Full wwPDB X-ray Structure Validation Report (i)

Mar 20, 2024 – 04:17 PM EDT

PDB ID	:	3D29
Title	:	Proteasome Inhibition by Fellutamide B
Authors	:	Groll, M.; Hines, J.; Fahnestock, M.; Crews, M.C.
Deposited on	:	2008-05-07
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

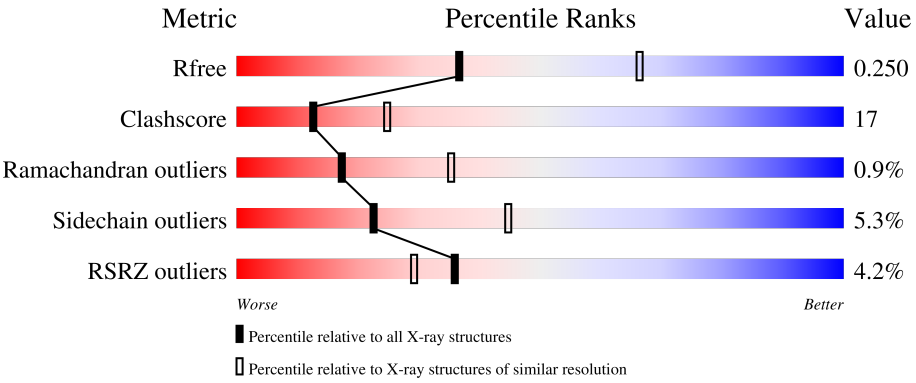
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	4% 74% 24% ·
1	O	250	6% 75% 24% ·
2	B	244	6% 59% 37% ·
2	P	244	6% 57% 40% ·
3	C	241	11% 61% 37% ·

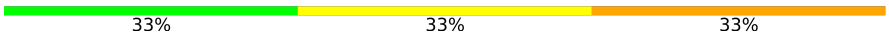
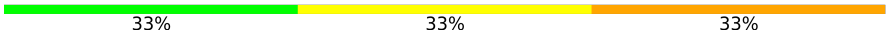
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Q	241	15% 61% 37%
4	D	242	7% 75% 22%
4	R	242	7% 73% 25%
5	E	233	4% 66% 29% 6%
5	S	233	3% 64% 31%
6	F	244	4% 69% 28%
6	T	244	3% 70% 27%
7	G	243	4% 68% 28%
7	U	243	3% 67% 28% 5%
8	H	222	% 69% 29%
8	V	222	% 72% 26%
9	I	204	2% 79% 19%
9	W	204	% 75% 23%
10	J	198	4% 65% 33%
10	X	198	3% 63% 36%
11	K	212	5% 70% 27%
11	Y	212	5% 71% 26%
12	L	222	3% 73% 24%
12	Z	222	5% 73% 23%
13	1	233	73% 25%
13	M	233	% 74% 24%
14	2	196	% 69% 28%
14	N	196	% 73% 24%
15	a	3	67% 33%
15	b	3	67% 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	c	3	
15	d	3	
15	e	3	
15	f	3	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 51114 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 PRE8 isoform 1.

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 PRE9 isoform 1.

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 PRE6 isoform 1.

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 PUP2 isoform 1.

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 PRE5 isoform 1.

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 PRE10 isoform 1.

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 SCL1 isoform 1.

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 endopeptidase complex.

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 PUP3 isoform 1.

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 subunit beta.

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 endopeptidase complex.

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 PRE7 isoform 1.

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 subunit beta.

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

- Molecule 15 is a protein called Fellutamide B.

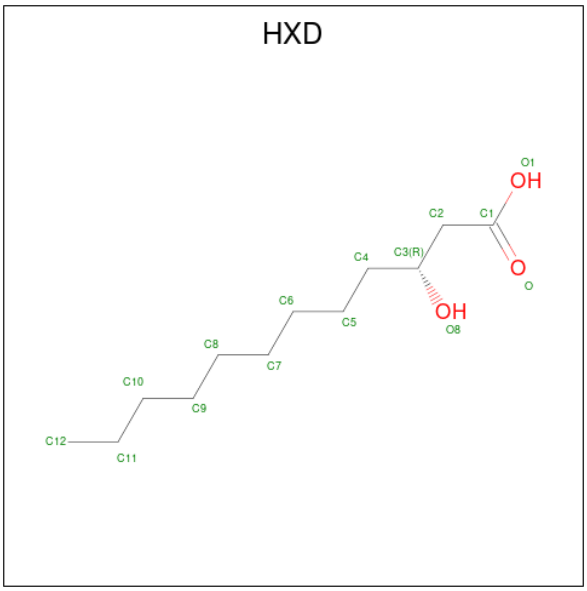
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	a	3	Total	C	N	O	0	0	0
			25	15	5	5			
15	b	3	Total	C	N	O	0	0	0
			25	15	5	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	c	3	Total C N O 25 15 5 5	0	0	0
15	d	3	Total C N O 25 15 5 5	0	0	0
15	e	3	Total C N O 25 15 5 5	0	0	0
15	f	3	Total C N O 25 15 5 5	0	0	0

- Molecule 16 is (3R)-3-HYDROXYDODECANOIC ACID (three-letter code: HXD) (formula: $C_{12}H_{24}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	a	1	Total C O 14 12 2	0	0
16	b	1	Total C O 14 12 2	0	0
16	c	1	Total C O 14 12 2	0	0
16	d	1	Total C O 14 12 2	0	0
16	e	1	Total C O 14 12 2	0	0
16	f	1	Total C O 14 12 2	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	55	Total O 55 55	0	0
17	B	36	Total O 36 36	0	0
17	C	46	Total O 46 46	0	0
17	D	42	Total O 42 42	0	0
17	E	23	Total O 23 23	0	0
17	F	46	Total O 46 46	0	0
17	G	62	Total O 62 62	0	0
17	H	51	Total O 51 51	0	0
17	I	66	Total O 66 66	0	0
17	J	53	Total O 53 53	0	0
17	K	42	Total O 42 42	0	0
17	L	56	Total O 56 56	0	0
17	M	68	Total O 68 68	0	0
17	N	59	Total O 59 59	0	0
17	O	35	Total O 35 35	0	0
17	P	29	Total O 29 29	0	0
17	Q	26	Total O 26 26	0	0
17	R	31	Total O 31 31	0	0
17	S	20	Total O 20 20	0	0
17	T	39	Total O 39 39	0	0
17	U	61	Total O 61 61	0	0
17	V	48	Total O 48 48	0	0

Continued on next page...

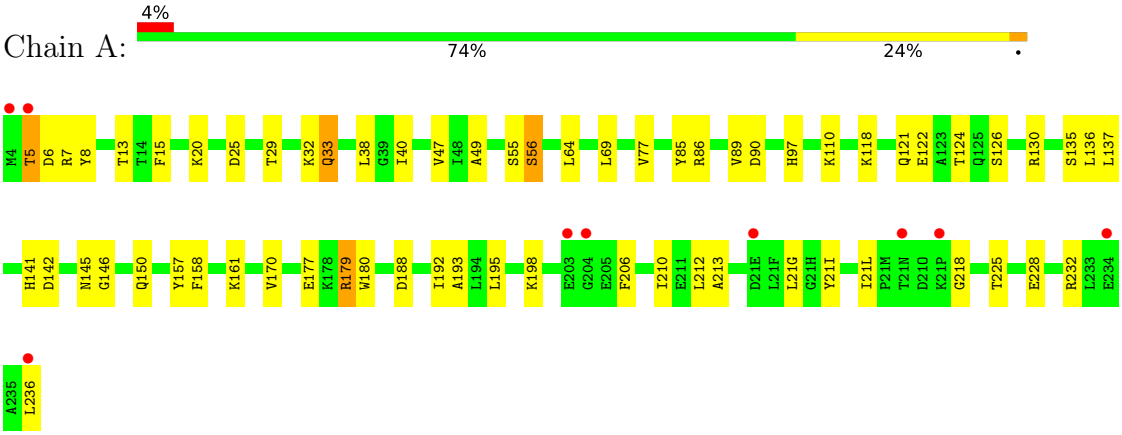
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	W	59	Total O 59 59	0	0
17	X	46	Total O 46 46	0	0
17	Y	48	Total O 48 48	0	0
17	Z	52	Total O 52 52	0	0
17	1	74	Total O 74 74	0	0
17	2	59	Total O 59 59	0	0

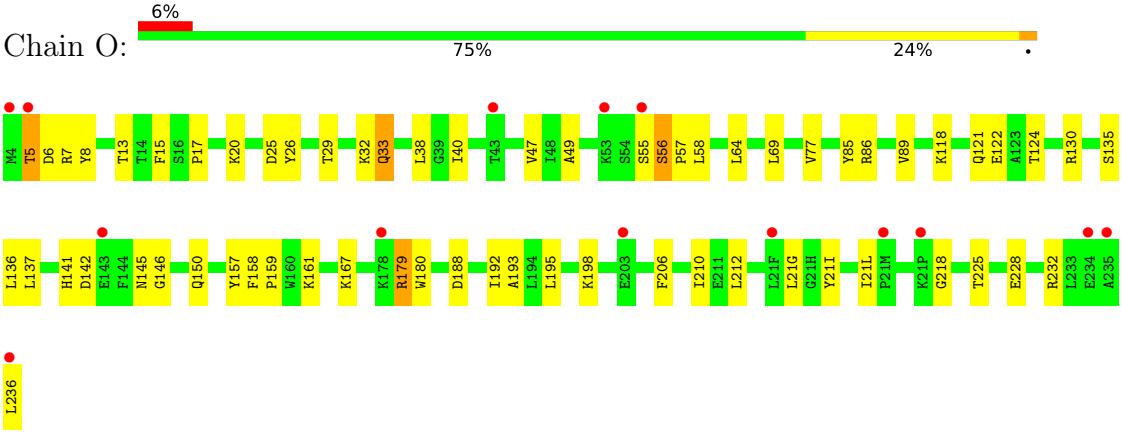
3 Residue-property plots (i)

