAL:O	13:M:143:ALA:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:78:ASN:ND2	13:M:81:ALA:HA	2.35	0.42
12:Z:174:TYR:CD1	12:Z:175:LEU:N	2.88	0.42
13:M:65:ARG:CD	16:M:336:HOH:O	2.67	0.42
12:L:220:LYS:HG3	16:L:352:HOH:O	2.19	0.42
5:E:181:ILE:HG21	5:E:187:GLU:CB	2.47	0.42
3:Q:95:ARG:HH11	3:Q:101:PRO:HB3	1.82	0.42
8:H:148:LYS:HD3	16:H:346:HOH:O	2.19	0.42
13:M:168:THR:HA	16:M:359:HOH:O	2.19	0.42
8:H:10:ASN:O	8:H:179:GLU:HG3	2.19	0.42
3:Q:225:GLU:O	3:Q:229:GLN:HG3	2.19	0.42
12:Z:89:ALA:O	12:Z:93:ILE:HG12	2.19	0.42
1:O:226:GLY:HA3	8:V:186:TYR:HB3	2.01	0.42
5:S:131:LEU:HB2	5:S:146:PHE:HB3	2.01	0.42
13:M:74:ASN:HB3	16:M:318:HOH:O	2.19	0.42
2:B:136:TYR:HB2	2:B:148:TYR:HB2	2.01	0.42
3:Q:27:ARG:CB	3:Q:27:ARG:NH1	2.83	0.42
5:S:131:LEU:HD12	5:S:146:PHE:CD2	2.54	0.42
9:I:148:MET:HE3	9:I:152:LEU:HD11	2.00	0.42
12:L:51:VAL:HG23	12:L:112:ALA:HB3	2.01	0.42
13:M:213:GLN:HE21	13:M:213:GLN:HB3	1.48	0.42
1:A:203:GLU:OE2	1:A:203:GLU:HA	2.18	0.42
6:T:34:ILE:HG22	6:T:160:ALA:HB1	1.96	0.42
4:R:159:TYR:HA	5:S:55:LEU:O	2.20	0.42
3:Q:164:ARG:O	3:Q:165:ASN:HB2	2.19	0.42
3:C:225:GLU:O	3:C:229:GLN:HG3	2.18	0.42
2:B:17:ARG:HH11	2:B:17:ARG:HG2	1.84	0.42
4:D:73:LEU:HD12	4:D:131:GLY:HA3	2.02	0.42
12:Z:98:TYR:CE2	12:Z:101:ARG:HD3	2.55	0.42
4:D:54:ASP:N	4:D:54:ASP:OD2	2.48	0.42
3:Q:46:ARG:HD2	3:Q:206:LYS:O	2.20	0.42
11:Y:12:ILE:HD13	11:Y:112:ILE:CD1	2.50	0.42
12:Z:3:ASN:HD22	12:Z:4:PRO:N	2.17	0.42
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.40	0.42
6:F:172:LEU:HD22	6:F:195:ILE:HD13	2.02	0.42
2:B:65:LEU:HD12	2:B:75:ALA:HA	2.01	0.42
2:B:159:TRP:CD2	2:B:162:ILE:HD13	2.54	0.42
1:A:28:VAL:HG11	1:A:133:SER:HB2	2.02	0.42
4:D:194:LYS:HE2	4:D:198:GLN:OE1	2.20	0.42
7:G:210:SER:O	7:G:236:LEU:HD21	2.19	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.42
4:R:194:LYS:HE2	4:R:198:GLN:OE1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:36:GLY:HA2	1:O:44:VAL:O	2.20	0.42
9:I:11:VAL:HG22	9:I:24:CYS:HB3	2.01	0.42
6:F:71:GLY:O	6:F:134:PHE:HA	2.19	0.42
3:C:107:LEU:O	3:C:107:LEU:HD13	2.19	0.42
12:Z:3:ASN:ND2	12:Z:3:ASN:C	2.72	0.42
4:R:37:GLY:HA2	4:R:145:TYR:CD1	2.54	0.42
2:B:234:ILE:O	2:B:238:LEU:HB2	2.20	0.42
2:B:180:LYS:O	2:B:183:MET:HG3	2.19	0.42
1:O:94:HIS:CD2	8:V:61:SER:OG	2.72	0.42
8:H:144:GLN:O	8:H:145:ASP:HB2	2.20	0.42
3:Q:131:THR:O	3:Q:147:GLN:HA	2.19	0.42
12:L:38:ARG:NH1	12:L:221:ARG:HB3	2.35	0.42
2:B:1:GLY:HA3	5:E:122:TYR:CE1	2.55	0.42
7:G:68:ARG:HB2	7:G:68:ARG:NH1	2.33	0.42
3:Q:101:PRO:HG2	3:Q:138:PRO:HG3	1.99	0.42
10:X:129:PRO:HB2	10:X:130:TYR:CD1	2.55	0.42
13:M:54:SER:OG	13:M:113:ALA:HB3	2.20	0.42
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.19	0.42
6:T:32:THR:CG2	6:T:47:GLU:OE2	2.67	0.42
6:F:34:ILE:HG22	6:F:160:ALA:HB1	1.99	0.42
4:R:193:LEU:HD12	4:R:193:LEU:HA	1.88	0.42
3:C:222:LEU:N	3:C:222:LEU:CD1	2.83	0.42
2:P:134:PHE:O	2:P:149:THR:HA	2.20	0.42
5:S:61:LYS:O	5:S:72:SER:HA	2.20	0.42
13:M:25:ASP:HA	13:M:195:PHE:CB	2.50	0.42
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.02	0.42
2:P:105:ILE:HG22	16:P:309:HOH:O	2.19	0.42
8:H:147:THR:HG23	8:H:150:GLU:OE1	2.20	0.42
5:E:49:LYS:HB3	5:E:58:TYR:HB3	2.01	0.42
5:S:33:VAL:HG22	5:S:34:THR:N	2.35	0.42
2:P:36:GLY:O	2:P:161:ALA:HA	2.20	0.42
2:P:57:GLU:OE1	2:P:57:GLU:HA	2.20	0.42
8:H:35:HIS:HB3	8:H:56:THR:HG21	2.01	0.42
2:B:189:ILE:HG23	2:B:212:PHE:CE2	2.55	0.42
9:I:141:ALA:HB2	9:I:177:ASP:HB2	2.02	0.42
4:R:85:ARG:O	4:R:89:VAL:HG23	2.20	0.42
2:P:239:VAL:HG12	2:P:240:LYS:N	2.35	0.42
6:F:123:ASN:C	6:F:123:ASN:HD22	2.22	0.42
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.19	0.42
9:W:11:VAL:HG22	9:W:24:CYS:HB3	2.01	0.42
