



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:36 PM UTC

PDB ID : 3D29 / pdb_00003d29
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

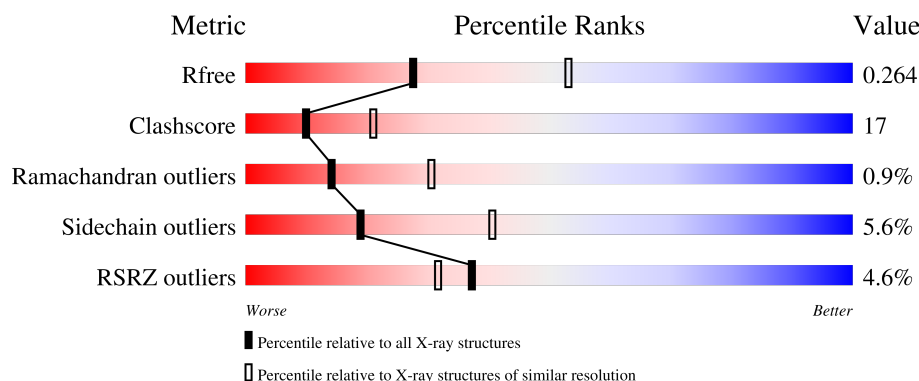
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	6% 72% 24% .
1	O	250	3% 73% 24% .
2	B	244	8% 54% 41% 5%
2	P	244	8% 54% 42% .
3	C	241	10% 59% 38% .

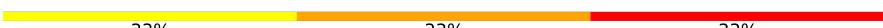
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Mol	Chain	Length	Quality of chain
3	Q	241	
4	D	242	
4	R	242	
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	
15	a	3	
15	b	3	

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Mol	Chain	Length	Quality of chain
15	c	3	 33% 33% 33%
15	d	3	 67% 33%
15	e	3	 67% 33%
15	f	3	 33% 33% 33%

2 Entry composition

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			

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

- Molecule 11 is a protein called proteasome 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.

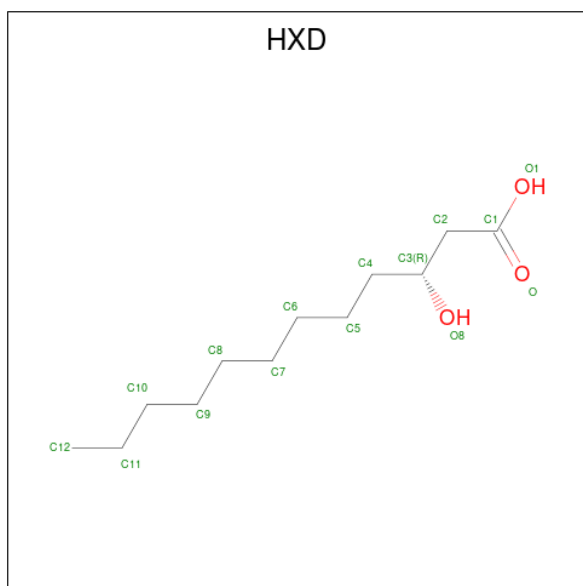
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	a	3	Total	C	N	O	0	0	0
			25	15	5	5			
15	b	3	Total	C	N	O	0	0	0
			25	15	5	5			

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

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



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

- 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

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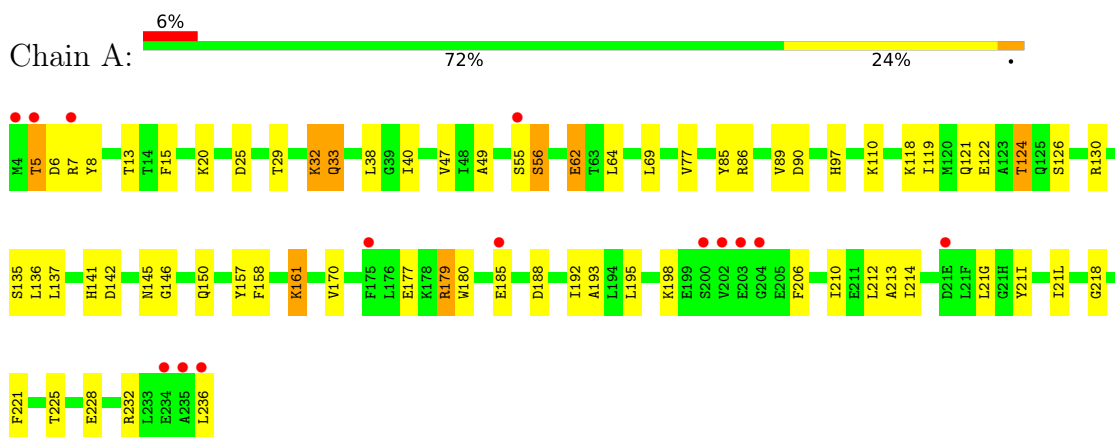
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	59	Total 59	O 59	0	0
17	X	46	Total 46	O 46	0	0
17	Y	48	Total 48	O 48	0	0
17	Z	52	Total 52	O 52	0	0
17	1	74	Total 74	O 74	0	0
17	2	59	Total 59	O 59	0	0

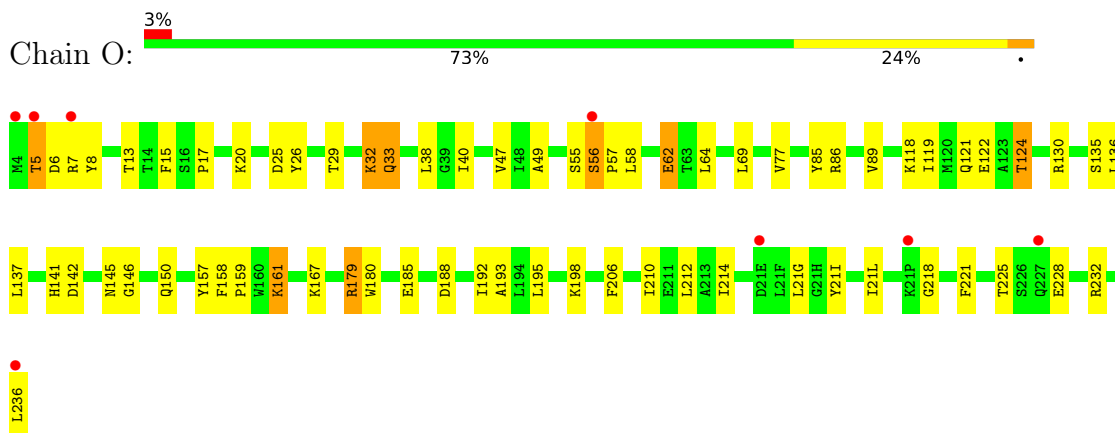
3 Residue-property plots [i](#)

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.