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

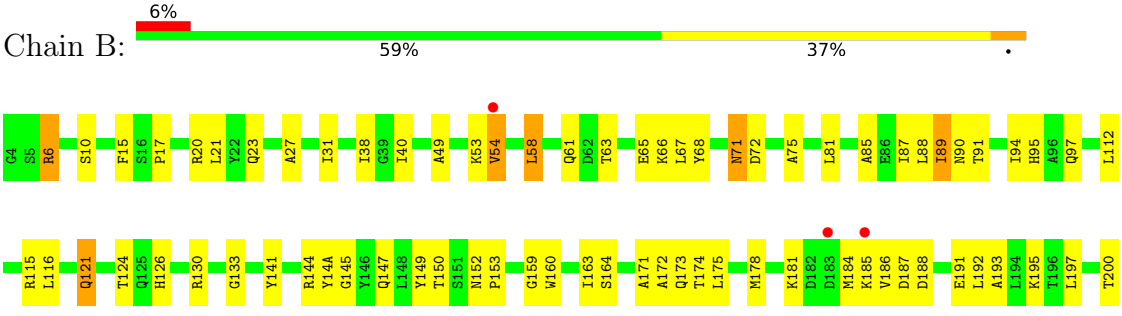
• Molecule 1: PRE8 isoform 1

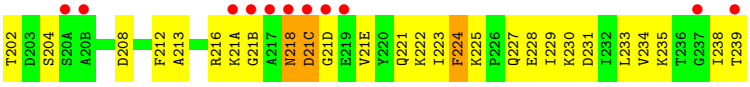


• Molecule 1: PRE8 isoform 1

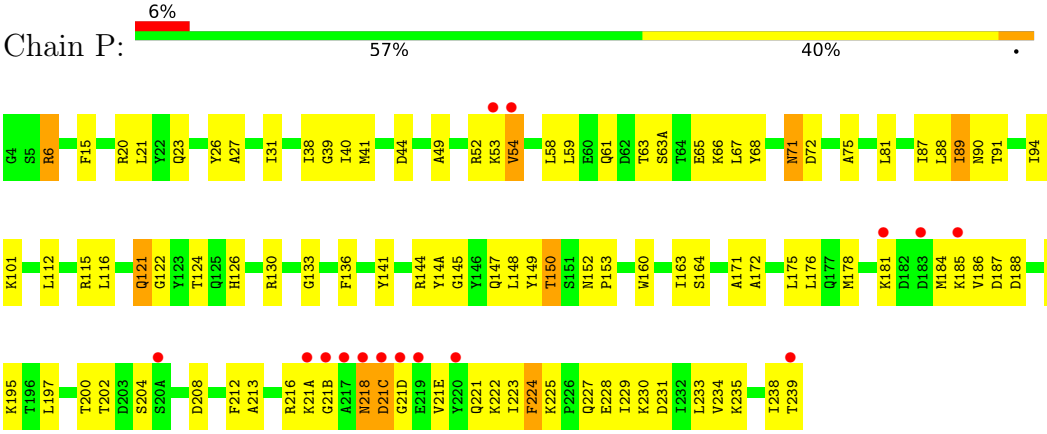


• Molecule 2: PRE9 isoform 1

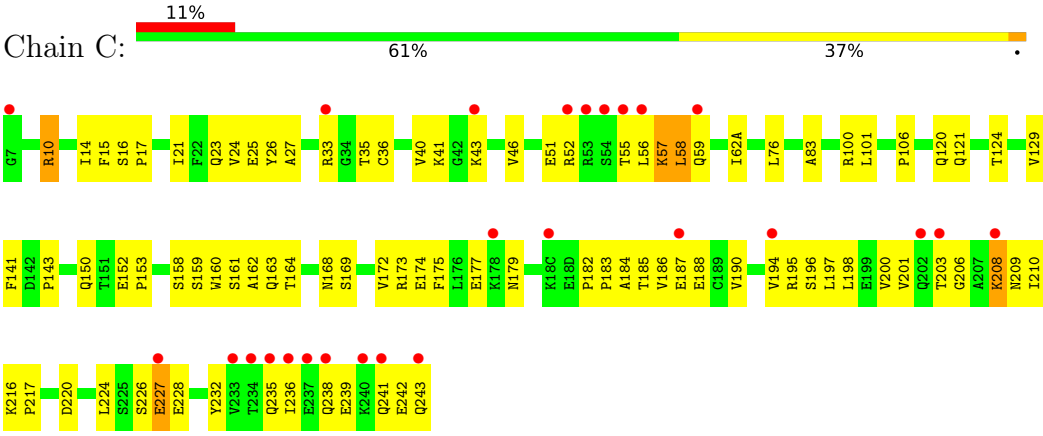




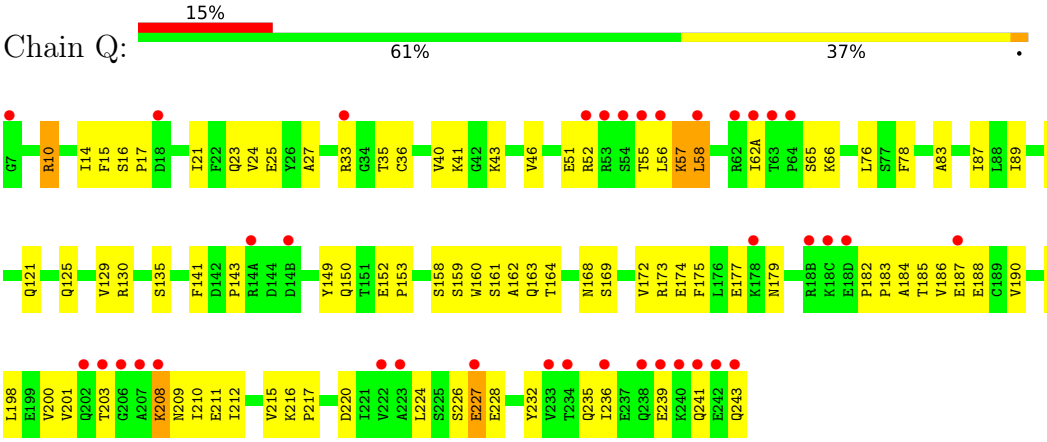
• Molecule 2: PRE9 isoform 1



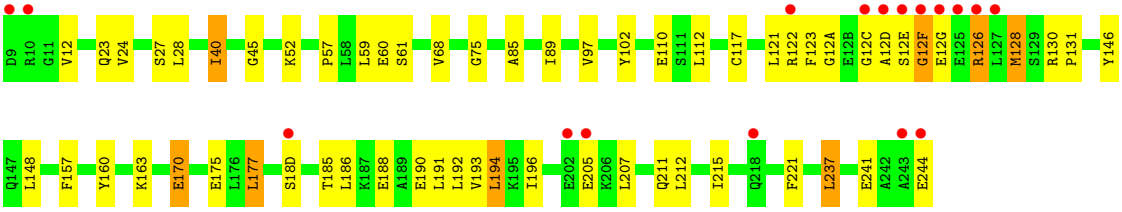
• Molecule 3: PRE6 isoform 1



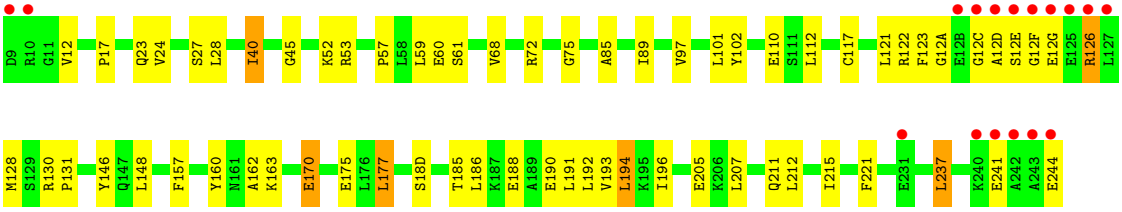
• Molecule 3: PRE6 isoform 1



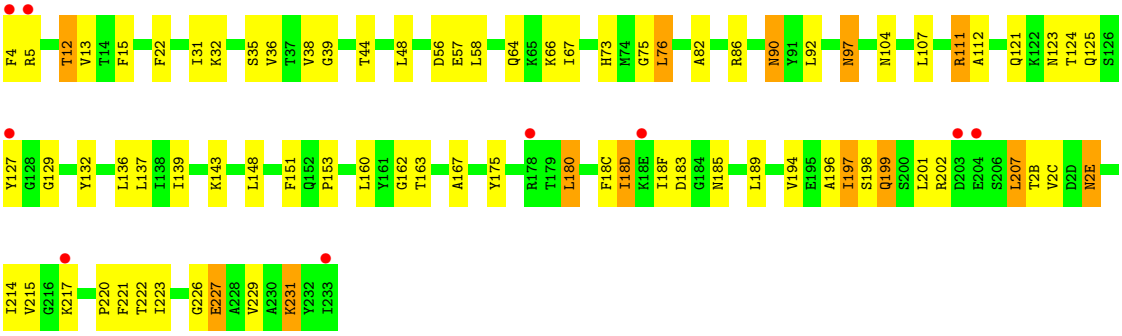
• Molecule 4: PUP2 isoform 1



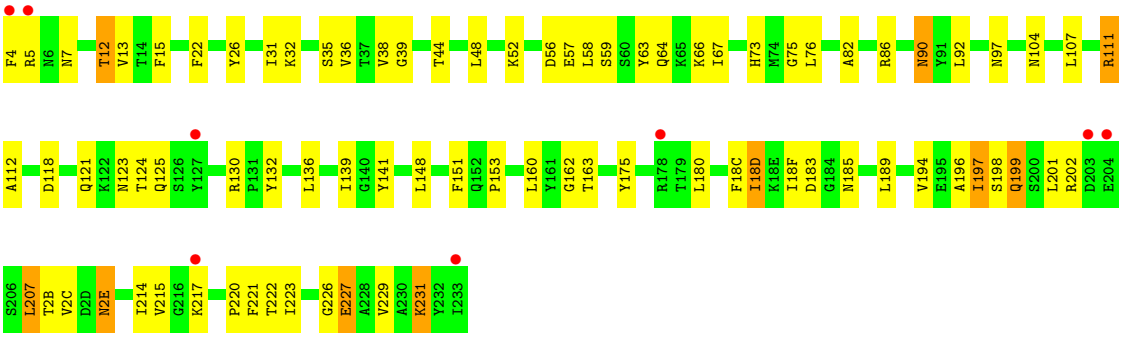
• Molecule 4: PUP2 isoform 1



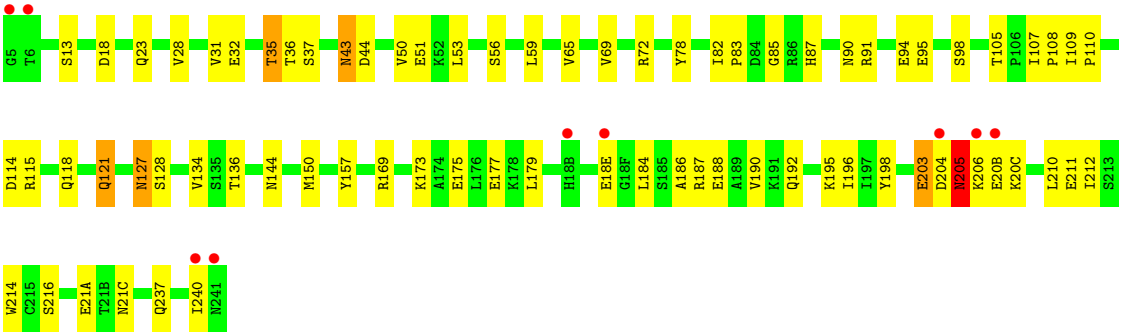
• Molecule 5: PRE5 isoform 1



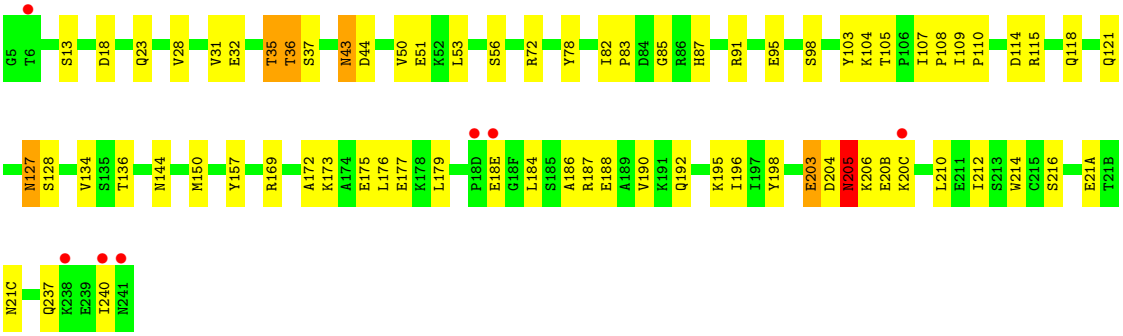
• Molecule 5: PRE5 isoform 1



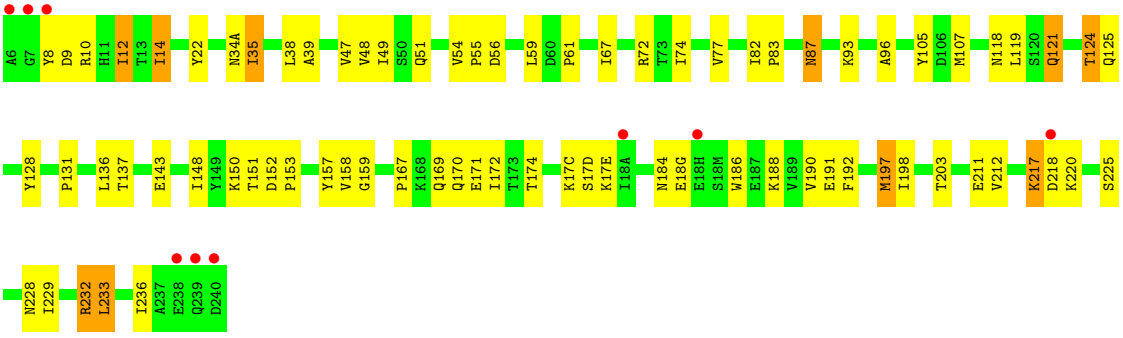
• Molecule 6: PRE10 isoform 1



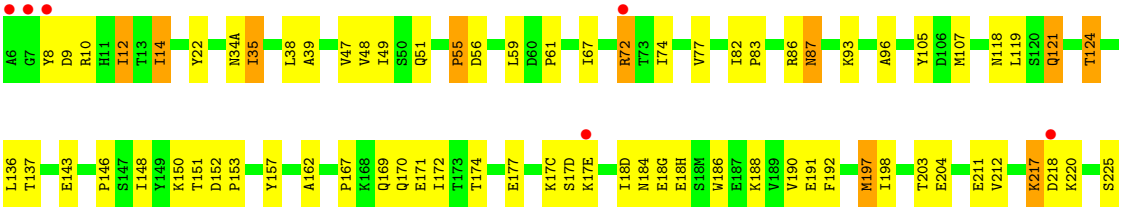
• Molecule 6: PRE10 isoform 1

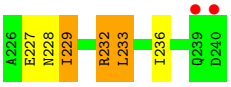


• Molecule 7: SCL1 isoform 1



• Molecule 7: SCL1 isoform 1



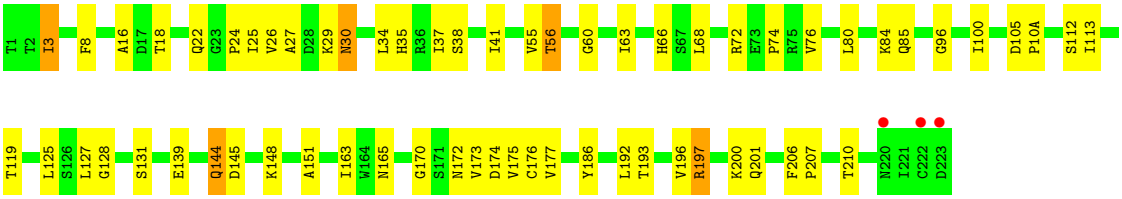


• Molecule 8: proteasome endopeptidase complex

Chain H:

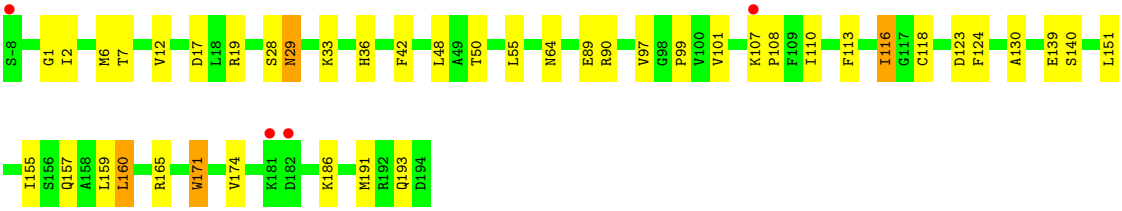
• Molecule 8: proteasome endopeptidase complex

Chain V:



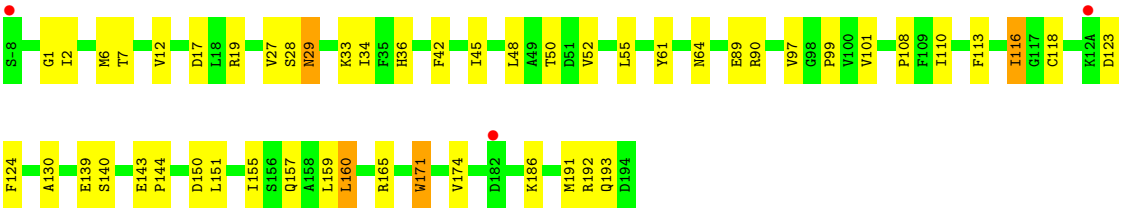
• Molecule 9: PUP3 isoform 1

Chain I:



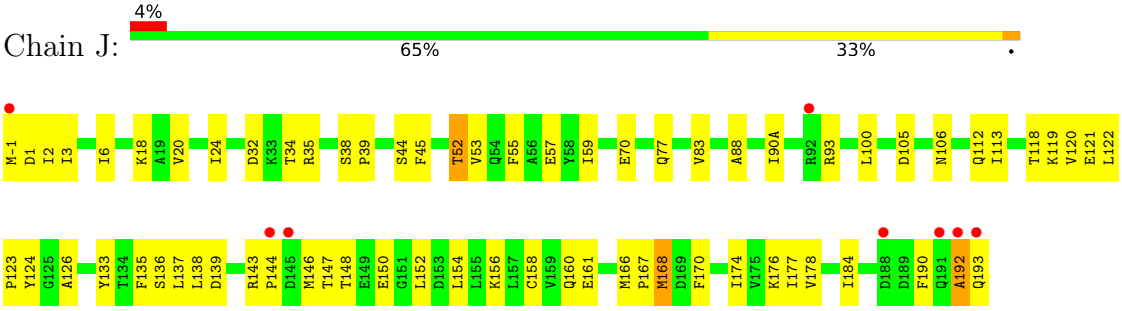
• Molecule 9: PUP3 isoform 1

Chain W:



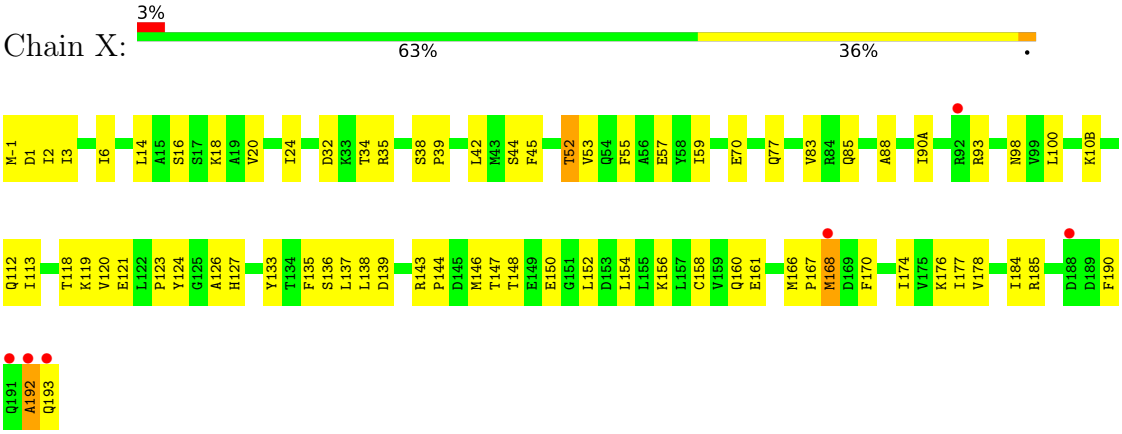
• Molecule 10: Proteasome subunit beta

Chain J:



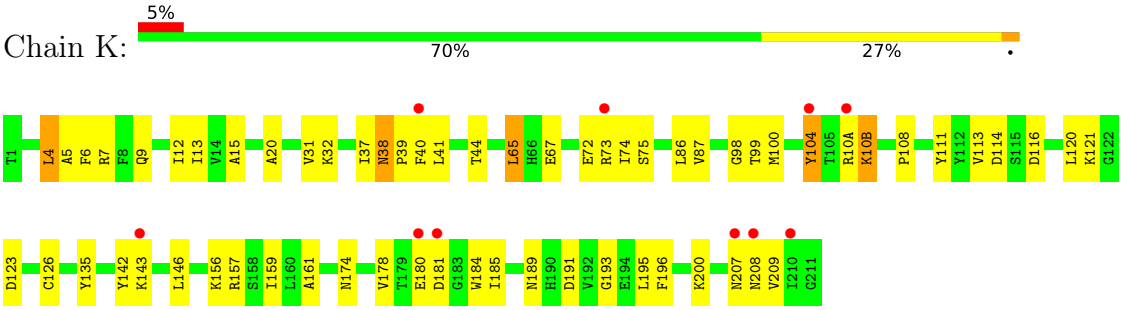
• Molecule 10: Proteasome subunit beta

Chain X:



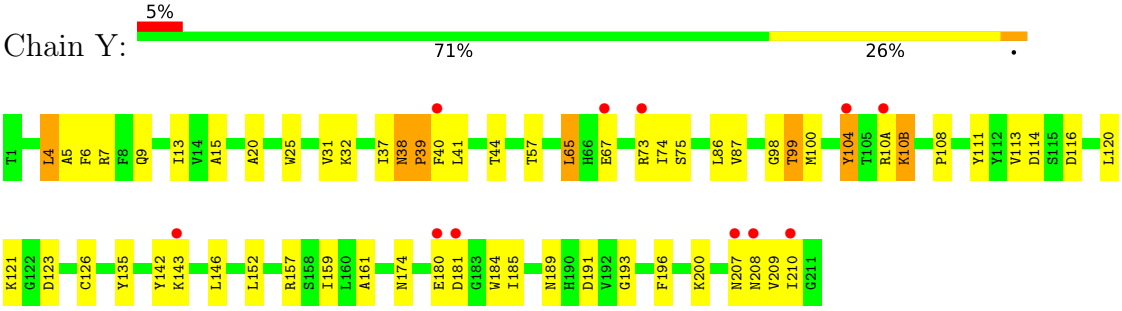
• Molecule 11: proteasome endopeptidase complex

Chain K:



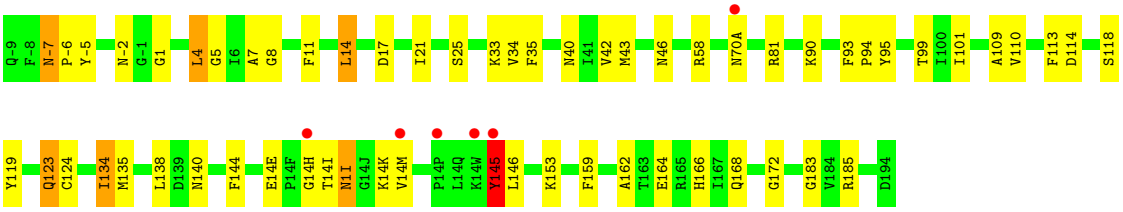
• Molecule 11: proteasome endopeptidase complex

Chain Y:



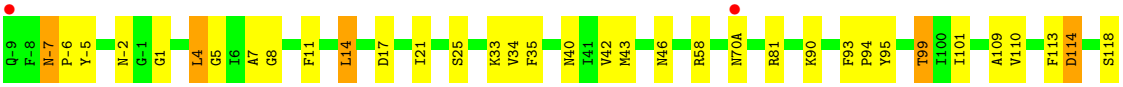
• Molecule 12: PRE7 isoform 1

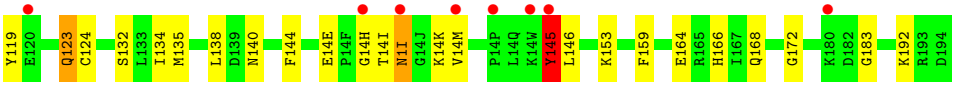
Chain L:



• Molecule 12: PRE7 isoform 1

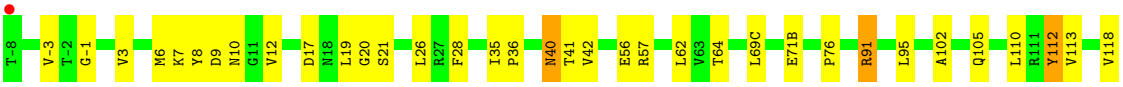
Chain Z:





• Molecule 13: Proteasome subunit beta

Chain M:

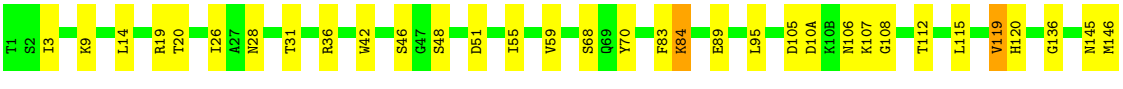


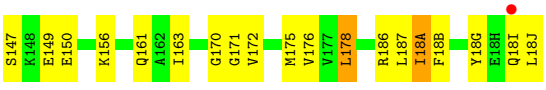
• Molecule 13: Proteasome subunit beta

Chain 1:

• Molecule 14: Proteasome subunit beta type-1

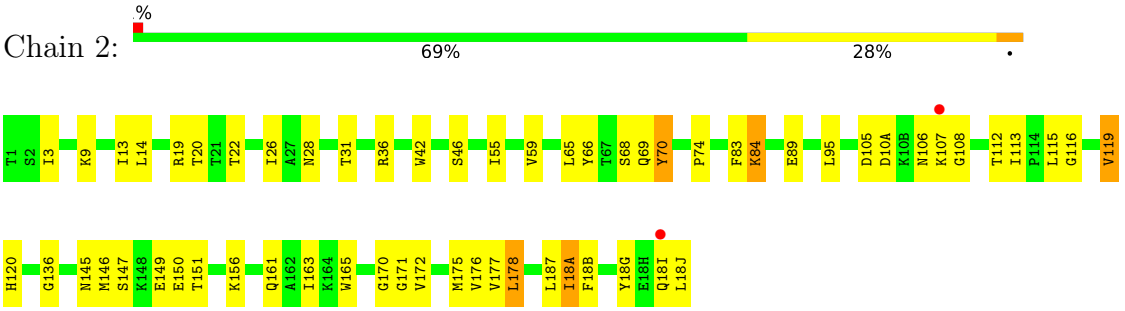
Chain N:





• Molecule 14: Proteasome subunit beta type-1

Chain 2:



• Molecule 15: Fellutamide B

Chain a:

• Molecule 15: Fellutamide B

Chain b:

• Molecule 15: Fellutamide B

Chain c:

• Molecule 15: Fellutamide B

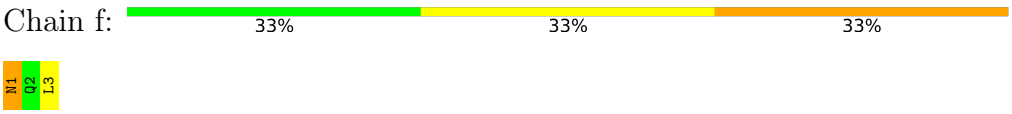
Chain d:

• Molecule 15: Fellutamide B

Chain e:

• Molecule 15: Fellutamide B

Chain f:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.27Å 301.58Å 143.45Å 90.00° 112.70° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 19.99 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.60) 98.0 (19.99-2.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.15 (at 2.56Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.266 0.227 , 0.250	Depositor DCC
R_{free} test set	15699 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	51114	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HXD

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	0.38	0/1952	0.63	0/2642
1	O	0.38	0/1952	0.63	0/2642
2	B	0.35	0/1935	0.62	0/2618
2	P	0.36	0/1935	0.62	0/2618
3	C	0.35	0/1920	0.60	0/2598
3	Q	0.35	0/1920	0.61	0/2598
4	D	0.35	0/1887	0.62	0/2541
4	R	0.35	0/1887	0.62	0/2541
5	E	0.36	0/1823	0.62	0/2463
5	S	0.36	0/1823	0.62	0/2463
6	F	0.38	0/1937	0.62	0/2614
6	T	0.39	0/1937	0.62	0/2614
7	G	0.42	0/1959	0.65	0/2652
7	U	0.41	0/1959	0.64	0/2652
8	H	0.39	0/1716	0.66	0/2326
8	V	0.39	0/1716	0.66	0/2326
9	I	0.40	0/1611	0.67	0/2174
9	W	0.41	0/1611	0.68	0/2174
10	J	0.39	0/1613	0.65	0/2173
10	X	0.39	0/1613	0.65	0/2173
11	K	0.42	0/1681	0.69	1/2274 (0.0%)
11	Y	0.43	0/1681	0.69	1/2274 (0.0%)
12	L	0.42	0/1795	0.70	1/2420 (0.0%)
12	Z	0.41	0/1795	0.69	1/2420 (0.0%)
13	1	0.40	0/1855	0.67	1/2514 (0.0%)
13	M	0.40	0/1855	0.67	1/2514 (0.0%)
14	2	0.41	0/1541	0.67	1/2087 (0.0%)
14	N	0.43	0/1541	0.67	0/2087
15	a	2.18	1/24 (4.2%)	1.10	0/30
15	b	2.37	1/24 (4.2%)	0.93	0/30
15	c	2.59	2/24 (8.3%)	1.32	0/30
15	d	2.10	1/24 (4.2%)	1.12	0/30