10:J:18:SER:HB2	10:J:176:PHE:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:106:ARG:HH11	5:E:106:ARG:HG2	1.84	0.42
11:Y:9:GLN:HE21	11:Y:9:GLN:HB3	1.70	0.42
10:X:194:ASP:O	10:X:198:GLN:HB2	2.18	0.41
2:B:140:ASP:OD2	2:B:146:GLN:NE2	2.45	0.41
6:F:165:ARG:O	6:F:169:LYS:HG3	2.20	0.41
3:Q:57:ILE:HD13	3:Q:57:ILE:H	1.85	0.41
9:W:137:VAL:HG11	9:W:145:LEU:HB3	2.00	0.41
12:L:213:ARG:NH1	12:L:213:ARG:HB3	2.35	0.41
2:P:35:ILE:HG12	2:P:196:LEU:HD21	2.01	0.41
5:S:181:ILE:HG21	5:S:187:GLU:CB	2.49	0.41
12:L:159:GLN:HG2	8:V:209:THR:CG2	2.48	0.41
9:W:104:VAL:HG23	9:W:106:PRO:HD3	2.02	0.41
7:G:78:ILE:N	7:G:79:PRO:HD2	2.35	0.41
13:M:162:GLU:O	13:M:165:ILE:HG13	2.20	0.41
4:R:24:LYS:O	4:R:166:SER:HA	2.20	0.41
7:U:230:GLU:HG2	16:U:356:HOH:O	2.19	0.41
5:S:49:LYS:HB3	5:S:58:TYR:HB3	2.01	0.41
2:P:234:ILE:O	2:P:238:LEU:HB2	2.20	0.41
4:R:88:ALA:HA	4:R:99:ILE:HG21	2.02	0.41
6:F:154:TRP:CZ3	7:G:60:VAL:HA	2.56	0.41
12:L:85:SER:HB2	12:L:87:ASN:OD1	2.20	0.41
8:H:139:GLU:HA	8:H:139:GLU:OE2	2.20	0.41
6:F:214:TRP:N	6:F:214:TRP:CD1	2.88	0.41
7:G:166:GLN:NE2	7:G:167:GLN:N	2.67	0.41
6:F:31:THR:CG2	6:F:32:THR:N	2.83	0.41
12:Z:20:PHE:CE1	12:Z:177:VAL:HA	2.55	0.41
1:A:89:SER:O	1:A:92:VAL:HG12	2.21	0.41
5:E:81:ARG:O	5:E:85:ASN:HB2	2.21	0.41
7:G:187:GLU:HG2	7:G:192:LYS:HB3	2.01	0.41
2:P:227:LYS:HZ1	2:P:233:GLU:CD	2.24	0.41
3:Q:11:PRO:HA	4:R:18:TYR:CE1	2.54	0.41
8:H:104:ASP:C	8:H:106:THR:H	2.23	0.41
6:F:112:LEU:O	6:F:116:VAL:HG23	2.20	0.41
9:W:26:LEU:CD2	9:W:40:GLU:HG2	2.49	0.41
7:U:231:ASN:N	7:U:231:ASN:HD22	2.17	0.41
3:C:69:VAL:HG13	3:C:104:VAL:HG22	2.01	0.41
14:N:159:LEU:O	14:N:163:ILE:CD1	2.68	0.41
6:T:200:HIS:O	6:T:200:HIS:CG	2.73	0.41
4:D:169:GLU:OE1	4:D:169:GLU:N	2.53	0.41
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.49	0.41
10:J:46:PHE:HB3	10:J:102:VAL:HG12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:38:ASN:HB2	11:K:39:PRO:HD2	2.02	0.41
5:S:84:SER:O	5:S:88:ARG:HG3	2.21	0.41
2:B:95:GLN:NE2	16:B:307:HOH:O	2.52	0.41
11:K:52:CYS:O	11:K:56:GLU:HB2	2.20	0.41
1:O:89:SER:O	1:O:92:VAL:HG12	2.20	0.41
4:D:85:ARG:HD2	16:D:304:HOH:O	2.20	0.41
9:I:30:SER:O	9:I:31:GLN:HB2	2.20	0.41
3:C:57:ILE:HG12	3:C:58:THR:N	2.35	0.41
2:B:18:LEU:O	2:B:22:GLU:HG2	2.21	0.41
7:G:49:LYS:O	7:G:51:PRO:HD3	2.21	0.41
6:F:191:GLN:HE21	6:F:194:LYS:CE	2.33	0.41
8:V:215:GLU:HG3	9:W:197:ARG:HG2	2.02	0.41
3:Q:107:LEU:O	3:Q:111:VAL:HG23	2.20	0.41
5:E:33:VAL:HG22	5:E:34:THR:N	2.36	0.41
6:T:115:TYR:O	6:T:118:ALA:HB3	2.20	0.41
8:V:144:GLN:O	8:V:145:ASP:HB2	2.20	0.41
11:K:8:PHE:HA	11:K:146:TRP:CE3	2.56	0.41
5:S:106:ARG:HH11	5:S:106:ARG:HG2	1.85	0.41
12:L:13:LEU:O	12:L:23:LEU:HD23	2.21	0.41
12:Z:3:ASN:HD22	12:Z:3:ASN:C	2.22	0.41
9:I:123:PHE:HA	9:I:128:CYS:O	2.20	0.41
6:T:41:GLY:CA	6:T:215:CYS:O	2.68	0.41
2:P:1:GLY:HA3	5:S:122:TYR:CE1	2.55	0.41
10:J:96:ARG:HH11	10:J:96:ARG:HG2	1.86	0.41
7:U:179:LYS:HB2	7:U:179:LYS:HE3	1.76	0.41
3:C:20:TYR:N	3:C:20:TYR:CD1	2.89	0.41
10:X:96:ARG:HG2	10:X:96:ARG:HH11	1.85	0.41
7:G:198:ILE:O	7:G:202:ILE:HG13	2.20	0.41
6:F:46:VAL:HG22	6:F:47:GLU:N	2.35	0.41
10:X:149:ARG:HA	10:X:150:PRO:HD3	1.93	0.41
2:B:6:ASP:OD1	3:C:4:ARG:HG3	2.20	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.56	0.41
6:T:103:ILE:HA	6:T:104:PRO:HD3	1.92	0.41
1:A:30:GLN:CA	1:A:30:GLN:HE21	2.25	0.41
11:K:106:ARG:HG2	11:K:106:ARG:NH1	2.36	0.41
7:G:78:ILE:HG22	7:G:79:PRO:HD3	2.02	0.41
2:B:65:LEU:HD13	7:U:93:ALA:CB	116.43	0.41
3:C:170:ARG:HB2	3:C:170:ARG:NH1	2.35	0.41
2:P:136:TYR:HB2	2:P:148:TYR:HB2	2.02	0.41
16:T:316:HOH:O	7:U:87:ARG:HB2	2.19	0.41
9:I:62:LEU:HD21	9:I:102:TYR:CD1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:185:TRP:C	11:K:186:ILE:HD13	2.41	0.41