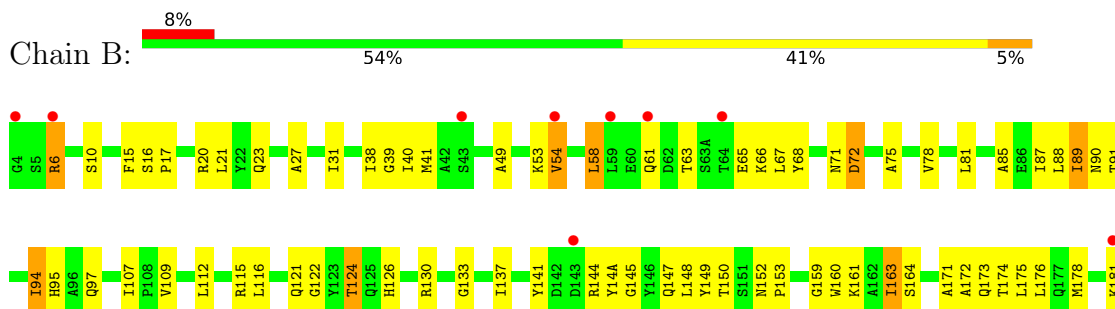
• Molecule 1: PRE8 isoform 1

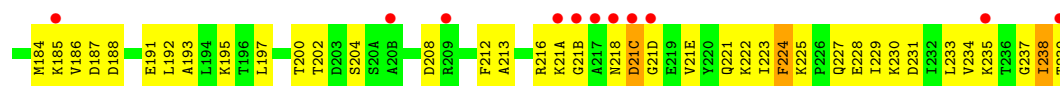


• Molecule 1: PRE8 isoform 1

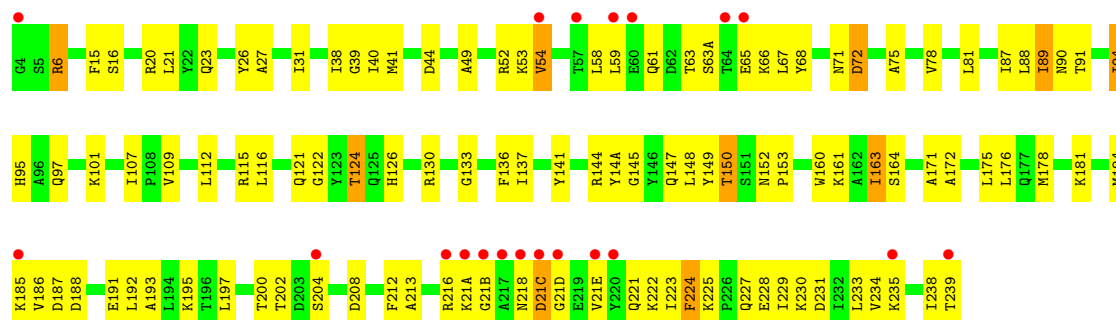


• Molecule 2: PRE9 isoform 1

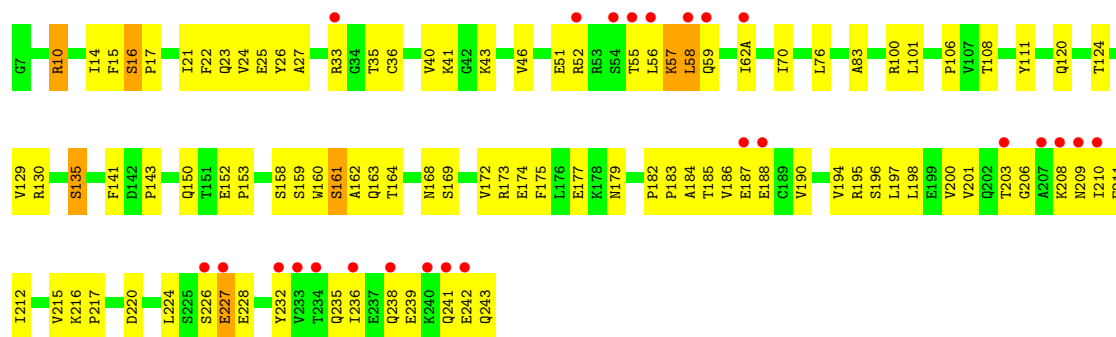




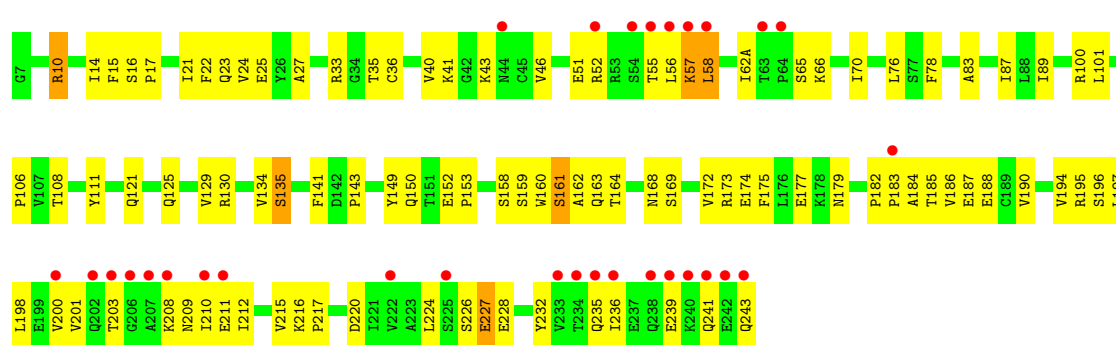
• Molecule 2: PRE9 isoform 1



• Molecule 3: PRE6 isoform 1

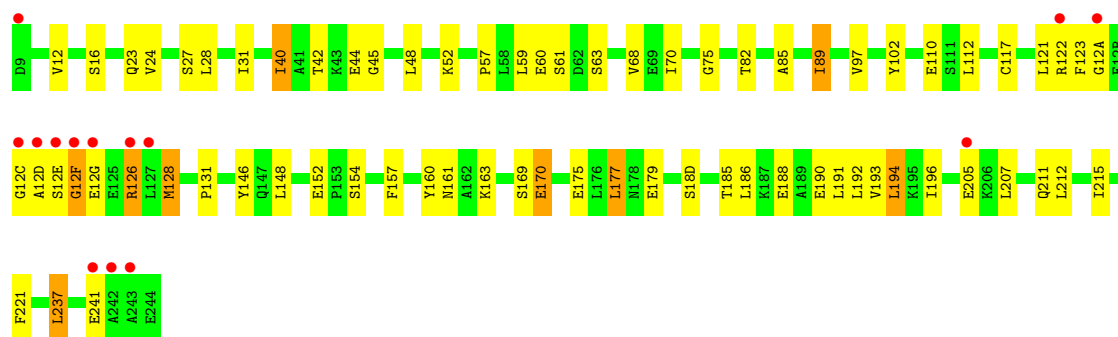


• Molecule 3: PRE6 isoform 1

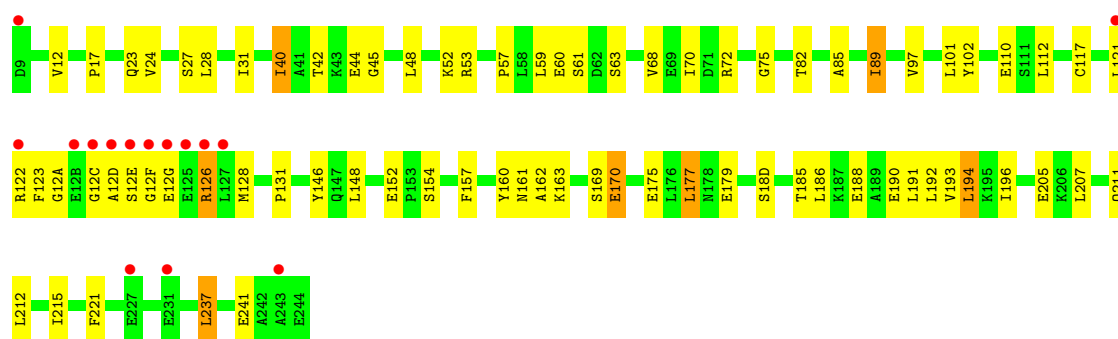


• Molecule 4: PUP2 isoform 1

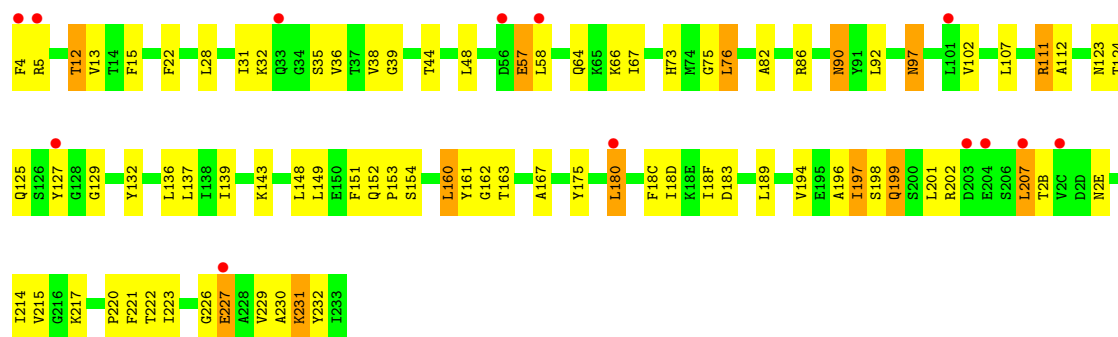




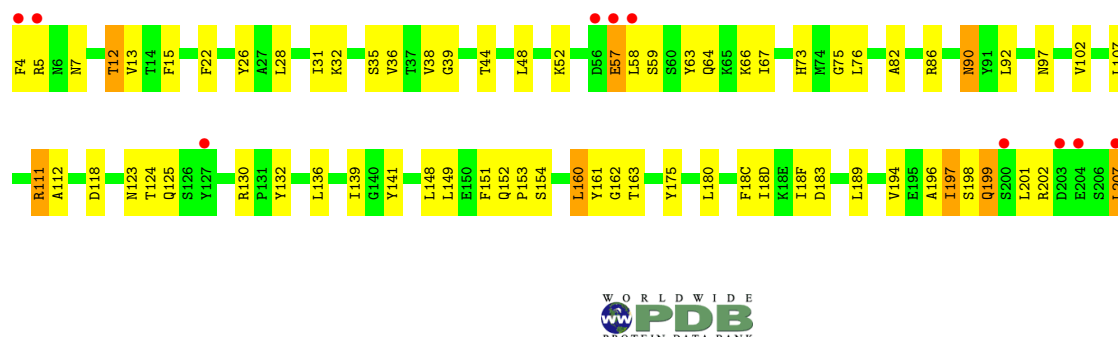
• Molecule 4: PUP2 isoform 1

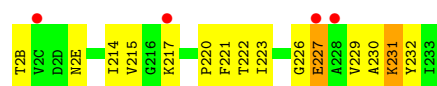


• Molecule 5: PRE5 isoform 1

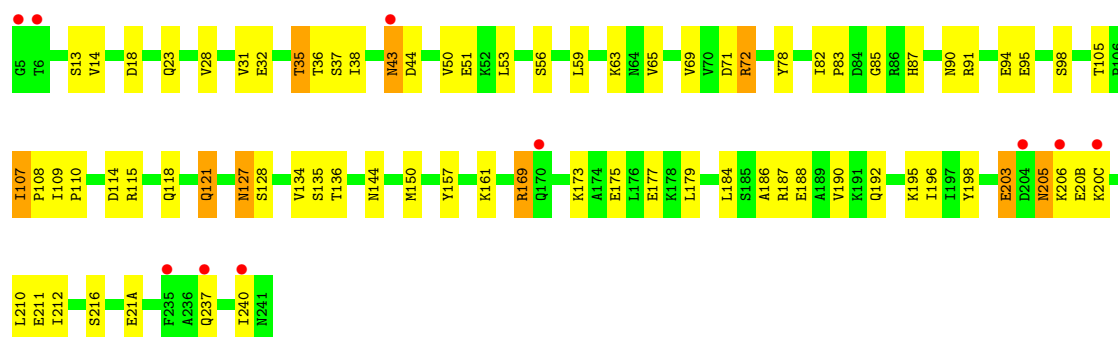


• Molecule 5: PRE5 isoform 1

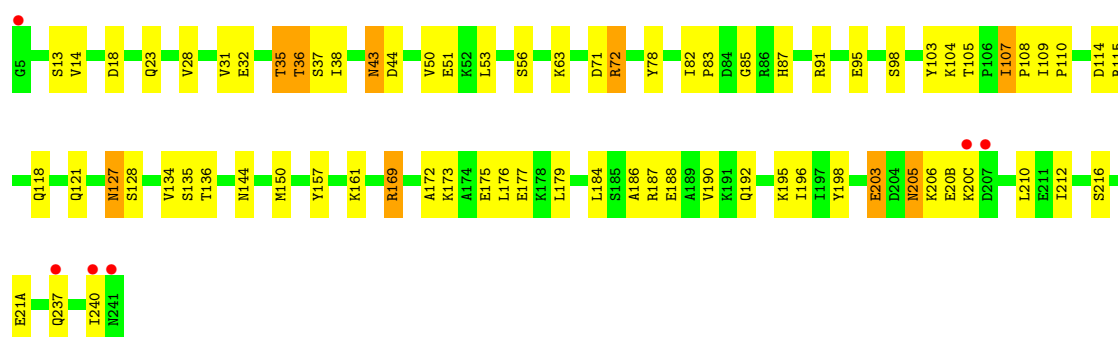




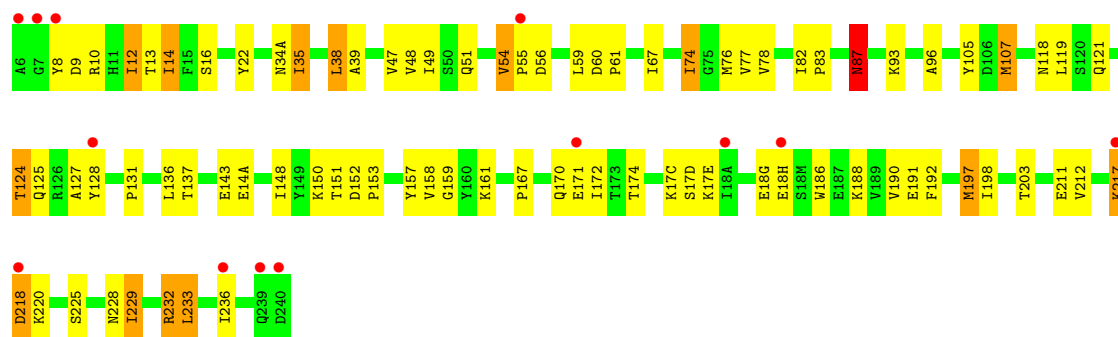
• Molecule 6: PRE10 isoform 1



• Molecule 6: PRE10 isoform 1

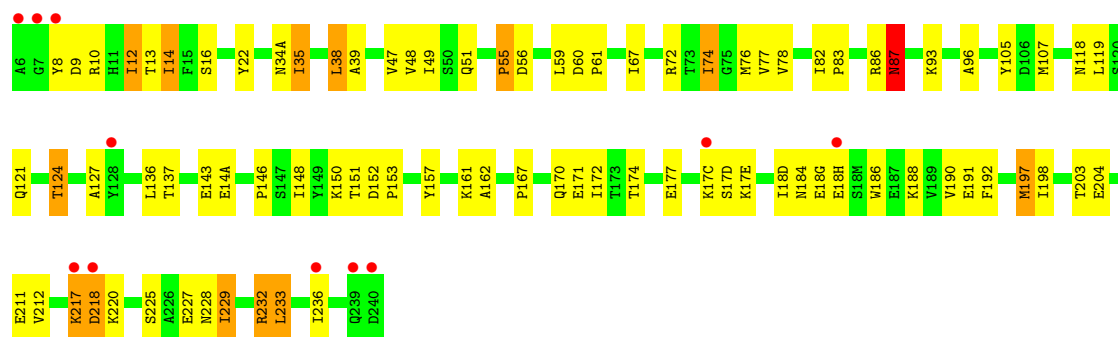


• Molecule 7: SCL1 isoform 1



• Molecule 7: SCL1 isoform 1

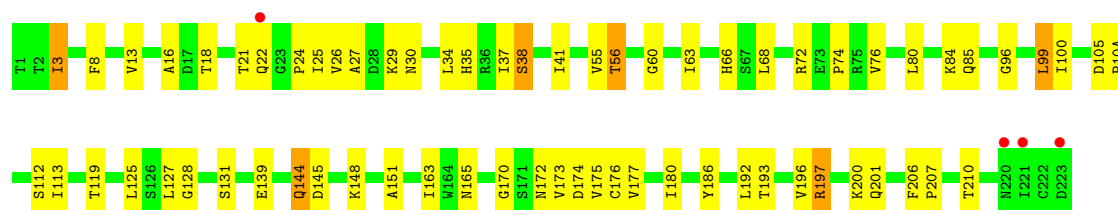




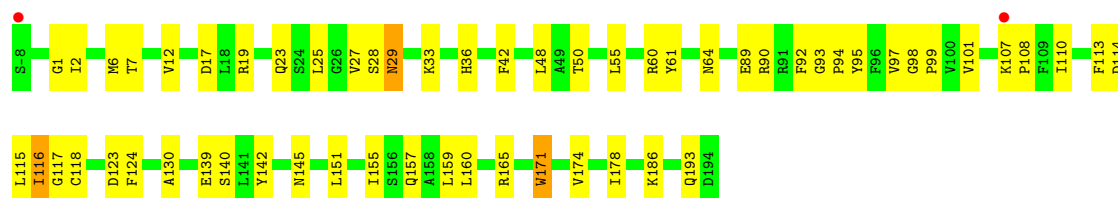
• Molecule 8: proteasome endopeptidase complex



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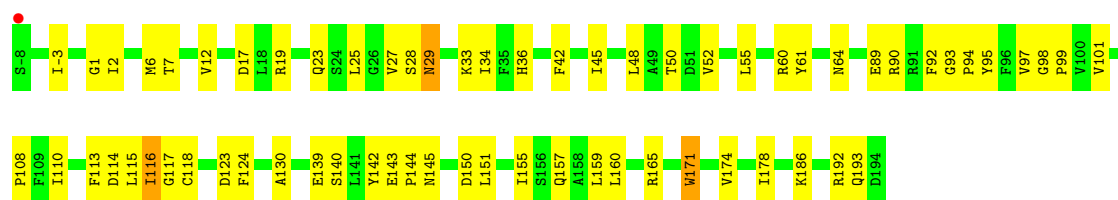