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
15	e	2.29	1/24 (4.2%)	0.92	0/30
15	f	2.69	2/24 (8.3%)	1.32	0/30
All	All	0.41	8/50594 (0.0%)	0.65	7/68372 (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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	3	LEU	C-OXT	10.55	1.43	1.23
15	f	3	LEU	C-OXT	10.28	1.42	1.23
15	e	3	LEU	C-OXT	9.99	1.42	1.23
15	c	3	LEU	C-OXT	9.83	1.42	1.23
15	a	3	LEU	C-OXT	9.48	1.41	1.23
15	d	3	LEU	C-OXT	9.03	1.40	1.23
15	f	1	ASN	N-CA	5.88	1.58	1.46
15	c	1	ASN	N-CA	5.76	1.57	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1	95	LEU	N-CA-C	-5.53	96.07	111.00
13	M	95	LEU	N-CA-C	-5.39	96.43	111.00
14	2	22	THR	N-CA-C	-5.16	97.07	111.00
11	K	98	GLY	N-CA-C	-5.16	100.21	113.10
11	Y	98	GLY	N-CA-C	-5.14	100.25	113.10
12	L	145	TYR	CA-CB-CG	-5.09	103.73	113.40
12	Z	145	TYR	CA-CB-CG	-5.09	103.73	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	59	0
1	O	1915	0	1926	58	0
2	B	1905	0	1901	97	0
2	P	1905	0	1901	91	0
3	C	1891	0	1900	107	0
3	Q	1891	0	1900	103	0
4	D	1862	0	1836	50	0
4	R	1862	0	1836	56	0
5	E	1795	0	1797	73	0
5	S	1795	0	1797	70	0
6	F	1897	0	1886	60	0
6	T	1897	0	1886	54	0
7	G	1921	0	1910	78	0
7	U	1921	0	1910	80	0
8	H	1685	0	1687	62	0
8	V	1685	0	1687	54	0
9	I	1581	0	1574	47	0
9	W	1581	0	1574	50	0
10	J	1585	0	1590	63	0
10	X	1585	0	1590	65	0
11	K	1644	0	1594	70	0
11	Y	1644	0	1594	71	0
12	L	1757	0	1711	52	0
12	Z	1757	0	1711	51	0
13	1	1824	0	1832	50	0
13	M	1824	0	1832	52	0
14	2	1512	0	1480	49	0
14	N	1512	0	1480	44	0
15	a	25	0	24	0	0
15	b	25	0	24	0	0
15	c	25	0	25	0	0
15	d	25	0	24	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	e	25	0	25	0	0
15	f	25	0	25	0	0
16	a	14	0	23	0	0
16	b	14	0	23	0	0
16	c	14	0	23	0	0
16	d	14	0	23	0	0
16	e	14	0	23	0	0
16	f	14	0	23	0	0
17	1	74	0	0	4	0
17	2	59	0	0	1	0
17	A	55	0	0	4	0
17	B	36	0	0	1	0
17	C	46	0	0	1	0
17	D	42	0	0	2	0
17	E	23	0	0	1	0
17	F	46	0	0	2	0
17	G	62	0	0	3	0
17	H	51	0	0	3	0
17	I	66	0	0	2	0
17	J	53	0	0	3	0
17	K	42	0	0	6	0
17	L	56	0	0	4	0
17	M	68	0	0	6	0
17	N	59	0	0	2	0
17	O	35	0	0	0	0
17	P	29	0	0	2	0
17	Q	26	0	0	2	0
17	R	31	0	0	3	0
17	S	20	0	0	1	0
17	T	39	0	0	2	0
17	U	61	0	0	6	0
17	V	48	0	0	3	0
17	W	59	0	0	1	0
17	X	46	0	0	6	0
17	Y	48	0	0	13	0
17	Z	52	0	0	3	0
All	All	51114	0	49533	1637	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 (1637) 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:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.10	1.16
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.33	1.10
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.33	1.10
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	1.10	1.09
11:Y:10(B):LYS:H	11:Y:10(B):LYS:HD2	1.11	1.09
3:C:201:VAL:HG21	3:C:210:ILE:HD11	1.10	1.06
4:D:175:GLU:HG2	4:D:196:ILE:HD12	1.36	1.06
7:U:9:ASP:HA	7:U:14:ILE:HD11	1.40	1.04
11:K:207:ASN:HD21	10:X:144:PRO:HG3	1.23	1.01
11:K:208:ASN:HD22	9:W:29:ASN:HD21	1.04	1.01
4:R:175:GLU:HG2	4:R:196:ILE:HD12	1.38	1.01
2:B:15:PHE:H	3:C:23:GLN:HE22	1.07	1.01
10:J:133:TYR:HD1	17:Y:232:HOH:O	1.44	1.00
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.10	0.99
7:G:9:ASP:HA	7:G:14:ILE:HD11	1.41	0.99
4:R:68:VAL:HG21	4:R:89:ILE:HD12	1.45	0.98
10:J:144:PRO:HG3	11:Y:207:ASN:HD21	1.25	0.98
10:J:133:TYR:HE1	17:X:225:HOH:O	1.45	0.97
3:C:100:ARG:NH1	3:C:106:PRO:HB3	1.80	0.97
1:A:15:PHE:H	2:B:23:GLN:HE22	1.11	0.96
3:C:163:GLN:NE2	3:C:164:THR:H	1.63	0.96
4:D:68:VAL:HG21	4:D:89:ILE:HD12	1.47	0.96
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.79	0.96
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.27	0.96
2:P:202:THR:HG22	2:P:204:SER:H	1.29	0.95
7:U:96:ALA:HA	7:U:107:MET:HE2	1.44	0.95
2:B:202:THR:HG22	2:B:204:SER:H	1.31	0.95
11:K:207:ASN:ND2	10:X:144:PRO:HG3	1.82	0.95
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.64	0.95
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.49	0.95
3:C:163:GLN:HE21	3:C:164:THR:N	1.66	0.94
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	1.68	0.93
7:G:96:ALA:HA	7:G:107:MET:HE2	1.48	0.93
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.67	0.93
9:I:29:ASN:HD21	11:Y:208:ASN:HD22	1.01	0.92
1:O:15:PHE:H	2:P:23:GLN:HE22	1.03	0.92
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.32	0.92
3:C:185:THR:HB	3:C:188:GLU:HG2	1.50	0.92
10:J:144:PRO:HG3	11:Y:207:ASN:ND2	1.85	0.92
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.13	0.92
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.35	0.91
12:L:123:GLN:HG3	12:L:145:TYR:OH	1.67	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:29:ASN:HD21	11:Y:208:ASN:ND2	1.69	0.91
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.52	0.91
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.53	0.91
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.37	0.90
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.11	0.90
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.51	0.90
11:Y:67:GLU:OE1	11:Y:73:ARG:HA	1.71	0.90
11:K:67:GLU:OE1	11:K:73:ARG:HA	1.72	0.89
5:S:2(B):THR:H	5:S:2(E):ASN:HD22	1.15	0.89
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.54	0.89
3:C:15:PHE:H	4:D:23:GLN:HE22	1.16	0.89
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.19	0.88
5:E:2(B):THR:H	5:E:2(E):ASN:HD22	1.15	0.88
3:Q:201:VAL:CG2	3:Q:210:ILE:HD11	2.03	0.88
11:K:99:THR:HG22	11:K:113:VAL:O	1.74	0.88
11:K:208:ASN:ND2	9:W:29:ASN:HD21	1.71	0.87
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.22	0.87
5:S:207:LEU:HD23	5:S:207:LEU:H	1.39	0.87
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.87	0.86
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.57	0.86
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.57	0.86
5:E:207:LEU:HD23	5:E:207:LEU:H	1.39	0.86
5:S:15:PHE:H	6:T:23:GLN:HE22	1.24	0.86
10:X:59:ILE:HD13	10:X:83:VAL:HG22	1.57	0.85
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.42	0.85
10:J:59:ILE:HD13	10:J:83:VAL:HG22	1.58	0.85
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.57	0.84
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.19	0.84
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.75	0.84
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.22	0.84
10:J:-1:MET:HG2	10:J:1:ASP:H	1.43	0.83
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.74	0.83
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.58	0.83
11:Y:210:ILE:HB	17:Y:248:HOH:O	1.78	0.83
3:C:201:VAL:CG2	3:C:210:ILE:HD11	2.03	0.83
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.43	0.83
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.44	0.83
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.44	0.82
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.44	0.82
11:Y:99:THR:HG22	11:Y:113:VAL:O	1.79	0.82
4:D:175:GLU:HG2	4:D:196:ILE:CD1	2.10	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:96:ALA:HA	7:G:107:MET:CE	2.08	0.82
7:U:96:ALA:HA	7:U:107:MET:CE	2.08	0.82
9:I:29:ASN:ND2	11:Y:208:ASN:HD22	1.77	0.81
5:E:15:PHE:H	6:F:23:GLN:HE22	1.28	0.81
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.46	0.81
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.62	0.80
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.45	0.80
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.77	0.80
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.94	0.80
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.63	0.80
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.65	0.79
3:C:185:THR:HG22	3:C:187:GLU:H	1.46	0.79
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.80	0.79
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.65	0.79
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.96	0.79
2:P:202:THR:HG22	2:P:204:SER:N	1.98	0.79
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.64	0.79
10:X:-1:MET:HG2	10:X:1:ASP:H	1.45	0.79
11:K:208:ASN:HD22	9:W:29:ASN:ND2	1.80	0.79
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.63	0.78
7:G:35:ILE:HG23	7:G:51:GLN:HB2	1.64	0.78
11:K:10(B):LYS:HD2	11:K:10(B):LYS:N	1.95	0.78
8:H:41:ILE:HD12	8:H:76:VAL:HG22	1.66	0.78
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.66	0.78
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.84	0.78
2:B:186:VAL:HG11	2:B:216:ARG:HD3	1.67	0.77
2:P:186:VAL:HG11	2:P:216:ARG:HD3	1.65	0.77
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.81	0.77
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.66	0.77
4:R:175:GLU:HG2	4:R:196:ILE:CD1	2.14	0.77
9:I:29:ASN:ND2	11:Y:208:ASN:ND2	2.32	0.77
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.99	0.77
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.85	0.76
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.67	0.76
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.68	0.76
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.00	0.76
5:S:18(D):ILE:HD13	5:S:18(D):ILE:O	1.86	0.76
2:B:202:THR:HG22	2:B:204:SER:N	1.99	0.76
2:B:160:TRP:CE2	2:B:163:ILE:HD12	2.21	0.76
6:F:192:GLN:O	6:F:196:ILE:HG12	1.85	0.76
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.67	0.75
12:L:166:HIS:HD2	12:L:168:GLN:H	1.33	0.75
2:P:160:TRP:CE2	2:P:163:ILE:HD12	2.21	0.75
11:Y:143:LYS:O	11:Y:146:LEU:HD13	1.85	0.75
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.32	0.75
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.67	0.75
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.33	0.75
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.68	0.75
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.50	0.74
4:R:52:LYS:HE3	4:R:211:GLN:HB2	1.68	0.74
4:R:185:THR:OG1	4:R:188:GLU:HG3	1.87	0.74
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.68	0.74
13:1:42:VAL:HG23	13:1:178:ILE:HD11	1.70	0.74
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.23	0.74
11:K:208:ASN:ND2	9:W:29:ASN:ND2	2.35	0.74
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.88	0.74
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:N	1.96	0.74
6:F:35:THR:HG21	6:F:51:GLU:O	1.88	0.73
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.71	0.73
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.87	0.73
4:D:52:LYS:HE3	4:D:211:GLN:HB2	1.69	0.73
8:H:201:GLN:HG3	12:Z:153:LYS:HG2	1.71	0.73
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.90	0.73
11:K:143:LYS:O	11:K:146:LEU:HD13	1.89	0.73
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.70	0.73
6:T:192:GLN:O	6:T:196:ILE:HG12	1.87	0.73
7:G:77:VAL:HG12	7:G:137:THR:HB	1.71	0.73
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.70	0.73
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.03	0.73
2:B:185:LYS:HD3	2:B:186:VAL:N	2.04	0.72
13:M:42:VAL:HG23	13:M:178:ILE:HD11	1.71	0.72
6:T:237:GLN:O	6:T:240:ILE:HG22	1.89	0.72
8:V:172:ASN:HD22	8:V:193:THR:HA	1.54	0.72
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.02	0.72
8:H:165:ASN:HD22	13:1:139:ARG:NH1	1.87	0.72
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.71	0.72
8:H:172:ASN:HD22	8:H:193:THR:HA	1.55	0.72
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.03	0.72
6:T:35:THR:HG21	6:T:51:GLU:O	1.89	0.72
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.88	0.72
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.23	0.72
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.52	0.72
5:E:18(D):ILE:HD13	5:E:18(D):ILE:O	1.89	0.72
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.70	0.72
8:V:41:ILE:HD12	8:V:76:VAL:HG22	1.72	0.72
8:H:3:ILE:HD11	8:H:127:LEU:CB	2.18	0.72
4:D:185:THR:OG1	4:D:188:GLU:HG3	1.89	0.71
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.72	0.71
7:G:217:LYS:HE3	7:G:217:LYS:HA	1.71	0.71
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.71	0.71
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.72	0.71
8:H:165:ASN:ND2	13:1:139:ARG:HH11	1.87	0.71
11:K:67:GLU:CD	11:K:73:ARG:HA	2.10	0.71
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.05	0.71
12:L:153:LYS:HG2	8:V:201:GLN:HG3	1.71	0.71
3:Q:163:GLN:HE21	3:Q:164:THR:H	0.82	0.71
8:V:3:ILE:HD11	8:V:127:LEU:CB	2.19	0.71
13:M:57:ARG:NE	17:M:244:HOH:O	2.23	0.71
2:P:185:LYS:HD3	2:P:186:VAL:N	2.06	0.70
6:F:237:GLN:O	6:F:240:ILE:HG22	1.91	0.70
3:C:185:THR:HG22	3:C:187:GLU:N	2.05	0.70
11:Y:67:GLU:CD	11:Y:73:ARG:HA	2.11	0.70
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.72	0.69
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.21	0.69
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.92	0.69
9:W:29:ASN:ND2	9:W:29:ASN:H	1.90	0.69
3:C:41:LYS:HG2	3:C:161:SER:O	1.91	0.69
5:E:207:LEU:H	5:E:207:LEU:CD2	2.06	0.69
10:J:146:MET:HE3	10:J:150:GLU:HB3	1.75	0.69
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.74	0.69
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.73	0.69
5:S:207:LEU:H	5:S:207:LEU:CD2	2.06	0.69
2:B:121:GLN:O	2:B:124:THR:HB	1.93	0.69
13:M:139:ARG:HH11	8:V:165:ASN:ND2	1.90	0.69
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.56	0.68
2:B:15:PHE:H	3:C:23:GLN:NE2	1.88	0.68
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.92	0.68
11:Y:38:ASN:ND2	17:Y:258:HOH:O	2.25	0.68
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.74	0.68
11:Y:181:ASP:N	17:Y:240:HOH:O	2.18	0.68
1:A:179:ARG:HH11	1:A:179:ARG:HB3	1.57	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:THR:HG22	10:J:53:VAL:N	2.09	0.67
4:R:192:LEU:O	4:R:196:ILE:HG12	1.95	0.67
7:U:77:VAL:HG12	7:U:137:THR:HB	1.75	0.67
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.04	0.67
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.77	0.67
9:I:2:ILE:HD13	9:I:159:LEU:CD1	2.24	0.67
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.41	0.67
9:I:6:MET:HE1	9:I:155:ILE:HA	1.76	0.67
13:M:139:ARG:NH1	8:V:165:ASN:HD22	1.91	0.67
10:J:112:GLN:NE2	17:J:234:HOH:O	2.26	0.67
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.77	0.67
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.23	0.67
2:B:149:TYR:OH	3:C:62(A):ILE:HB	1.95	0.67
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.43	0.67
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.41	0.67
1:A:21(G):LEU:HD13	1:A:218:GLY:HA2	1.75	0.67
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.94	0.67
7:G:87:ASN:C	7:G:87:ASN:HD22	1.98	0.67
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.76	0.67
9:I:2:ILE:HD13	9:I:159:LEU:HD11	1.75	0.66
7:G:77:VAL:CG1	7:G:137:THR:HB	2.26	0.66
7:U:87:ASN:C	7:U:87:ASN:HD22	1.99	0.66
5:S:227:GLU:CD	5:S:227:GLU:H	1.98	0.66
13:1:40:ASN:H	13:1:40:ASN:HD22	1.42	0.66
1:O:21(G):LEU:HD13	1:O:218:GLY:HA2	1.78	0.66
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.77	0.66
11:Y:10(B):LYS:H	11:Y:10(B):LYS:CD	1.91	0.66
14:2:18(A):ILE:HD13	14:2:18(B):PHE:N	2.11	0.66
12:L:135:MET:CE	9:W:165:ARG:NH2	2.58	0.66
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.95	0.66
10:X:52:THR:HG22	10:X:53:VAL:N	2.11	0.66
8:H:3:ILE:HD13	8:H:3:ILE:O	1.96	0.66
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.78	0.66
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.25	0.66
9:W:2:ILE:HD13	9:W:159:LEU:CD1	2.26	0.66
9:W:2:ILE:HD13	9:W:159:LEU:HD11	1.76	0.66
13:M:7:LYS:HG3	13:M:14(G):ILE:HD12	1.77	0.65
3:Q:197:LEU:O	3:Q:201:VAL:HG23	1.95	0.65
10:X:146:MET:HE3	10:X:150:GLU:HB3	1.77	0.65
13:M:40:ASN:H	13:M:40:ASN:HD22	1.43	0.65
9:I:29:ASN:ND2	9:I:29:ASN:H	1.93	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:179:ARG:HB3	1:O:179:ARG:NH1	2.12	0.65
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.45	0.65
8:V:3:ILE:HD13	8:V:3:ILE:O	1.97	0.65
11:K:73:ARG:NH2	11:K:104:TYR:O	2.30	0.65
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.26	0.65
5:E:227:GLU:CD	5:E:227:GLU:H	1.98	0.65
10:X:-1:MET:HG2	10:X:1:ASP:N	2.12	0.65
10:J:6:ILE:HD11	10:J:154:LEU:HD23	1.79	0.65
5:S:132:TYR:O	5:S:153:PRO:HB3	1.98	0.65
2:B:160:TRP:HA	3:C:59:GLN:HA	1.78	0.64
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.78	0.64
8:H:24:PRO:HG2	8:H:25:ILE:HD12	1.78	0.64
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.79	0.64
3:C:175:PHE:O	3:C:179:ASN:HB2	1.96	0.64
10:J:-1:MET:HG2	10:J:1:ASP:N	2.10	0.64
6:T:173:LYS:O	6:T:177:GLU:HG3	1.97	0.64
7:U:121:GLN:O	7:U:124:THR:HB	1.97	0.64
2:P:121:GLN:O	2:P:124:THR:HB	1.96	0.64
2:P:181:LYS:O	2:P:184:MET:HG3	1.96	0.64
2:B:181:LYS:O	2:B:184:MET:HG3	1.98	0.64
7:G:198:ILE:HG23	7:G:203:THR:O	1.97	0.64
14:N:18(A):ILE:HD13	14:N:18(B):PHE:N	2.13	0.64
6:T:127:ASN:HD22	6:T:128:SER:N	1.96	0.64
12:Z:99:THR:HG23	17:Z:201:HOH:O	1.98	0.64
12:Z:109:ALA:HA	17:Z:205:HOH:O	1.97	0.64
6:T:179:LEU:HD21	6:T:192:GLN:HG2	1.80	0.64
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.28	0.64
6:F:127:ASN:HD22	6:F:128:SER:N	1.95	0.64
10:J:133:TYR:OH	10:X:24:ILE:O	2.16	0.64
8:V:24:PRO:HG2	8:V:25:ILE:HD12	1.78	0.64
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.79	0.63
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.79	0.63
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.29	0.63
7:G:55:PRO:HG2	7:G:56:ASP:H	1.63	0.63
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.64	0.63
7:U:55:PRO:HG2	7:U:56:ASP:H	1.64	0.63
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.28	0.63
3:C:41:LYS:HD3	3:C:161:SER:HA	1.80	0.63
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.62	0.63
3:Q:65:SER:HB2	17:Q:246:HOH:O	1.96	0.63
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.81	0.63
1:O:188:ASP:O	1:O:192:ILE:HG12	1.99	0.63
10:X:6:ILE:HD11	10:X:154:LEU:HD23	1.80	0.63
11:Y:73:ARG:NH2	11:Y:104:TYR:O	2.31	0.63
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.79	0.63
1:A:188:ASP:O	1:A:192:ILE:HG12	1.98	0.63
3:Q:175:PHE:O	3:Q:179:ASN:HB2	1.99	0.63
3:C:197:LEU:O	3:C:201:VAL:HG23	1.98	0.62
10:J:24:ILE:O	10:X:133:TYR:OH	2.17	0.62
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.79	0.62
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.95	0.62
7:U:77:VAL:CG1	7:U:137:THR:HB	2.28	0.62
11:Y:67:GLU:OE2	17:Y:255:HOH:O	2.16	0.62
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.79	0.62
5:E:2(B):THR:N	5:E:2(E):ASN:HD22	1.95	0.62
5:E:226:GLY:O	5:E:229:VAL:HG22	2.00	0.62
3:Q:190:VAL:O	3:Q:194:VAL:HG23	1.99	0.62
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.34	0.62
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.14	0.62
3:C:190:VAL:O	3:C:194:VAL:HG23	2.00	0.62
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.29	0.62
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.30	0.62
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.81	0.62
6:F:173:LYS:O	6:F:177:GLU:HG3	1.99	0.62
6:F:175:GLU:HB3	6:F:196:ILE:HD12	1.82	0.62
9:I:2:ILE:CD1	9:I:159:LEU:HD11	2.30	0.62
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.47	0.62
11:K:181:ASP:N	17:K:239:HOH:O	2.32	0.62
5:S:207:LEU:HD23	5:S:207:LEU:N	2.14	0.62
4:D:192:LEU:O	4:D:196:ILE:HG12	2.00	0.62
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.00	0.62
1:A:110:LYS:HG2	17:A:245:HOH:O	2.00	0.61
10:J:147:THR:OG1	10:J:150:GLU:HG3	2.00	0.61
11:Y:40:PHE:HB3	11:Y:73:ARG:HH21	1.64	0.61
13:1:12:VAL:HG21	13:1:102:ALA:HB1	1.82	0.61
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.00	0.61
11:K:40:PHE:HB3	11:K:73:ARG:HH21	1.65	0.61
4:R:237:LEU:HD22	4:R:241:GLU:HG3	1.82	0.61
11:K:44:THR:OG1	11:K:100:MET:HB2	2.00	0.61
10:X:156:LYS:O	10:X:160:GLN:HG3	2.01	0.61
10:J:55:PHE:CZ	10:J:59:ILE:HD11	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.81	0.61
6:T:175:GLU:HB3	6:T:196:ILE:HD12	1.82	0.61
7:U:198:ILE:HG23	7:U:203:THR:O	2.01	0.61
2:B:202:THR:CG2	2:B:204:SER:H	2.10	0.61
4:D:186:LEU:O	4:D:190:GLU:HG3	2.01	0.61
12:L:109:ALA:HA	17:L:233:HOH:O	1.99	0.61
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.49	0.61
10:J:178:VAL:HG22	10:J:184:ILE:HG12	1.83	0.61
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.66	0.61
9:W:174:VAL:HG21	9:W:186:LYS:HE3	1.82	0.61
5:E:207:LEU:HD23	5:E:207:LEU:N	2.14	0.61
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.82	0.61
5:E:132:TYR:O	5:E:153:PRO:HB3	1.99	0.61
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.82	0.61
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.83	0.61
2:B:163:ILE:HG12	2:B:164:SER:N	2.15	0.61
5:E:12:THR:HG21	5:E:124:THR:HA	1.83	0.61
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.01	0.61
13:1:148:VAL:HG23	17:1:228:HOH:O	2.01	0.61
5:E:198:SER:HA	5:E:201:LEU:HG	1.83	0.60
2:P:163:ILE:HG12	2:P:164:SER:N	2.15	0.60
6:T:184:LEU:HD11	6:T:188:GLU:HB3	1.83	0.60
10:X:6:ILE:CD1	10:X:154:LEU:HD23	2.31	0.60
7:G:121:GLN:O	7:G:124:THR:HB	2.00	0.60
5:E:2(B):THR:OG1	5:E:2(E):ASN:HB3	2.00	0.60
10:J:6:ILE:CD1	10:J:154:LEU:HD23	2.31	0.60
10:J:146:MET:CE	10:J:150:GLU:HB3	2.31	0.60
17:P:250:HOH:O	3:Q:87:ILE:HD11	2.00	0.60
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.01	0.60
5:S:12:THR:HG21	5:S:124:THR:HA	1.83	0.60
4:D:112:LEU:C	4:D:112:LEU:HD13	2.21	0.60
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.83	0.60
2:P:202:THR:CG2	2:P:204:SER:H	2.10	0.60
4:D:237:LEU:HD22	4:D:241:GLU:HG3	1.82	0.60
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.84	0.60
6:F:184:LEU:HD11	6:F:188:GLU:HB3	1.84	0.60
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.83	0.60
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.83	0.60
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.84	0.60
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.83	0.60
6:F:179:LEU:HD21	6:F:192:GLN:HG2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.32	0.60
13:M:12:VAL:HG21	13:M:102:ALA:HB1	1.82	0.60
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.37	0.60
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.83	0.60
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.83	0.60
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.84	0.60
3:C:46:VAL:O	3:C:215:VAL:HG12	2.02	0.60
3:Q:197:LEU:HD13	3:Q:210:ILE:HD12	1.82	0.60
5:S:2(B):THR:OG1	5:S:2(E):ASN:HB3	2.02	0.59
7:U:67:ILE:CD1	7:U:211:GLU:HG2	2.31	0.59
10:X:146:MET:CE	10:X:150:GLU:HB3	2.32	0.59
11:Y:104:TYR:CE1	11:Y:180:GLU:OE2	2.55	0.59
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.38	0.59
8:H:72:ARG:HG3	8:H:72:ARG:HH11	1.68	0.59
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.83	0.59
9:I:174:VAL:HG21	9:I:186:LYS:HE3	1.84	0.59
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.00	0.59
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.33	0.59
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.84	0.59
9:W:2:ILE:CD1	9:W:159:LEU:HD11	2.32	0.59
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.37	0.59
3:C:197:LEU:HD13	3:C:210:ILE:HD12	1.83	0.59
5:S:2(B):THR:N	5:S:2(E):ASN:HD22	1.95	0.59
6:T:186:ALA:O	6:T:190:VAL:HG23	2.02	0.59
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.67	0.59
9:W:48:LEU:HG	9:W:50:THR:HG22	1.84	0.59
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.02	0.59
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.37	0.59
10:J:-1:MET:N	17:J:246:HOH:O	2.32	0.59
5:S:226:GLY:O	5:S:229:VAL:HG22	2.03	0.59
2:P:186:VAL:HG11	2:P:216:ARG:CD	2.33	0.59
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.36	0.59
8:V:84:LYS:HG3	8:V:85:GLN:N	2.17	0.59
3:C:186:VAL:O	3:C:190:VAL:HG23	2.03	0.59
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.49	0.59
8:V:172:ASN:ND2	8:V:193:THR:HA	2.17	0.59
3:C:163:GLN:HE21	3:C:164:THR:H	0.80	0.58
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.33	0.58
8:H:128:GLY:O	8:H:131:SER:HB2	2.02	0.58
10:J:156:LYS:O	10:J:160:GLN:HG3	2.03	0.58
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:178:VAL:HG22	10:X:184:ILE:HG12	1.84	0.58
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.85	0.58
9:I:48:LEU:HG	9:I:50:THR:HG22	1.85	0.58
12:Z:-7:ASN:C	12:Z:-7:ASN:HD22	2.07	0.58
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.34	0.58
13:M:35:ILE:HG12	13:M:56:GLU:CG	2.34	0.58
5:S:221:PHE:CE1	5:S:223:ILE:HD11	2.39	0.58
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.39	0.58
5:S:198:SER:HA	5:S:201:LEU:HG	1.84	0.58
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.84	0.58
10:X:44:SER:OG	10:X:100:LEU:HB2	2.04	0.58
13:1:76:PRO:HD2	13:1:105:GLN:OE1	2.04	0.58
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.49	0.58
8:H:172:ASN:ND2	8:H:193:THR:HA	2.18	0.58
14:N:107:LYS:HG2	14:N:108:GLY:N	2.18	0.58
13:1:149:GLN:H	13:1:149:GLN:NE2	2.02	0.58
2:B:234:VAL:HA	2:B:239:THR:HA	1.85	0.58
4:R:121:LEU:HA	4:R:123:PHE:CE1	2.39	0.58
5:S:35:SER:HB3	5:S:66:LYS:HZ3	1.68	0.58
7:U:228:ASN:HB3	17:U:242:HOH:O	2.03	0.58
5:E:175:TYR:CD2	5:E:196:ALA:HA	2.39	0.58
7:G:67:ILE:CD1	7:G:211:GLU:HG2	2.33	0.58
5:S:227:GLU:CD	5:S:227:GLU:N	2.57	0.58
3:C:57:LYS:O	3:C:58:LEU:HB2	2.02	0.58
4:D:85:ALA:O	4:D:89:ILE:HG12	2.03	0.58
6:F:186:ALA:O	6:F:190:VAL:HG23	2.04	0.58
10:J:44:SER:OG	10:J:100:LEU:HB2	2.04	0.58
11:K:104:TYR:CE1	11:K:180:GLU:OE2	2.57	0.58
1:O:86:ARG:NE	7:U:118:ASN:HD21	1.98	0.58
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.04	0.58
5:S:175:TYR:CD2	5:S:196:ALA:HA	2.39	0.58
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.19	0.58
13:M:149:GLN:NE2	13:M:149:GLN:H	2.02	0.57
14:N:9:LYS:HA	14:N:145:ASN:HD22	1.69	0.57
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.04	0.57
2:B:71:ASN:ND2	2:B:72:ASP:H	2.02	0.57
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.04	0.57
3:C:227:GLU:N	3:C:227:GLU:OE1	2.37	0.57
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.85	0.57
1:O:21(L):ILE:N	1:O:21(L):ILE:HD12	2.19	0.57
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.14	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:PHE:N	3:C:23:GLN:HE22	1.89	0.57
5:E:221:PHE:CE1	5:E:223:ILE:HD11	2.40	0.57
7:G:212:VAL:HG23	7:G:229:ILE:HD13	1.85	0.57
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.85	0.57
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.70	0.57
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.86	0.57
11:Y:114:ASP:OD1	11:Y:116:ASP:HB2	2.04	0.57
5:E:227:GLU:CD	5:E:227:GLU:N	2.57	0.57
12:L:123:GLN:CG	12:L:145:TYR:OH	2.47	0.57
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.19	0.57
2:P:234:VAL:HA	2:P:239:THR:HA	1.85	0.57
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.87	0.57
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.86	0.57
12:L:166:HIS:CD2	12:L:168:GLN:H	2.20	0.57
4:R:112:LEU:HD13	4:R:112:LEU:C	2.25	0.57
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.70	0.57
7:G:233:LEU:O	7:G:236:ILE:HG13	2.05	0.57
2:P:75:ALA:HB2	2:P:221:GLN:NE2	2.20	0.57
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.87	0.57
8:H:41:ILE:CD1	8:H:76:VAL:HG22	2.34	0.57
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.85	0.57
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.87	0.57
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.04	0.57
14:2:107:LYS:HG2	14:2:108:GLY:N	2.19	0.57
4:D:122:ARG:HH11	4:D:122:ARG:HG2	1.70	0.57
8:H:200:LYS:HE3	9:I:140:SER:O	2.05	0.57
13:M:19:LEU:HD12	13:M:28:PHE:O	2.05	0.57
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.35	0.57
7:U:212:VAL:HG23	7:U:229:ILE:HD13	1.85	0.57
2:B:75:ALA:HB2	2:B:221:GLN:NE2	2.20	0.57
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.87	0.57
12:Z:123:GLN:CG	12:Z:145:TYR:OH	2.47	0.57
10:J:93:ARG:HG2	10:J:93:ARG:HH11	1.71	0.56
8:V:128:GLY:O	8:V:131:SER:HB2	2.04	0.56
5:E:36:VAL:HG13	5:E:197:ILE:HD11	1.87	0.56
5:E:167:ALA:HB3	17:E:253:HOH:O	2.06	0.56
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.34	0.56
6:F:175:GLU:HB3	6:F:196:ILE:CD1	2.36	0.56
9:I:116:ILE:HD13	9:I:116:ILE:H	1.70	0.56
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.20	0.56
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:71:ASN:ND2	2:P:72:ASP:H	2.02	0.56
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.87	0.56
8:V:72:ARG:HG3	8:V:72:ARG:HH11	1.69	0.56
13:1:35:ILE:HG12	13:1:56:GLU:CG	2.34	0.56
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.40	0.56
5:S:36:VAL:HG13	5:S:197:ILE:HD11	1.86	0.56
6:T:175:GLU:HB3	6:T:196:ILE:CD1	2.35	0.56
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.87	0.56
5:S:220:PRO:O	5:S:222:THR:HG23	2.06	0.56
8:V:200:LYS:HE3	9:W:140:SER:O	2.05	0.56