7:G:19:VAL:O	7:G:23:PHE:HD2	2.04	0.41
9:I:122:GLY:O	9:I:130:ASP:HB3	2.21	0.41
8:V:139:GLU:OE2	8:V:139:GLU:HA	2.21	0.41
6:F:200:HIS:CG	6:F:200:HIS:O	2.73	0.41
2:P:128:ARG:HA	2:P:129:PRO:HD3	1.94	0.41
7:U:103:MET:HE3	7:U:108:LEU:HB2	2.03	0.41
12:L:126:ASP:HB2	12:L:130:SER:N	2.30	0.41
6:F:105:ILE:CG2	6:F:143:HIS:HB2	2.48	0.41
6:T:28:GLU:HB3	6:T:165:ARG:NH2	2.36	0.41
3:Q:170:ARG:NH1	3:Q:170:ARG:HB2	2.35	0.41
9:I:41:LYS:O	9:I:51:GLY:HA2	2.21	0.41
14:N:163:ILE:HG23	14:N:170:GLY:HA2	2.01	0.41
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.03	0.41
11:K:199:LYS:N	16:K:338:HOH:O	2.53	0.41
12:L:31:THR:O	12:L:32:ASP:HB2	2.21	0.41
9:I:53:THR:OG1	9:I:138:SER:OG	2.38	0.41
11:Y:185:TRP:C	11:Y:186:ILE:HD13	2.41	0.41
11:K:6:PHE:HA	11:K:125:ASP:O	2.21	0.41
5:E:9:THR:HG21	5:E:126:PRO:HG3	2.03	0.41
10:J:23:ARG:HA	10:J:23:ARG:HD3	1.95	0.41
7:G:179:LYS:HE3	7:G:179:LYS:HB2	1.76	0.41
4:D:159:TYR:CD2	4:D:162:LYS:HD3	2.53	0.41
3:Q:9:PHE:CE1	3:Q:15:ILE:HD11	2.56	0.41
3:Q:46:ARG:HB2	3:Q:207:ASN:HA	2.03	0.41
12:L:3:ASN:HD22	12:L:4:PRO:N	2.19	0.41
7:U:49:LYS:O	7:U:51:PRO:HD3	2.21	0.41
11:Y:106:ARG:HH11	11:Y:106:ARG:HG2	1.84	0.41
9:W:154:GLU:O	9:W:157:LEU:HG	2.21	0.41
2:B:237:ILE:O	2:B:237:ILE:HG13	2.21	0.41
4:D:37:GLY:HA2	4:D:145:TYR:CD1	2.56	0.41
2:B:134:PHE:O	2:B:149:THR:HA	2.20	0.41
8:V:156:SER:HB3	16:V:318:HOH:O	2.21	0.41
9:I:137:VAL:HG11	9:I:145:LEU:HB3	2.03	0.41
6:F:41:GLY:CA	6:F:215:CYS:O	2.69	0.41
14:N:82:PHE:HB3	14:N:113:ILE:HD12	2.02	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.03	0.41
1:A:36:GLY:HA2	1:A:44:VAL:O	2.21	0.41
8:H:40:LYS:HE2	8:H:183:ASP:HA	2.03	0.41
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.02	0.41
9:I:37:ASN:HD22	9:I:38:LYS:HG3	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:3:ILE:HD11	8:H:127:LEU:HB2	2.02	0.41
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.55	0.41
4:R:168:SER:O	4:R:172:GLN:HB2	2.21	0.41
4:D:82:GLU:OE1	11:K:69:ARG:HD2	2.21	0.41
11:K:13:ILE:HG13	11:K:153:ALA:HB1	2.03	0.41
4:R:169:GLU:OE1	4:R:169:GLU:N	2.54	0.41
8:V:35:HIS:HB3	8:V:56:THR:HG21	2.02	0.41
6:T:105:ILE:CG2	6:T:143:HIS:HB2	2.49	0.41
3:C:157:TRP:NE1	4:D:51:LEU:HD23	2.35	0.41
4:R:155:THR:HG22	5:S:77:ALA:HB3	2.02	0.41
1:A:4:ARG:HD3	5:E:122:TYR:CD2	2.56	0.41
4:D:44:LYS:HB2	4:D:208:ASN:C	2.41	0.41
11:Y:38:ASN:HB2	11:Y:39:PRO:HD2	2.03	0.41
3:Q:110:TYR:O	3:Q:114:VAL:HG23	2.20	0.41
10:J:150:PRO:HG2	11:Y:208:ASN:HD21	1.86	0.41
12:Z:108:HIS:HE1	12:Z:124:SER:HB2	1.85	0.41
2:B:36:GLY:O	2:B:161:ALA:HA	2.21	0.40
7:G:114:ASN:HD22	7:G:114:ASN:HA	1.62	0.40
2:B:41:ASP:OD2	2:B:41:ASP:N	2.52	0.40
6:T:214:TRP:CH2	6:T:219:GLU:HB3	2.56	0.40
12:Z:49:ASN:HA	12:Z:49:ASN:HD22	1.73	0.40
6:T:201:GLU:C	6:T:203:ASN:H	2.24	0.40
9:I:37:ASN:ND2	9:I:37:ASN:H	2.19	0.40
6:F:178:HIS:O	6:F:179:HIS:CG	2.74	0.40
7:U:210:SER:O	7:U:236:LEU:HD21	2.21	0.40
3:C:57:ILE:H	3:C:57:ILE:HD13	1.86	0.40
1:A:174:PHE:O	1:A:178:ARG:HG2	2.21	0.40
13:M:129:TYR:O	13:M:136:THR:HA	2.20	0.40
11:K:4:LEU:C	11:K:4:LEU:HD22	2.41	0.40
13:M:169:THR:HG23	16:M:359:HOH:O	2.21	0.40
9:I:65:MET:O	9:I:68:TYR:HB3	2.21	0.40
6:T:237:ASP:O	6:T:238:PHE:C	2.60	0.40
4:R:44:LYS:HB2	4:R:208:ASN:C	2.42	0.40
8:V:78:SER:O	8:V:82:MET:HG3	2.21	0.40
6:T:171:GLU:OE1	6:T:198:LEU:HD23	2.21	0.40
10:J:26:SER:HB2	11:K:133:GLN:NE2	2.36	0.40
3:C:178:ASP:OD1	3:C:180:LYS:HB2	2.21	0.40
12:L:5:TYR:CE2	12:L:106:TYR:HB2	2.56	0.40
6:F:83:HIS:CD2	6:F:128:PHE:HE2	2.37	0.40
6:T:214:TRP:N	6:T:214:TRP:CD1	2.87	0.40
6:F:17:ASN:ND2	6:F:20:VAL:HG23	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:4:VAL:HG23	4:D:116:GLY:HA2	2.03	0.40