• Molecule 9: PUP3 isoform 1

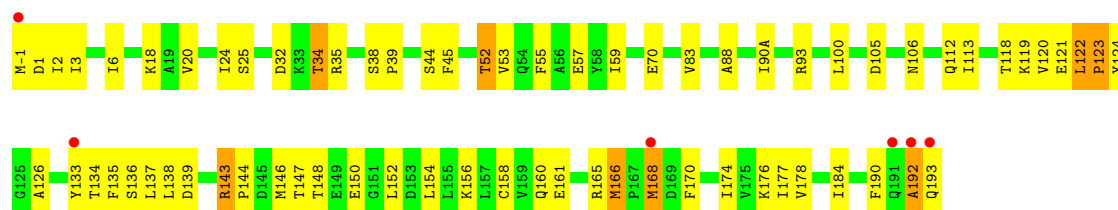


• Molecule 9: PUP3 isoform 1

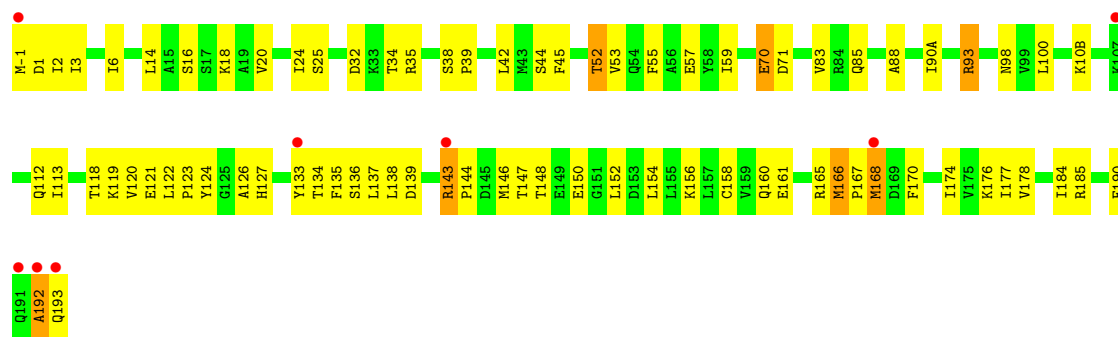




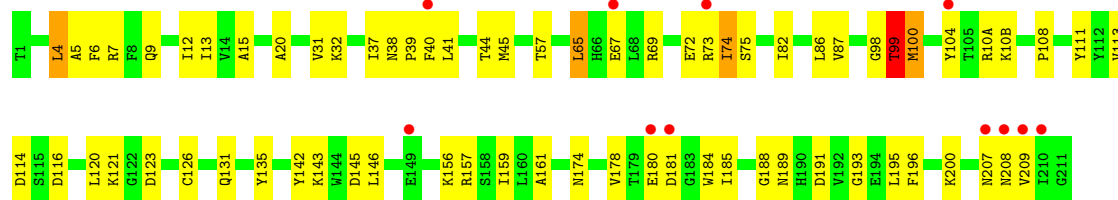
• Molecule 10: Proteasome subunit beta



• Molecule 10: Proteasome subunit beta



• Molecule 11: proteasome endopeptidase complex

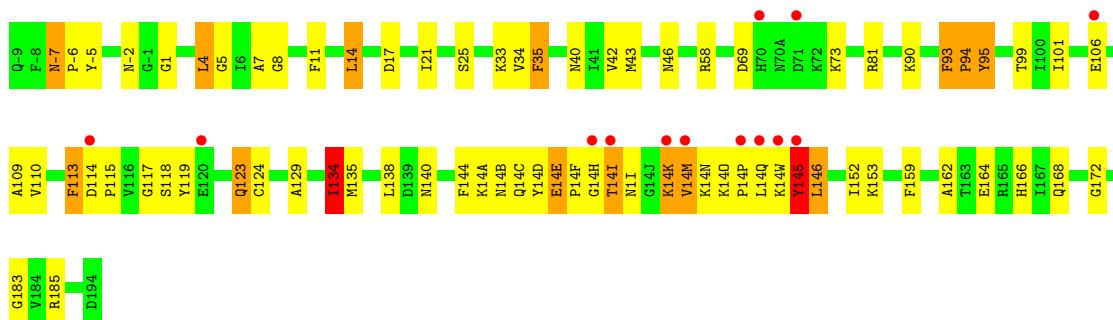


• Molecule 11: proteasome endopeptidase complex

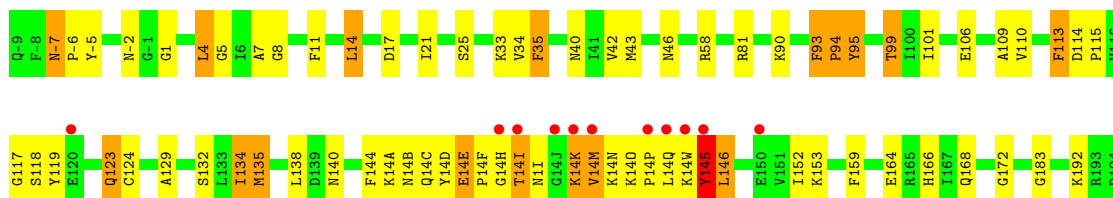




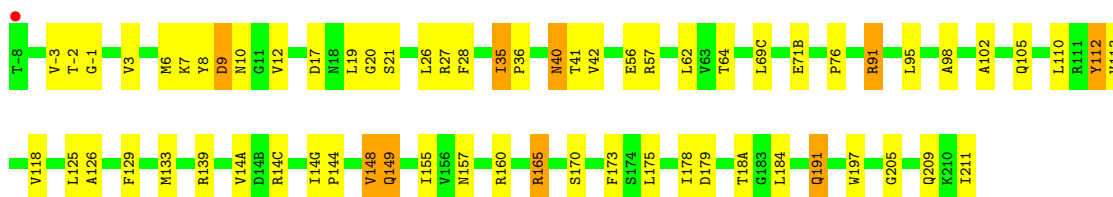
- Molecule 12: PRE7 isoform 1



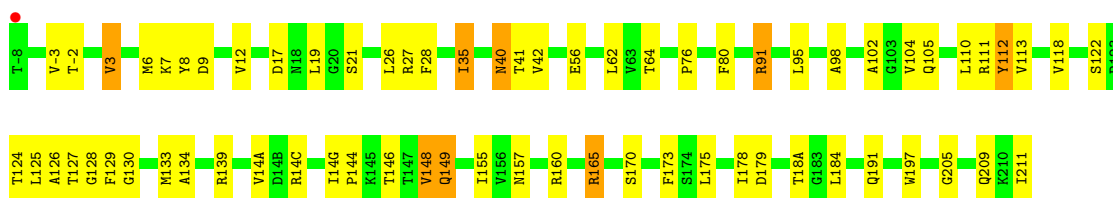
- Molecule 12: PRE7 isoform 1



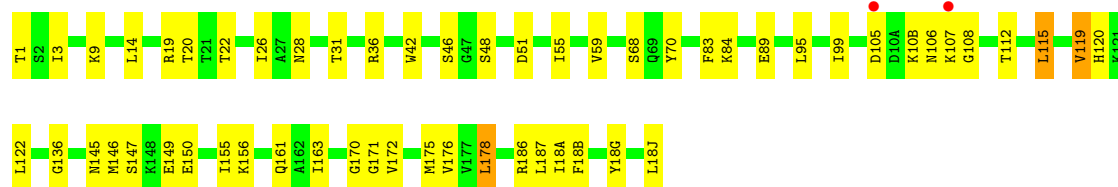
- Molecule 13: Proteasome subunit beta



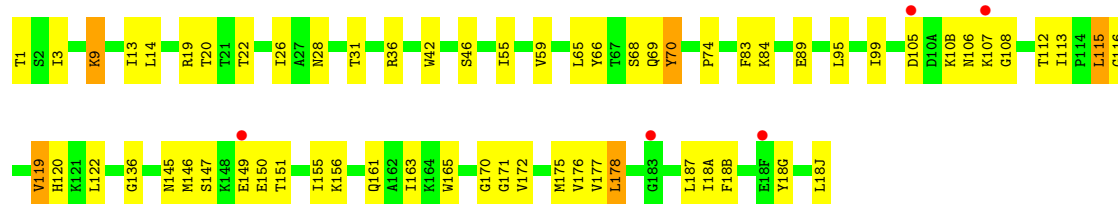
- Molecule 13: Proteasome subunit beta



- Molecule 14: Proteasome subunit beta type-1



• Molecule 14: Proteasome subunit beta type-1



• Molecule 15: Fellutamide B



• Molecule 15: Fellutamide B



• Molecule 15: Fellutamide B



• Molecule 15: Fellutamide B



• Molecule 15: Fellutamide B



• Molecule 15: Fellutamide B



4 Data and refinement statistics

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 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (15.00-2.60) 97.7 (15.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.56Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.266 0.239 , 0.264	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)	0.37 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.44	0/1952	0.91	2/2642 (0.1%)
1	O	0.41	0/1952	0.92	2/2642 (0.1%)
2	B	0.42	0/1935	0.92	9/2618 (0.3%)
2	P	0.43	0/1935	0.91	8/2618 (0.3%)
3	C	0.41	0/1920	0.90	7/2598 (0.3%)
3	Q	0.40	0/1920	0.90	6/2598 (0.2%)
4	D	0.41	0/1887	0.88	8/2541 (0.3%)
4	R	0.41	0/1887	0.88	7/2541 (0.3%)
5	E	0.42	0/1823	0.93	6/2463 (0.2%)
5	S	0.42	0/1823	0.93	6/2463 (0.2%)
6	F	0.44	0/1937	0.94	7/2614 (0.3%)
6	T	0.45	0/1937	0.95	7/2614 (0.3%)
7	G	0.49	1/1959 (0.1%)	0.97	11/2652 (0.4%)
7	U	0.47	0/1959	0.96	9/2652 (0.3%)
8	H	0.47	0/1716	0.94	4/2326 (0.2%)
8	V	0.45	0/1716	0.94	4/2326 (0.2%)
9	I	0.45	0/1611	1.05	15/2174 (0.7%)
9	W	0.46	0/1611	1.05	14/2174 (0.6%)
10	J	0.47	0/1613	0.99	9/2173 (0.4%)
10	X	0.46	0/1613	1.00	10/2173 (0.5%)
11	K	0.47	0/1681	0.97	7/2274 (0.3%)
11	Y	0.47	0/1681	0.98	6/2274 (0.3%)
12	L	0.47	0/1795	1.05	14/2420 (0.6%)
12	Z	0.46	1/1795 (0.1%)	1.04	13/2420 (0.5%)
13	1	0.47	0/1855	0.96	8/2514 (0.3%)
13	M	0.47	0/1855	0.95	7/2514 (0.3%)
14	2	0.48	0/1541	0.96	5/2087 (0.2%)
14	N	0.49	0/1541	0.98	4/2087 (0.2%)
15	a	2.24	1/24 (4.2%)	1.75	0/30
15	b	2.41	1/24 (4.2%)	1.56	0/30
15	c	2.70	2/24 (8.3%)	2.01	0/30
15	d	2.16	1/24 (4.2%)	1.74	0/30

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
15	e	2.33	1/24 (4.2%)	1.53	0/30
15	f	2.75	2/24 (8.3%)	2.05	0/30
All	All	0.47	10/50594 (0.0%)	0.96	215/68372 (0.3%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	b	3	LEU	C-OXT	9.92	1.43	1.23
15	f	3	LEU	C-OXT	9.67	1.42	1.23
15	e	3	LEU	C-OXT	9.39	1.42	1.23
15	c	3	LEU	C-OXT	9.24	1.42	1.23
15	a	3	LEU	C-OXT	8.90	1.41	1.23
15	d	3	LEU	C-OXT	8.48	1.40	1.23
15	f	1	ASN	N-CA	6.24	1.58	1.46
15	c	1	ASN	N-CA	6.12	1.57	1.46
7	G	107	MET	SD-CE	-5.54	1.65	1.79
12	Z	135	MET	SD-CE	-5.37	1.66	1.79