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.34	0.56
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.05	0.56
2:B:224:PHE:H	2:B:224:PHE:HD2	1.54	0.56
5:E:86:ARG:O	5:E:90:ASN:HB2	2.05	0.56
9:I:29:ASN:ND2	9:I:29:ASN:N	2.53	0.56
7:U:143:GLU:HA	7:U:217:LYS:NZ	2.21	0.56
9:W:29:ASN:ND2	9:W:29:ASN:N	2.51	0.56
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.70	0.56
3:C:35:THR:HB	3:C:51:GLU:HG3	1.87	0.56
4:D:40:ILE:HG13	4:D:193:VAL:CG2	2.35	0.56
8:H:84:LYS:HG3	8:H:85:GLN:N	2.18	0.56
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.86	0.56
10:X:55:PHE:CZ	10:X:59:ILE:HD11	2.39	0.56
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.41	0.56
4:D:121:LEU:HA	4:D:123:PHE:CE1	2.40	0.56
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.06	0.56
4:R:186:LEU:O	4:R:190:GLU:HG3	2.06	0.56
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.88	0.56
1:A:21(L):ILE:N	1:A:21(L):ILE:HD12	2.21	0.56
13:M:14(C):ARG:HG3	13:M:14(C):ARG:HH11	1.71	0.56
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.88	0.56
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.87	0.56
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.87	0.56
14:2:9:LYS:HA	14:2:145:ASN:HD22	1.71	0.56
11:K:114:ASP:OD1	11:K:116:ASP:HB2	2.06	0.56
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.21	0.56
5:E:207:LEU:HA	5:E:2(E):ASN:HD21	1.70	0.55
11:K:6:PHE:HA	11:K:123:ASP:O	2.05	0.55
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.06	0.55
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.06	0.55
5:S:73:HIS:HE1	5:S:107:LEU:O	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:86:ARG:O	5:S:90:ASN:HB2	2.06	0.55
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.35	0.55
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.87	0.55
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.88	0.55
8:H:153:LYS:HD2	17:H:251:HOH:O	2.05	0.55
10:J:161:GLU:HA	10:J:161:GLU:OE2	2.06	0.55
4:R:85:ALA:O	4:R:89:ILE:HG12	2.07	0.55
8:V:34:LEU:HB2	17:V:238:HOH:O	2.07	0.55
13:1:19:LEU:HD12	13:1:28:PHE:O	2.06	0.55
13:1:113:VAL:HA	13:1:118:VAL:O	2.06	0.55
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.70	0.55
6:F:175:GLU:CB	6:F:196:ILE:HD12	2.37	0.55
1:O:57:PRO:HG3	7:U:177:GLU:CD	2.26	0.55
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.87	0.55
9:W:116:ILE:HD13	9:W:116:ILE:H	1.70	0.55
8:H:34:LEU:HB2	17:H:247:HOH:O	2.05	0.55
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.22	0.55
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.20	0.55
11:Y:41:LEU:HB2	17:Y:258:HOH:O	2.05	0.55
5:E:220:PRO:O	5:E:222:THR:HG23	2.07	0.55
8:H:84:LYS:HE2	8:H:119:THR:HG23	1.88	0.55
11:K:142:TYR:O	11:K:143:LYS:HD2	2.07	0.55
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.40	0.55
5:S:207:LEU:HA	5:S:2(E):ASN:HD21	1.70	0.55
4:D:12(F):GLY:HA3	17:D:267:HOH:O	2.07	0.55
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.22	0.55
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.88	0.55
14:N:163:ILE:O	17:N:188:HOH:O	2.18	0.55
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.20	0.55
3:C:15:PHE:CD1	3:C:21:ILE:HD11	2.42	0.55
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.88	0.55
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.87	0.55
2:P:160:TRP:CD2	2:P:163:ILE:HD12	2.42	0.55
5:S:15:PHE:H	6:T:23:GLN:NE2	1.98	0.55
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.88	0.55
13:M:157:ASN:ND2	17:M:279:HOH:O	2.39	0.55
4:R:12:VAL:CG2	4:R:12(A):GLY:HA2	2.37	0.55
10:X:113:ILE:HA	10:X:118:THR:O	2.07	0.55
11:Y:191:ASP:OD2	11:Y:193:GLY:N	2.40	0.55
5:E:73:HIS:HE1	5:E:107:LEU:O	1.89	0.55
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:-7:ASN:HD22	12:L:-7:ASN:C	2.10	0.55
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.89	0.55
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.42	0.55
2:B:186:VAL:HG11	2:B:216:ARG:CD	2.35	0.55
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.54	0.55
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG13	1.89	0.55
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.42	0.55
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG13	1.89	0.54
8:H:3:ILE:CD1	8:H:127:LEU:O	2.55	0.54
17:L:199:HOH:O	9:W:192:ARG:HG3	2.07	0.54
14:N:107:LYS:HG2	14:N:108:GLY:H	1.72	0.54
1:O:150:GLN:O	1:O:157:TYR:HA	2.07	0.54
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.90	0.54
2:P:223:ILE:HD12	2:P:223:ILE:N	2.22	0.54
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.89	0.54
2:B:160:TRP:CD2	2:B:163:ILE:HD12	2.41	0.54
2:B:223:ILE:N	2:B:223:ILE:HD12	2.22	0.54
6:F:179:LEU:HD21	6:F:192:GLN:CG	2.37	0.54
7:G:143:GLU:HA	7:G:217:LYS:NZ	2.22	0.54
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.72	0.54
6:T:175:GLU:CB	6:T:196:ILE:HD12	2.36	0.54
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.88	0.54
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.89	0.54
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.23	0.54
12:L:1:GLY:HA3	12:L:33:LYS:HZ2	1.72	0.54
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.89	0.54
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.42	0.54
2:P:239:THR:OXT	2:P:239:THR:HG22	2.07	0.54
6:T:179:LEU:HD21	6:T:192:GLN:CG	2.36	0.54
17:I:224:HOH:O	10:J:122:LEU:HD13	2.06	0.54
11:K:191:ASP:OD2	11:K:193:GLY:N	2.40	0.54
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.20	0.54
1:O:141:HIS:HA	1:O:146:GLY:O	2.07	0.54
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.89	0.54
2:P:186:VAL:CG1	2:P:216:ARG:HD3	2.37	0.54
9:W:34:ILE:HB	17:W:215:HOH:O	2.08	0.54
13:M:113:VAL:HA	13:M:118:VAL:O	2.07	0.54
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.73	0.54
7:U:14:ILE:HD13	7:U:14:ILE:H	1.73	0.54
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.42	0.54
2:B:27:ALA:O	2:B:31:ILE:HG12	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12:VAL:CG2	4:D:12(A):GLY:HA2	2.38	0.54
10:J:52:THR:CG2	10:J:53:VAL:N	2.71	0.54
2:P:224:PHE:H	2:P:224:PHE:HD2	1.54	0.54
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.89	0.54
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.72	0.54
13:1:6:MET:HG2	13:1:155:ILE:HD11	1.89	0.54
3:C:101:LEU:HD11	10:J:57:GLU:HB3	1.90	0.54
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.89	0.54
5:S:160:LEU:HD13	5:S:163:THR:HB	1.90	0.54
9:W:29:ASN:H	9:W:29:ASN:HD22	1.55	0.54
4:R:40:ILE:HG13	4:R:193:VAL:CG2	2.37	0.53
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.90	0.53
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.89	0.53
10:J:52:THR:HG22	10:J:53:VAL:HG23	1.89	0.53
3:Q:216:LYS:HD2	3:Q:220:ASP:OD1	2.09	0.53
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.20	0.53
1:A:69:LEU:C	1:A:69:LEU:HD23	2.28	0.53
1:A:141:HIS:HA	1:A:146:GLY:O	2.09	0.53
2:B:239:THR:HG22	2:B:239:THR:OXT	2.09	0.53
5:E:86:ARG:HG3	5:E:86:ARG:HH11	1.72	0.53
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.21	0.53
1:O:69:LEU:C	1:O:69:LEU:HD23	2.29	0.53
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.91	0.53
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.39	0.53
5:E:35:SER:HB3	5:E:66:LYS:NZ	2.23	0.53
7:G:151:THR:HG22	7:G:157:TYR:CB	2.38	0.53
8:V:41:ILE:CD1	8:V:76:VAL:HG22	2.38	0.53
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.90	0.53
17:D:273:HOH:O	5:E:86:ARG:HD3	2.08	0.53
7:G:87:ASN:C	7:G:87:ASN:ND2	2.61	0.53
11:Y:142:TYR:O	11:Y:143:LYS:HD2	2.09	0.53
1:A:150:GLN:O	1:A:157:TYR:HA	2.08	0.53
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.90	0.53
5:S:67:ILE:HG21	5:S:223:ILE:HD12	1.90	0.53
7:U:9:ASP:HA	7:U:14:ILE:CD1	2.28	0.53
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.90	0.53
5:S:86:ARG:HG3	5:S:86:ARG:HH11	1.74	0.53
7:U:87:ASN:C	7:U:87:ASN:ND2	2.61	0.53
11:Y:38:ASN:O	11:Y:40:PHE:N	2.42	0.53
3:C:216:LYS:HD2	3:C:220:ASP:OD1	2.09	0.53
7:G:12:ILE:HD13	7:G:12:ILE:H	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:35:ILE:HG12	13:M:56:GLU:HG3	1.89	0.53
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.74	0.53
9:I:113:PHE:HA	9:I:118:CYS:O	2.08	0.53
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.23	0.53
8:V:35:HIS:CB	8:V:56:THR:HG21	2.39	0.53
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	1.91	0.53
4:D:170:GLU:OE1	4:D:170:GLU:N	2.41	0.53
5:E:15:PHE:H	6:F:23:GLN:NE2	2.03	0.53
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.38	0.53
3:Q:182:PRO:O	3:Q:184:ALA:N	2.42	0.53
4:R:205:GLU:HA	4:R:205:GLU:OE2	2.09	0.53
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.23	0.53
7:U:8:TYR:C	7:U:10:ARG:H	2.13	0.53
7:U:233:LEU:O	7:U:236:ILE:HG13	2.08	0.53
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.90	0.53
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.09	0.53
3:C:241:GLN:C	3:C:243:GLN:H	2.13	0.52
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.24	0.52
1:O:159:PRO:O	2:P:59:LEU:HD12	2.08	0.52
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.44	0.52
3:Q:241:GLN:C	3:Q:243:GLN:H	2.13	0.52
10:X:190:PHE:C	10:X:192:ALA:H	2.12	0.52
1:A:198:LYS:HE3	1:A:236:LEU:HD11	1.91	0.52
8:H:35:HIS:CB	8:H:56:THR:HG21	2.39	0.52
10:X:53:VAL:HB	17:Y:237:HOH:O	2.10	0.52
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	1.90	0.52
4:R:170:GLU:N	4:R:170:GLU:OE1	2.42	0.52
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.91	0.52
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.91	0.52
4:D:205:GLU:OE2	4:D:205:GLU:HA	2.08	0.52
7:U:186:TRP:O	7:U:190:VAL:HG23	2.09	0.52
14:2:107:LYS:HG2	14:2:108:GLY:H	1.73	0.52
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.45	0.52
2:B:186:VAL:CG1	2:B:216:ARG:HD3	2.38	0.52
3:C:224:LEU:HD12	3:C:224:LEU:N	2.24	0.52
10:X:93:ARG:HG2	10:X:93:ARG:HH11	1.73	0.52
3:C:182:PRO:O	3:C:184:ALA:N	2.42	0.52
6:F:28:VAL:O	6:F:32:GLU:HG3	2.10	0.52
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.92	0.52
10:J:113:ILE:HA	10:J:118:THR:O	2.09	0.52
11:K:99:THR:CG2	11:K:113:VAL:HB	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.91	0.52
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.90	0.52
11:K:184:TRP:O	11:K:185:ILE:HD13	2.08	0.52
13:M:184:LEU:HD23	13:M:184:LEU:C	2.30	0.52
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.10	0.52
9:W:113:PHE:HA	9:W:118:CYS:O	2.08	0.52
10:X:135:PHE:HZ	17:X:216:HOH:O	1.91	0.52
2:B:21(A):LYS:HE2	2:B:21(D):GLY:O	2.10	0.52
7:G:38:LEU:C	7:G:38:LEU:HD12	2.30	0.52
7:G:39:ALA:HB1	7:G:148:ILE:HD12	1.91	0.52
13:M:40:ASN:H	13:M:40:ASN:ND2	2.07	0.52
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.96	0.52
8:V:3:ILE:HD13	8:V:127:LEU:H	1.73	0.52
10:X:16:SER:HB2	17:X:233:HOH:O	2.08	0.52
7:G:172:ILE:HD13	7:G:197:MET:CE	2.40	0.52
7:G:186:TRP:O	7:G:190:VAL:HG23	2.10	0.52
11:K:161:ALA:HB1	10:X:136:SER:HB2	1.92	0.52
14:N:146:MET:HE3	14:N:150:GLU:HB3	1.91	0.52
2:P:172:ALA:HB2	2:P:200:THR:HG21	1.91	0.52
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.25	0.52
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.09	0.52
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.90	0.52
10:X:52:THR:CG2	10:X:53:VAL:N	2.72	0.52
14:N:106:ASN:O	14:N:107:LYS:HB3	2.09	0.52
2:P:21(A):LYS:HE2	2:P:21(D):GLY:O	2.10	0.52
9:W:19:ARG:HB2	9:W:171:TRP:HB2	1.92	0.52
7:G:14:ILE:HD13	7:G:14:ILE:H	1.74	0.51
1:O:121:GLN:O	1:O:124:THR:HB	2.10	0.51
4:R:24:VAL:O	4:R:27:SER:HB3	2.10	0.51
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.91	0.51
14:2:106:ASN:O	14:2:107:LYS:HB3	2.08	0.51
3:C:36:CYS:N	3:C:51:GLU:HG2	2.25	0.51
7:G:8:TYR:C	7:G:10:ARG:H	2.12	0.51
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.75	0.51
11:K:143:LYS:HB2	11:K:146:LEU:HD11	1.92	0.51
1:O:225:THR:OG1	1:O:228:GLU:HG3	2.10	0.51
2:P:27:ALA:O	2:P:31:ILE:HG12	2.09	0.51
3:Q:100:ARG:HH12	3:Q:106:PRO:HB3	1.70	0.51
5:S:35:SER:HB3	5:S:66:LYS:NZ	2.26	0.51
9:W:174:VAL:HG21	9:W:186:LYS:CE	2.41	0.51
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.92	0.51
5:E:160:LEU:HD13	5:E:163:THR:HB	1.92	0.51
3:Q:15:PHE:CD1	3:Q:21:ILE:HD11	2.45	0.51
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.23	0.51
6:F:91:ARG:O	6:F:95:GLU:HB2	2.10	0.51
7:G:12:ILE:HD11	7:G:14:ILE:HD12	1.92	0.51
8:H:3:ILE:HG12	8:H:100:ILE:HD12	1.92	0.51
7:U:18(G):GLU:HG2	7:U:188:LYS:HB3	1.93	0.51
11:Y:38:ASN:CG	17:Y:258:HOH:O	2.49	0.51
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.37	0.51
13:1:40:ASN:HD22	13:1:40:ASN:N	2.05	0.51
2:B:231:ASP:O	2:B:235:LYS:HG2	2.11	0.51
7:G:93:LYS:HD3	14:N:68:SER:HB3	1.90	0.51
8:V:22:GLN:HG3	8:V:27:ALA:HB2	1.92	0.51
8:H:3:ILE:HD13	8:H:127:LEU:H	1.76	0.51
11:K:38:ASN:O	11:K:40:PHE:N	2.43	0.51
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.20	0.51
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.93	0.51
10:J:190:PHE:C	10:J:192:ALA:H	2.13	0.51
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.41	0.51
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.46	0.51
10:J:143:ARG:HB2	10:J:146:MET:HG3	1.92	0.51
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.26	0.51
2:B:172:ALA:HB2	2:B:200:THR:HG21	1.91	0.51
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.45	0.51
4:R:122:ARG:HG2	4:R:122:ARG:HH11	1.75	0.51
1:A:33:GLN:HE21	1:A:33:GLN:HA	1.76	0.50
3:C:100:ARG:HH12	3:C:106:PRO:HB3	1.72	0.50
5:E:67:ILE:HG21	5:E:223:ILE:HD12	1.93	0.50
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.26	0.50
11:K:40:PHE:CB	11:K:73:ARG:NH2	2.74	0.50
7:U:38:LEU:C	7:U:38:LEU:HD12	2.32	0.50
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.93	0.50
11:Y:99:THR:CG2	11:Y:113:VAL:HB	2.41	0.50
14:2:3:ILE:HD13	14:2:46:SER:HB3	1.93	0.50
3:C:173:ARG:O	3:C:177:GLU:HG3	2.11	0.50
8:H:22:GLN:HG3	8:H:27:ALA:HB2	1.92	0.50
6:T:91:ARG:O	6:T:95:GLU:HB2	2.11	0.50
7:U:39:ALA:HB1	7:U:148:ILE:HD12	1.92	0.50
9:W:89:GLU:O	9:W:90:ARG:NH1	2.45	0.50
10:X:52:THR:HG22	10:X:53:VAL:HG23	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.11	0.50
11:Y:143:LYS:HB2	11:Y:146:LEU:HD11	1.92	0.50
13:1:184:LEU:C	13:1:184:LEU:HD23	2.31	0.50
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.46	0.50
3:C:55:THR:O	3:C:56:LEU:HD22	2.12	0.50
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.11	0.50
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.92	0.50
3:C:211:GLU:C	3:C:212:ILE:HD12	2.32	0.50
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.37	0.50
9:I:193:GLN:HG3	11:Y:196:PHE:CE1	2.46	0.50
11:K:142:TYR:C	11:K:143:LYS:HD2	2.31	0.50
5:S:31:ILE:HD11	5:S:153:PRO:HG2	1.93	0.50
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.93	0.50
8:V:148:LYS:HE3	8:V:177:VAL:HG11	1.92	0.50
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.32	0.50
13:1:40:ASN:H	13:1:40:ASN:ND2	2.06	0.50
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.12	0.50
2:B:186:VAL:CG2	2:B:216:ARG:HD3	2.42	0.50
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.93	0.50
9:I:89:GLU:O	9:I:90:ARG:NH1	2.45	0.50
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.47	0.50
10:J:135:PHE:HZ	17:J:234:HOH:O	1.93	0.50
14:N:20:THR:HG23	14:N:31:THR:OG1	2.12	0.50
9:W:27:VAL:HG13	17:X:216:HOH:O	2.12	0.50
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.46	0.50
11:Y:40:PHE:CB	11:Y:73:ARG:HH21	2.25	0.50
3:C:236:ILE:HA	3:C:239:GLU:HG2	1.93	0.50
7:G:172:ILE:CD1	7:G:197:MET:HE1	2.41	0.50
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.75	0.50
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.77	0.50
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.12	0.50
2:B:88:LEU:HB3	2:B:116:LEU:HD21	1.94	0.50
4:D:24:VAL:O	4:D:27:SER:HB3	2.12	0.50
7:G:9:ASP:HA	7:G:14:ILE:CD1	2.28	0.50
7:G:188:LYS:HD3	7:G:191:GLU:OE2	2.12	0.50
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.41	0.50
11:K:4:LEU:HD22	11:K:4:LEU:C	2.32	0.50
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.94	0.50
11:Y:40:PHE:CB	11:Y:73:ARG:NH2	2.74	0.50
1:A:206:PHE:CD1	1:A:210:ILE:HD11	2.46	0.50
10:X:143:ARG:HB2	10:X:146:MET:HG3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:157:ARG:HG3	11:Y:157:ARG:HH11	1.76	0.50
6:F:69:VAL:HG12	17:F:248:HOH:O	2.11	0.49
6:F:127:ASN:HD22	6:F:127:ASN:C	2.15	0.49
14:N:186:ARG:HD3	17:N:234:HOH:O	2.11	0.49
6:T:179:LEU:CD2	6:T:192:GLN:HG2	2.42	0.49
7:U:72:ARG:HG2	17:U:271:HOH:O	2.11	0.49
8:V:25:ILE:HD12	8:V:25:ILE:N	2.27	0.49
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.94	0.49
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.50	0.49
11:Y:184:TRP:O	11:Y:185:ILE:HD13	2.12	0.49
1:A:85:TYR:O	1:A:89:VAL:HG23	2.13	0.49
2:P:186:VAL:HG21	2:P:216:ARG:CD	2.40	0.49
1:A:5:THR:O	1:A:7:ARG:HG2	2.13	0.49
8:H:148:LYS:HE3	8:H:177:VAL:HG11	1.92	0.49
4:R:207:LEU:C	4:R:207:LEU:HD23	2.32	0.49
1:A:121:GLN:O	1:A:124:THR:HB	2.12	0.49
9:I:29:ASN:H	9:I:29:ASN:HD22	1.59	0.49
11:K:208:ASN:HB3	17:K:237:HOH:O	2.12	0.49
10:X:2:ILE:HD13	10:X:170:PHE:CG	2.47	0.49
2:B:90:ASN:O	2:B:94:ILE:HD12	2.12	0.49
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.95	0.49
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.78	0.49
9:I:174:VAL:HG21	9:I:186:LYS:CE	2.42	0.49
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.43	0.49
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.42	0.49
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.93	0.49
2:B:224:PHE:N	2:B:224:PHE:CD2	2.81	0.49
3:C:212:ILE:HG22	3:C:224:LEU:HD13	1.95	0.49
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.47	0.49
4:D:112:LEU:HD13	4:D:112:LEU:O	2.13	0.49
9:I:19:ARG:HB2	9:I:171:TRP:HB2	1.94	0.49
6:T:72:ARG:HD2	13:1:64:THR:OG1	2.13	0.49
7:U:12:ILE:HD13	7:U:12:ILE:H	1.76	0.49
6:F:136:THR:O	6:F:150:MET:HA	2.13	0.49
6:F:179:LEU:HD11	6:F:192:GLN:CG	2.42	0.49
1:O:55:SER:O	1:O:56:SER:HB2	2.13	0.49
2:P:202:THR:CG2	2:P:204:SER:HB2	2.43	0.49
7:U:151:THR:HG22	7:U:157:TYR:CB	2.42	0.49
13:1:35:ILE:HG12	13:1:56:GLU:HG3	1.93	0.49
3:C:232:TYR:O	3:C:236:ILE:HG13	2.13	0.49
6:F:179:LEU:CD2	6:F:192:GLN:HG2	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:197:ARG:NH2	9:I:139:GLU:O	2.46	0.49
12:L:1(I):ASN:O	12:L:14(K):LYS:HG2	2.12	0.49
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.93	0.49
11:Y:135:TYR:HB2	17:Y:232:HOH:O	2.12	0.49
2:P:231:ASP:O	2:P:235:LYS:HG2	2.12	0.49
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.48	0.49
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.95	0.49
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.48	0.49
10:X:190:PHE:HA	10:X:193:GLN:HB2	1.95	0.49
4:D:12(E):SER:O	5:E:123:ASN:OD1	2.31	0.49
5:E:31:ILE:HD11	5:E:153:PRO:HG2	1.95	0.49
10:J:190:PHE:HA	10:J:193:GLN:HB2	1.95	0.49
1:O:198:LYS:HE3	1:O:236:LEU:HD11	1.94	0.49
3:Q:14:ILE:C	3:Q:14:ILE:HD12	2.33	0.49
3:Q:33:ARG:NH1	3:Q:33:ARG:HB2	2.28	0.49
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.43	0.49
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.48	0.49
5:S:111:ARG:HH11	5:S:111:ARG:HG2	1.77	0.49
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.27	0.49
8:V:3:ILE:HG12	8:V:100:ILE:HD12	1.94	0.49
10:X:88:ALA:O	10:X:90(A):ILE:HG22	2.12	0.49
10:X:185:ARG:NH1	17:X:222:HOH:O	2.41	0.49
13:1:8:TYR:CE2	13:1:148:VAL:HG22	2.48	0.49
1:A:126:SER:HB3	17:A:253:HOH:O	2.12	0.48
3:C:163:GLN:HE22	3:C:173:ARG:NE	2.11	0.48
5:E:143:LYS:HB2	17:M:258:HOH:O	2.11	0.48
6:F:53:LEU:HD11	6:F:205:ASN:OD1	2.13	0.48
11:K:7:ARG:HD2	11:K:108:PRO:O	2.12	0.48
1:O:85:TYR:O	1:O:89:VAL:HG23	2.12	0.48
2:P:163:ILE:HG12	2:P:164:SER:H	1.78	0.48
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.66	0.48
6:F:20(B):GLU:CD	6:F:20(C):LYS:HE3	2.33	0.48
13:M:148:VAL:HG23	17:M:239:HOH:O	2.12	0.48
5:S:107:LEU:HD11	5:S:111:ARG:HG2	1.96	0.48
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.95	0.48
8:V:175:VAL:HG12	8:V:176:CYS:N	2.28	0.48
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.95	0.48
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.95	0.48
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.48	0.48
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.81	0.48
2:B:238:ILE:O	2:B:239:THR:O	2.31	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.49	0.48
10:J:45:PHE:CE1	10:J:52:THR:HG23	2.49	0.48
11:K:86:LEU:C	11:K:86:LEU:HD13	2.34	0.48
1:O:5:THR:O	1:O:7:ARG:HG2	2.14	0.48
3:Q:236:ILE:HA	3:Q:239:GLU:HG2	1.93	0.48
6:T:136:THR:O	6:T:150:MET:HA	2.12	0.48
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.34	0.48
11:K:38:ASN:C	11:K:38:ASN:OD1	2.51	0.48
12:L:145:TYR:CD1	12:L:146:LEU:N	2.80	0.48
6:T:28:VAL:O	6:T:32:GLU:HG3	2.14	0.48
12:Z:1(I):ASN:O	12:Z:14(K):LYS:HG2	2.14	0.48
2:B:17:PRO:HA	3:C:26:TYR:CE1	2.48	0.48
3:C:169:SER:HA	3:C:172:VAL:CG1	2.43	0.48
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.48	0.48
4:D:177:LEU:CD2	5:E:58:LEU:HD13	2.41	0.48
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.28	0.48
7:G:131:PRO:HB3	17:G:243:HOH:O	2.13	0.48
1:O:33:GLN:HE21	1:O:33:GLN:HA	1.77	0.48
1:O:47:VAL:HG23	1:O:212:LEU:HD21	1.94	0.48
2:P:224:PHE:N	2:P:224:PHE:CD2	2.81	0.48
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.47	0.48
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.34	0.48
12:Z:114:ASP:HB2	12:Z:118:SER:N	2.28	0.48
13:1:14(A):VAL:HG23	13:1:14(A):VAL:O	2.14	0.48
1:A:55:SER:O	1:A:56:SER:HB2	2.13	0.48
10:J:2:ILE:HD13	10:J:170:PHE:CG	2.49	0.48
10:J:52:THR:HG22	10:J:53:VAL:H	1.78	0.48
12:L:5:GLY:O	12:L:124:CYS:HA	2.13	0.48
2:P:88:LEU:HB3	2:P:116:LEU:HD21	1.96	0.48
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.56	0.48
6:T:20(B):GLU:CD	6:T:20(C):LYS:HE3	2.33	0.48
7:U:227:GLU:HG2	17:U:295:HOH:O	2.14	0.48
3:C:33:ARG:NH1	3:C:33:ARG:HB2	2.29	0.48
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.67	0.48
13:M:40:ASN:HD22	13:M:40:ASN:N	2.05	0.48
1:O:29:THR:O	1:O:33:GLN:HG2	2.14	0.48
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.14	0.48
8:V:3:ILE:CD1	8:V:127:LEU:O	2.61	0.48
8:H:25:ILE:HD12	8:H:25:ILE:N	2.28	0.48
11:K:10(B):LYS:N	11:K:10(B):LYS:CD	2.67	0.48
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.35	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.96	0.48
7:G:228:ASN:HB3	17:G:253:HOH:O	2.14	0.48
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.41	0.48
14:N:3:ILE:HD13	14:N:46:SER:HB3	1.96	0.48
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.62	0.48
3:Q:101:LEU:HD11	10:X:57:GLU:HB3	1.95	0.48
5:S:15:PHE:N	6:T:23:GLN:HE22	2.02	0.48
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.40	0.47
8:H:26:VAL:HG11	8:H:29:LYS:HG2	1.94	0.47
3:Q:24:VAL:O	3:Q:27:ALA:HB3	2.13	0.47
10:X:52:THR:HG22	10:X:53:VAL:H	1.78	0.47
14:2:3:ILE:CD1	14:2:46:SER:HB3	2.43	0.47
1:A:21(G):LEU:HG	1:A:21(I):TYR:CE1	2.49	0.47
4:D:40:ILE:HG13	4:D:193:VAL:HG22	1.95	0.47
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.12	0.47
13:M:3:VAL:O	13:M:126:ALA:HA	2.14	0.47
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.13	0.47
4:R:53:ARG:HD2	17:R:264:HOH:O	2.14	0.47
2:B:163:ILE:HG12	2:B:164:SER:H	1.79	0.47
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.27	0.47
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.96	0.47
7:G:212:VAL:HG23	7:G:229:ILE:CD1	2.45	0.47
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.96	0.47
12:Z:99:THR:CG2	17:Z:201:HOH:O	2.61	0.47
14:2:20:THR:HG23	14:2:31:THR:OG1	2.14	0.47
3:C:24:VAL:O	3:C:27:ALA:HB3	2.14	0.47
5:E:15:PHE:N	6:F:23:GLN:HE22	2.06	0.47
9:I:90:ARG:HD2	17:I:257:HOH:O	2.14	0.47
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.26	0.47
3:Q:211:GLU:C	3:Q:212:ILE:HD12	2.34	0.47
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.41	0.47
10:X:45:PHE:CE1	10:X:52:THR:HG23	2.50	0.47
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.11	0.47
13:1:128:GLY:N	17:1:281:HOH:O	2.46	0.47
12:L:114:ASP:HB2	12:L:118:SER:N	2.29	0.47
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.50	0.47
4:R:72:ARG:HG3	17:R:275:HOH:O	2.14	0.47
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.38	0.47
7:U:188:LYS:HD3	7:U:191:GLU:OE2	2.14	0.47
2:B:224:PHE:HD2	2:B:224:PHE:N	2.12	0.47
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:136:SER:HB2	11:Y:161:ALA:HB1	1.95	0.47
2:P:90:ASN:O	2:P:94:ILE:HD12	2.14	0.47
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.49	0.47
6:T:127:ASN:HD22	6:T:127:ASN:C	2.17	0.47
7:U:10:ARG:HG2	7:U:22:TYR:CD2	2.50	0.47
8:V:197:ARG:NH2	9:W:139:GLU:O	2.46	0.47
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.29	0.47
2:B:186:VAL:HG21	2:B:216:ARG:CD	2.42	0.47
3:C:14:ILE:C	3:C:14:ILE:HD12	2.35	0.47
4:D:207:LEU:HD23	4:D:207:LEU:C	2.33	0.47
5:E:35:SER:HB3	5:E:66:LYS:HZ3	1.80	0.47
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.15	0.47
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.96	0.47
10:J:45:PHE:CD1	10:J:52:THR:HG23	2.50	0.47
13:M:14(A):VAL:HG23	13:M:14(A):VAL:O	2.14	0.47
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.50	0.47
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.11	0.47
2:P:186:VAL:CG2	2:P:216:ARG:HD3	2.40	0.47
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.96	0.47
7:U:12:ILE:HD11	7:U:14:ILE:HD12	1.97	0.47
1:A:38:LEU:HD12	1:A:38:LEU:O	2.15	0.47
1:A:198:LYS:HE3	1:A:236:LEU:CD1	2.45	0.47
2:B:202:THR:CG2	2:B:204:SER:HB2	2.45	0.47
3:C:36:CYS:H	3:C:51:GLU:HG2	1.80	0.47
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.44	0.47
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.30	0.47
4:R:40:ILE:HG13	4:R:193:VAL:HG22	1.96	0.47
6:T:114:ASP:O	6:T:118:GLN:HG2	2.15	0.47
14:2:107:LYS:CG	14:2:108:GLY:H	2.28	0.47
1:A:177:GLU:CG	2:B:58:LEU:HD22	2.44	0.47
4:D:12(E):SER:HB2	5:E:123:ASN:OD1	2.15	0.47
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.30	0.47
9:I:6:MET:CE	9:I:155:ILE:HA	2.44	0.47
3:Q:228:GLU:O	3:Q:232:TYR:HD1	1.97	0.47
8:V:37:ILE:HG23	8:V:60:GLY:HA2	1.97	0.47
10:X:34:THR:HG21	10:X:176:LYS:HZ2	1.80	0.47
8:H:3:ILE:HD12	8:H:127:LEU:O	2.15	0.47
12:L:140:ASN:O	12:L:144:PHE:HA	2.15	0.47
2:P:224:PHE:HD2	2:P:224:PHE:N	2.12	0.47
3:Q:159:SER:O	4:R:59:LEU:HD22	2.15	0.47
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.15	0.47
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.12	0.46
11:K:67:GLU:OE2	17:K:241:HOH:O	2.19	0.46
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.96	0.46
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.15	0.46
8:H:175:VAL:HG12	8:H:176:CYS:N	2.31	0.46
10:J:168:MET:HE1	10:X:167:PRO:CB	2.45	0.46
2:P:229:ILE:O	2:P:233:LEU:HB2	2.15	0.46
7:U:74:ILE:HD13	17:U:287:HOH:O	2.15	0.46
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.50	0.46
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.96	0.46
8:H:38:SER:OG	8:H:41:ILE:HG12	2.16	0.46
10:J:93:ARG:HG2	10:J:93:ARG:NH1	2.30	0.46
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.98	0.46
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.80	0.46
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.97	0.46
7:U:59:LEU:O	7:U:61:PRO:HD3	2.15	0.46
7:U:17(C):LYS:HB2	7:U:17(C):LYS:HE3	1.75	0.46
12:L:93:PHE:N	12:L:94:PRO:HD3	2.30	0.46
1:O:40:ILE:HD12	1:O:193:ALA:HB2	1.96	0.46
3:Q:169:SER:HA	3:Q:172:VAL:HG12	1.98	0.46
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.77	0.46
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.30	0.46
3:C:16:SER:HB2	3:C:17:PRO:HD2	1.96	0.46
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.97	0.46
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.50	0.46
3:Q:159:SER:HB2	17:Q:264:HOH:O	2.16	0.46
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.46	0.46
9:W:6:MET:CE	9:W:155:ILE:HA	2.45	0.46
10:X:193:GLN:OXT	10:X:193:GLN:HG2	2.16	0.46
2:B:144:ARG:O	2:B:144:ARG:HG2	2.16	0.46
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.79	0.46
13:M:17:ASP:HA	13:M:173:PHE:CB	2.45	0.46
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.98	0.46
11:Y:135:TYR:CB	17:Y:232:HOH:O	2.63	0.46
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.96	0.46
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.15	0.46
3:Q:16:SER:HB2	3:Q:17:PRO:HD2	1.97	0.46
17:T:273:HOH:O	14:2:70:TYR:HE2	1.98	0.46
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.97	0.46
5:E:194:VAL:HG13	5:E:207:LEU:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.97	0.46
6:F:121:GLN:NE2	17:F:258:HOH:O	2.48	0.46
10:J:167:PRO:CB	10:X:168:MET:HE1	2.46	0.46
2:P:63:THR:HG22	2:P:63:THR:O	2.16	0.46
