Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:06 AM GMT

PDB ID	:	2FAK
Title	:	Crystal structure of Salinosporamide A in complex with the yeast 20S proteasome
Authors	:	Groll, M.; Potts, B.C.
Deposited on	:	2005-12-07
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

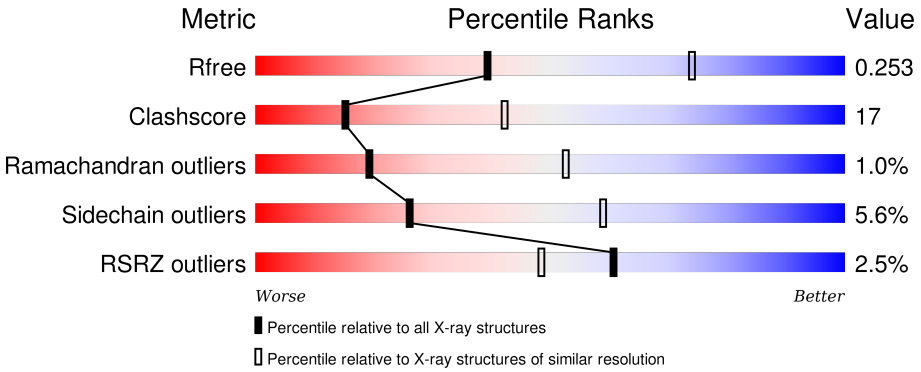
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 75% 23%
1	O	250	4% 74% 24%
2	B	244	5% 58% 36% 6%
2	P	244	6% 58% 36% 6%
3	C	241	5% 58% 39%

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Mol	Chain	Length	Quality of chain
3	Q	241	7% 59% 38%
4	D	242	5% 69% 27%
4	R	242	5% 68% 27% 5%
5	E	233	3% 59% 35% 6%
5	S	233	7% 58% 36% 6%
6	F	244	2% 63% 34%
6	T	244	2% 61% 35%
7	G	243	% 67% 28% 5%
7	U	243	2% 62% 33% 5%
8	H	222	% 73% 27%
8	V	222	% 72% 27%
9	I	204	74% 25%
9	W	204	71% 26%
10	J	198	2% 67% 31%
10	X	198	3% 68% 30%
11	K	212	75% 23%
11	Y	212	73% 25%
12	L	222	% 69% 26% 5%
12	Z	222	2% 68% 27% 5%
13	1	233	% 66% 31%
13	M	233	66% 32%
14	2	196	% 66% 31%
14	N	196	68% 28%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 50685 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome component Y7.

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

- Molecule 2 is a protein called Proteasome component Y13.

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

- Molecule 3 is a protein called Proteasome component PRE6.

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

- Molecule 4 is a protein called Proteasome component PUP2.

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

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

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

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

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

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

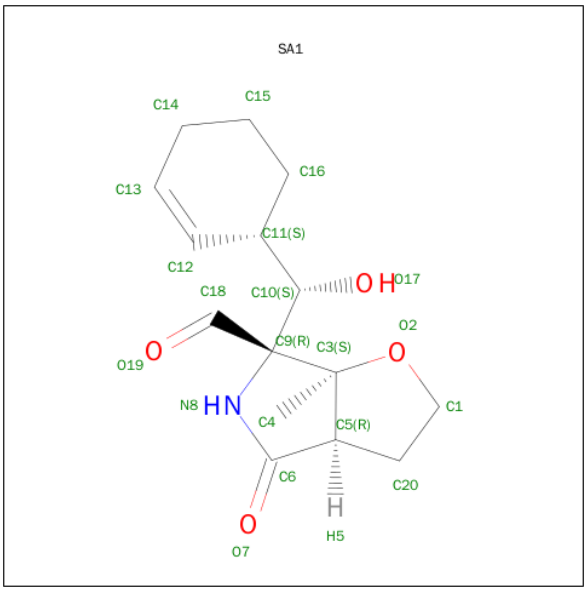
- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