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	27	ARG	N-CA-C	11.70	123.58	111.07
13	M	27	ARG	N-CA-C	11.41	123.28	111.07
11	Y	188	GLY	N-CA-C	9.44	124.58	112.68
12	L	93	PHE	CA-C-N	9.18	129.25	119.89
12	L	93	PHE	C-N-CA	9.18	129.25	119.89
12	Z	93	PHE	CA-C-N	9.03	129.09	119.89
12	Z	93	PHE	C-N-CA	9.03	129.09	119.89
6	F	107	ILE	N-CA-C	8.83	118.58	108.96
6	T	107	ILE	N-CA-C	8.47	118.19	108.96
9	W	142	TYR	N-CA-C	7.68	120.80	110.35
13	1	95	LEU	N-CA-C	-7.67	96.07	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	169	SER	N-CA-C	7.55	119.15	111.07
11	K	188	GLY	N-CA-C	7.55	124.69	112.61
3	Q	161	SER	N-CA-C	-7.49	103.14	111.82
13	M	95	LEU	N-CA-C	-7.44	96.43	108.41
9	I	142	TYR	N-CA-C	7.41	120.43	110.35
3	C	161	SER	N-CA-C	-7.40	103.24	111.82
7	U	161	LYS	N-CA-C	-7.38	102.62	111.69
4	R	169	SER	N-CA-C	7.32	118.90	111.07
7	G	161	LYS	N-CA-C	-7.28	102.74	111.69
5	E	57	GLU	N-CA-C	-7.19	104.07	112.92
6	T	161	LYS	N-CA-C	-7.19	102.46	112.45
1	O	161	LYS	N-CA-C	-7.18	102.47	112.45
5	S	57	GLU	N-CA-C	-7.11	104.18	112.92
10	X	166	MET	CA-C-N	7.08	126.33	118.97
10	X	166	MET	C-N-CA	7.08	126.33	118.97
12	L	134	ILE	N-CA-C	7.05	117.66	110.82
4	R	70	ILE	N-CA-C	-7.05	104.89	111.45
6	F	63	LYS	N-CA-C	6.99	121.94	113.41
1	A	161	LYS	N-CA-C	-6.98	102.74	112.45
10	J	166	MET	CA-C-N	6.94	126.19	118.97
10	J	166	MET	C-N-CA	6.94	126.19	118.97
6	T	135	SER	N-CA-C	-6.94	98.09	109.40
6	T	63	LYS	N-CA-C	6.92	121.85	113.41
6	F	161	LYS	N-CA-C	-6.90	102.86	112.45
4	D	70	ILE	N-CA-C	-6.88	105.06	111.45
14	N	122	LEU	CA-C-N	6.83	126.43	119.19
14	N	122	LEU	C-N-CA	6.83	126.43	119.19
10	J	122	LEU	N-CA-C	6.82	116.16	108.25
2	B	238	ILE	N-CA-C	-6.82	106.66	113.20
12	Z	134	ILE	N-CA-C	6.76	117.38	110.82
9	W	117	GLY	N-CA-C	6.74	123.68	114.92
9	W	60	ARG	N-CA-C	-6.73	103.87	111.14
13	1	-2	THR	N-CA-C	6.73	120.13	109.50
9	I	117	GLY	N-CA-C	6.70	123.63	114.92
2	P	16	SER	N-CA-C	-6.61	102.53	110.13
6	F	135	SER	N-CA-C	-6.59	98.66	109.40
13	M	-2	THR	N-CA-C	6.58	119.90	109.50
6	T	14	VAL	N-CA-C	6.58	117.57	108.89
14	N	99	ILE	N-CA-C	6.55	117.92	108.48
7	U	16	SER	N-CA-C	-6.55	101.82	110.40
7	G	13	THR	N-CA-C	6.55	120.85	110.70
10	X	122	LEU	N-CA-C	6.54	115.84	108.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	16	SER	N-CA-C	-6.53	101.84	110.40
14	2	99	ILE	N-CA-C	6.53	117.88	108.48
2	B	16	SER	N-CA-C	-6.52	102.63	110.13
2	P	161	LYS	N-CA-C	-6.47	103.46	112.45
2	B	137	ILE	N-CA-C	-6.46	98.32	107.75
2	B	161	LYS	N-CA-C	-6.38	103.58	112.45
13	M	98	ALA	N-CA-C	-6.35	98.54	108.90
5	E	152	GLN	CA-C-N	6.31	126.00	119.82
5	E	152	GLN	C-N-CA	6.31	126.00	119.82
5	E	161	TYR	N-CA-C	-6.25	104.72	112.90
3	C	70	ILE	N-CA-C	-6.22	104.99	111.58
7	U	13	THR	N-CA-C	6.20	120.31	110.70
10	X	165	ARG	N-CA-C	6.20	120.97	113.41
12	L	117	GLY	N-CA-C	6.19	123.30	114.64
3	Q	70	ILE	N-CA-C	-6.17	105.04	111.58
12	L	115	PRO	N-CA-C	-6.16	106.16	113.86
9	I	60	ARG	N-CA-C	-6.16	104.49	111.14
9	W	95	TYR	N-CA-C	-6.12	100.53	110.20
1	A	185	GLU	N-CA-C	-6.11	101.73	110.59
12	Z	35	PHE	N-CA-C	6.09	119.12	109.50
12	Z	115	PRO	N-CA-C	-6.08	106.26	113.86
1	O	185	GLU	N-CA-C	-6.07	101.78	110.59
13	1	98	ALA	N-CA-C	-6.07	99.01	108.90
12	L	35	PHE	N-CA-C	6.04	119.05	109.50
7	G	127	ALA	N-CA-C	6.03	117.94	111.36
4	D	128	MET	N-CA-C	-6.03	97.96	110.80
3	C	108	THR	N-CA-C	-6.02	101.61	110.52
4	R	128	MET	N-CA-C	-6.02	97.99	110.80
10	J	165	ARG	N-CA-C	6.00	120.73	113.41
7	U	218	ASP	N-CA-C	5.94	119.84	112.24
14	N	115	LEU	N-CA-C	5.93	118.23	111.11
12	Z	117	GLY	N-CA-C	5.92	122.93	114.64
2	P	137	ILE	N-CA-C	-5.91	99.13	107.75
5	S	152	GLN	CA-C-N	5.88	125.59	119.82
5	S	152	GLN	C-N-CA	5.88	125.59	119.82
7	U	127	ALA	N-CA-C	5.86	117.75	111.36
14	2	122	LEU	CA-C-N	5.86	125.40	119.19
14	2	122	LEU	C-N-CA	5.86	125.40	119.19
4	R	161	ASN	N-CA-C	-5.83	104.89	112.23
7	G	218	ASP	N-CA-C	5.82	119.69	112.24
14	2	115	LEU	N-CA-C	5.79	118.06	111.11
12	L	94	PRO	N-CA-C	5.79	120.31	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	14	VAL	N-CA-C	5.77	117.06	109.21
9	W	23	GLN	CB-CA-C	-5.77	109.39	117.23
4	D	161	ASN	N-CA-C	-5.77	104.96	112.23
9	I	23	GLN	CB-CA-C	-5.73	109.44	117.23
13	1	9	ASP	N-CA-C	5.71	117.51	111.28
12	Z	94	PRO	N-CA-C	5.70	120.18	111.11
12	Z	129	ALA	N-CA-C	5.68	117.93	111.11
11	K	45	MET	N-CA-C	5.67	118.14	108.90
8	V	38	SER	N-CA-C	-5.66	103.03	108.07
9	W	93	GLY	CA-C-N	5.66	125.98	119.92
9	W	93	GLY	C-N-CA	5.66	125.98	119.92
9	I	145	ASN	N-CA-C	5.66	119.23	111.54
12	Z	145	TYR	CA-CB-CG	-5.65	103.73	113.90
12	L	145	TYR	CA-CB-CG	-5.65	103.73	113.90
12	L	129	ALA	N-CA-C	5.63	117.87	111.11
12	L	146	LEU	N-CA-C	5.63	118.61	110.28
9	I	178	ILE	N-CA-C	5.61	116.03	108.17
12	L	95	TYR	N-CA-C	-5.60	100.67	109.25
12	L	113	PHE	N-CA-C	5.60	118.20	109.52
6	F	38	ILE	N-CA-C	5.59	116.76	108.65
10	X	93	ARG	CA-C-N	5.59	125.54	119.78
10	X	93	ARG	C-N-CA	5.59	125.54	119.78
6	T	38	ILE	N-CA-C	5.59	116.75	108.65
10	X	134	THR	N-CA-C	5.58	119.27	112.23
13	M	165	ARG	N-CA-C	5.58	120.97	113.72
3	Q	108	THR	N-CA-C	-5.57	101.46	110.32
9	W	145	ASN	N-CA-C	5.55	119.08	111.54
9	I	95	TYR	N-CA-C	-5.54	101.45	110.20
4	R	63	SER	N-CA-C	-5.51	106.15	112.92
12	Z	146	LEU	N-CA-C	5.50	118.41	110.28
5	S	161	TYR	N-CA-C	-5.49	105.71	112.90
5	S	102	VAL	N-CA-C	5.49	116.98	111.00
5	S	154	SER	N-CA-C	-5.49	106.54	113.18
11	K	131	GLN	N-CA-C	5.48	117.69	111.11
12	Z	95	TYR	N-CA-C	-5.47	100.87	109.25
11	K	98	GLY	N-CA-C	-5.47	100.21	113.18
2	B	107	ILE	N-CA-C	5.47	114.31	108.95
13	1	165	ARG	N-CA-C	5.47	120.83	113.72
11	Y	45	MET	N-CA-C	5.46	117.98	108.76
11	Y	98	GLY	N-CA-C	-5.46	100.25	113.18
9	W	178	ILE	N-CA-C	5.45	115.70	107.80
8	V	99	LEU	N-CA-C	5.44	117.46	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	72	ASP	N-CA-C	-5.43	106.50	113.23
2	P	109	VAL	N-CA-C	5.43	116.06	110.36
9	I	94	PRO	N-CA-C	5.43	119.75	111.34
8	H	99	LEU	N-CA-C	5.42	117.43	109.24
13	M	9	ASP	N-CA-C	5.42	117.19	111.28
6	F	71	ASP	CB-CA-C	-5.42	110.35	116.63
9	W	25	LEU	N-CA-C	5.42	116.95	109.15
3	Q	135	SER	N-CA-C	-5.40	100.60	109.40
13	1	35	ILE	N-CA-C	5.40	113.37	107.60
13	M	35	ILE	N-CA-C	5.38	113.36	107.60
3	Q	22	PHE	N-CA-C	5.38	117.84	111.33
9	I	114	ASP	N-CA-C	-5.38	102.03	110.36
13	1	3	VAL	N-CA-C	-5.37	99.78	107.78
4	R	179	GLU	N-CA-C	5.34	117.10	111.28
9	I	25	LEU	N-CA-C	5.34	116.84	109.15
3	C	135	SER	N-CA-C	-5.33	100.71	109.40
9	I	98	GLY	CA-C-N	5.33	125.27	119.78
9	I	98	GLY	C-N-CA	5.33	125.27	119.78
8	H	38	SER	N-CA-C	-5.32	103.33	108.07
12	L	69	ASP	N-CA-C	5.32	117.83	111.71
11	Y	57	THR	N-CA-C	-5.32	105.48	111.28
11	K	57	THR	N-CA-C	-5.31	105.49	111.28
5	E	102	VAL	N-CA-C	5.31	116.79	111.00
3	C	22	PHE	N-CA-C	5.31	117.75	111.33
10	X	25	SER	N-CA-C	5.29	118.03	109.40
2	B	109	VAL	N-CA-C	5.28	115.91	110.36
2	B	163	ILE	N-CA-C	5.28	114.14	107.70
11	K	99	THR	N-CA-C	5.28	117.70	109.52
4	D	63	SER	N-CA-C	-5.28	106.43	112.92
4	D	82	THR	N-CA-C	5.27	118.49	111.75
9	W	94	PRO	N-CA-C	5.27	119.50	111.34
10	J	25	SER	N-CA-C	5.26	117.98	109.40
11	Y	99	THR	N-CA-C	5.25	117.66	109.52
4	R	82	THR	N-CA-C	5.25	118.47	111.75
7	U	74	ILE	N-CA-C	5.25	115.86	108.36
10	X	143	ARG	CA-C-N	5.25	124.87	119.05
10	X	143	ARG	C-N-CA	5.25	124.87	119.05
11	K	145	ASP	N-CA-C	5.24	119.38	112.25
9	W	114	ASP	N-CA-C	-5.24	102.24	110.36
10	J	134	THR	N-CA-C	5.24	118.83	112.23
2	P	78	VAL	N-CA-C	5.23	116.11	108.53
2	P	107	ILE	N-CA-C	5.23	114.08	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	180	ILE	N-CA-C	5.22	120.21	109.34
2	B	72	ASP	N-CA-C	-5.22	106.76	113.23
8	H	21	THR	N-CA-C	5.21	117.10	109.24
8	V	180	ILE	N-CA-C	5.20	120.17	109.34
14	2	9	LYS	N-CA-C	5.20	117.35	111.11
7	G	87	ASN	N-CA-C	-5.20	105.50	111.07
4	D	16	SER	N-CA-C	-5.18	104.17	110.13
12	Z	113	PHE	N-CA-C	5.18	117.54	109.52
10	J	143	ARG	CA-C-N	5.14	124.76	119.05
10	J	143	ARG	C-N-CA	5.14	124.76	119.05
11	Y	145	ASP	N-CA-C	5.14	119.24	112.25
7	G	60	ASP	CA-C-N	5.13	125.42	119.47
7	G	60	ASP	C-N-CA	5.13	125.42	119.47
7	U	60	ASP	CA-C-N	5.13	125.42	119.47
7	U	60	ASP	C-N-CA	5.13	125.42	119.47
5	E	154	SER	N-CA-C	-5.12	106.99	113.18
9	I	93	GLY	CA-C-N	5.11	125.39	119.92
9	I	93	GLY	C-N-CA	5.11	125.39	119.92
3	Q	134	VAL	N-CA-C	5.11	115.09	108.35
7	G	74	ILE	N-CA-C	5.11	115.66	108.36
8	V	21	THR	N-CA-C	5.10	116.94	109.24
2	P	163	ILE	N-CA-C	5.08	113.90	107.70
7	U	87	ASN	N-CA-C	-5.08	105.63	111.07
12	L	145	TYR	N-CA-C	5.08	117.68	109.40
6	T	71	ASP	CB-CA-C	-5.07	110.75	116.63
4	D	179	GLU	N-CA-C	5.06	116.80	111.28
7	G	54	VAL	CA-C-N	5.05	126.15	119.84
7	G	54	VAL	C-N-CA	5.05	126.15	119.84
10	J	123	PRO	N-CA-C	-5.03	106.98	113.57
9	W	98	GLY	CA-C-N	5.03	124.96	119.78
9	W	98	GLY	C-N-CA	5.03	124.96	119.78
9	I	27	VAL	N-CA-C	5.02	115.88	111.56
12	Z	145	TYR	N-CA-C	5.02	117.58	109.40
2	B	78	VAL	N-CA-C	5.02	115.80	108.53
3	C	16	SER	CA-C-N	5.00	126.09	119.84
3	C	16	SER	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	145	TYR	Sidechain