11:Y:8:PHE:HA	11:Y:146:TRP:CE3	2.56	0.40
5:S:85:ASN:O	5:S:89:GLN:HG3	2.21	0.40
10:X:46:PHE:HB3	10:X:102:VAL:HG12	2.03	0.40
4:R:109:CYS:HB3	4:R:154:GLY:O	2.21	0.40
4:R:109:CYS:SG	4:R:156:PHE:HB3	2.62	0.40
10:J:60:ILE:HD13	10:J:60:ILE:HA	1.94	0.40
13:M:206:LEU:C	13:M:206:LEU:HD23	2.42	0.40
2:B:223:GLU:CG	2:B:224:VAL:N	2.85	0.40
5:E:206:THR:H	5:E:209:ASN:HD22	1.69	0.40
3:Q:66:ASP:OD1	3:Q:95:ARG:NH1	2.55	0.40
3:C:66:ASP:OD1	3:C:95:ARG:NH1	2.54	0.40
6:T:105:ILE:N	6:T:105:ILE:CD1	2.84	0.40
12:Z:5:TYR:CE2	12:Z:106:TYR:HB2	2.57	0.40
6:T:186:ARG:CG	6:T:186:ARG:HH11	2.34	0.40
10:J:174:MET:HE3	10:X:174:MET:HG2	2.04	0.40
6:F:176:VAL:HG21	7:G:54:LEU:HD23	2.04	0.40
8:V:18:THR:CB	8:V:30:ASN:HD22	2.34	0.40
2:B:172:GLN:HG2	3:C:50:LEU:HD12	2.04	0.40
7:U:87:ARG:CZ	7:U:115:LEU:HD21	2.52	0.40
10:X:18:SER:HB2	10:X:176:PHE:HB2	2.03	0.40
1:A:158:PRO:HG2	2:B:57:GLU:HB3	2.03	0.40
14:N:15:GLY:HA2	14:N:174:ARG:O	2.22	0.40
6:F:115:TYR:O	6:F:118:ALA:HB3	2.21	0.40
7:G:87:ARG:CZ	7:G:115:LEU:HD21	2.52	0.40
12:Z:80:ASN:HA	12:Z:80:ASN:HD22	1.63	0.40
7:G:103:MET:HE3	7:G:108:LEU:HD13	2.02	0.40
12:L:20:PHE:CE1	12:L:177:VAL:HA	2.57	0.40
3:Q:213:VAL:O	3:Q:213:VAL:HG13	2.21	0.40
3:Q:197:LEU:HD13	3:Q:208:ILE:HG23	2.03	0.40
6:F:123:ASN:HD22	6:F:123:ASN:N	2.18	0.40
11:Y:176:ASN:HD22	11:Y:176:ASN:HA	1.69	0.40
5:E:167:ALA:CB	5:E:195:ALA:O	2.69	0.40
12:L:165:ASN:O	12:L:167:LYS:HG2	2.21	0.40
12:Z:165:ASN:O	12:Z:167:LYS:HG2	2.22	0.40
11:Y:52:CYS:O	11:Y:56:GLU:HB2	2.22	0.40
4:R:59:ILE:HD12	4:R:210:GLN:HE21	1.86	0.40
4:R:38:VAL:HG11	4:R:137:ALA:HB1	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%)	226 (91%)	17 (7%)	5 (2%)	9	30
1	O	248/250 (99%)	226 (91%)	18 (7%)	4 (2%)	12	38
2	B	242/244 (99%)	212 (88%)	24 (10%)	6 (2%)	7	24
2	P	242/244 (99%)	213 (88%)	23 (10%)	6 (2%)	7	24
3	C	239/241 (99%)	218 (91%)	15 (6%)	6 (2%)	7	24
3	Q	239/241 (99%)	217 (91%)	16 (7%)	6 (2%)	7	24
4	D	240/242 (99%)	218 (91%)	17 (7%)	5 (2%)	9	29
4	R	240/242 (99%)	218 (91%)	17 (7%)	5 (2%)	9	29
5	E	231/233 (99%)	207 (90%)	15 (6%)	9 (4%)	4	12
5	S	231/233 (99%)	204 (88%)	20 (9%)	7 (3%)	5	18
6	F	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	24	58
6	T	242/244 (99%)	222 (92%)	18 (7%)	2 (1%)	24	58
7	G	241/243 (99%)	223 (92%)	15 (6%)	3 (1%)	16	47
7	U	241/243 (99%)	221 (92%)	17 (7%)	3 (1%)	16	47
8	H	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	21	55
8	V	220/222 (99%)	201 (91%)	16 (7%)	3 (1%)	14	42
9	I	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	34	69
9	W	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	34	69
10	J	196/198 (99%)	183 (93%)	11 (6%)	2 (1%)	19	52
10	X	196/198 (99%)	182 (93%)	13 (7%)	1 (0%)	34	69
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	34	69
11	Y	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	34	69
12	L	220/222 (99%)	199 (90%)	20 (9%)	1 (0%)	34	69
12	Z	220/222 (99%)	199 (90%)	20 (9%)	1 (0%)	34	69
13	M	231/233 (99%)	215 (93%)	15 (6%)	1 (0%)	39	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	231/233 (99%)	213 (92%)	16 (7%)	2 (1%)	21	55
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	b	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6312/6368 (99%)	5794 (92%)	432 (7%)	86 (1%)	14	42

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	SER
2	B	51	VAL
2	B	221	ASP
3	C	52	LEU
3	C	203	THR
4	D	122	GLU
5	E	2	ARG
7	G	242	GLN
1	O	53	SER
2	P	51	VAL
2	P	221	ASP
3	Q	52	LEU
4	R	122	GLU
5	S	2	ARG
7	U	242	GLN
2	B	62	THR
2	B	218	GLY
3	C	183	PRO
4	D	181	SER
5	E	175	LEU
5	E	201	ARG
5	E	217	LYS
9	I	191	LYS
10	J	193	ASP
12	L	81	ASP
2	P	62	THR
2	P	218	GLY
3	Q	183	PRO
3	Q	203	THR
4	R	181	SER
5	S	175	LEU
5	S	201	ARG