1:A:13:THR:O	2:B:130:ARG:HD3	2.16	0.46
13:M:14(G):ILE:HB	13:M:144:PRO:CD	2.45	0.46
14:N:14:LEU:O	14:N:175:MET:HA	2.16	0.46
7:U:212:VAL:HG23	7:U:229:ILE:CD1	2.46	0.46
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.97	0.46
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.96	0.46
12:L:1:GLY:N	17:L:224:HOH:O	2.49	0.46
14:N:3:ILE:CD1	14:N:46:SER:HB3	2.46	0.46
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.51	0.46
7:U:83:PRO:HG2	17:U:265:HOH:O	2.15	0.46
10:X:14:LEU:HD12	10:X:42:LEU:HD23	1.98	0.46
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.16	0.46
6:F:50:VAL:HG22	6:F:51:GLU:N	2.31	0.45
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.97	0.45
3:Q:141:PHE:CD1	3:Q:217:PRO:HG3	2.51	0.45
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.98	0.45
5:S:67:ILE:CG2	5:S:223:ILE:HD12	2.47	0.45
8:V:63:ILE:HD13	8:V:63:ILE:HA	1.85	0.45
2:B:53:LYS:HG2	2:B:54:VAL:HG23	1.99	0.45
2:B:229:ILE:O	2:B:233:LEU:HB2	2.15	0.45
3:C:163:GLN:HG3	3:C:164:THR:N	2.30	0.45
3:C:224:LEU:N	3:C:224:LEU:CD1	2.80	0.45
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.98	0.45
9:I:55:LEU:CD1	9:I:97:VAL:HG21	2.46	0.45
11:K:5:ALA:HA	11:K:13:ILE:O	2.17	0.45
2:P:144:ARG:O	2:P:144:ARG:HG2	2.16	0.45
5:S:64:GLN:NE2	5:S:82:ALA:HB2	2.31	0.45
6:T:78:TYR:CE1	6:T:85:GLY:HA3	2.51	0.45
7:U:171:GLU:OE1	7:U:171:GLU:N	2.47	0.45
1:A:29:THR:O	1:A:33:GLN:HG2	2.15	0.45
2:B:191:GLU:O	2:B:195:LYS:HG2	2.16	0.45
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.98	0.45
8:H:144:GLN:O	8:H:145:ASP:HB2	2.16	0.45
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.98	0.45
1:A:8:TYR:HD2	7:G:128:TYR:HB3	1.81	0.45
1:A:47:VAL:HG23	1:A:212:LEU:HD21	1.97	0.45
3:C:141:PHE:CD1	3:C:217:PRO:HG3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.43	0.45
5:E:125:GLN:HE22	6:F:87:HIS:CD2	2.34	0.45
6:F:203:GLU:C	6:F:205:ASN:H	2.19	0.45
7:G:96:ALA:CA	7:G:107:MET:CE	2.89	0.45
3:Q:57:LYS:HG2	3:Q:208:LYS:NZ	2.32	0.45
4:R:68:VAL:CG2	4:R:89:ILE:HD12	2.33	0.45
8:V:26:VAL:HG11	8:V:29:LYS:HG2	1.97	0.45
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.15	0.45
7:G:172:ILE:HD13	7:G:197:MET:HE1	1.98	0.45
7:G:218:ASP:O	7:G:220:LYS:HB2	2.16	0.45
10:J:88:ALA:O	10:J:90(A):ILE:HG22	2.16	0.45
6:T:203:GLU:C	6:T:205:ASN:H	2.19	0.45
7:U:47:VAL:HG12	7:U:49:ILE:CD1	2.47	0.45
7:U:146:PRO:HD2	17:U:299:HOH:O	2.16	0.45
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.99	0.45
1:A:21(L):ILE:HD11	8:H:186:TYR:CD2	2.52	0.45
5:E:64:GLN:NE2	5:E:82:ALA:HB2	2.32	0.45
8:H:37:ILE:HG23	8:H:60:GLY:HA2	1.98	0.45
12:L:4:LEU:HD23	12:L:159:PHE:CE1	2.52	0.45
1:O:21(G):LEU:HG	1:O:21(I):TYR:CE1	2.51	0.45
8:V:38:SER:OG	8:V:41:ILE:HG12	2.16	0.45
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.98	0.45
7:G:105:TYR:OH	8:H:66:HIS:HE1	2.00	0.45
11:K:40:PHE:CB	11:K:73:ARG:HH21	2.25	0.45
11:K:74:ILE:HG13	11:K:75:SER:N	2.30	0.45
11:K:99:THR:HG22	11:K:113:VAL:HB	1.99	0.45
13:M:-3:VAL:HA	13:M:21:SER:O	2.17	0.45
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.12	0.45
8:V:196:VAL:HG23	17:V:242:HOH:O	2.16	0.45
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.98	0.45
5:E:197:ILE:HG23	5:E:198:SER:N	2.32	0.45
7:G:47:VAL:HG12	7:G:49:ILE:CD1	2.47	0.45
10:J:193:GLN:OXT	10:J:193:GLN:HG2	2.16	0.45
12:L:14(E):GLU:HB2	12:L:14(M):VAL:HB	1.98	0.45
3:C:57:LYS:HG2	3:C:208:LYS:NZ	2.32	0.45
6:F:43:ASN:HD22	6:F:44:ASP:N	2.15	0.45
13:M:57:ARG:CD	17:M:244:HOH:O	2.64	0.45
9:W:101:VAL:O	9:W:110:ILE:HA	2.17	0.45
10:X:45:PHE:CD1	10:X:52:THR:HG23	2.52	0.45
10:X:112:GLN:NE2	10:X:126:ALA:H	2.15	0.45
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:14(G):ILE:HB	13:1:144:PRO:CD	2.46	0.45
13:1:146:THR:HA	17:1:233:HOH:O	2.17	0.45
3:C:228:GLU:O	3:C:232:TYR:HD1	1.99	0.45
7:G:151:THR:HG22	7:G:157:TYR:HB3	1.98	0.45
12:L:-2:ASN:HA	12:L:21:ILE:O	2.16	0.45
12:L:4:LEU:HD23	12:L:159:PHE:HE1	1.82	0.45
4:R:102:TYR:O	12:Z:81:ARG:HG3	2.16	0.45
4:R:112:LEU:HD13	4:R:112:LEU:O	2.16	0.45
5:S:111:ARG:HG2	5:S:111:ARG:NH1	2.32	0.45
8:V:144:GLN:O	8:V:145:ASP:HB2	2.16	0.45
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.52	0.45
11:Y:74:ILE:HG13	11:Y:75:SER:N	2.32	0.45
12:Z:14(E):GLU:HB2	12:Z:14(M):VAL:HB	1.99	0.45
13:1:-3:VAL:HA	13:1:21:SER:O	2.17	0.45
1:A:38:LEU:HD12	1:A:38:LEU:C	2.37	0.44
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.32	0.44
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	1.99	0.44
10:J:-1:MET:CG	10:J:1:ASP:H	2.23	0.44
11:K:157:ARG:HH11	11:K:157:ARG:HG3	1.82	0.44
12:L:4:LEU:HD12	12:L:5:GLY:N	2.32	0.44
5:S:125:GLN:HE22	6:T:87:HIS:CD2	2.34	0.44
5:S:197:ILE:HG23	5:S:198:SER:N	2.31	0.44
7:U:218:ASP:O	7:U:220:LYS:HB2	2.17	0.44
12:Z:1:GLY:HA3	12:Z:33:LYS:NZ	2.32	0.44
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.98	0.44
14:2:116:GLY:HA3	17:2:191:HOH:O	2.15	0.44
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.16	0.44
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.51	0.44
6:F:78:TYR:CE1	6:F:85:GLY:HA3	2.52	0.44
2:P:87:ILE:O	2:P:91:THR:HG23	2.16	0.44
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.18	0.44
3:Q:14:ILE:HD12	3:Q:14:ILE:O	2.17	0.44
4:R:177:LEU:CD2	5:S:58:LEU:HD13	2.43	0.44
7:U:172:ILE:HD13	7:U:197:MET:CE	2.47	0.44
12:Z:1:GLY:HA3	12:Z:33:LYS:HZ2	1.81	0.44
12:Z:114:ASP:HB2	12:Z:118:SER:H	1.83	0.44
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.46	0.44
3:C:43:LYS:O	3:C:43:LYS:HG2	2.17	0.44
10:J:112:GLN:NE2	10:J:126:ALA:H	2.15	0.44
13:M:19:LEU:HD12	13:M:20:GLY:H	1.83	0.44
1:O:198:LYS:HE3	1:O:236:LEU:CD1	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.46	0.44
14:2:146:MET:HB3	14:2:150:GLU:HB2	1.98	0.44
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.17	0.44
7:G:59:LEU:O	7:G:61:PRO:HD3	2.16	0.44
7:G:136:LEU:O	7:G:150:LYS:HA	2.17	0.44
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.52	0.44
1:O:38:LEU:HD12	1:O:38:LEU:O	2.18	0.44
2:P:53:LYS:HG2	2:P:54:VAL:HG23	1.99	0.44
7:U:34(A):ASN:HA	7:U:167:PRO:HG2	2.00	0.44
2:B:63:THR:HG22	2:B:63:THR:O	2.17	0.44
2:B:85:ALA:O	2:B:89:ILE:HG13	2.18	0.44
5:S:44:THR:HG23	5:S:183:ASP:HB3	2.00	0.44
11:Y:99:THR:HG22	11:Y:113:VAL:HB	1.99	0.44
3:C:33:ARG:O	3:C:33:ARG:HG2	2.17	0.44
3:C:169:SER:HA	3:C:172:VAL:HG12	1.97	0.44
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.88	0.44
2:P:191:GLU:O	2:P:195:LYS:HG2	2.16	0.44
6:T:50:VAL:HG22	6:T:51:GLU:N	2.32	0.44
10:X:93:ARG:HG2	10:X:93:ARG:NH1	2.33	0.44
2:B:6:ARG:HG2	3:C:10:ARG:NH2	2.33	0.44
4:D:122:ARG:HG2	4:D:122:ARG:NH1	2.32	0.44
11:K:4:LEU:HD11	11:K:15:ALA:HB3	2.00	0.44
14:N:107:LYS:CG	14:N:108:GLY:H	2.28	0.44
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.99	0.44
9:W:2:ILE:HD11	9:W:17:ASP:HB3	2.00	0.44
9:W:7:THR:HG23	9:W:110:ILE:HD13	2.00	0.44
11:Y:200:LYS:HE2	17:Y:239:HOH:O	2.17	0.44
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.52	0.44
13:1:17:ASP:HA	13:1:173:PHE:CB	2.47	0.44
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.52	0.44
1:A:21(I):TYR:HE2	1:A:21(L):ILE:HD13	1.83	0.44
2:B:171:ALA:O	2:B:175:LEU:HG	2.17	0.44
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.37	0.44
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.18	0.44
5:E:44:THR:HG23	5:E:183:ASP:HB3	2.00	0.44
7:G:12:ILE:HD13	7:G:12:ILE:N	2.33	0.44
7:G:17(C):LYS:HE3	7:G:17(C):LYS:HB2	1.75	0.44
10:J:133:TYR:HE2	10:J:166:MET:SD	2.41	0.44
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.98	0.44
11:K:67:GLU:HG2	11:K:72:GLU:O	2.18	0.44
1:O:58:LEU:HB3	7:U:162:ALA:O	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:186:VAL:CB	2:P:216:ARG:HD3	2.48	0.44
6:T:109:ILE:HB	6:T:110:PRO:HD3	2.00	0.44
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.18	0.44
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	2.00	0.44
11:Y:40:PHE:CG	11:Y:73:ARG:NH2	2.86	0.44
11:Y:208:ASN:O	11:Y:209:VAL:C	2.56	0.44
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.18	0.44
2:B:112:LEU:HD23	2:B:112:LEU:C	2.39	0.43
2:B:126:HIS:HA	17:C:267:HOH:O	2.17	0.43
3:C:235:GLN:O	3:C:239:GLU:HG2	2.18	0.43
8:H:3:ILE:HG22	8:H:16:ALA:CB	2.47	0.43
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.39	0.43
11:K:32:LYS:HD2	11:K:32:LYS:N	2.33	0.43
12:L:114:ASP:HB2	12:L:118:SER:H	1.83	0.43
2:P:95:HIS:CD2	2:P:115:ARG:HG2	2.53	0.43
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.99	0.43
14:2:14:LEU:O	14:2:175:MET:HA	2.18	0.43
7:G:188:LYS:HD3	7:G:188:LYS:HA	1.87	0.43
9:I:1:GLY:HA2	9:I:17:ASP:OD1	2.18	0.43
1:O:38:LEU:HD12	1:O:38:LEU:C	2.38	0.43
1:O:86:ARG:NE	7:U:118:ASN:ND2	2.55	0.43
3:Q:163:GLN:HE22	3:Q:173:ARG:NE	2.12	0.43
13:1:40:ASN:N	13:1:40:ASN:ND2	2.65	0.43
5:E:4:PHE:CG	5:E:5:ARG:N	2.86	0.43
9:I:160:LEU:HD12	9:I:191:MET:HE3	2.00	0.43
10:J:138:LEU:HD21	10:J:158:CYS:SG	2.59	0.43
4:R:128:MET:HE3	4:R:130:ARG:O	2.19	0.43
6:T:172:ALA:O	6:T:176:LEU:HD23	2.18	0.43
6:T:210:LEU:HD21	6:T:212:ILE:HD11	2.00	0.43
8:V:22:GLN:CG	8:V:27:ALA:HB2	2.48	0.43
11:Y:32:LYS:HD2	11:Y:32:LYS:N	2.32	0.43
12:Z:17:ASP:HA	12:Z:172:GLY:O	2.18	0.43
13:1:3:VAL:O	13:1:126:ALA:HA	2.18	0.43
14:2:59:VAL:HG11	14:2:83:PHE:CE2	2.54	0.43
3:C:57:LYS:HG2	3:C:208:LYS:HZ3	1.83	0.43
8:H:18:THR:HB	8:H:30:ASN:HD22	1.84	0.43
9:I:2:ILE:HD11	9:I:17:ASP:HB3	2.00	0.43
9:I:7:THR:HG23	9:I:110:ILE:HD13	2.00	0.43
13:M:165:ARG:HA	14:2:26:ILE:HB	2.00	0.43
3:Q:33:ARG:O	3:Q:33:ARG:HG2	2.17	0.43
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.18	0.43
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.54	0.43
6:T:18:ASP:OD2	6:T:18:ASP:N	2.43	0.43
6:T:37:SER:HB3	6:T:50:VAL:HG23	2.00	0.43
17:V:264:HOH:O	9:W:150:ASP:HA	2.19	0.43
13:1:12:VAL:CG2	13:1:102:ALA:HB1	2.48	0.43
1:A:170:VAL:HB	17:A:252:HOH:O	2.19	0.43
2:B:184:MET:HE2	2:B:188:ASP:HB3	1.99	0.43
3:C:194:VAL:O	3:C:198:LEU:HG	2.17	0.43
12:L:135:MET:HE2	9:W:165:ARG:NH2	2.31	0.43
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.32	0.43
2:P:112:LEU:C	2:P:112:LEU:HD23	2.39	0.43
2:P:122:GLY:C	2:P:124:THR:H	2.22	0.43
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.39	0.43
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.88	0.43
7:U:136:LEU:O	7:U:150:LYS:HA	2.17	0.43
12:Z:4:LEU:HD23	12:Z:159:PHE:HE1	1.82	0.43
13:1:148:VAL:CG2	17:1:228:HOH:O	2.62	0.43
14:2:105:ASP:OD2	14:2:106:ASN:N	2.45	0.43
2:B:184:MET:CE	2:B:188:ASP:HB3	2.49	0.43
6:F:90:ASN:O	6:F:94:GLU:HG3	2.19	0.43
10:J:32:ASP:OD2	10:J:34:THR:HG22	2.18	0.43
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.39	0.43
14:N:19:ARG:CZ	14:N:26:ILE:HD11	2.48	0.43
2:P:68:TYR:CG	2:P:89:ILE:HD12	2.52	0.43
2:P:238:ILE:O	2:P:239:THR:O	2.37	0.43
5:S:5:ARG:HG3	5:S:22:PHE:CZ	2.54	0.43
5:S:199:GLN:CA	5:S:199:GLN:HE21	2.32	0.43
9:W:123:ASP:OD1	9:W:124:PHE:N	2.46	0.43
12:Z:4:LEU:HD12	12:Z:5:GLY:N	2.33	0.43
2:B:227:GLN:OE1	2:B:230:LYS:HD3	2.19	0.43
3:C:152:GLU:HB2	3:C:153:PRO:HD2	2.00	0.43
6:F:37:SER:HB3	6:F:50:VAL:HG23	2.00	0.43
10:J:133:TYR:CD1	17:Y:232:HOH:O	2.34	0.43
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.49	0.43
10:X:138:LEU:HD21	10:X:158:CYS:SG	2.58	0.43
14:2:146:MET:CE	14:2:150:GLU:HB3	2.49	0.43
2:B:87:ILE:O	2:B:91:THR:HG23	2.18	0.43
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	2.01	0.43
9:I:101:VAL:O	9:I:110:ILE:HA	2.19	0.43
11:K:4:LEU:CD1	11:K:159:ILE:CD1	2.94	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.53	0.43
2:P:136:PHE:O	2:P:150:THR:HA	2.19	0.43
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.82	0.43
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.54	0.43
5:S:4:PHE:CG	5:S:5:ARG:N	2.86	0.43
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.17	0.43
2:B:95:HIS:CD2	2:B:115:ARG:HG2	2.53	0.43
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.19	0.43
7:G:12:ILE:CD1	7:G:14:ILE:HD12	2.49	0.43
8:H:201:GLN:HG2	12:Z:153:LYS:HA	2.00	0.43
11:K:40:PHE:CG	11:K:73:ARG:NH2	2.87	0.43
11:K:184:TRP:C	11:K:185:ILE:HD13	2.38	0.43
11:K:208:ASN:O	11:K:209:VAL:C	2.57	0.43
14:N:36:ARG:HG3	14:N:42:TRP:CZ2	2.54	0.43
14:N:146:MET:CE	14:N:150:GLU:HB3	2.49	0.43
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.18	0.43
8:V:139:GLU:HA	8:V:139:GLU:OE2	2.19	0.43
12:Z:4:LEU:HD23	12:Z:159:PHE:CE1	2.53	0.43
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.83	0.43
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.99	0.43
3:C:195:ARG:CG	3:C:236:ILE:HD13	2.46	0.43
7:G:8:TYR:C	7:G:10:ARG:N	2.73	0.43
1:O:77:VAL:HG12	1:O:137:LEU:HB2	2.00	0.43
3:Q:43:LYS:O	3:Q:43:LYS:HG2	2.19	0.43
7:U:96:ALA:CA	7:U:107:MET:CE	2.89	0.43
3:C:206:GLY:HA3	3:C:209:ASN:HD22	1.84	0.42
8:H:22:GLN:CG	8:H:27:ALA:HB2	2.48	0.42
11:K:67:GLU:CB	17:K:241:HOH:O	2.67	0.42
12:L:17:ASP:HA	12:L:172:GLY:O	2.19	0.42
14:N:59:VAL:HG11	14:N:83:PHE:CE2	2.54	0.42
1:O:21(I):TYR:HE2	1:O:21(L):ILE:HD13	1.84	0.42
2:P:184:MET:CE	2:P:188:ASP:HB3	2.49	0.42
11:Y:40:PHE:CG	11:Y:73:ARG:CZ	3.02	0.42
14:2:36:ARG:HG3	14:2:42:TRP:NE1	2.33	0.42
2:B:40:ILE:HD12	2:B:193:ALA:HB2	2.01	0.42
3:C:58:LEU:HA	3:C:58:LEU:HD12	1.77	0.42
6:F:31:VAL:HG22	6:F:134:VAL:HA	2.01	0.42
11:K:111:TYR:CE1	11:K:121:LYS:HB2	2.55	0.42
12:L:185:ARG:NH1	17:L:242:HOH:O	2.51	0.42
14:N:147:SER:OG	14:N:150:GLU:HG3	2.18	0.42
1:O:15:PHE:H	2:P:23:GLN:NE2	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:41:MET:HE2	17:P:244:HOH:O	2.19	0.42
2:P:227:GLN:OE1	2:P:230:LYS:HD3	2.18	0.42
3:Q:76:LEU:C	3:Q:76:LEU:HD23	2.40	0.42
7:U:12:ILE:HD13	7:U:12:ILE:N	2.33	0.42
7:U:39:ALA:CB	7:U:148:ILE:HD12	2.49	0.42
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.50	0.42
14:2:147:SER:OG	14:2:150:GLU:HG3	2.19	0.42
1:A:90:ASP:OD1	17:A:244:HOH:O	2.22	0.42
4:D:128:MET:HE3	4:D:130:ARG:O	2.19	0.42
4:D:148:LEU:HB3	4:D:160:TYR:O	2.19	0.42
5:E:5:ARG:HG3	5:E:22:PHE:CZ	2.54	0.42
7:G:191:GLU:HG3	7:G:232:ARG:HG3	2.01	0.42
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.16	0.42
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.54	0.42
13:M:191:GLN:HE21	13:M:191:GLN:HB3	1.61	0.42
14:N:107:LYS:NZ	14:N:145:ASN:HD21	2.17	0.42
4:R:121:LEU:HA	4:R:123:PHE:HE1	1.84	0.42
7:U:18(D):ILE:O	7:U:18(G):GLU:N	2.50	0.42
7:U:225:SER:O	7:U:229:ILE:HG13	2.19	0.42
5:E:67:ILE:CG2	5:E:223:ILE:HD12	2.49	0.42
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.49	0.42
7:G:74:ILE:HD13	17:G:246:HOH:O	2.20	0.42
14:N:146:MET:HB3	14:N:150:GLU:HB2	2.00	0.42
2:P:141:TYR:CE2	2:P:145:GLY:HA2	2.55	0.42
5:S:52:LYS:HB3	5:S:63:TYR:HB3	2.02	0.42
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.55	0.42
6:T:43:ASN:HD22	6:T:44:ASP:N	2.17	0.42
6:T:157:TYR:CD1	6:T:157:TYR:C	2.92	0.42
11:Y:39:PRO:HG3	17:Y:256:HOH:O	2.19	0.42
1:A:130:ARG:HG2	7:G:125:GLN:HG3	2.02	0.42
3:C:33:ARG:NH1	3:C:33:ARG:CB	2.83	0.42
1:O:142:ASP:OD1	1:O:145:ASN:HB2	2.20	0.42
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.19	0.42
6:T:172:ALA:O	6:T:176:LEU:CD2	2.68	0.42
7:U:191:GLU:HG3	7:U:232:ARG:HG3	2.02	0.42
1:A:40:ILE:HD12	1:A:193:ALA:HB2	2.01	0.42
1:A:142:ASP:OD1	1:A:145:ASN:HB2	2.20	0.42
4:D:68:VAL:CG2	4:D:89:ILE:HD12	2.35	0.42
5:E:199:GLN:CA	5:E:199:GLN:HE21	2.32	0.42
12:L:21:ILE:C	12:L:21:ILE:HD12	2.40	0.42
13:M:12:VAL:CG2	13:M:102:ALA:HB1	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.20	0.42
8:V:206:PHE:CZ	9:W:157:GLN:HG3	2.55	0.42
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.54	0.42
10:X:3:ILE:HD13	10:X:3:ILE:HA	1.90	0.42
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	2.14	0.42
1:A:97:HIS:HD2	8:H:61:SER:OG	2.03	0.42
4:D:102:TYR:O	12:L:81:ARG:HG3	2.20	0.42
5:E:111:ARG:HG2	5:E:111:ARG:NH1	2.33	0.42
8:H:139:GLU:OE2	8:H:139:GLU:HA	2.19	0.42
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.55	0.42
9:I:123:ASP:OD1	9:I:124:PHE:N	2.50	0.42
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	2.00	0.42
3:Q:224:LEU:CD1	3:Q:224:LEU:H	2.32	0.42
4:R:59:LEU:C	4:R:59:LEU:HD13	2.40	0.42
12:Z:14(I):THR:HB	12:Z:14(M):VAL:HG23	2.01	0.42
2:B:213:ALA:HA	2:B:222:LYS:O	2.20	0.42
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.55	0.42
8:H:206:PHE:CZ	9:I:157:GLN:HG3	2.55	0.42
14:N:48:SER:HB3	14:N:51:ASP:HB2	2.02	0.42
1:O:49:ALA:HB2	1:O:212:LEU:HG	2.00	0.42
4:R:17:PRO:HA	5:S:26:TYR:CD1	2.54	0.42
6:T:31:VAL:HG22	6:T:134:VAL:HA	2.02	0.42
7:U:93:LYS:HD3	14:2:68:SER:HB3	2.01	0.42
7:G:17(D):SER:O	7:G:17(E):LYS:HB2	2.20	0.42
11:K:10(A):ARG:HH11	11:K:10(A):ARG:HG2	1.85	0.42
12:L:1:GLY:HA3	12:L:33:LYS:NZ	2.34	0.42
2:P:52:ARG:HH22	2:P:63(A):SER:HB3	1.85	0.42
3:Q:194:VAL:O	3:Q:198:LEU:HG	2.19	0.42
3:Q:212:ILE:HG22	3:Q:224:LEU:HD13	2.00	0.42
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.20	0.42
8:V:18:THR:HB	8:V:30:ASN:HD22	1.85	0.42
11:Y:10(A):ARG:HG2	11:Y:10(A):ARG:HH11	1.85	0.42
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.55	0.42
2:B:184:MET:HE2	2:B:188:ASP:CB	2.50	0.42
2:B:186:VAL:CB	2:B:216:ARG:HD3	2.50	0.42
3:C:76:LEU:HD23	3:C:76:LEU:C	2.40	0.42
5:E:44:THR:CG2	5:E:183:ASP:HB3	2.50	0.42
7:G:158:VAL:HG22	7:G:159:GLY:N	2.35	0.42
9:I:28:SER:HB2	10:J:120:VAL:HG21	2.01	0.42
10:J:190:PHE:C	10:J:192:ALA:N	2.74	0.42
13:M:14(G):ILE:HB	13:M:144:PRO:HD3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:55:ILE:O	14:N:59:VAL:HG23	2.20	0.42
1:O:13:THR:O	2:P:130:ARG:HD3	2.19	0.42
1:O:32:LYS:HE2	1:O:32:LYS:HA	2.01	0.42
2:P:213:ALA:HA	2:P:222:LYS:O	2.20	0.42
5:S:7:ASN:HD22	5:S:7:ASN:HA	1.64	0.42
7:U:18(H):GLU:H	7:U:18(H):GLU:CD	2.23	0.42
2:B:141:TYR:CE2	2:B:145:GLY:HA2	2.54	0.41
3:C:159:SER:O	4:D:59:LEU:HD22	2.20	0.41
7:G:225:SER:O	7:G:229:ILE:HG13	2.20	0.41
2:P:149:TYR:OH	3:Q:62(A):ILE:HB	2.20	0.41
5:S:118:ASP:HA	17:S:234:HOH:O	2.20	0.41
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.49	0.41
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.84	0.41
9:W:28:SER:HB2	10:X:120:VAL:HG21	2.02	0.41
14:2:19:ARG:CZ	14:2:26:ILE:HD11	2.50	0.41
14:2:113:ILE:HG12	14:2:119:VAL:HG13	2.01	0.41
1:A:212:LEU:HD23	1:A:213:ALA:N	2.35	0.41
2:B:68:TYR:CG	2:B:89:ILE:HD12	2.55	0.41
3:C:55:THR:C	3:C:56:LEU:HD22	2.41	0.41
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.56	0.41
12:L:113:PHE:CD2	12:L:119:TYR:HB3	2.55	0.41
7:U:212:VAL:CG2	7:U:229:ILE:HD13	2.49	0.41
11:Y:143:LYS:HB2	11:Y:146:LEU:HD12	2.01	0.41
12:Z:21:ILE:C	12:Z:21:ILE:HD12	2.41	0.41
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.55	0.41
1:A:212:LEU:HD23	1:A:212:LEU:C	2.41	0.41
2:B:225:LYS:N	2:B:228:GLU:OE1	2.48	0.41
3:C:52:ARG:HD2	3:C:208:LYS:O	2.20	0.41
4:D:59:LEU:HD13	4:D:59:LEU:C	2.40	0.41
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.73	0.41
5:E:214:ILE:HG12	5:E:215:VAL:N	2.35	0.41
7:G:39:ALA:CB	7:G:148:ILE:HD12	2.49	0.41
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.51	0.41
8:H:40:LYS:HB2	17:H:238:HOH:O	2.20	0.41
8:H:52:THR:O	8:H:56:THR:HB	2.20	0.41
12:L:35:PHE:O	12:L:42:VAL:HA	2.20	0.41
4:R:122:ARG:HG2	4:R:122:ARG:NH1	2.35	0.41
5:S:194:VAL:O	5:S:197:ILE:HG22	2.20	0.41
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.49	0.41
10:X:98:ASN:HB3	10:X:127:HIS:CD2	2.55	0.41
10:X:190:PHE:C	10:X:192:ALA:N	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:ARG:NH1	2:B:20:ARG:HG2	2.35	0.41
2:B:71:ASN:HD22	2:B:72:ASP:H	1.69	0.41
5:E:125:GLN:HE22	6:F:87:HIS:HD2	1.68	0.41
6:F:157:TYR:CD1	6:F:157:TYR:C	2.92	0.41
7:G:55:PRO:HG2	7:G:56:ASP:N	2.33	0.41
7:G:212:VAL:CG2	7:G:229:ILE:HD13	2.50	0.41
9:I:165:ARG:NH2	12:Z:135:MET:HE2	2.35	0.41
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	2.02	0.41
4:R:148:LEU:HB3	4:R:160:TYR:O	2.21	0.41
5:S:38:VAL:HG12	5:S:39:GLY:N	2.35	0.41
7:U:39:ALA:HA	7:U:47:VAL:O	2.21	0.41
13:1:112:TYR:CE1	13:1:127:THR:HG22	2.55	0.41
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.50	0.41
2:B:14(A):TYR:HB2	2:B:147:GLN:NE2	2.36	0.41
6:F:18:ASP:OD2	6:F:18:ASP:N	2.46	0.41
6:F:35:THR:CG2	6:F:51:GLU:O	2.63	0.41
10:J:148:THR:CG2	10:J:177:ILE:HD13	2.50	0.41
10:J:154:LEU:HD12	10:J:154:LEU:HA	1.89	0.41
12:L:14:LEU:HD13	12:L:34:VAL:CG1	2.44	0.41
4:R:85:ALA:O	4:R:89:ILE:CG1	2.68	0.41
5:S:214:ILE:HG12	5:S:215:VAL:N	2.34	0.41
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.85	0.41
14:2:172:VAL:HB	14:2:18(A):ILE:HD11	2.02	0.41
3:C:14:ILE:HD12	3:C:14:ILE:O	2.19	0.41
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.60	0.41
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.84	0.41
11:K:200:LYS:HE2	17:K:244:HOH:O	2.21	0.41
14:N:26:ILE:HB	13:1:165:ARG:HA	2.01	0.41
1:O:136:LEU:O	1:O:150:GLN:HA	2.21	0.41
3:Q:208:LYS:O	3:Q:208:LYS:HD2	2.21	0.41
7:U:172:ILE:CD1	7:U:197:MET:HE1	2.50	0.41
7:U:192:PHE:CD1	7:U:192:PHE:C	2.93	0.41
13:1:122:SER:HB3	13:1:124:THR:O	2.20	0.41
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.55	0.41
14:2:107:LYS:CG	14:2:108:GLY:N	2.82	0.41
5:E:160:LEU:HD23	6:F:59:LEU:HA	2.03	0.41
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.86	0.41
11:K:40:PHE:CG	11:K:73:ARG:CZ	3.04	0.41
13:M:69(C):LEU:HD13	13:M:71(B):GLU:HB2	2.03	0.41
13:M:112:TYR:CD2	13:M:112:TYR:C	2.94	0.41
2:P:40:ILE:HD12	2:P:193:ALA:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:225:LYS:N	2:P:228:GLU:OE1	2.49	0.41
9:W:61:TYR:CD1	9:W:61:TYR:C	2.94	0.41
1:A:49:ALA:HB2	1:A:212:LEU:HG	2.03	0.41
1:A:77:VAL:HG12	1:A:137:LEU:HB2	2.02	0.41
3:C:175:PHE:CZ	3:C:195:ARG:HB3	2.56	0.41
3:C:215:VAL:O	3:C:215:VAL:HG13	2.20	0.41
3:C:238:GLN:O	3:C:242:GLU:HG3	2.21	0.41
6:F:65:VAL:HA	6:F:211:GLU:OE2	2.20	0.41
6:F:179:LEU:HD11	6:F:192:GLN:HG3	2.02	0.41
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.51	0.41
8:H:34:LEU:HD22	8:H:174:ASP:HB3	2.03	0.41
10:J:3:ILE:HD12	10:J:44:SER:HB2	2.01	0.41
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.20	0.41
11:K:156:LYS:HD3	11:K:195:LEU:HD11	2.03	0.41
3:Q:125:GLN:NE2	17:R:263:HOH:O	2.54	0.41
7:U:203:THR:HG22	7:U:204:GLU:O	2.21	0.41
8:V:34:LEU:HD22	8:V:174:ASP:HB3	2.02	0.41
11:Y:111:TYR:CE1	11:Y:121:LYS:HB2	2.55	0.41
1:A:195:LEU:HD23	1:A:236:LEU:HD21	2.03	0.41
2:B:10:SER:HB2	17:B:248:HOH:O	2.21	0.41
3:C:57:LYS:HD2	3:C:58:LEU:N	2.35	0.41
3:C:158:SER:CB	4:D:59:LEU:HD21	2.51	0.41
5:E:38:VAL:HG12	5:E:39:GLY:N	2.35	0.41
7:G:10:ARG:HG2	7:G:22:TYR:CD2	2.55	0.41
7:G:47:VAL:CG1	7:G:49:ILE:CD1	2.99	0.41
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.21	0.41
11:K:12:ILE:HB	11:K:178:VAL:HB	2.03	0.41
12:L:14(I):THR:HB	12:L:14(M):VAL:HG23	2.02	0.41
13:M:40:ASN:ND2	13:M:40:ASN:N	2.64	0.41
14:N:36:ARG:HG3	14:N:42:TRP:NE1	2.34	0.41
3:Q:215:VAL:HG13	3:Q:215:VAL:O	2.20	0.41
4:R:117:CYS:SG	4:R:157:PHE:HB3	2.60	0.41
6:T:103:TYR:O	6:T:104:LYS:HB3	2.21	0.41
7:U:82:ILE:CG2	7:U:83:PRO:HD3	2.51	0.41
7:U:105:TYR:OH	8:V:66:HIS:HE1	2.03	0.41
9:W:160:LEU:HD12	9:W:191:MET:HE3	2.03	0.41
14:2:107:LYS:NZ	14:2:145:ASN:HD21	2.18	0.41
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.18	0.41
1:A:136:LEU:O	1:A:150:GLN:HA	2.21	0.41
2:B:149:TYR:CZ	3:C:62(A):ILE:HB	2.56	0.41
3:C:120:GLN:O	3:C:124:THR:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:171:GLU:OE1	7:G:171:GLU:N	2.47	0.41
8:H:63:ILE:HD13	8:H:63:ILE:HA	1.83	0.41
13:M:9:ASP:OD1	13:M:10:ASN:N	2.54	0.41
1:O:26:TYR:N	1:O:26:TYR:CD1	2.88	0.41
1:O:77:VAL:CG1	1:O:137:LEU:HB2	2.51	0.41
2:P:14(A):TYR:HB2	2:P:147:GLN:NE2	2.36	0.41
3:Q:76:LEU:HD22	3:Q:89:ILE:HG12	2.03	0.41
4:R:121:LEU:HD13	5:S:130:ARG:HH21	1.86	0.41
9:W:45:ILE:HB	9:W:52:VAL:HG13	2.03	0.41
10:X:3:ILE:O	10:X:126:ALA:HA	2.20	0.41
10:X:136:SER:HA	10:X:139:ASP:HB2	2.03	0.41
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.56	0.41
12:Z:35:PHE:O	12:Z:42:VAL:HA	2.21	0.41
1:A:32:LYS:HE2	1:A:32:LYS:HA	2.03	0.40
1:A:77:VAL:CG1	1:A:137:LEU:HB2	2.52	0.40
2:B:20:ARG:NH2	3:C:33:ARG:HE	2.19	0.40
2:B:174:THR:O	2:B:178:MET:HB2	2.21	0.40
4:D:121:LEU:HA	4:D:123:PHE:HE1	1.83	0.40
7:G:192:PHE:CD1	7:G:192:PHE:C	2.94	0.40
12:L:134:ILE:HD11	12:L:162:ALA:HB2	2.03	0.40
13:M:-1:GLY:HA2	17:M:214:HOH:O	2.20	0.40
2:P:39:GLY:O	2:P:148:LEU:HD21	2.21	0.40
2:P:176:LEU:C	2:P:178:MET:H	2.24	0.40
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.36	0.40
3:Q:66:LYS:HE2	3:Q:78:PHE:CZ	2.57	0.40
9:W:6:MET:HE1	9:W:155:ILE:HA	2.03	0.40
13:1:80:PHE:CE1	13:1:111:ARG:HD3	2.56	0.40
14:2:161:GLN:HE22	14:2:165:TRP:HE1	1.69	0.40
4:D:123:PHE:CZ	4:D:131:PRO:HG3	2.56	0.40
5:E:221:PHE:HE1	5:E:223:ILE:HD11	1.84	0.40
9:I:2:ILE:HD12	9:I:2:ILE:O	2.21	0.40
11:K:180:GLU:N	17:K:239:HOH:O	2.53	0.40
2:P:44:ASP:OD2	2:P:44:ASP:N	2.54	0.40
17:T:244:HOH:O	7:U:86:ARG:HD2	2.19	0.40
10:X:10(B):LYS:HB2	10:X:10(B):LYS:NZ	2.36	0.40
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	2.02	0.40
14:2:13:ILE:HD12	14:2:151:THR:CG2	2.52	0.40
2:B:159:GLY:O	3:C:59:GLN:HB3	2.21	0.40
13:M:35:ILE:HA	13:M:36:PRO:HD3	1.93	0.40
14:N:172:VAL:HB	14:N:18(A):ILE:HD11	2.04	0.40
1:O:206:PHE:CE1	1:O:210:ILE:HD11	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:71:ASN:HD22	2:P:72:ASP:H	1.69	0.40
3:Q:195:ARG:CG	3:Q:236:ILE:HD13	2.47	0.40
4:R:123:PHE:CZ	4:R:131:PRO:HG3	2.56	0.40
5:S:44:THR:CG2	5:S:183:ASP:HB3	2.50	0.40
10:X:3:ILE:HD12	10:X:44:SER:HB2	2.02	0.40
10:X:166:MET:HA	10:X:167:PRO:HD3	1.79	0.40
5:E:76:LEU:HB2	5:E:137:LEU:O	2.21	0.40
6:F:114:ASP:O	6:F:118:GLN:HG2	2.21	0.40
7:G:54:VAL:HA	7:G:55:PRO:HD2	1.96	0.40
8:H:3:ILE:CD1	8:H:3:ILE:H	2.35	0.40
9:I:107:LYS:HA	9:I:108:PRO:HD3	1.84	0.40
11:K:143:LYS:HB2	11:K:146:LEU:HD12	2.03	0.40
14:N:105:ASP:OD2	14:N:106:ASN:N	2.46	0.40
1:O:195:LEU:HD23	1:O:236:LEU:HD21	2.03	0.40
1:O:21(L):ILE:HD11	8:V:186:TYR:CD2	2.57	0.40
2:P:67:LEU:HD23	2:P:213:ALA:HB2	2.03	0.40
2:P:171:ALA:O	2:P:175:LEU:HG	2.20	0.40
4:R:121:LEU:HD23	4:R:123:PHE:HE1	1.87	0.40
4:R:12(E):SER:O	5:S:123:ASN:OD1	2.39	0.40
10:X:3:ILE:HB	17:X:234:HOH:O	2.20	0.40
10:X:148:THR:CG2	10:X:177:ILE:HD13	2.51	0.40
11:Y:25:TRP:CH2	12:Z:132:SER:HA	2.57	0.40
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.17	0.40
2:B:67:LEU:HD23	2:B:213:ALA:HB2	2.02	0.40
6:F:179:LEU:HD11	6:F:192:GLN:HG2	2.04	0.40
8:H:24:PRO:HG2	8:H:25:ILE:CD1	2.50	0.40
8:H:84:LYS:HE2	8:H:119:THR:CG2	2.51	0.40
10:J:105:ASP:O	10:J:106:ASN:N	2.55	0.40
10:J:136:SER:HA	10:J:139:ASP:HB2	2.04	0.40
12:L:43:MET:CB	12:L:101:ILE:HG22	2.51	0.40
2:P:20:ARG:HG2	2:P:20:ARG:NH1	2.37	0.40
2:P:163:ILE:CG1	2:P:164:SER:N	2.82	0.40
2:P:185:LYS:O	2:P:188:ASP:HB2	2.22	0.40
3:Q:175:PHE:CZ	3:Q:195:ARG:HB3	2.56	0.40
8:V:84:LYS:HE2	8:V:119:THR:CG2	2.49	0.40
9:W:143:GLU:HA	9:W:144:PRO:HD3	1.89	0.40
13:1:130:GLY:O	13:1:134:ALA:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	231 (93%)	15 (6%)	2 (1%)	19	39
1	O	248/250 (99%)	232 (94%)	13 (5%)	3 (1%)	13	27
2	B	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	9	18
2	P	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	9	18
3	C	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	12	24
3	Q	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	12	24
4	D	240/242 (99%)	221 (92%)	12 (5%)	7 (3%)	4	7
4	R	240/242 (99%)	221 (92%)	13 (5%)	6 (2%)	5	9
5	E	231/233 (99%)	214 (93%)	13 (6%)	4 (2%)	9	18
5	S	231/233 (99%)	213 (92%)	16 (7%)	2 (1%)	17	35
6	F	242/244 (99%)	230 (95%)	9 (4%)	3 (1%)	13	27
6	T	242/244 (99%)	230 (95%)	9 (4%)	3 (1%)	13	27
7	G	241/243 (99%)	229 (95%)	12 (5%)	0	100	100
7	U	241/243 (99%)	229 (95%)	11 (5%)	1 (0%)	34	57
8	H	220/222 (99%)	210 (96%)	8 (4%)	2 (1%)	17	35
8	V	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	29	52
9	I	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
9	W	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
10	J	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	29	52
10	X	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	29	52
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	29	52
11	Y	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	29	52
12	L	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	29	52
12	Z	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	29	52
13	1	231/233 (99%)	217 (94%)	14 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/233 (99%)	217 (94%)	14 (6%)	0	100	100
14	2	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
15	a	1/3 (33%)	1 (100%)	0	0	100	100
15	b	1/3 (33%)	1 (100%)	0	0	100	100
15	c	1/3 (33%)	1 (100%)	0	0	100	100
15	d	1/3 (33%)	1 (100%)	0	0	100	100
15	e	1/3 (33%)	1 (100%)	0	0	100	100
15	f	1/3 (33%)	1 (100%)	0	0	100	100
All	All	6318/6386 (99%)	5954 (94%)	310 (5%)	54 (1%)	17	35