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Mol	Chain	Res	Type	Group
12	Z	145	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	62	0
1	O	1915	0	1926	62	0
2	B	1905	0	1901	104	0
2	P	1905	0	1901	97	0
3	C	1891	0	1900	109	0
3	Q	1891	0	1900	107	0
4	D	1862	0	1836	53	0
4	R	1862	0	1836	58	0
5	E	1795	0	1797	75	0
5	S	1795	0	1797	72	0
6	F	1897	0	1886	62	0
6	T	1897	0	1886	56	0
7	G	1921	0	1910	83	0
7	U	1921	0	1910	88	0
8	H	1685	0	1687	63	0
8	V	1685	0	1687	55	0
9	I	1581	0	1574	49	0
9	W	1581	0	1574	51	0
10	J	1585	0	1590	66	0
10	X	1585	0	1590	68	0
11	K	1644	0	1594	71	0
11	Y	1644	0	1594	74	0
12	L	1757	0	1711	52	0
12	Z	1757	0	1711	50	0
13	1	1824	0	1832	53	0
13	M	1824	0	1832	54	0
14	2	1512	0	1480	58	0
14	N	1512	0	1480	51	0
15	a	25	0	24	0	0
15	b	25	0	24	0	0
15	c	25	0	25	7	0
15	d	25	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	e	25	0	25	0	0
15	f	25	0	25	6	0
16	a	14	0	23	3	0
16	b	14	0	23	0	0
16	c	14	0	23	1	0
16	d	14	0	23	3	0
16	e	14	0	23	0	0
16	f	14	0	23	1	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	2	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	4	0
17	K	42	0	0	6	0
17	L	56	0	0	5	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	1729	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 (1729) 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
10:J:168:MET:HE3	10:X:168:MET:HE3	1.33	1.08
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
7:U:96:ALA:HA	7:U:107:MET:HE2	1.43	0.96
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:G:96:ALA:HA	7:G: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:123:GLN:HG3	12:L:145:TYR:OH	1.67	0.91
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:175:GLU:HG2	4:D:196:ILE:CD1	2.10	0.82
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
7:G:172:ILE:HD13	7:G:197:MET:HE1	1.61	0.81
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
7:U:172:ILE:HD13	7:U:197:MET:HE1	1.67	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
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.00	0.76
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
11:K:67:GLU:CD	11:K:73:ARG:HA	2.10	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:18(D):ILE:O	5:S:18(D):ILE:HD13	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
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
11:Y:67:GLU:CD	11:Y:73:ARG:HA	2.11	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
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O	5:E:18(D):ILE:HD13	1.89	0.72
7:U:217:LYS:HA	7:U:217:LYS:HE3	1.70	0.72
8:V:41:ILE:HD12	8:V:76:VAL:HG22	1.72	0.72
15:c:2:GLN:HG3	16:c:4:HXD:H91	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:HA	7:G:217:LYS:HE3	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
15:f:2:GLN:HG3	16:f:4:HXD:H91	1.71	0.71
7:G:87:ASN:C	7:G:87:ASN:HD22	1.98	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
7:U:87:ASN:C	7:U:87:ASN:HD22	1.99	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
5:S:227:GLU:H	5:S:227:GLU:CD	1.98	0.71
14:N:22:THR:HG22	15:c:1:ASN:ND2	2.06	0.70
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
14:2:22:THR:HG22	15:f:1:ASN:ND2	2.06	0.70
3:C:185:THR:HG22	3:C:187:GLU:N	2.05	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
3:C:41:LYS:HG2	3:C:161:SER:O	1.91	0.69
5:E:227:GLU:H	5:E:227:GLU:CD	1.98	0.69
5:E:207:LEU:H	5:E:207:LEU:CD2	2.06	0.69
13:1:7:LYS:HG3	13:1:14(G):ILE:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB3	1:O:179:ARG:HH11	1.56	0.68
2:B:15:PHE:H	3:C:23:GLN:NE2	1.88	0.68
14:2:22:THR:CG2	15:f:1:ASN:ND2	2.57	0.68
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.92	0.68
9:W:29:ASN:ND2	9:W:29:ASN:H	1.90	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:HB3	1:A:179:ARG:HH11	1.57	0.68
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
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.76	0.67
14:2:20:THR:HG22	15:f:3:LEU:HD23	1.75	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
14:N:22:THR:CG2	15:c:1:ASN:ND2	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	8:H:3:ILE:HD13	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:HD11	1.76	0.66
9:W:2:ILE:HD13	9:W:159:LEU:CD1	2.26	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
13:M:40:ASN:HD22	13:M:40:ASN:H	1.43	0.65
9:I:29:ASN:ND2	9:I:29:ASN:H	1.93	0.65
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
4:D:112:LEU:C	4:D:112:LEU:HD13	2.21	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
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
2:P:41:MET:HE3	17:P:244:HOH:O	1.96	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
14:N:20:THR:HG22	15:c:3:LEU:HD23	1.77	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
9:W:6:MET:HE1	9:W:155:ILE:HA	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
12:Z:-7:ASN:C	12:Z:-7:ASN:HD22	2.07	0.63
3:C:41:LYS:HD3	3:C:161:SER:HA	1.80	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
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
5:E:227:GLU:CD	5:E:227:GLU:N	2.57	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
5:S:227:GLU:CD	5:S:227:GLU:N	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:R:112:LEU:HD13	4:R:112:LEU:C	2.25	0.62
5:S:207:LEU:HD23	5:S:207:LEU:N	2.14	0.62
14:2:155:ILE:HG22	14:2:175:MET:HE2	1.82	0.62
4:D:192:LEU:O	4:D:196:ILE:HG12	2.00	0.62
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.62	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
15:f:1:ASN:HD22	15:f:1:ASN:N	1.98	0.61
7:G:172:ILE:CD1	7:G:197:MET:HE1	2.29	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
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.81	0.61
15:c:1:ASN:HD22	15:c:1:ASN:N	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:J:146:MET:CE	10:J:150:GLU:HB3	2.31	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
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
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
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
1:O:57:PRO:HG3	7:U:177:GLU:CD	2.26	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:HH11	8:H:72:ARG:HG3	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
7:U:172:ILE:CD1	7:U:197:MET:HE1	2.33	0.59
10:X:147:THR:OG1	10:X:150:GLU:HG3	2.00	0.59
12:L:-7:ASN:HD22	12:L:-7:ASN:C	2.10	0.59
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	13:1:14(C):ARG:HG3	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:OE1	3:Q:227:GLU:N	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
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
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:69:LEU:HD23	1:A:69:LEU:C	2.28	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
1:O:69:LEU:C	1:O:69:LEU:HD23	2.29	0.58
13:1:149:GLN:NE2	13:1:149:GLN:H	2.02	0.58
2:B:234:VAL:HA	2:B:239:THR:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
10:X:190:PHE:C	10:X:192:ALA:H	2.12	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
7:U:87:ASN:C	7:U:87:ASN:ND2	2.61	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:OE1	3:C:227:GLU:N	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
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:HH11	1:O:232:ARG:HG3	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
3:C:241:GLN:C	3:C:243:GLN:H	2.13	0.57
12:L:123:GLN:CG	12:L:145:TYR:OH	2.47	0.57
7:U:8:TYR:C	7:U:10:ARG:H	2.13	0.57
2:P:234:VAL:HA	2:P:239:THR:HA	1.85	0.57
3:Q:241:GLN:C	3:Q:243:GLN:H	2.13	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
14:2:22:THR:HG22	15:f:1:ASN:HD22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:41:MET:HE3	17:B:240:HOH:O	2.03	0.57
4:D:122:ARG:HG2	4:D:122:ARG:HH11	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
14:2:107:LYS:HG2	14:2:108:GLY:N	2.19	0.57
7:G:38:LEU:C	7:G:38:LEU:HD12	2.30	0.56
10:J:93:ARG:HG2	10:J:93:ARG:HH11	1.71	0.56
13:M:184:LEU:HD23	13:M:184:LEU:C	2.30	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
5:E:35:SER:HB3	5:E:66:LYS:HZ3	1.70	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
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:HH11	8:V:72:ARG:HG3	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
14:N:155:ILE:HG22	14:N:175:MET:HE2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:W:115:LEU:HD21	16:d:4:HxD:H42	1.88	0.56
10:X:146:MET:HE3	10:X:150:GLU:HB3	1.88	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
14:N:22:THR:HG22	15:c:1:ASN:HD22	1.70	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
7:G:8:TYR:C	7:G:10:ARG:H	2.12	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:HD12	1:A:21(L):ILE:N	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
10:J:168:MET:CE	10:X:168:MET:HE3	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:115:LEU:HD21	16:a:4:HxD:H42	1.89	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
7:G:87:ASN:C	7:G:87:ASN:ND2	2.61	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
7:U:38:LEU:C	7:U:38:LEU:HD12	2.32	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
13:1:184:LEU:C	13:1:184:LEU:HD23	2.31	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
11:K:142:TYR:C	11:K:143:LYS:HD2	2.31	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
3:C:211:GLU:C	3:C:212:ILE:HD12	2.32	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:142:TYR:C	11:Y:143:LYS:HD2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.88	0.55
10:J:168:MET:HE3	10:X:168:MET:CE	2.24	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
10:J:146:MET:HE3	10:J:150:GLU:HB3	1.89	0.54
11:K:4:LEU:HD22	11:K:4:LEU:C	2.32	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:HD12	2:B:223:ILE:N	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
11:K:44:THR:HG1	11:K:100:MET:HB2	1.71	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:127:ASN:HD22	6:F:127:ASN:C	2.15	0.54
10:J:190:PHE:C	10:J:192:ALA:H	2.13	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:HG22	2:P:239:THR:OXT	2.07	0.54
6:T:179:LEU:HD21	6:T:192:GLN:CG	2.36	0.54
11:Y:38:ASN:C	11:Y:38:ASN:OD1	2.50	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
4:R:207:LEU:HD23	4:R:207:LEU:C	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:34:ILE:HB	17:W:215:HOH:O	2.08	0.54
11:Y:38:ASN:CG	17:Y:258:HOH:O	2.49	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
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: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:HH11	5:E:86:ARG:HG3	1.72	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
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
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.23	0.53
11:K:86:LEU:HD13	11:K:86:LEU:C	2.34	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
11:K:38:ASN:C	11:K:38:ASN:OD1	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.90	0.53
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.74	0.53
11:Y:38:ASN:O	11:Y:40:PHE:N	2.42	0.53
13:1:133:MET:HE1	13:1:165:ARG:HG3	1.90	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
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
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.34	0.53
6:F:20(B):GLU:CD	6:F:20(C):LYS:HE3	2.33	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
6:T:20(B):GLU:CD	6:T:20(C):LYS:HE3	2.33	0.53
8:V:35:HIS:CB	8:V:56:THR:HG21	2.39	0.53
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.34	0.53
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	1.91	0.53
4:D:170:GLU:N	4:D:170:GLU:OE1	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:14:ILE:C	3:Q:14:ILE:HD12	2.33	0.53
3:Q:182:PRO:O	3:Q:184:ALA:N	2.42	0.53
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.23	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
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
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:OE1	4:R:170:GLU:N	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:HA	4:D:205:GLU:OE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:207:LEU:C	4:D:207:LEU:HD23	2.33	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
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
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
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.66	0.52
2:B:21(A):LYS:HE2	2:B:21(D):GLY:O	2.10	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: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
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
6:T:127:ASN:HD22	6:T:127:ASN:C	2.17	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
3:C:14:ILE:HD12	3:C:14:ILE:C	2.35	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:6:MET:HE3	9:W:155:ILE:HG13	1.91	0.52
9:W:19:ARG:HB2	9:W:171:TRP:HB2	1.92	0.52
7:G:14:ILE:H	7:G:14:ILE:HD13	1.74	0.51
1:O:121:GLN:O	1:O:124:THR:HB	2.10	0.51
3:Q:211:GLU:C	3:Q:212:ILE:HD12	2.34	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
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:R:205:GLU:HA	4:R:205:GLU:OE2	2.09	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
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.40	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
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
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
9:W:92:PHE:HD2	16:d:4:HXD:H122	1.76	0.51
1:A:33:GLN:HA	1:A:33:GLN:HE21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:O:206:PHE:CD1	1:O:210:ILE:HD11	2.46	0.50
7:U:76:MET:HE3	7:U:78:VAL:CG2	2.41	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
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
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
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
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
6:F:203:GLU:C	6:F:205:ASN:H	2.19	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
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:T:203:GLU:C	6:T:205:ASN:H	2.19	0.50
10:X:143:ARG:HB2	10:X:146:MET:HG3	1.94	0.50
11:Y:44:THR:HG1	11:Y:100:MET:HB2	1.74	0.50
11:Y:157:ARG:HH11	11:Y:157:ARG:HG3	1.76	0.50
6:F:69:VAL:HG12	17:F:248:HOH:O	2.11	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: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
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.67	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
13:M:133:MET:HE1	13:M:165:ARG:HG3	1.92	0.49
10:X:2:ILE:HD13	10:X:170:PHE:CG	2.47	0.49
1:A:38:LEU:C	1:A:38:LEU:HD12	2.37	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
12:L:73:LYS:NZ	17:L:231:HOH:O	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:146:MET:HE2	14:N:150:GLU:HB3	1.95	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
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:33:ARG:HB2	3:Q:33:ARG:NH1	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:HG2	5:S:111:ARG:HH11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:Y:208:ASN:O	11:Y:209:VAL:C	2.56	0.48
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.81	0.48
2:B:112:LEU:HD23	2:B:112:LEU:C	2.39	0.48
2:B:238:ILE:O	2:B:239:THR:O	2.31	0.48
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.49	0.48
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.39	0.48
10:J:45:PHE:CE1	10:J:52:THR:HG23	2.49	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
12:L:145:TYR:CD1	12:L:146:LEU:N	2.80	0.48
1:O:38:LEU:C	1:O:38:LEU:HD12	2.38	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
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
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
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
2:P:112:LEU:HD23	2:P:112:LEU:C	2.39	0.48
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.39	0.48
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.39	0.48
2:P:122:GLY:C	2:P:124:THR:H	2.22	0.48
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.35	0.48
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
7:G:8:TYR:C	7:G:10:ARG:N	2.73	0.47
11:K:184:TRP:C	11:K:185:ILE:HD13	2.38	0.47
11:K:208:ASN:O	11:K:209:VAL:C	2.57	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
2:P:184:MET:HE2	2:P:188:ASP:HB3	1.96	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
10:J:146:MET:HE2	10:J:150:GLU:HB3	1.97	0.47
3:Q:33:ARG:CB	3:Q:33:ARG:HH11	2.26	0.47
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:I:92:PHE:HD2	16:a:4:HXD:H122	1.80	0.47
12:L:114:ASP:HB2	12:L:118:SER:N	2.29	0.47
3:Q:76:LEU:C	3:Q:76:LEU:HD23	2.40	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
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
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
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: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
6:T:157:TYR:CD1	6:T:157:TYR:C	2.92	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
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
14:2:146:MET:HE2	14:2:150:GLU:HB3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:21:ILE:C	12:L:21:ILE:HD12	2.40	0.47
3:Q:228:GLU:O	3:Q:232:TYR:HD1	1.97	0.47
4:R:59:LEU:HD13	4:R:59:LEU:C	2.40	0.47
8:V:37:ILE:HG23	8:V:60:GLY:HA2	1.97	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
9:W:116:ILE:HD12	16:d:4:HXD:H41	1.96	0.47
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
3:C:76:LEU:HD23	3:C:76:LEU:C	2.40	0.46
8:H:175:VAL:HG12	8:H:176:CYS:N	2.31	0.46
10:J:190:PHE:C	10:J:192:ALA:N	2.74	0.46
13:M:14(A):VAL:HG23	13:M:14(A):VAL:O	2.14	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
7:U:18(H):GLU:CD	7:U:18(H):GLU:H	2.23	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
3:C:55:THR:C	3:C:56:LEU:HD22	2.41	0.46
12:L:17:ASP:OD2	12:L:33:LYS:NZ	2.48	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
12:Z:21:ILE:C	12:Z:21:ILE:HD12	2.41	0.46
1:A:212:LEU:HD23	1:A:212:LEU:C	2.41	0.46
3:C:16:SER:HB2	3:C:17:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:59:LEU:HD13	4:D:59:LEU:C	2.40	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
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.30	0.46
4:R:101:LEU:CD1	11:Y:57:THR:HG22	2.46	0.46
10:X:193:GLN:HG2	10:X:193:GLN:OXT	2.16	0.46
2:B:144:ARG:O	2:B:144:ARG:HG2	2.16	0.46
6:F:157:TYR:CD1	6:F:157:TYR:C	2.92	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
2:B:184:MET:HE2	2:B:188:ASP:HB3	1.96	0.46
5:E:194:VAL:HG13	5:E:207:LEU:HD11	1.98	0.46
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
2:P:63:THR:O	2:P:63:THR:HG22	2.16	0.46
7:U:192:PHE:CD1	7:U:192:PHE:C	2.93	0.46
1:A:13:THR:O	2:B:130:ARG:HD3	2.16	0.46
13:M:112:TYR:C	13:M:112:TYR:CD2	2.94	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
9:W:61:TYR:CD1	9:W:61:TYR:C	2.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:172:ILE:HD13	7:G:197:MET:CE	2.40	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
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
7:G:96:ALA:CA	7:G:107:MET:CE	2.89	0.45
7:G:192:PHE:C	7:G:192:PHE:CD1	2.94	0.45
2:P:176:LEU:C	2:P:178:MET:H	2.24	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: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
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
9:W:6:MET:CE	9:W:155:ILE:HA	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:T:205:ASN:C	6:T:20(B):GLU:H	2.25	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
4:R:42:THR:C	4:R:44:GLU:H	2.25	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
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
6:F:205:ASN:C	6:F:20(B):GLU:H	2.25	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
4:R:170:GLU:CD	4:R:170:GLU:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:10(B):LYS:HD3	14:2:10(B):LYS:C	2.42	0.45
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.32	0.44
2:B:141:TYR:CD1	2:B:141:TYR:C	2.95	0.44
4:D:152:GLU:C	4:D:154:SER:H	2.25	0.44
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	1.99	0.44
7:G:18(H):GLU:CD	7:G:18(H):GLU:H	2.25	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
12:Z:17:ASP:OD2	12:Z:33:LYS:NZ	2.51	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
1:A:236:LEU:C	1:A:236:LEU:HD13	2.43	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
2:P:184:MET:HE2	2:P:188:ASP:CB	2.48	0.44
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
2:B:122:GLY:C	2:B:124:THR:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:THR:O	2:B:63:THR:HG22	2.17	0.44
2:B:85:ALA:O	2:B:89:ILE:HG13	2.18	0.44
1:O:236:LEU:C	1:O:236:LEU:HD13	2.42	0.44
3:Q:241:GLN:C	3:Q:243:GLN:N	2.75	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:HG2	3:C:33:ARG:O	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
2:B:184:MET:HE2	2:B:188:ASP:CB	2.48	0.44
4:D:122:ARG:HG2	4:D:122:ARG:NH1	2.32	0.44
5:E:230:ALA:C	5:E:232:TYR:H	2.26	0.44
8:H:3:ILE:HD13	8:H:3:ILE:C	2.41	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
10:X:34:THR:HG21	10:X:176:LYS:HZ2	1.83	0.44
10:X:190:PHE:C	10:X:192:ALA:N	2.73	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
2:P:141:TYR:CD1	2:P:141:TYR:C	2.95	0.44
2:P:186:VAL:CB	2:P:216:ARG:HD3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.18	0.44
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
11:K:32:LYS:N	11:K:32:LYS:HD2	2.33	0.43
12:L:114:ASP:HB2	12:L:118:SER:H	1.83	0.43
13:M:175:LEU:HD23	13:M:175:LEU:C	2.43	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
9:I:116:ILE:HD12	16:a:4:HXD:H41	1.99	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
10:J:138:LEU:HD21	10:J:158:CYS:SG	2.59	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:N	11:Y:32:LYS:HD2	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
2:B:176:LEU:C	2:B:178:MET:H	2.26	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:HG2	3:Q:33:ARG:O	2.17	0.43
3:Q:58:LEU:HD12	3:Q:58:LEU:HA	1.76	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:194:VAL:O	3:C:198:LEU:HG	2.17	0.43
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.32	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
14:N:19:ARG:CZ	14:N:26:ILE:HD11	2.48	0.43
14:N:10(B):LYS:C	14:N:10(B):LYS:HD3	2.44	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
7:G:143:GLU:HA	7:G:217:LYS:HZ3	1.84	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
13:1:112:TYR:CD2	13:1:112:TYR:C	2.96	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
2:B:122:GLY:C	2:B:124:THR:N	2.77	0.43
4:D:170:GLU:H	4:D:170:GLU:CD	2.25	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:70:GLU:O	10:X:71:ASP:C	2.62	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
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
5:E:18(D):ILE:HD13	5:E:18(D):ILE:C	2.44	0.43
1:O:77:VAL:HG12	1:O:137:LEU:HB2	2.00	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
4:D:42:THR:C	4:D:44:GLU:H	2.26	0.42
6:F:31:VAL:HG22	6:F:134:VAL:HA	2.01	0.42
7:G:48:VAL:C	7:G:49:ILE:HD12	2.44	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
1:O:212:LEU:HD23	1:O:212:LEU:C	2.44	0.42
2:P:227:GLN:OE1	2:P:230:LYS:HD3	2.18	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:HD13	8:V:3:ILE:C	2.44	0.42
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:127:ASN:C	6:T:127:ASN:ND2	2.77	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
2:P:122:GLY:C	2:P:124:THR:N	2.76	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
11:Y:184:TRP:C	11:Y:185:ILE:HD13	2.44	0.42
13:1:175:LEU:HD23	13:1:175:LEU:C	2.45	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
13:M:12:VAL:CG2	13:M:102:ALA:HB1	2.48	0.42
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.20	0.42
1:O:221:PHE:CD2	1:O:221:PHE:C	2.97	0.42
5:S:230:ALA:C	5:S:232:TYR:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:57:LYS:HD2	3:C:57:LYS:C	2.45	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:HA	8:H:139:GLU:OE2	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
7:U:184:ASN:C	7:U:184:ASN:HD22	2.27	0.42
12:Z:14(I):THR:HB	12:Z:14(M):VAL:HG23	2.01	0.42
14:2:20:THR:HG1	14:2:28:ASN:HB3	1.84	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
6:F:127:ASN:C	6:F:127:ASN:ND2	2.76	0.42
8:H:206:PHE:CZ	9:I:157:GLN:HG3	2.55	0.42
9:I:61:TYR:CD1	9:I:61:TYR:C	2.98	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:U:197:MET:HA	7:U:197:MET:HE3	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:HG2	11:K:10(A):ARG:HH11	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
8:V:18:THR:HB	8:V:30:ASN:HD22	1.85	0.42
10:X:146:MET:HE2	10:X:150:GLU:HB3	1.99	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
14:2:107:LYS:HZ2	14:2:145:ASN:HD21	1.67	0.42
2:B:186:VAL:CB	2:B:216:ARG:HD3	2.50	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
13:M:14(G):ILE:HB	13:M:144:PRO:HD3	2.02	0.42