5	S	217	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	139	LYS
9	W	191	LYS
10	X	193	ASP
12	Z	81	ASP
2	B	183	MET
3	C	202	GLN
4	D	121	GLY
5	E	176	ASP
5	E	221	PHE
6	F	139	LYS
6	F	203	ASN
7	G	51	PRO
1	O	166	LYS
2	P	183	MET
3	Q	202	GLN
4	R	120	SER
4	R	121	GLY
5	S	176	ASP
5	S	221	PHE
6	T	203	ASN
7	U	51	PRO
1	A	2	THR
1	A	166	LYS
1	A	249	ALA
3	C	47	ARG
4	D	120	SER
8	H	105	PRO
10	J	186	LYS
1	O	2	THR
1	O	249	ALA
3	Q	47	ARG
8	V	91	GLN
8	V	105	PRO
1	A	3	ASP
5	E	227	GLU
8	H	91	GLN
13	M	10	SER
13	a	111	TRP
4	D	118	GLY
5	E	231	LYS
7	G	2	GLY
4	R	118	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	9	ASN
13	a	10	SER
5	S	181	ILE
7	U	2	GLY
5	E	181	ILE
11	Y	39	PRO
2	B	243	ILE
3	C	204	GLY
11	K	39	PRO
2	P	243	ILE
3	Q	204	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%)	203 (97%)	6 (3%)	50	83
1	O	209/209 (100%)	203 (97%)	6 (3%)	50	83
2	B	203/203 (100%)	191 (94%)	12 (6%)	24	57
2	P	203/203 (100%)	192 (95%)	11 (5%)	27	60
3	C	213/213 (100%)	202 (95%)	11 (5%)	29	62
3	Q	213/213 (100%)	202 (95%)	11 (5%)	29	62
4	D	198/198 (100%)	186 (94%)	12 (6%)	23	55
4	R	198/198 (100%)	186 (94%)	12 (6%)	23	55
5	E	192/192 (100%)	179 (93%)	13 (7%)	20	49
5	S	192/192 (100%)	178 (93%)	14 (7%)	17	44
6	F	201/201 (100%)	180 (90%)	21 (10%)	9	25
6	T	201/201 (100%)	180 (90%)	21 (10%)	9	25
7	G	207/207 (100%)	196 (95%)	11 (5%)	28	61
7	U	207/207 (100%)	197 (95%)	10 (5%)	31	66
8	H	181/181 (100%)	171 (94%)	10 (6%)	27	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V	181/181 (100%)	171 (94%)	10 (6%)	27	59
9	I	172/172 (100%)	164 (95%)	8 (5%)	32	67
9	W	172/172 (100%)	164 (95%)	8 (5%)	32	67
10	J	175/175 (100%)	171 (98%)	4 (2%)	58	88
10	X	175/175 (100%)	171 (98%)	4 (2%)	58	88
11	K	169/169 (100%)	162 (96%)	7 (4%)	37	72
11	Y	169/169 (100%)	161 (95%)	8 (5%)	32	67
12	L	185/185 (100%)	173 (94%)	12 (6%)	21	52
12	Z	185/185 (100%)	173 (94%)	12 (6%)	21	52
13	M	199/199 (100%)	190 (96%)	9 (4%)	34	68
13	a	199/199 (100%)	189 (95%)	10 (5%)	30	64
14	N	162/162 (100%)	155 (96%)	7 (4%)	35	70
14	b	162/162 (100%)	155 (96%)	7 (4%)	35	70
15	c	1/1 (100%)	1 (100%)	0	100	100
15	d	1/1 (100%)	1 (100%)	0	100	100
15	e	1/1 (100%)	1 (100%)	0	100	100
15	f	1/1 (100%)	1 (100%)	0	100	100
All	All	5336/5336 (100%)	5049 (95%)	287 (5%)	27	60

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	30	GLN
1	A	122	THR
1	A	157	PHE
1	A	178	ARG
1	A	213	ILE
2	B	65	LEU
2	B	69	ASN
2	B	70	ASP
2	B	119	GLN
2	B	149	THR
2	B	155	ASN
2	B	157	THR
2	B	184	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	191	LEU
2	B	212	PHE
2	B	220	ASN
2	B	239	VAL
3	C	4	ARG
3	C	51	LYS
3	C	55	THR
3	C	57	ILE
3	C	61	LYS
3	C	69	VAL
3	C	116	GLN
3	C	147	GLN
3	C	160	GLN
3	C	206	LYS
3	C	225	GLU
4	D	20	LEU
4	D	40	LEU
4	D	68	CYS
4	D	99	ILE
4	D	102	GLU
4	D	124	ARG
4	D	143	ASP
4	D	169	GLU
4	D	176	LEU
4	D	182	SER
4	D	183	LEU
4	D	214	ILE
5	E	9	THR
5	E	29	LYS
5	E	53	ASP
5	E	59	GLN
5	E	71	LEU
5	E	92	ASN
5	E	116	GLN
5	E	179	ILE
5	E	184	ASN
5	E	205	LEU
5	E	222	THR
5	E	227	GLU
5	E	231	LYS
6	F	7	SER
6	F	32	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	39	ASN
6	F	68	ARG
6	F	78	ILE
6	F	94	SER
6	F	101	THR
6	F	103	ILE
6	F	117	GLN
6	F	123	ASN
6	F	131	SER
6	F	165	ARG
6	F	181	GLU
6	F	186	ARG
6	F	201	GLU
6	F	202	ASP
6	F	203	ASN
6	F	208	PHE
6	F	214	TRP
6	F	221	ASN
6	F	243	ILE
7	G	24	LYS
7	G	68	ARG
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	166	GLN
7	G	186	ASN
7	G	201	MET
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
8	H	30	ASN
8	H	31	CYS
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	156	SER
8	H	196	ARG
9	I	37	ASN
9	I	52	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	68	TYR