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	56	SER
3	C	58	LEU
4	D	12(G)	GLU
10	J	192	ALA
1	O	5	THR
1	O	56	SER
3	Q	58	LEU
4	R	12(G)	GLU
10	X	192	ALA
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	183	PRO
3	C	203	THR
4	D	18(D)	SER
2	P	54	VAL
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	203	THR
4	R	18(D)	SER
4	D	12(F)	GLY
5	E	202	ARG
6	F	206	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	39	PRO
2	P	6	ARG
4	R	12(F)	GLY
5	S	202	ARG
6	T	206	LYS
11	Y	39	PRO
2	B	6	ARG
5	E	231	LYS
6	F	205	ASN
5	S	231	LYS
6	T	205	ASN
4	D	60	GLU
4	D	61	SER
4	R	60	GLU
4	R	61	SER
4	D	12(C)	GLY
4	D	128	MET
5	E	180	LEU
5	E	217	LYS
6	F	13	SER
1	O	167	LYS
4	R	12(C)	GLY
6	T	13	SER
8	V	96	GLY
8	H	180	ILE
12	L	14(H)	GLY
8	H	96	GLY
7	U	55	PRO
12	Z	14(H)	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/209 (100%)	204 (98%)	5 (2%)	49 74
1	O	209/209 (100%)	204 (98%)	5 (2%)	49 74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	203/203 (100%)	195 (96%)	8 (4%)	32 58
2	P	203/203 (100%)	195 (96%)	8 (4%)	32 58
3	C	213/213 (100%)	204 (96%)	9 (4%)	30 55
3	Q	213/213 (100%)	204 (96%)	9 (4%)	30 55
4	D	198/198 (100%)	187 (94%)	11 (6%)	21 42
4	R	198/198 (100%)	187 (94%)	11 (6%)	21 42
5	E	192/192 (100%)	171 (89%)	21 (11%)	6 11
5	S	192/192 (100%)	171 (89%)	21 (11%)	6 11
6	F	201/201 (100%)	186 (92%)	15 (8%)	13 27
6	T	201/201 (100%)	185 (92%)	16 (8%)	12 24
7	G	207/207 (100%)	193 (93%)	14 (7%)	16 32
7	U	207/207 (100%)	192 (93%)	15 (7%)	14 29
8	H	181/181 (100%)	173 (96%)	8 (4%)	28 53
8	V	181/181 (100%)	174 (96%)	7 (4%)	32 58
9	I	172/172 (100%)	168 (98%)	4 (2%)	50 75
9	W	172/172 (100%)	168 (98%)	4 (2%)	50 75
10	J	175/175 (100%)	168 (96%)	7 (4%)	31 57
10	X	175/175 (100%)	168 (96%)	7 (4%)	31 57
11	K	169/169 (100%)	162 (96%)	7 (4%)	30 56
11	Y	169/169 (100%)	161 (95%)	8 (5%)	26 50
12	L	185/185 (100%)	174 (94%)	11 (6%)	19 39
12	Z	185/185 (100%)	173 (94%)	12 (6%)	17 34
13	1	199/199 (100%)	189 (95%)	10 (5%)	24 47
13	M	199/199 (100%)	190 (96%)	9 (4%)	27 52
14	2	162/162 (100%)	152 (94%)	10 (6%)	18 37
14	N	162/162 (100%)	152 (94%)	10 (6%)	18 37
15	a	3/3 (100%)	3 (100%)	0	100 100
15	b	3/3 (100%)	3 (100%)	0	100 100
15	c	3/3 (100%)	2 (67%)	1 (33%)	0 0
15	d	3/3 (100%)	3 (100%)	0	100 100
15	e	3/3 (100%)	3 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	f	3/3 (100%)	2 (67%)	1 (33%)	0 0
All	All	5350/5350 (100%)	5066 (95%)	284 (5%)	22 45