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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
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
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:113:PHE:CD2	12:Z:119:TYR:HB3	2.55	0.41
1:A:221:PHE:CD2	1:A:221:PHE:C	2.98	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:121:GLN:NE2	2:P:121:GLN:C	2.79	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
7:U:143:GLU:HA	7:U:217:LYS:HZ3	1.85	0.41
7:U:18(H):GLU:CD	7:U:18(H):GLU:N	2.79	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
3:Q:43:LYS:O	3:Q:43:LYS:HG2	2.19	0.41
4:R:85:ALA:O	4:R:89:ILE:CG1	2.68	0.41
5:S:18(D):ILE:HD13	5:S:18(D):ILE:C	2.43	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
3:C:241:GLN:C	3:C:243:GLN:N	2.75	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
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
1:A:62:GLU:CD	1:A:62:GLU:H	2.29	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
2:P:40:ILE:HD12	2:P:193:ALA:HB2	2.02	0.41
2:P:225:LYS:N	2:P:228:GLU:OE1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:P:39:GLY:C	2:P:148:LEU:HD21	2.46	0.41
3:Q:111:TYR:CD2	3:Q:111:TYR:C	2.99	0.41
3:Q:125:GLN:NE2	17:R:263:HOH:O	2.54	0.41
7:U:48:VAL:C	7:U:49:ILE:HD12	2.45	0.41
7:U:17(D):SER:O	7:U:17(E):LYS:HB2	2.20	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:111:TYR:CD2	3:C:111:TYR:C	2.99	0.41
3:C:158:SER:CB	4:D:59:LEU:HD21	2.51	0.41
4:D:112:LEU:C	4:D:112:LEU:CD1	2.91	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
1:O:62:GLU:CD	1:O:62:GLU:H	2.29	0.41
3:Q:57:LYS:HD2	3:Q:57:LYS:C	2.46	0.41
4:R:117:CYS:SG	4:R:157:PHE:HB3	2.60	0.41
4:R:152:GLU:C	4:R:154:SER:H	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
10:J:133:TYR:C	17:J:198:HOH:O	2.63	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
3:Q:215:VAL:O	3:Q:215:VAL:HG13	2.20	0.41
4:R:121:LEU:HD13	5:S:130:ARG:HH21	1.86	0.41
7:U:184:ASN:C	7:U:184:ASN:ND2	2.79	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:39:GLY:C	2:B:148:LEU:HD21	2.46	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
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
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
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
14:N:20:THR:HA	15:c:2:GLN:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:235:LYS:C	2:B:237:GLY:N	2.79	0.40
7:G:197:MET:HA	7:G:197:MET:HE3	2.03	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
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
3:Q:121:GLN:C	3:Q:121:GLN:NE2	2.80	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
7:U:8:TYR:C	7:U:10:ARG:N	2.74	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
11:Y:114:ASP:OD1	11:Y:114:ASP:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	16	34
1	O	248/250 (99%)	232 (94%)	13 (5%)	3 (1%)	10	23
2	B	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	7	15
2	P	242/244 (99%)	225 (93%)	13 (5%)	4 (2%)	7	15
3	C	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	9	21
3	Q	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	9	21
4	D	240/242 (99%)	221 (92%)	12 (5%)	7 (3%)	3	6
4	R	240/242 (99%)	221 (92%)	13 (5%)	6 (2%)	4	8
5	E	231/233 (99%)	214 (93%)	13 (6%)	4 (2%)	7	15
5	S	231/233 (99%)	213 (92%)	16 (7%)	2 (1%)	14	30
6	F	242/244 (99%)	230 (95%)	9 (4%)	3 (1%)	10	23
6	T	242/244 (99%)	230 (95%)	9 (4%)	3 (1%)	10	23
7	G	241/243 (99%)	229 (95%)	12 (5%)	0	100	100
7	U	241/243 (99%)	229 (95%)	11 (5%)	1 (0%)	30	51
8	H	220/222 (99%)	210 (96%)	8 (4%)	2 (1%)	14	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	24	46
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%)	24	46
10	X	196/198 (99%)	184 (94%)	11 (6%)	1 (0%)	24	46
11	K	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	24	46
11	Y	210/212 (99%)	202 (96%)	7 (3%)	1 (0%)	24	46
12	L	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	24	46
12	Z	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	24	46
13	1	231/233 (99%)	217 (94%)	14 (6%)	0	100	100
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%)	14	30