9	I	123	PHE
9	I	166	ILE
9	I	171	LEU
9	I	182	TRP
9	I	202	ARG
10	J	71	GLU
10	J	78	GLN
10	J	92	ILE
10	J	189	ILE
11	K	4	LEU
11	K	8	PHE
11	K	9	GLN
11	K	17	ASP
11	K	104	TYR
11	K	107	LYS
11	K	147	ASP
12	L	1	GLN
12	L	3	ASN
12	L	23	LEU
12	L	49	ASN
12	L	70	ASN
12	L	71	SER
12	L	80	ASN
12	L	108	HIS
12	L	109	THR
12	L	126	ASP
12	L	132	GLU
12	L	165	ASN
13	M	37	ASN
13	M	48	ASN
13	M	69	ASP
13	M	70	LEU
13	M	104	ARG
13	M	159	VAL
13	M	161	ARG
13	M	171	GLN
13	M	226	LYS
14	N	36	ARG
14	N	83	LYS
14	N	88	GLU
14	N	104	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	105	LYS
14	N	115	LEU
14	N	144	GLU
1	O	4	ARG
1	O	30	GLN
1	O	122	THR
1	O	157	PHE
1	O	178	ARG
1	O	213	ILE
2	P	65	LEU
2	P	69	ASN
2	P	119	GLN
2	P	149	THR
2	P	155	ASN
2	P	157	THR
2	P	184	LYS
2	P	191	LEU
2	P	212	PHE
2	P	220	ASN
2	P	239	VAL
3	Q	4	ARG
3	Q	51	LYS
3	Q	55	THR
3	Q	57	ILE
3	Q	61	LYS
3	Q	69	VAL
3	Q	116	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	206	LYS
3	Q	225	GLU
4	R	20	LEU
4	R	40	LEU
4	R	68	CYS
4	R	99	ILE
4	R	102	GLU
4	R	124	ARG
4	R	143	ASP
4	R	169	GLU
4	R	176	LEU
4	R	182	SER
4	R	183	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	R	214	ILE
5	S	9	THR
5	S	29	LYS
5	S	53	ASP
5	S	59	GLN
5	S	71	LEU
5	S	92	ASN
5	S	116	GLN
5	S	179	ILE
5	S	184	ASN
5	S	197	SER
5	S	205	LEU
5	S	222	THR
5	S	227	GLU
5	S	231	LYS
6	T	7	SER
6	T	32	THR
6	T	39	ASN
6	T	68	ARG
6	T	78	ILE
6	T	94	SER
6	T	101	THR
6	T	103	ILE
6	T	117	GLN
6	T	123	ASN
6	T	131	SER
6	T	165	ARG
6	T	181	GLU
6	T	186	ARG
6	T	201	GLU
6	T	202	ASP
6	T	203	ASN
6	T	208	PHE
6	T	214	TRP
6	T	221	ASN
6	T	243	ILE
7	U	68	ARG
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	166	GLN
7	U	186	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	201	MET
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
8	V	30	ASN
8	V	31	CYS
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	156	SER
8	V	196	ARG
9	W	37	ASN
9	W	52	ILE
9	W	68	TYR
9	W	123	PHE
9	W	166	ILE
9	W	171	LEU
9	W	182	TRP
9	W	202	ARG
10	X	71	GLU
10	X	78	GLN
10	X	92	ILE
10	X	189	ILE
11	Y	4	LEU
11	Y	8	PHE
11	Y	9	GLN
11	Y	17	ASP
11	Y	104	TYR
11	Y	107	LYS
11	Y	118	ASP
11	Y	147	ASP
12	Z	1	GLN
12	Z	3	ASN
12	Z	23	LEU
12	Z	49	ASN
12	Z	70	ASN
12	Z	71	SER
12	Z	80	ASN
12	Z	108	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Z	109	THR
12	Z	126	ASP
12	Z	132	GLU
12	Z	165	ASN
13	a	37	ASN
13	a	48	ASN
13	a	69	ASP
13	a	70	LEU
13	a	82	ASP
13	a	104	ARG
13	a	159	VAL
13	a	161	ARG
13	a	171	GLN
13	a	226	LYS
14	b	36	ARG
14	b	83	LYS
14	b	88	GLU
14	b	104	ASP
14	b	105	LYS
14	b	115	LEU
14	b	144	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (197) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
1	A	143	ASN
2	B	20	GLN
2	B	58	GLN
2	B	69	ASN
2	B	93	HIS
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	220	ASN
2	B	232	GLN
3	C	17	GLN
3	C	77	ASN
3	C	92	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
3	C	241	GLN
4	D	15	GLN
4	D	100	ASN
4	D	139	HIS
4	D	160	ASN
4	D	210	GLN
4	D	225	ASN
5	E	4	ASN
5	E	30	GLN
5	E	59	GLN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
5	E	198	GLN
5	E	209	ASN
6	F	19	GLN
6	F	39	ASN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	186	ASN
7	G	231	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	172	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	189	ASN
8	H	219	ASN
9	I	37	ASN
9	I	71	ASN
9	I	88	GLN
9	I	156	ASN
10	J	55	GLN
10	J	78	GLN
10	J	86	GLN
10	J	118	GLN
10	J	146	HIS
10	J	147	HIS
10	J	191	GLN
10	J	198	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	176	ASN
11	K	208	ASN
11	K	209	ASN
12	L	1	GLN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	80	ASN
12	L	95	HIS
12	L	152	ASN
12	L	153	GLN