All (284) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	135	SER
1	A	158	PHE
1	A	179	ARG
2	B	58	LEU
2	B	71	ASN
2	B	89	ILE
2	B	121	GLN
2	B	150	THR
2	B	192	LEU
2	B	218	ASN
2	B	224	PHE
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	174	GLU
3	C	208	LYS
3	C	227	GLU
4	D	28	LEU
4	D	40	ILE
4	D	110	GLU
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
4	D	244	GLU
5	E	12	THR
5	E	13	VAL
5	E	32	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	56	ASP
5	E	57	GLU
5	E	76	LEU
5	E	90	ASN
5	E	97	ASN
5	E	104	ASN
5	E	111	ARG
5	E	121	GLN
5	E	18(D)	ILE
5	E	185	ASN
5	E	189	LEU
5	E	197	ILE
5	E	199	GLN
5	E	207	LEU
5	E	2(C)	VAL
5	E	2(E)	ASN
5	E	227	GLU
5	E	231	LYS
6	F	35	THR
6	F	43	ASN
6	F	56	SER
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
6	F	21(C)	ASN
7	G	12	ILE
7	G	14	ILE
7	G	35	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	169	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	184	ASN
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	3	ILE
8	H	30	ASN
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	99	LEU
8	H	144	GLN
8	H	197	ARG
9	I	29	ASN
9	I	116	ILE
9	I	160	LEU
9	I	171	TRP
10	J	35	ARG
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	121	GLU
10	J	137	LEU
10	J	168	MET
11	K	4	LEU
11	K	9	GLN
11	K	38	ASN
11	K	65	LEU
11	K	87	VAL
11	K	104	TYR
11	K	10(B)	LYS
12	L	-7	ASN
12	L	4	LEU
12	L	14	LEU
12	L	25	SER
12	L	58	ARG
12	L	70(A)	ASN
12	L	99	THR
12	L	123	GLN
12	L	134	ILE
12	L	1(I)	ASN
12	L	145	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	112	TYR
13	M	129	PHE
13	M	14(C)	ARG
13	M	149	GLN
13	M	204	LYS
13	M	211	ILE
14	N	70	TYR
14	N	84	LYS
14	N	89	GLU
14	N	10(A)	ASP
14	N	115	LEU
14	N	119	VAL
14	N	149	GLU
14	N	178	LEU
14	N	18(A)	ILE
14	N	18(I)	GLN
1	O	33	GLN
1	O	64	LEU
1	O	135	SER
1	O	158	PHE
1	O	179	ARG
2	P	58	LEU
2	P	71	ASN
2	P	89	ILE
2	P	121	GLN
2	P	150	THR
2	P	192	LEU
2	P	218	ASN
2	P	224	PHE
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	174	GLU
3	Q	208	LYS
3	Q	227	GLU
4	R	28	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	R	40	ILE
4	R	110	GLU
4	R	126	ARG
4	R	170	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
4	R	244	GLU
5	S	12	THR
5	S	13	VAL
5	S	32	LYS
5	S	56	ASP
5	S	57	GLU
5	S	76	LEU
5	S	90	ASN
5	S	97	ASN
5	S	104	ASN
5	S	111	ARG
5	S	121	GLN
5	S	18(D)	ILE
5	S	185	ASN
5	S	189	LEU
5	S	197	ILE
5	S	199	GLN
5	S	207	LEU
5	S	2(C)	VAL
5	S	2(E)	ASN
5	S	227	GLU
5	S	231	LYS
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	56	SER
6	T	98	SER
6	T	105	THR
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	18(E)	GLU
6	T	187	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
6	T	21(C)	ASN
7	U	12	ILE
7	U	14	ILE
7	U	35	ILE
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	169	GLN
7	U	184	ASN
7	U	197	MET
7	U	217	LYS
7	U	229	ILE
7	U	232	ARG
7	U	233	LEU
8	V	3	ILE
8	V	30	ASN
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	144	GLN
8	V	197	ARG
9	W	29	ASN
9	W	116	ILE
9	W	160	LEU
9	W	171	TRP
10	X	35	ARG
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	121	GLU
10	X	137	LEU
10	X	168	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	38	ASN
11	Y	65	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Y	87	VAL
11	Y	99	THR
11	Y	104	TYR
11	Y	10(B)	LYS
12	Z	-7	ASN
12	Z	4	LEU
12	Z	14	LEU
12	Z	25	SER
12	Z	58	ARG
12	Z	70(A)	ASN
12	Z	99	THR
12	Z	114	ASP
12	Z	123	GLN
12	Z	134	ILE
12	Z	1(I)	ASN
12	Z	145	TYR
13	1	39	ASP
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	112	TYR
13	1	129	PHE
13	1	14(C)	ARG
13	1	149	GLN
13	1	204	LYS
13	1	211	ILE
14	2	70	TYR
14	2	84	LYS
14	2	89	GLU
14	2	10(A)	ASP
14	2	115	LEU
14	2	119	VAL
14	2	149	GLU
14	2	178	LEU
14	2	18(A)	ILE
14	2	18(I)	GLN
15	c	1	ASN
15	f	1	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	218	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
7	G	34(A)	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	10	ASN
8	H	30	ASN
8	H	66	HIS
8	H	91	GLN
8	H	114	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
9	I	81	GLN
10	J	36	GLN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	53	GLN
11	K	66	HIS
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	40	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	1(I)	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	69	GLN
14	N	145	ASN
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	33	GLN
5	S	64	GLN
5	S	73	HIS
5	S	97	ASN
5	S	104	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	185	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	192	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	10	ASN
8	V	30	ASN
8	V	66	HIS
8	V	91	GLN
8	V	114	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	81	GLN
10	X	36	GLN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	53	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	Y	66	HIS
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	85	HIS
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	69	GLN
14	2	141	ASN
14	2	145	ASN
14	2	161	GLN
15	c	1	ASN
15	f	1	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	HXD	b	4	15	13,13,14	0.86	0	13,13,15	0.70	0
16	HXD	e	4	15	13,13,14	0.83	0	13,13,15	0.66	0
16	HXD	d	4	15	13,13,14	0.63	0	13,13,15	0.81	1 (7%)
16	HXD	a	4	15	13,13,14	0.71	0	13,13,15	0.82	1 (7%)
16	HXD	f	4	15	13,13,14	1.99	2 (15%)	13,13,15	1.00	1 (7%)
16	HXD	c	4	15	13,13,14	2.01	2 (15%)	13,13,15	1.03	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	HXD	b	4	15	-	5/12/12/13	-
16	HXD	e	4	15	-	5/12/12/13	-
16	HXD	d	4	15	-	2/12/12/13	-
16	HXD	a	4	15	-	2/12/12/13	-
16	HXD	f	4	15	-	3/12/12/13	-
16	HXD	c	4	15	-	3/12/12/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	c	4	HXD	C2-C3	6.18	1.61	1.53
16	f	4	HXD	C2-C3	6.15	1.61	1.53
16	f	4	HXD	C5-C4	2.06	1.61	1.52
16	c	4	HXD	C5-C4	2.02	1.60	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	d	4	HXD	C3-C2-C1	2.27	116.74	112.75
16	a	4	HXD	C3-C2-C1	2.26	116.73	112.75
16	f	4	HXD	O-C1-C2	-2.14	119.19	125.43
16	c	4	HXD	O-C1-C2	-2.04	119.48	125.43