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
12	Z	14(H)	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	199 (95%)	10 (5%)	23	47
1	O	209/209 (100%)	199 (95%)	10 (5%)	23	47
2	B	203/203 (100%)	196 (97%)	7 (3%)	32	60
2	P	203/203 (100%)	196 (97%)	7 (3%)	32	60
3	C	213/213 (100%)	206 (97%)	7 (3%)	33	61
3	Q	213/213 (100%)	206 (97%)	7 (3%)	33	61
4	D	198/198 (100%)	185 (93%)	13 (7%)	15	34
4	R	198/198 (100%)	185 (93%)	13 (7%)	15	34
5	E	192/192 (100%)	175 (91%)	17 (9%)	9	20
5	S	192/192 (100%)	175 (91%)	17 (9%)	9	20
6	F	201/201 (100%)	189 (94%)	12 (6%)	17	37
6	T	201/201 (100%)	188 (94%)	13 (6%)	15	35
7	G	207/207 (100%)	194 (94%)	13 (6%)	16	36
7	U	207/207 (100%)	194 (94%)	13 (6%)	16	36
8	H	181/181 (100%)	172 (95%)	9 (5%)	22	46
8	V	181/181 (100%)	173 (96%)	8 (4%)	25	50
9	I	172/172 (100%)	168 (98%)	4 (2%)	44	71
9	W	172/172 (100%)	167 (97%)	5 (3%)	37	65
10	J	175/175 (100%)	168 (96%)	7 (4%)	28	55
10	X	175/175 (100%)	169 (97%)	6 (3%)	32	60
11	K	169/169 (100%)	160 (95%)	9 (5%)	20	43
11	Y	169/169 (100%)	159 (94%)	10 (6%)	18	38
12	L	185/185 (100%)	160 (86%)	25 (14%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	185/185 (100%)	160 (86%)	25 (14%)	4	7
13	1	199/199 (100%)	190 (96%)	9 (4%)	24	50
13	M	199/199 (100%)	190 (96%)	9 (4%)	24	50
14	2	162/162 (100%)	155 (96%)	7 (4%)	26	51
14	N	162/162 (100%)	155 (96%)	7 (4%)	26	51
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
15	f	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	5350/5350 (100%)	5049 (94%)	301 (6%)	19	40

All (301) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	33	GLN
1	A	62	GLU
1	A	64	LEU
1	A	119	ILE
1	A	124	THR
1	A	135	SER
1	A	158	PHE
1	A	179	ARG
1	A	214	ILE
2	B	58	LEU
2	B	89	ILE
2	B	94	ILE
2	B	124	THR
2	B	150	THR
2	B	192	LEU
2	B	224	PHE
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	135	SER
3	C	150	GLN

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Mol	Chain	Res	Type
3	C	174	GLU
3	C	227	GLU
4	D	28	LEU
4	D	31	ILE
4	D	40	ILE
4	D	48	LEU
4	D	89	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
5	E	12	THR
5	E	13	VAL
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	90	ASN
5	E	97	ASN
5	E	111	ARG
5	E	149	LEU
5	E	160	LEU
5	E	189	LEU
5	E	197	ILE
5	E	199	GLN
5	E	207	LEU
5	E	227	GLU
5	E	231	LYS
6	F	35	THR
6	F	43	ASN
6	F	56	SER
6	F	72	ARG
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	169	ARG

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Mol	Chain	Res	Type
6	F	187	ARG
6	F	203	GLU
7	G	12	ILE
7	G	14	ILE
7	G	35	ILE
7	G	38	LEU
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
7	G	14(A)	GLU
7	G	197	MET
7	G	217	LYS
7	G	229	ILE
7	G	232	ARG
7	G	233	LEU
8	H	3	ILE
8	H	13	VAL
8	H	34	LEU
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	34	THR
10	J	35	ARG
10	J	52	THR
10	J	70	GLU
10	J	121	GLU
10	J	137	LEU
10	J	168	MET
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	69	ARG
11	K	74	ILE
11	K	82	ILE
11	K	87	VAL

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Mol	Chain	Res	Type
11	K	99	THR
11	K	100	MET
12	L	-7	ASN
12	L	4	LEU
12	L	14	LEU
12	L	25	SER
12	L	58	ARG
12	L	99	THR
12	L	106	GLU
12	L	123	GLN
12	L	134	ILE
12	L	14(A)	LYS
12	L	14(B)	ASN
12	L	14(C)	GLN
12	L	14(D)	TYR
12	L	14(E)	GLU
12	L	14(F)	PRO
12	L	14(I)	THR
12	L	14(K)	LYS
12	L	14(M)	VAL
12	L	14(N)	LYS
12	L	14(O)	LYS
12	L	14(P)	PRO
12	L	14(Q)	LEU
12	L	14(W)	LYS
12	L	145	TYR
12	L	152	ILE
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	112	TYR
13	M	129	PHE
13	M	148	VAL
13	M	149	GLN
13	M	191	GLN
13	M	211	ILE
14	N	1	THR
14	N	70	TYR
14	N	89	GLU
14	N	115	LEU
14	N	119	VAL
14	N	149	GLU

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Mol	Chain	Res	Type
14	N	178	LEU
1	O	32	LYS
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	119	ILE
1	O	124	THR
1	O	135	SER
1	O	158	PHE
1	O	179	ARG
1	O	214	ILE
2	P	58	LEU
2	P	89	ILE
2	P	94	ILE
2	P	124	THR
2	P	150	THR
2	P	192	LEU
2	P	224	PHE
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	135	SER
3	Q	150	GLN
3	Q	174	GLU
3	Q	227	GLU
4	R	28	LEU
4	R	31	ILE
4	R	40	ILE
4	R	48	LEU
4	R	89	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
5	S	12	THR
5	S	13	VAL
5	S	28	LEU
5	S	32	LYS

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Mol	Chain	Res	Type
5	S	57	GLU
5	S	76	LEU
5	S	90	ASN
5	S	97	ASN
5	S	111	ARG
5	S	149	LEU
5	S	160	LEU
5	S	189	LEU
5	S	197	ILE
5	S	199	GLN
5	S	207	LEU
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	72	ARG
6	T	98	SER
6	T	105	THR
6	T	121	GLN
6	T	127	ASN
6	T	144	ASN
6	T	169	ARG
6	T	187	ARG
6	T	203	GLU
7	U	12	ILE
7	U	14	ILE
7	U	35	ILE
7	U	38	LEU
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	14(A)	GLU
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	13	VAL
8	V	55	VAL

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Mol	Chain	Res	Type
8	V	56	THR
8	V	68	LEU
8	V	99	LEU
8	V	144	GLN
8	V	197	ARG
9	W	-3	ILE
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	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
11	Y	69	ARG
11	Y	74	ILE
11	Y	82	ILE
11	Y	87	VAL
11	Y	99	THR
11	Y	100	MET
12	Z	-7	ASN
12	Z	4	LEU
12	Z	14	LEU
12	Z	25	SER
12	Z	58	ARG
12	Z	99	THR
12	Z	106	GLU
12	Z	123	GLN
12	Z	134	ILE
12	Z	14(A)	LYS
12	Z	14(B)	ASN
12	Z	14(C)	GLN
12	Z	14(D)	TYR
12	Z	14(E)	GLU
12	Z	14(F)	PRO
12	Z	14(I)	THR

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Mol	Chain	Res	Type
12	Z	14(K)	LYS
12	Z	14(M)	VAL
12	Z	14(N)	LYS
12	Z	14(O)	LYS
12	Z	14(P)	PRO
12	Z	14(Q)	LEU
12	Z	14(W)	LYS
12	Z	145	TYR
12	Z	152	ILE
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	112	TYR
13	1	129	PHE
13	1	148	VAL
13	1	149	GLN
13	1	191	GLN
13	1	211	ILE
14	2	1	THR
14	2	70	TYR
14	2	89	GLU
14	2	115	LEU
14	2	119	VAL
14	2	149	GLU
14	2	178	LEU
15	c	1	ASN
15	f	1	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (223) 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	95	HIS
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN

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Mol	Chain	Res	Type
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	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	64	GLN
5	E	73	HIS
5	E	95	GLN
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	152	GLN
5	E	199	GLN
5	E	2(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	184	ASN
7	G	208	ASN
7	G	228	ASN

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Mol	Chain	Res	Type
8	H	10	ASN
8	H	30	ASN
8	H	66	HIS
8	H	91	GLN
8	H	114	HIS
8	H	141	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
8	H	195	ASN
8	H	201	GLN
9	I	29	ASN
9	I	56	ASN
9	I	81	GLN
9	I	193	GLN
10	J	36	GLN
10	J	54	GLN
10	J	62	ASN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	24	ASN
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	27	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	82	ASN
12	L	14(B)	ASN

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Mol	Chain	Res	Type
12	L	1(I)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	54	HIS
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	106	ASN
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	90	ASN
2	P	95	HIS
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	226	ASN
5	S	7	ASN
5	S	33	GLN

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Mol	Chain	Res	Type
5	S	64	GLN
5	S	73	HIS
5	S	95	GLN
5	S	97	ASN
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	152	GLN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	192	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	184	ASN
7	U	228	ASN
8	V	10	ASN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS
8	V	91	GLN
8	V	114	HIS
8	V	141	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
8	V	195	ASN
8	V	201	GLN
9	W	29	ASN
9	W	56	ASN
9	W	81	GLN

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Mol	Chain	Res	Type
9	W	193	GLN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	64	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	186	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	24	ASN
11	Y	53	GLN
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	27	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	14(B)	ASN
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	10	ASN
13	1	40	ASN
13	1	54	HIS
13	1	89	GLN
13	1	93	ASN
13	1	132	HIS
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	69	GLN
14	2	106	ASN
14	2	145	ASN
14	2	161	GLN

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Mol	Chain	Res	Type
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	a	4	15	12,13,14	0.62	0	13,13,15	0.85	1 (7%)
16	HXD	d	4	15	12,13,14	0.59	0	13,13,15	0.84	1 (7%)
16	HXD	e	4	15	12,13,14	0.74	0	13,13,15	0.67	0
16	HXD	c	4	15	12,13,14	1.14	1 (8%)	13,13,15	1.05	1 (7%)
16	HXD	f	4	15	12,13,14	1.13	2 (16%)	13,13,15	1.00	1 (7%)
16	HXD	b	4	15	12,13,14	0.77	0	13,13,15	0.71	0

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	f	4	HXD	C5-C6	-2.21	1.40	1.51
16	f	4	HXD	C5-C4	2.10	1.61	1.52
16	c	4	HXD	C5-C4	2.06	1.60	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	d	4	HXD	C3-C2-C1	2.37	116.74	112.70
16	a	4	HXD	C3-C2-C1	2.37	116.73	112.70
16	f	4	HXD	O-C1-C2	-2.13	119.19	125.38
16	c	4	HXD	O-C1-C2	-2.03	119.48	125.38