12	L	165	ASN
12	L	195	HIS
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	171	GLN
13	M	179	ASN
13	M	213	GLN
14	N	145	ASN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	143	ASN
2	P	20	GLN
2	P	58	GLN
2	P	69	ASN
2	P	93	HIS
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN
2	P	220	ASN
2	P	232	GLN
3	Q	17	GLN
3	Q	77	ASN
3	Q	92	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	241	GLN
4	R	15	GLN
4	R	100	ASN
4	R	139	HIS
4	R	160	ASN
4	R	210	GLN
4	R	225	ASN
5	S	4	ASN
5	S	59	GLN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
5	S	198	GLN
5	S	209	ASN
6	T	19	GLN
6	T	39	ASN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
7	U	30	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
7	U	231	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	172	ASN
8	V	189	ASN
8	V	219	ASN
9	W	37	ASN
9	W	88	GLN
9	W	156	ASN
10	X	55	GLN
10	X	63	ASN
10	X	78	GLN
10	X	86	GLN
10	X	118	GLN
10	X	146	HIS
10	X	147	HIS
10	X	191	GLN
10	X	198	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	176	ASN
11	Y	208	ASN
11	Y	209	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	95	HIS
12	Z	152	ASN
12	Z	153	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	Z	159	GLN
12	Z	165	ASN
12	Z	195	HIS
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	171	GLN
13	a	179	ASN
13	a	213	GLN
14	b	145	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	LYO	c	3	15	8,9,10	0.95	0	7,10,12	1.00	1 (14%)
15	OW6	c	4	8,15	6,6,7	1.32	1 (16%)	4,6,8	0.65	0
15	LYO	d	3	15	8,9,10	0.88	0	7,10,12	1.28	1 (14%)
15	OW6	d	4	11,15	6,6,7	1.14	0	4,6,8	0.73	0
15	LYO	e	3	15	8,9,10	0.97	0	7,10,12	0.95	1 (14%)
15	OW6	e	4	8,15	6,6,7	1.01	0	4,6,8	0.69	0
15	LYO	f	3	15	8,9,10	0.87	0	7,10,12	1.25	1 (14%)
15	OW6	f	4	11,15	6,6,7	1.12	0	4,6,8	0.68	0

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	LYO	c	3	15	-	0/7/9/11	0/0/0/0
15	OW6	c	4	8,15	-	0/3/4/5	0/0/0/0
15	LYO	d	3	15	-	0/7/9/11	0/0/0/0
15	OW6	d	4	11,15	-	0/3/4/5	0/0/0/0
15	LYO	e	3	15	-	0/7/9/11	0/0/0/0
15	OW6	e	4	8,15	-	0/3/4/5	0/0/0/0
15	LYO	f	3	15	-	0/7/9/11	0/0/0/0
15	OW6	f	4	11,15	-	0/3/4/5	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	c	4	OW6	C17-C15	2.60	1.56	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	d	3	LYO	O-C-CA	-2.56	118.83	125.49
15	f	3	LYO	O-C-CA	-2.48	119.04	125.49
15	c	3	LYO	O-C-CA	-2.41	119.22	125.49
15	e	3	LYO	O-C-CA	-2.29	119.52	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.23	6 (2%) 62 50	44, 65, 95, 118	0
1	O	250/250 (100%)	-0.26	7 (2%) 56 44	43, 66, 96, 118	0
2	B	244/244 (100%)	-0.07	8 (3%) 50 38	45, 67, 107, 132	0
2	P	244/244 (100%)	-0.10	11 (4%) 37 26	46, 68, 107, 133	0
3	C	241/241 (100%)	-0.01	14 (5%) 26 16	48, 71, 119, 140	0
3	Q	241/241 (100%)	0.02	13 (5%) 29 19	49, 74, 120, 140	0
4	D	242/242 (100%)	0.02	7 (2%) 55 43	50, 72, 105, 139	0
4	R	242/242 (100%)	0.02	11 (4%) 37 26	51, 73, 106, 139	0
5	E	233/233 (100%)	-0.07	10 (4%) 39 27	51, 77, 102, 124	0
5	S	233/233 (100%)	0.07	8 (3%) 49 36	51, 77, 103, 124	0
6	F	244/244 (100%)	-0.17	5 (2%) 68 58	47, 67, 103, 117	0
6	T	244/244 (100%)	-0.01	9 (3%) 45 33	47, 67, 102, 117	0
7	G	243/243 (100%)	-0.28	5 (2%) 67 56	43, 63, 92, 124	0
7	U	243/243 (100%)	-0.25	2 (0%) 87 81	45, 63, 92, 123	0
8	H	222/222 (100%)	-0.47	3 (1%) 78 69	41, 57, 79, 118	0
8	V	222/222 (100%)	-0.50	3 (1%) 78 69	43, 58, 79, 117	0
9	I	204/204 (100%)	-0.52	1 (0%) 91 88	40, 59, 80, 97	0
9	W	204/204 (100%)	-0.48	1 (0%) 91 88	40, 59, 81, 97	0
10	J	198/198 (100%)	-0.41	3 (1%) 76 68	41, 57, 77, 137	0
10	X	198/198 (100%)	-0.44	4 (2%) 68 58	42, 58, 78, 137	0
11	K	212/212 (100%)	-0.42	1 (0%) 91 88	41, 58, 79, 86	0