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	c	4	HXD	C1-C2-C3-C4
16	c	4	HXD	C1-C2-C3-O8
16	f	4	HXD	C1-C2-C3-C4
16	f	4	HXD	C1-C2-C3-O8
16	b	4	HXD	O8-C3-C4-C5
16	e	4	HXD	C11-C10-C9-C8
16	b	4	HXD	C11-C10-C9-C8
16	e	4	HXD	O8-C3-C4-C5
16	d	4	HXD	C9-C10-C11-C12
16	a	4	HXD	C9-C10-C11-C12
16	b	4	HXD	C2-C3-C4-C5
16	e	4	HXD	C2-C3-C4-C5
16	e	4	HXD	C9-C10-C11-C12
16	b	4	HXD	C9-C10-C11-C12
16	d	4	HXD	C7-C8-C9-C10
16	a	4	HXD	C7-C8-C9-C10
16	e	4	HXD	C7-C8-C9-C10
16	b	4	HXD	C7-C8-C9-C10
16	c	4	HXD	C3-C4-C5-C6
16	f	4	HXD	C3-C4-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.09	9 (3%)	42	35	34, 52, 85, 106	0
1	O	250/250 (100%)	-0.01	14 (5%)	24	19	35, 54, 85, 105	0
2	B	244/244 (100%)	0.18	14 (5%)	23	18	37, 56, 89, 116	0
2	P	244/244 (100%)	0.19	15 (6%)	21	16	40, 56, 89, 116	0
3	C	241/241 (100%)	0.41	26 (10%)	5	3	39, 61, 110, 124	0
3	Q	241/241 (100%)	0.54	37 (15%)	2	1	41, 62, 110, 124	0
4	D	242/242 (100%)	0.22	17 (7%)	16	12	43, 58, 94, 121	0
4	R	242/242 (100%)	0.29	17 (7%)	16	12	44, 59, 95, 122	0
5	E	233/233 (100%)	0.02	9 (3%)	39	32	42, 55, 82, 109	0
5	S	233/233 (100%)	-0.03	8 (3%)	45	38	41, 54, 82, 109	0
6	F	244/244 (100%)	-0.17	9 (3%)	41	34	36, 50, 89, 106	0
6	T	244/244 (100%)	-0.18	7 (2%)	51	45	34, 50, 89, 106	0
7	G	243/243 (100%)	-0.18	9 (3%)	41	34	33, 47, 75, 112	0
7	U	243/243 (100%)	-0.12	8 (3%)	46	39	33, 47, 75, 111	0
8	H	222/222 (100%)	-0.36	3 (1%)	75	71	30, 44, 62, 100	0
8	V	222/222 (100%)	-0.41	3 (1%)	75	71	29, 45, 63, 100	0
9	I	204/204 (100%)	-0.37	4 (1%)	65	60	35, 45, 63, 80	0
9	W	204/204 (100%)	-0.35	3 (1%)	73	70	36, 46, 64, 80	0
10	J	198/198 (100%)	-0.09	8 (4%)	38	31	38, 49, 69, 122	0
10	X	198/198 (100%)	-0.10	6 (3%)	50	43	38, 49, 69, 122	0
11	K	212/212 (100%)	-0.12	10 (4%)	31	25	34, 47, 72, 86	0
11	Y	212/212 (100%)	-0.15	11 (5%)	27	21	35, 47, 74, 86	0
12	L	222/222 (100%)	-0.18	6 (2%)	54	48	33, 48, 74, 89	0
12	Z	222/222 (100%)	-0.23	10 (4%)	33	26	34, 47, 74, 89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	233/233 (100%)	-0.47	1 (0%) 92 91	31, 43, 57, 61	0
13	M	233/233 (100%)	-0.40	2 (0%) 84 82	32, 43, 57, 63	0
14	2	196/196 (100%)	-0.40	2 (1%) 82 80	31, 41, 61, 81	0
14	N	196/196 (100%)	-0.40	1 (0%) 91 89	31, 40, 60, 81	0
15	a	3/3 (100%)	-0.86	0 100 100	41, 41, 44, 46	0
15	b	3/3 (100%)	-0.46	0 100 100	34, 34, 42, 47	0
15	c	3/3 (100%)	-0.26	0 100 100	43, 43, 48, 51	0
15	d	3/3 (100%)	-0.55	0 100 100	44, 44, 44, 47	0
15	e	3/3 (100%)	-0.30	0 100 100	37, 37, 44, 50	0
15	f	3/3 (100%)	0.08	0 100 100	43, 43, 50, 51	0
All	All	6386/6386 (100%)	-0.10	269 (4%) 36 29	29, 50, 84, 124	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	12(C)	GLY	13.2
3	C	55	THR	12.6
4	R	12(E)	SER	11.7
4	D	12(E)	SER	10.0
10	X	192	ALA	9.8
7	U	240	ASP	9.8
4	R	12(C)	GLY	9.6
4	R	12(F)	GLY	9.2
4	D	12(D)	ALA	9.0
10	J	192	ALA	8.9
4	R	12(D)	ALA	8.4
3	Q	55	THR	7.9
2	B	217	ALA	7.7
7	G	240	ASP	7.4
2	B	54	VAL	7.3
2	B	218	ASN	7.3
3	C	56	LEU	7.0
6	F	5	GLY	6.9
4	D	12(F)	GLY	6.7
10	X	193	GLN	6.7
10	J	191	GLN	6.6
7	U	6	ALA	6.5
7	G	6	ALA	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	240	LYS	6.4
1	A	5	THR	6.3
2	P	218	ASN	6.2
1	O	5	THR	6.2
10	X	191	GLN	6.2
1	O	4	MET	6.1
11	Y	208	ASN	6.0
2	P	21(A)	LYS	6.0
1	A	4	MET	6.0
12	L	145	TYR	5.9
10	J	193	GLN	5.9
2	P	54	VAL	5.8
11	K	208	ASN	5.7
2	P	217	ALA	5.6
12	Z	145	TYR	5.6
4	R	126	ARG	5.5
5	S	203	ASP	5.4
3	C	240	LYS	5.3
3	Q	242	GLU	5.3
2	P	219	GLU	5.2
5	E	203	ASP	5.2
3	Q	203	THR	5.2
3	Q	243	GLN	5.1
5	E	4	PHE	5.0
2	P	21(C)	ASP	4.9
3	Q	56	LEU	4.9
8	H	223	ASP	4.9
4	D	125	GLU	4.8
8	V	223	ASP	4.7
9	W	-8	SER	4.7
2	B	21(A)	LYS	4.7
3	Q	54	SER	4.7
4	R	242	ALA	4.6
12	L	14(P)	PRO	4.6
5	S	5	ARG	4.6
3	C	241	GLN	4.5
5	S	4	PHE	4.5
1	O	53	LYS	4.4
3	Q	241	GLN	4.4
4	R	243	ALA	4.3
1	A	236	LEU	4.3
6	T	240	ILE	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	R	127	LEU	4.3
1	O	21(P)	LYS	4.2
9	I	-8	SER	4.2
3	Q	64	PRO	4.2
4	R	125	GLU	4.2
4	D	127	LEU	4.1
3	Q	207	ALA	4.1
3	Q	236	ILE	4.0
2	B	21(B)	GLY	4.0
4	D	126	ARG	4.0
5	E	5	ARG	4.0
11	K	207	ASN	3.9
13	1	-8	THR	3.9
8	V	222	CYS	3.9
2	B	219	GLU	3.9
7	G	239	GLN	3.9
11	K	210	ILE	3.9
12	L	14(H)	GLY	3.8
11	Y	104	TYR	3.8
5	S	178	ARG	3.8
3	Q	63	THR	3.7
6	F	204	ASP	3.7
3	C	43	LYS	3.7
6	F	241	ASN	3.7
11	K	104	TYR	3.7
12	L	14(M)	VAL	3.7
11	K	143	LYS	3.6
4	D	244	GLU	3.6
2	P	21(B)	GLY	3.6
11	Y	210	ILE	3.6
1	O	235	ALA	3.6
3	C	243	GLN	3.6
3	Q	18(C)	LYS	3.6
6	F	20(B)	GLU	3.6
11	Y	10(A)	ARG	3.6
10	J	92	ARG	3.5
12	Z	14(W)	LYS	3.5
7	U	8	TYR	3.4
5	S	217	LYS	3.4
8	H	220	ASN	3.4
11	Y	207	ASN	3.4
1	A	203	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	T	241	ASN	3.4
5	S	127	TYR	3.4
2	P	239	THR	3.3
2	P	53	LYS	3.3
3	Q	53	ARG	3.3
4	R	12(G)	GLU	3.3
3	Q	7	GLY	3.3
13	M	-8	THR	3.3
3	Q	202	GLN	3.3
8	H	222	CYS	3.3
2	B	21(C)	ASP	3.3
3	C	33	ARG	3.3
11	Y	67	GLU	3.3
14	N	18(I)	GLN	3.3
7	G	8	TYR	3.3
8	V	220	ASN	3.3
1	O	236	LEU	3.3
2	P	185	LYS	3.2
7	U	7	GLY	3.2
6	F	240	ILE	3.2
11	Y	181	ASP	3.2
14	2	18(I)	GLN	3.2
2	B	20(B)	ALA	3.2
7	G	7	GLY	3.2
10	J	-1	MET	3.2
2	B	239	THR	3.2
3	Q	178	LYS	3.2
4	D	243	ALA	3.2
3	Q	208	LYS	3.2
4	D	12(G)	GLU	3.2
11	K	40	PHE	3.1
12	L	14(W)	LYS	3.1
3	Q	239	GLU	3.1
3	Q	223	ALA	3.1
3	Q	222	VAL	3.1
6	T	6	THR	3.0
5	E	127	TYR	3.0
12	Z	-9	GLN	3.0
2	P	220	TYR	3.0
10	X	92	ARG	3.0
9	W	182	ASP	3.0
3	C	203	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	K	10(A)	ARG	3.0
6	F	6	THR	3.0
3	Q	206	GLY	3.0
3	C	52	ARG	2.9
5	E	233	ILE	2.9
7	G	218	ASP	2.9
12	Z	14(P)	PRO	2.9
7	G	18(A)	ILE	2.9
11	K	73	ARG	2.9
1	O	21(F)	LEU	2.9
2	P	183	ASP	2.9
9	I	181	LYS	2.8
6	T	18(E)	GLU	2.8
3	Q	62	ARG	2.8
1	O	43	THR	2.8
3	Q	62(A)	ILE	2.8
4	R	9	ASP	2.8
6	F	18(E)	GLU	2.8
3	Q	238	GLN	2.8
5	S	204	GLU	2.8
12	Z	14(H)	GLY	2.8
3	C	238	GLN	2.7
11	Y	180	GLU	2.7
7	G	18(H)	GLU	2.7
3	C	194	VAL	2.7
7	U	218	ASP	2.7
11	K	181	ASP	2.7
4	D	218	GLN	2.7
3	C	237	GLU	2.7
3	Q	14(B)	ASP	2.7
3	Q	18(D)	GLU	2.7
2	P	21(D)	GLY	2.7
6	F	206	LYS	2.7
12	L	70(A)	ASN	2.7
3	Q	187	GLU	2.7
4	R	244	GLU	2.7
2	B	237	GLY	2.6
2	P	20(A)	SER	2.6
3	C	53	ARG	2.6
12	Z	14(M)	VAL	2.6
2	P	181	LYS	2.6
4	D	9	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	234	THR	2.6
11	Y	73	ARG	2.6
3	C	233	VAL	2.5
7	U	239	GLN	2.5
5	E	217	LYS	2.5
5	S	233	ILE	2.5
3	Q	33	ARG	2.5
5	E	204	GLU	2.5
1	O	143	GLU	2.5
2	B	20(A)	SER	2.5
4	D	10	ARG	2.5
3	C	227	GLU	2.4
4	R	241	GLU	2.4
11	K	180	GLU	2.4
10	X	188	ASP	2.4
1	A	21(P)	LYS	2.4
3	C	208	LYS	2.4
6	T	20(C)	LYS	2.4
4	R	12(B)	GLU	2.4
2	B	183	ASP	2.4
1	A	21(N)	THR	2.3
3	C	234	THR	2.3
2	B	21(D)	GLY	2.3
1	O	55	SER	2.3
4	D	18(D)	SER	2.3
10	J	188	ASP	2.3
1	O	178	LYS	2.3
1	A	234	GLU	2.3
1	O	234	GLU	2.3
3	Q	14(A)	ARG	2.3
3	Q	18(B)	ARG	2.3
3	C	54	SER	2.2
3	C	202	GLN	2.2
7	G	238	GLU	2.2
9	I	182	ASP	2.2
4	R	10	ARG	2.2
3	Q	233	VAL	2.2
7	U	17(E)	LYS	2.2
3	Q	58	LEU	2.2
6	T	238	LYS	2.2
9	W	12(A)	LYS	2.2
4	D	205	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	M	211	ILE	2.2
1	O	203	GLU	2.2
1	A	204	GLY	2.2
1	O	21(M)	PRO	2.2
4	D	122	ARG	2.2
7	U	72	ARG	2.2
3	Q	227	GLU	2.1
4	D	202	GLU	2.1
12	Z	70(A)	ASN	2.1
12	Z	120	GLU	2.1
3	C	235	GLN	2.1
3	Q	52	ARG	2.1
11	Y	40	PHE	2.1
1	A	21(E)	ASP	2.1
2	B	185	LYS	2.1
5	E	178	ARG	2.1
10	J	144	PRO	2.1
5	E	18(E)	LYS	2.1
3	C	236	ILE	2.1
4	R	231	GLU	2.1
6	F	18(B)	HIS	2.1
6	T	18(D)	PRO	2.1
10	X	168	MET	2.1
12	Z	1(I)	ASN	2.1
3	C	178	LYS	2.1
4	R	240	LYS	2.1
3	C	59	GLN	2.0
3	C	187	GLU	2.0
10	J	145	ASP	2.0
14	2	107	LYS	2.0
3	C	18(C)	LYS	2.0
9	I	107	LYS	2.0
12	Z	180	LYS	2.0
3	C	7	GLY	2.0
3	Q	18	ASP	2.0
11	Y	143	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	HXD	c	4	14/15	0.87	0.29	49,58,60,61	0
16	HXD	d	4	14/15	0.87	0.30	43,45,60,63	0
16	HXD	e	4	14/15	0.89	0.26	34,39,56,58	0
16	HXD	f	4	14/15	0.89	0.40	50,59,61,65	0
16	HXD	a	4	14/15	0.91	0.25	43,47,59,63	0
16	HXD	b	4	14/15	0.91	0.23	37,41,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.