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	b	4	HXD	C2-C3-C4-C5
16	e	4	HXD	C2-C3-C4-C5
16	d	4	HXD	C9-C10-C11-C12
16	a	4	HXD	C9-C10-C11-C12
16	e	4	HXD	C9-C10-C11-C12
16	b	4	HXD	C9-C10-C11-C12
16	d	4	HXD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
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.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	a	4	HXD	3	0
16	d	4	HXD	3	0
16	c	4	HXD	1	0
16	f	4	HXD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	250/250 (100%)	0.20	14 (5%)	30	24	34, 52, 85, 106	0
1	O	250/250 (100%)	0.20	8 (3%)	50	44	35, 54, 85, 105	0
2	B	244/244 (100%)	0.46	20 (8%)	17	14	37, 56, 89, 116	0
2	P	244/244 (100%)	0.46	20 (8%)	17	14	40, 56, 89, 116	0
3	C	241/241 (100%)	0.68	25 (10%)	11	9	39, 61, 110, 124	0
3	Q	241/241 (100%)	0.76	30 (12%)	8	6	41, 62, 110, 124	0
4	D	242/242 (100%)	0.49	14 (5%)	29	23	43, 58, 94, 121	0
4	R	242/242 (100%)	0.50	15 (6%)	26	21	44, 59, 95, 122	0
5	E	233/233 (100%)	0.37	13 (5%)	30	24	42, 55, 82, 109	0
5	S	233/233 (100%)	0.37	14 (6%)	27	22	41, 54, 82, 109	0
6	F	244/244 (100%)	0.19	10 (4%)	41	36	36, 50, 89, 106	0
6	T	244/244 (100%)	0.12	6 (2%)	58	52	34, 50, 89, 106	0
7	G	243/243 (100%)	0.02	13 (5%)	32	26	33, 47, 75, 112	0
7	U	243/243 (100%)	0.10	11 (4%)	38	32	33, 47, 75, 111	0
8	H	222/222 (100%)	-0.18	4 (1%)	67	63	30, 44, 62, 100	0
8	V	222/222 (100%)	-0.16	4 (1%)	67	63	29, 45, 63, 100	0
9	I	204/204 (100%)	-0.17	2 (0%)	79	76	35, 45, 63, 80	0
9	W	204/204 (100%)	-0.15	1 (0%)	87	85	36, 46, 64, 80	0
10	J	198/198 (100%)	0.02	6 (3%)	52	47	38, 49, 69, 122	0
10	X	198/198 (100%)	0.06	8 (4%)	42	37	38, 49, 69, 122	0
11	K	212/212 (100%)	0.11	11 (5%)	33	27	34, 47, 72, 86	0
11	Y	212/212 (100%)	0.19	14 (6%)	24	19	35, 47, 74, 86	0
12	L	222/222 (100%)	0.10	13 (5%)	28	23	33, 48, 74, 89	0
12	Z	222/222 (100%)	0.07	11 (4%)	34	28	34, 47, 74, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.32	1 (0%) 88 86	31, 43, 57, 61	0
13	M	233/233 (100%)	-0.20	1 (0%) 88 86	32, 43, 57, 63	0
14	2	196/196 (100%)	-0.27	5 (2%) 57 51	31, 41, 61, 81	0
14	N	196/196 (100%)	-0.27	2 (1%) 79 76	31, 40, 60, 81	0
15	a	3/3 (100%)	-0.23	0 100 100	41, 41, 44, 46	0
15	b	3/3 (100%)	0.17	0 100 100	34, 34, 42, 47	0
15	c	3/3 (100%)	0.20	0 100 100	43, 43, 48, 51	0
15	d	3/3 (100%)	-0.09	0 100 100	44, 44, 44, 47	0
15	e	3/3 (100%)	-0.12	0 100 100	37, 37, 44, 50	0
15	f	3/3 (100%)	0.15	0 100 100	43, 43, 50, 51	0
All	All	6386/6386 (100%)	0.15	296 (4%) 37 32	29, 50, 84, 124	0

All (296) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	145	TYR	8.2
4	R	12(E)	SER	8.0
3	Q	56	LEU	7.4
11	K	208	ASN	7.4
3	C	56	LEU	7.3
11	Y	208	ASN	6.7
12	Z	145	TYR	6.5
7	U	240	ASP	6.5
2	B	217	ALA	6.4
10	J	192	ALA	6.3
11	Y	67	GLU	6.2
3	C	55	THR	6.2
4	D	12(D)	ALA	6.2
4	D	12(E)	SER	6.1
2	B	21(A)	LYS	6.0
10	X	192	ALA	6.0
4	R	12(D)	ALA	5.8
11	Y	104	TYR	5.5
4	D	12(C)	GLY	5.3
6	F	5	GLY	5.1
11	K	73	ARG	5.1
11	K	207	ASN	5.1
2	B	21(B)	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
5	S	4	PHE	5.0
12	L	14(H)	GLY	5.0
1	A	203	GLU	4.9
4	D	127	LEU	4.8
4	R	12(C)	GLY	4.8
1	A	5	THR	4.7
10	J	193	GLN	4.7
10	J	-1	MET	4.6
11	K	180	GLU	4.5
11	K	104	TYR	4.5
3	C	54	SER	4.5
10	J	191	GLN	4.5
2	B	54	VAL	4.5
7	G	6	ALA	4.5
4	R	127	LEU	4.5
2	P	21(B)	GLY	4.5
5	E	4	PHE	4.5
3	Q	58	LEU	4.4
1	O	5	THR	4.4
11	Y	180	GLU	4.4
3	C	207	ALA	4.2
10	X	-1	MET	4.2
3	Q	208	LYS	4.2
11	Y	207	ASN	4.2
3	C	240	LYS	4.2
11	K	210	ILE	4.2
2	P	4	GLY	4.1
2	P	21(D)	GLY	4.1
3	Q	55	THR	4.1
2	P	54	VAL	4.0
9	I	-8	SER	4.0
3	C	52	ARG	4.0
10	X	191	GLN	4.0
12	Z	120	GLU	4.0
4	D	126	ARG	4.0
12	L	120	GLU	3.9
3	C	59	GLN	3.9
10	X	193	GLN	3.9
11	Y	210	ILE	3.9
2	B	218	ASN	3.8
2	B	239	THR	3.8
1	O	56	SER	3.8

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Mol	Chain	Res	Type	RSRZ
2	P	217	ALA	3.8
3	Q	240	LYS	3.8
13	1	-8	THR	3.8
1	O	4	MET	3.8
4	D	242	ALA	3.8
9	W	-8	SER	3.7
4	R	243	ALA	3.7
3	C	238	GLN	3.7
12	L	14(M)	VAL	3.7
1	A	202	VAL	3.6
11	Y	73	ARG	3.6
8	H	22	GLN	3.6
4	D	12(F)	GLY	3.6
3	Q	54	SER	3.6
3	Q	203	THR	3.5
5	E	203	ASP	3.5
3	C	208	LYS	3.5
14	2	107	LYS	3.5
7	U	6	ALA	3.5
11	K	67	GLU	3.5
3	Q	236	ILE	3.5
4	R	12(F)	GLY	3.5
4	R	126	ARG	3.5
14	N	107	LYS	3.4
5	S	127	TYR	3.3
2	P	21(A)	LYS	3.3
3	Q	207	ALA	3.3
11	Y	181	ASP	3.3
2	P	239	THR	3.3
12	Z	14(Q)	LEU	3.3
3	Q	241	GLN	3.3
11	K	40	PHE	3.3
3	C	236	ILE	3.3
5	S	5	ARG	3.3
7	U	239	GLN	3.3
11	Y	40	PHE	3.3
6	F	240	ILE	3.3
12	Z	14(H)	GLY	3.2
12	L	14(P)	PRO	3.2
7	G	239	GLN	3.2
5	S	203	ASP	3.2
3	C	33	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
3	Q	57	LYS	3.2
3	C	233	VAL	3.1
8	V	220	ASN	3.1
8	V	223	ASP	3.1
1	A	236	LEU	3.1
3	C	234	THR	3.1
8	H	223	ASP	3.1
1	A	4	MET	3.1
1	A	204	GLY	3.0
7	G	7	GLY	3.0
5	E	127	TYR	3.0
7	U	17(C)	LYS	3.0
5	S	204	GLU	3.0
3	Q	233	VAL	3.0
7	G	240	ASP	2.9
7	G	236	ILE	2.9
1	O	21(P)	LYS	2.9
7	U	8	TYR	2.9
1	A	235	ALA	2.9
5	E	33	GLN	2.9
6	T	241	ASN	2.9
2	B	21(D)	GLY	2.9
12	Z	14(P)	PRO	2.9
12	Z	14(I)	THR	2.9
12	Z	14(W)	LYS	2.8
4	R	121	LEU	2.8
10	X	168	MET	2.8
3	Q	202	GLN	2.8
6	F	237	GLN	2.8
7	G	18(A)	ILE	2.8
6	F	20(C)	LYS	2.8
12	L	14(Q)	LEU	2.8
3	C	188	GLU	2.8
12	L	14(W)	LYS	2.8
5	E	227	GLU	2.8
2	B	4	GLY	2.8
3	Q	206	GLY	2.8
7	G	218	ASP	2.8
1	O	7	ARG	2.8
3	C	241	GLN	2.7
4	D	241	GLU	2.7
3	Q	64	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	210	ILE	2.7
3	Q	44	ASN	2.7
2	B	20(B)	ALA	2.7
4	D	243	ALA	2.7
12	Z	14(M)	VAL	2.7
3	Q	238	GLN	2.7
2	B	59	LEU	2.7
1	A	200	SER	2.7
5	E	2(C)	VAL	2.7
13	M	-8	THR	2.7
7	G	18(H)	GLU	2.6
6	F	43	ASN	2.6
10	J	168	MET	2.6
2	P	65	GLU	2.6
12	Z	14(J)	GLY	2.6
3	C	203	THR	2.6
8	H	220	ASN	2.6
2	P	220	TYR	2.6
3	Q	52	ARG	2.6
7	U	7	GLY	2.6
2	P	218	ASN	2.6
4	R	122	ARG	2.5
1	A	185	GLU	2.5
5	S	56	ASP	2.5
2	P	59	LEU	2.5
5	E	207	LEU	2.5
2	P	64	THR	2.5
5	S	227	GLU	2.5
7	U	128	TYR	2.5
8	V	22	GLN	2.5
1	A	175	PHE	2.5
2	B	181	LYS	2.4
3	Q	63	THR	2.4
5	S	58	LEU	2.4
14	2	18(F)	GLU	2.4
3	Q	183	PRO	2.4
3	Q	234	THR	2.4
5	E	101	LEU	2.4
1	A	21(E)	ASP	2.4
5	E	56	ASP	2.4
3	C	187	GLU	2.4
6	T	5	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	Q	210	ILE	2.4
6	T	207	ASP	2.4
4	D	122	ARG	2.4
7	G	8	TYR	2.4
6	T	240	ILE	2.4
5	S	57	GLU	2.4
2	B	143	ASP	2.4
4	D	9	ASP	2.4
6	F	204	ASP	2.4
3	C	62(A)	ILE	2.3
4	R	9	ASP	2.3
7	G	217	LYS	2.3
5	S	2(C)	VAL	2.3
4	R	12(B)	GLU	2.3
4	R	12(G)	GLU	2.3
2	P	216	ARG	2.3
11	Y	183	GLY	2.3
10	J	133	TYR	2.3
1	A	234	GLU	2.3
2	B	235	LYS	2.3
5	S	217	LYS	2.3
2	P	21(C)	ASP	2.3
14	2	183	GLY	2.3
11	Y	209	VAL	2.3
5	S	207	LEU	2.3
3	Q	239	GLU	2.3
12	Z	150	GLU	2.3
1	A	7	ARG	2.3
4	R	227	GLU	2.2
4	R	231	GLU	2.2
11	Y	149	GLU	2.2
12	L	106	GLU	2.2
10	X	133	TYR	2.2
2	B	21(C)	ASP	2.2
3	Q	225	SER	2.2
6	T	237	GLN	2.2
7	U	218	ASP	2.2
4	D	12(A)	GLY	2.2
3	C	58	LEU	2.2
3	Q	242	GLU	2.2
5	E	204	GLU	2.2
3	Q	243	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
11	Y	145	ASP	2.2
12	L	71	ASP	2.2
11	K	209	VAL	2.2
4	D	12(G)	GLU	2.2
7	U	18(H)	GLU	2.2
6	T	20(C)	LYS	2.2
14	2	105	ASP	2.2
2	P	21(E)	VAL	2.2
3	C	227	GLU	2.2
4	D	205	GLU	2.2
2	P	57	THR	2.2
11	Y	39	PRO	2.2
5	E	180	LEU	2.2
3	C	226	SER	2.2
3	C	242	GLU	2.1
2	B	64	THR	2.1
5	E	5	ARG	2.1
2	P	185	LYS	2.1
3	C	209	ASN	2.1
3	Q	235	GLN	2.1
6	F	206	LYS	2.1
7	G	128	TYR	2.1
10	X	107	LYS	2.1
2	P	204	SER	2.1
3	Q	200	VAL	2.1
6	F	235	PHE	2.1
4	R	125	GLU	2.1
7	G	171	GLU	2.1
10	X	143	ARG	2.1
6	F	6	THR	2.1
2	B	185	LYS	2.1
12	L	14(K)	LYS	2.1
12	Z	14(K)	LYS	2.1
3	Q	222	VAL	2.1
8	H	221	ILE	2.1
8	V	221	ILE	2.1
11	K	181	ASP	2.1
12	L	114	ASP	2.1
14	N	105	ASP	2.1
5	S	200	SER	2.1
5	S	228	ALA	2.1
2	P	60	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	Q	211	GLU	2.1
11	K	149	GLU	2.1
14	2	149	GLU	2.1
9	I	107	LYS	2.1
2	B	61	GLN	2.1
7	U	236	ILE	2.1
1	O	21(E)	ASP	2.1
2	B	209	ARG	2.1
1	O	227	GLN	2.1
1	O	236	LEU	2.1
3	C	232	TYR	2.1
2	B	6	ARG	2.0
1	A	55	SER	2.0
12	L	14(I)	THR	2.0
7	G	55	PRO	2.0
5	E	58	LEU	2.0
6	F	170	GLN	2.0
2	P	235	LYS	2.0
7	U	217	LYS	2.0
2	B	43	SER	2.0
12	L	70	HIS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	HXD	f	4	14/15	0.85	0.12	50,59,61,65	0
16	HXD	d	4	14/15	0.86	0.13	43,45,60,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	HXD	c	4	14/15	0.86	0.14	49,58,60,61	0
16	HXD	a	4	14/15	0.87	0.12	43,47,59,63	0
16	HXD	e	4	14/15	0.88	0.15	34,39,56,58	0
16	HXD	b	4	14/15	0.88	0.12	37,41,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.