11	Y	212/212 (100%)	-0.44	1 (0%) 91 88	40, 58, 80, 87	0
12	L	222/222 (100%)	-0.47	2 (0%) 85 79	41, 60, 84, 108	0
12	Z	222/222 (100%)	-0.44	2 (0%) 85 79	40, 60, 84, 108	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/233 (100%)	-0.49	1 (0%) 93 90	39, 59, 76, 83	0
13	a	233/233 (100%)	-0.46	1 (0%) 93 90	39, 58, 76, 82	0
14	N	196/196 (100%)	-0.52	0 100 100	36, 54, 78, 90	0
14	b	196/196 (100%)	-0.49	1 (0%) 91 88	37, 54, 78, 90	0
15	c	1/4 (25%)	-0.30	0 100 100	63, 63, 63, 63	0
15	d	1/4 (25%)	0.03	0 100 100	53, 53, 53, 53	0
15	e	1/4 (25%)	-0.21	0 100 100	64, 64, 64, 64	0
15	f	1/4 (25%)	-0.67	0 100 100	53, 53, 53, 53	0
All	All	6372/6384 (99%)	-0.27	140 (2%) 65 54	36, 63, 99, 140	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	120	SER	8.0
4	D	121	GLY	7.8
2	B	220	ASN	7.7
4	R	121	GLY	7.4
7	U	243	ASP	7.2
4	R	120	SER	7.1
3	C	49	THR	6.9
3	C	50	LEU	6.8
2	P	220	ASN	6.8
10	X	198	GLN	6.5
4	D	118	GLY	6.2
2	P	219	ALA	5.6
4	D	122	GLU	5.5
5	E	202	ASP	5.4
10	X	197	ALA	5.4
10	J	198	GLN	5.2
2	B	51	VAL	5.2
6	F	1	GLY	5.1
3	Q	49	THR	5.1
5	S	2	ARG	4.9
4	D	119	ALA	4.9
4	R	118	GLY	4.9
8	H	221	CYS	4.9
3	Q	50	LEU	4.9
7	G	243	ASP	4.9
10	J	197	ALA	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	1	ALA	4.6
5	E	1	PHE	4.5
8	V	222	ASP	4.4
1	O	2	THR	4.4
2	B	219	ALA	4.3
4	R	119	ALA	4.2
1	O	1	MET	4.1
5	S	1	PHE	4.1
2	B	244	THR	4.1
6	T	1	GLY	4.1
7	U	1	ALA	4.0
3	Q	48	SER	3.9
5	E	2	ARG	3.9
12	L	174	TYR	3.8
5	S	202	ASP	3.8
2	P	223	GLU	3.7
1	A	2	THR	3.7
9	I	1	SER	3.7
12	Z	173	LYS	3.7
13	M	1	THR	3.6
10	X	196	GLN	3.5
13	a	1	THR	3.5
6	F	202	ASP	3.5
1	A	1	MET	3.4
6	T	2	THR	3.4
12	Z	174	TYR	3.4
8	H	222	ASP	3.4
1	A	250	LEU	3.4
3	Q	241	GLN	3.4
3	C	241	GLN	3.4
8	V	221	CYS	3.3
1	O	249	ALA	3.3
3	Q	240	GLU	3.3
4	R	124	ARG	3.3
3	Q	239	GLN	3.3
2	P	60	THR	3.2
10	J	196	GLN	3.2
3	Q	203	THR	3.2
3	Q	58	THR	3.2
2	P	221	ASP	3.1
4	D	124	ARG	3.1
4	R	49	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	221	ASP	2.9
5	S	173	ARG	2.9
5	S	36	GLY	2.9
1	O	230	ASP	2.9
6	T	51	THR	2.9
6	F	2	THR	2.9
6	T	53	LYS	2.9
4	R	125	LEU	2.9
3	Q	236	GLN	2.8
3	C	240	GLU	2.8
5	E	3	ASN	2.8
5	S	45	LEU	2.8
1	O	52	SER	2.8
1	O	250	LEU	2.7
3	C	48	SER	2.7
8	V	219	ASN	2.7
5	S	233	ILE	2.7
7	G	3	TYR	2.7
5	E	233	ILE	2.7
3	C	202	GLN	2.7
6	T	244	ASN	2.7
5	E	203	GLU	2.6
12	L	173	LYS	2.6
2	P	218	GLY	2.6
6	T	178	HIS	2.6
4	R	123	GLU	2.5
2	P	59	ASP	2.5
3	Q	202	GLN	2.5
2	B	223	GLU	2.5
3	Q	47	ARG	2.5
6	T	181	GLU	2.4
3	C	193	THR	2.4
4	R	240	ALA	2.4
1	A	36	GLY	2.4
3	C	33	GLY	2.4
11	Y	24	ASN	2.4
1	A	248	GLU	2.4
5	E	30	GLN	2.4
2	P	50	LYS	2.4
5	E	36	GLY	2.4
4	D	31	GLY	2.4
6	T	35	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	R	31	GLY	2.3
9	W	1	SER	2.3
11	K	212	GLY	2.3
1	O	231	LYS	2.3
3	C	43	GLY	2.3
4	R	122	GLU	2.3
3	C	53	GLN	2.3
2	P	51	VAL	2.2
14	b	195	GLN	2.2
5	E	54	GLU	2.2
2	B	218	GLY	2.2
5	E	201	ARG	2.2
7	G	240	ALA	2.2
5	S	134	ILE	2.2
6	F	241	LYS	2.2
2	P	244	THR	2.2
3	C	207	ASN	2.2
3	Q	57	ILE	2.2
2	B	217	LYS	2.1
1	A	51	SER	2.1
6	F	243	ILE	2.1
10	X	194	ASP	2.1
3	Q	207	ASN	2.0
7	G	180	SER	2.0
8	H	198	GLU	2.0
3	C	239	GLN	2.0
2	P	203	SER	2.0
6	T	180	PRO	2.0
3	C	238	LYS	2.0
3	C	203	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
15	LYO	e	3	10/11	0.93	0.17	-	60,61,62,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	LYO	c	3	10/11	0.95	0.17	-	59,60,63,63	0
15	0W6	c	4	7/8	0.93	0.14	-	57,58,61,63	0
15	0W6	f	4	7/8	0.95	0.13	-	49,50,56,56	0
15	0W6	d	4	7/8	0.96	0.11	-	49,50,56,56	0
15	0W6	e	4	7/8	0.95	0.15	-	57,59,61,62	0
15	LYO	d	3	10/11	0.95	0.17	-	48,51,53,54	0
15	LYO	f	3	10/11	0.96	0.16	-	48,51,53,54	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.