- Molecule 15 is (3AR,6R,6AS)-6-((S)-((S)-CYCLOHEX-2-ENYL)(HYDROXY)METHYL)-6A-METHYL-4-OXO-HEXAHYDRO-2H-FURO[3,2-C]PYRROLE-6-CARBALDEHYDE (three-letter code: SA1) (formula: $C_{15}H_{21}NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total C N O 20 15 1 4	0	0
15	K	1	Total C N O 20 15 1 4	0	0
15	N	1	Total C N O 20 15 1 4	0	0
15	V	1	Total C N O 20 15 1 4	0	0
15	Y	1	Total C N O 20 15 1 4	0	0
15	2	1	Total C N O 20 15 1 4	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	42	Total O 42 42	0	0
16	B	29	Total O 29 29	0	0
16	C	35	Total O 35 35	0	0
16	D	27	Total O 27 27	0	0
16	E	10	Total O 10 10	0	0
16	F	35	Total O 35 35	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	50	Total O 50 50	0	0
16	H	40	Total O 40 40	0	0
16	I	49	Total O 49 49	0	0
16	J	43	Total O 43 43	0	0
16	K	30	Total O 30 30	0	0
16	L	36	Total O 36 36	0	0
16	M	49	Total O 49 49	0	0
16	N	51	Total O 51 51	0	0
16	O	28	Total O 28 28	0	0
16	P	20	Total O 20 20	0	0
16	Q	20	Total O 20 20	0	0
16	R	23	Total O 23 23	0	0
16	S	17	Total O 17 17	0	0
16	T	31	Total O 31 31	0	0
16	U	47	Total O 47 47	0	0
16	V	42	Total O 42 42	0	0
16	W	41	Total O 41 41	0	0
16	X	37	Total O 37 37	0	0
16	Y	34	Total O 34 34	0	0
16	Z	46	Total O 46 46	0	0
16	1	59	Total O 59 59	0	0

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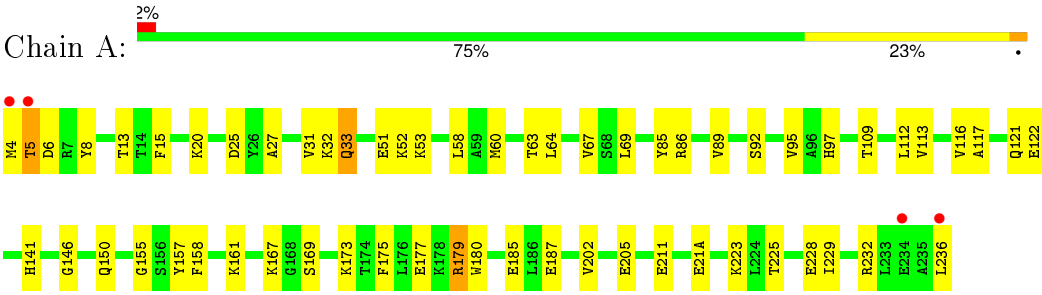
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	2	46	Total	O	0	0
			46	46		

3 Residue-property plots (i)

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

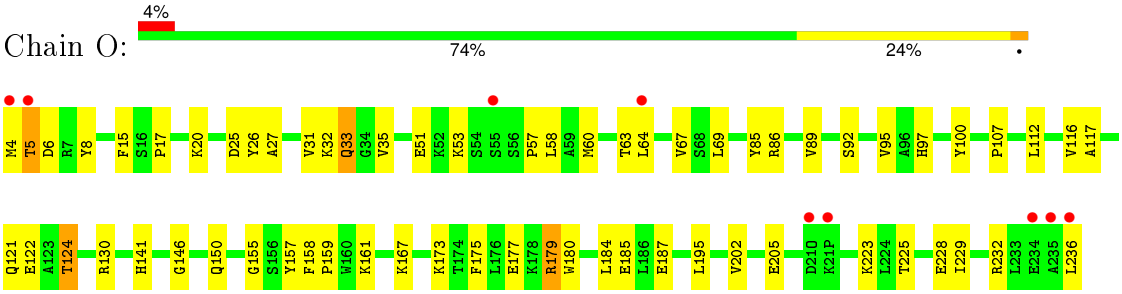
- Molecule 1: Proteasome component Y7

Chain A:



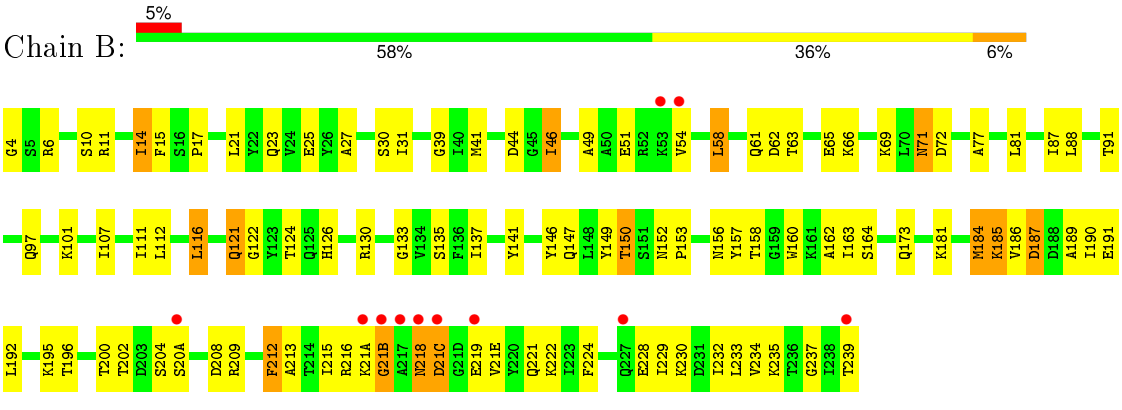
- Molecule 1: Proteasome component Y7

Chain O:



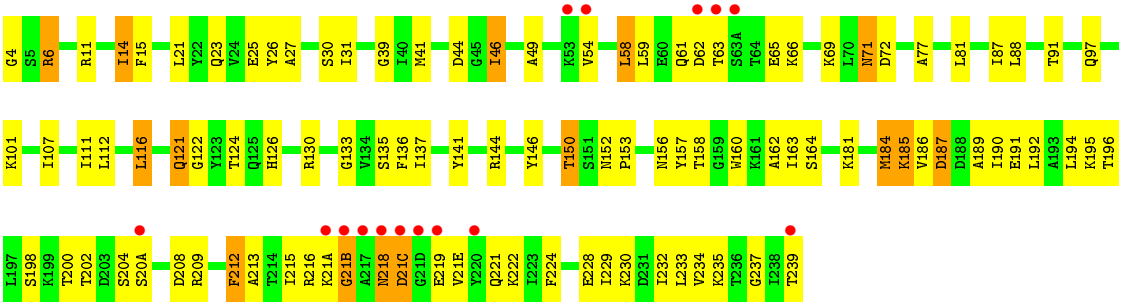
- Molecule 2: Proteasome component Y13

Chain B:



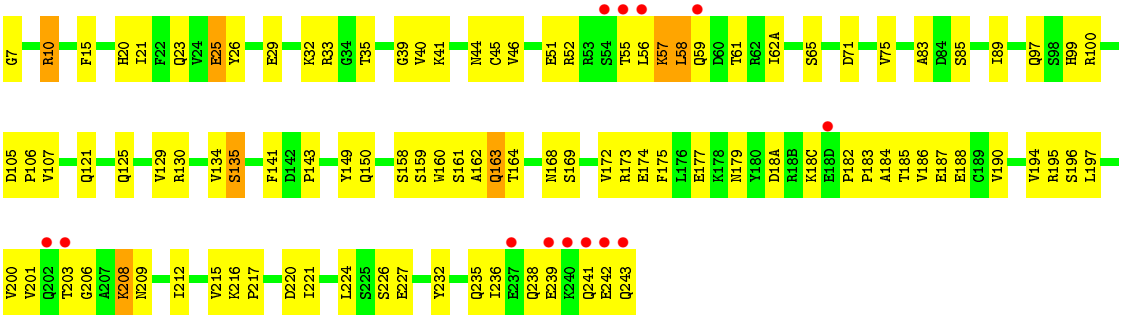
- Molecule 2: Proteasome component Y13

Chain P:



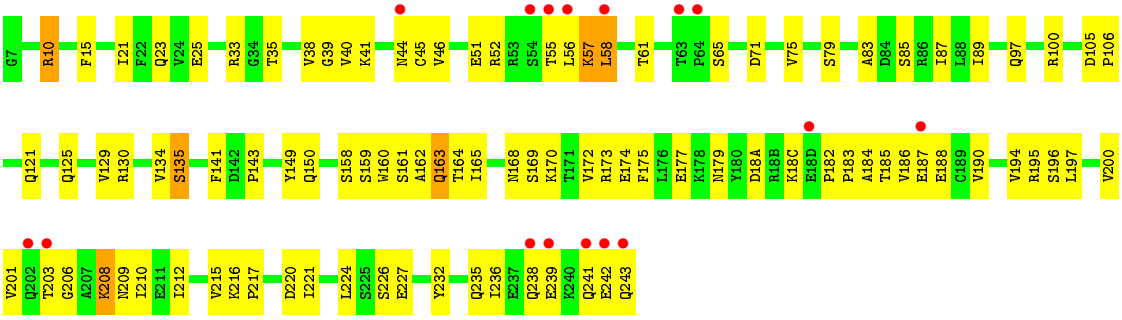
• Molecule 3: Proteasome component PRE6

Chain C:



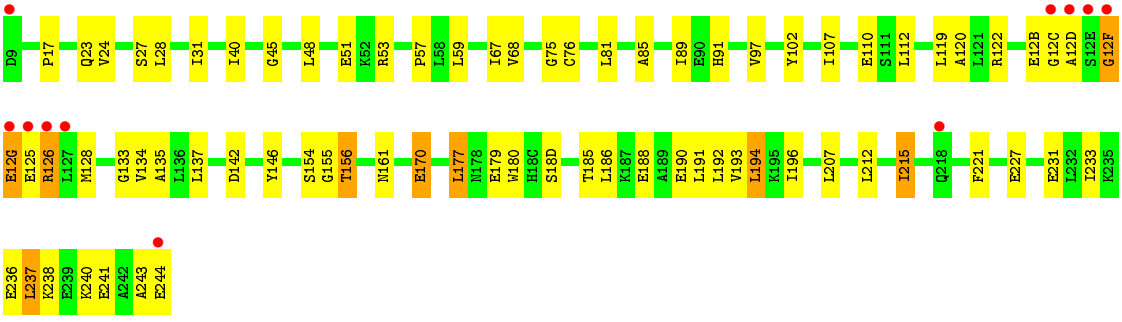
• Molecule 3: Proteasome component PRE6

Chain Q:



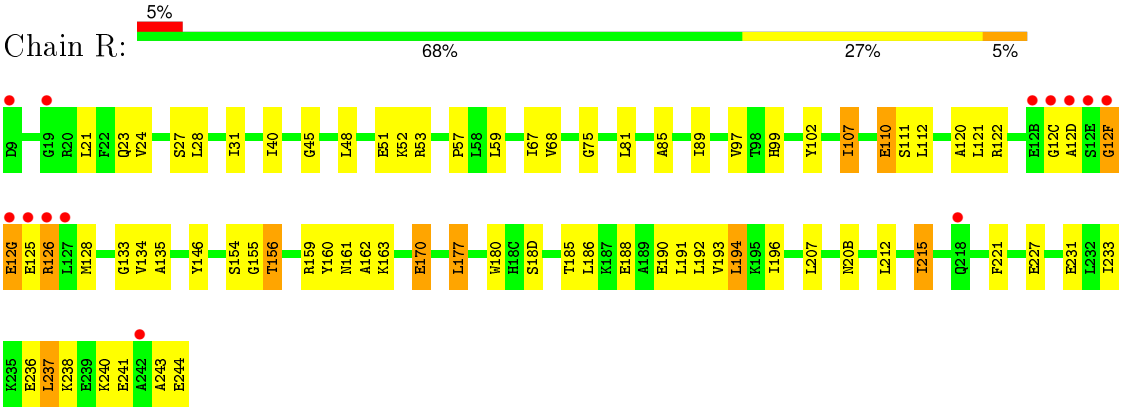
• Molecule 4: Proteasome component PUP2

Chain D:



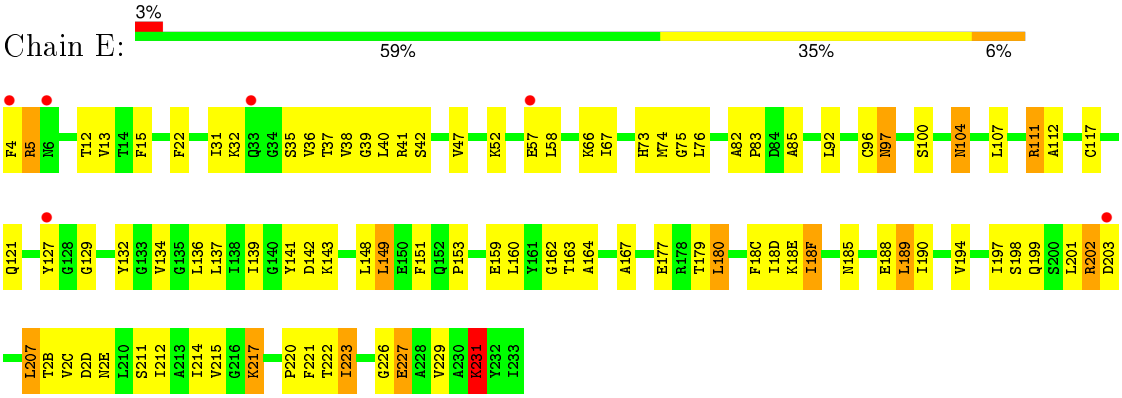
• Molecule 4: Proteasome component PUP2

Chain R:



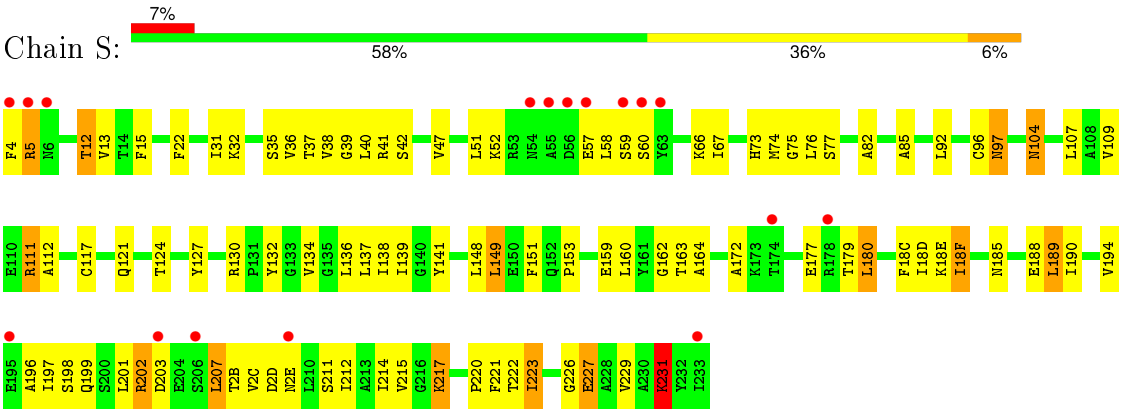
• Molecule 5: Proteasome component PRE5

Chain E:



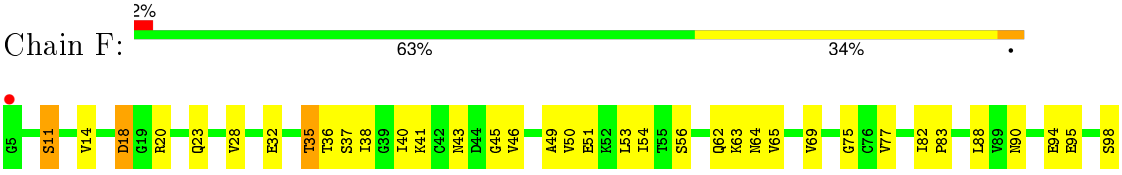
• Molecule 5: Proteasome component PRE5

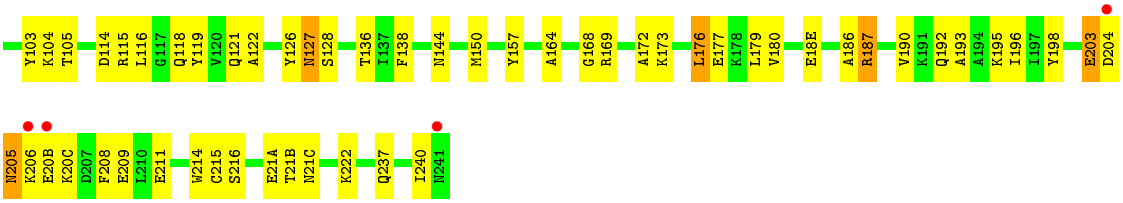
Chain S:



• Molecule 6: Proteasome component C1

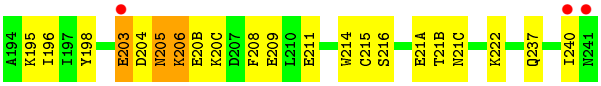
Chain F:





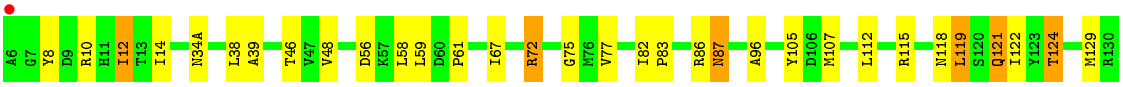
• Molecule 6: Proteasome component C1

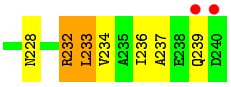
Chain T:



• Molecule 7: Proteasome component C7-alpha

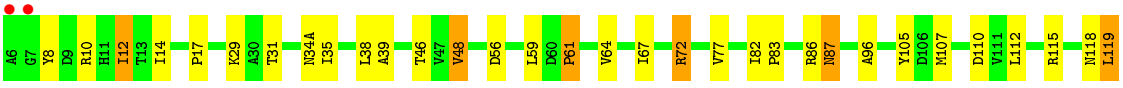
Chain G:

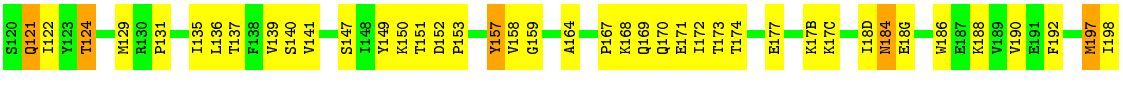


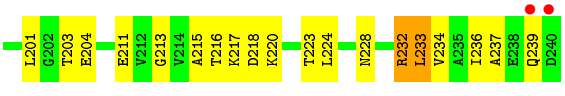


• Molecule 7: Proteasome component C7-alpha

Chain U:

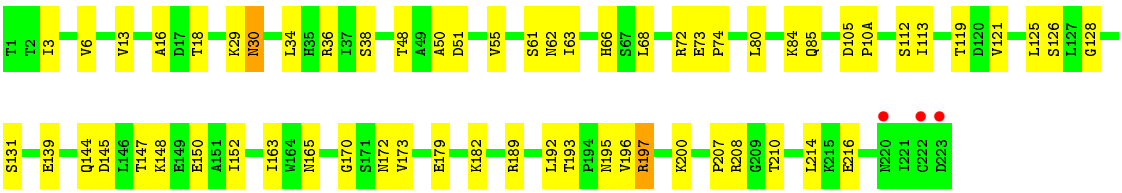




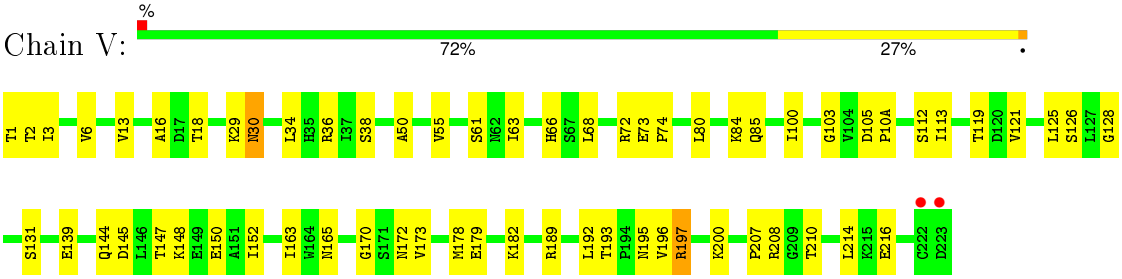


• Molecule 8: Proteasome component PUP1

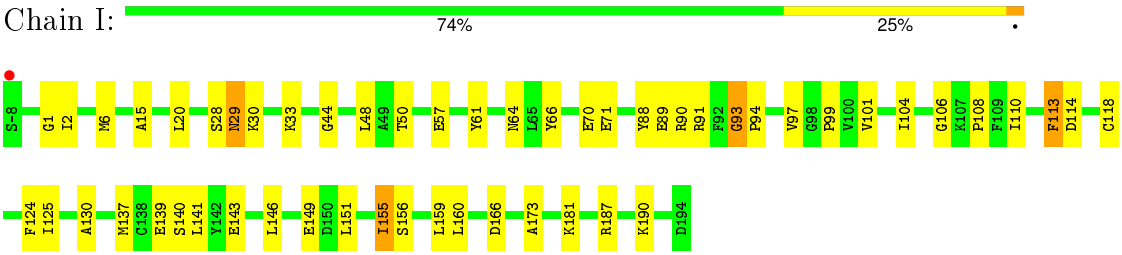
Chain H:



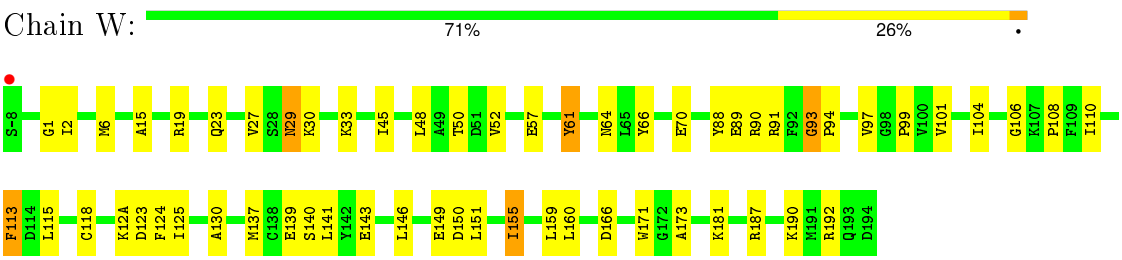
• Molecule 8: Proteasome component PUP1



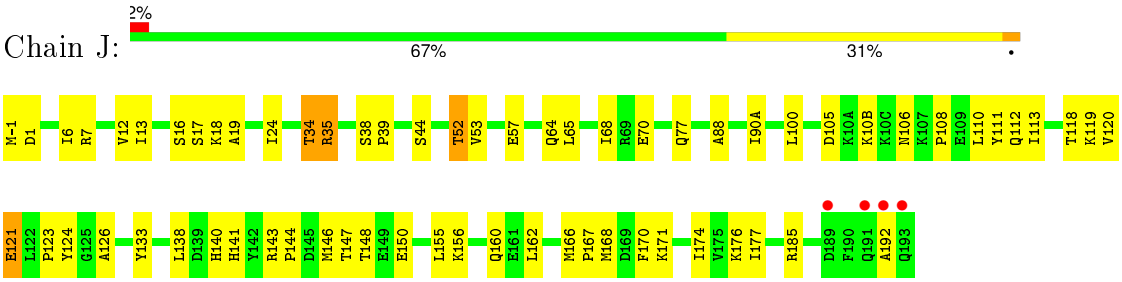
• Molecule 9: Proteasome component PUP3



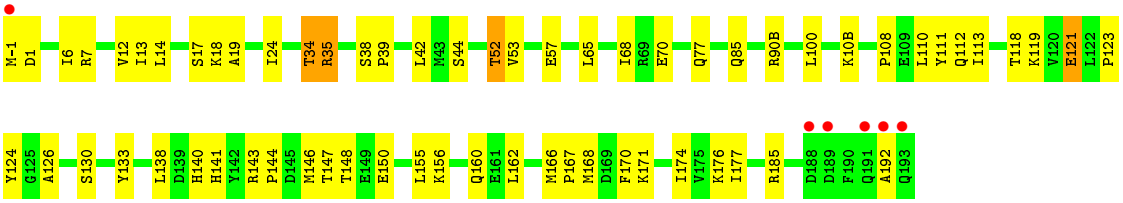
• Molecule 9: Proteasome component PUP3



• Molecule 10: Proteasome component C11

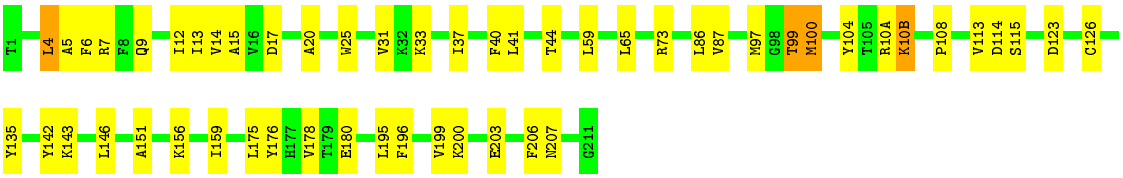


• Molecule 10: Proteasome component C11



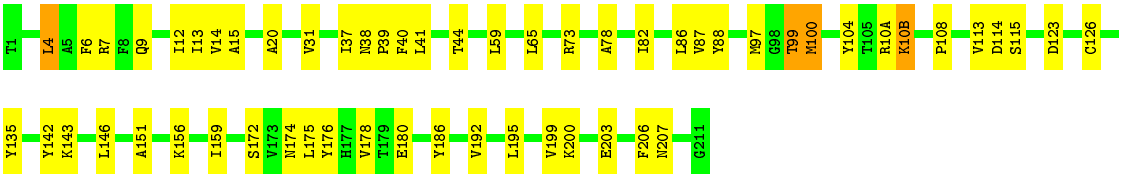
• Molecule 11: Proteasome component PRE2

Chain K:



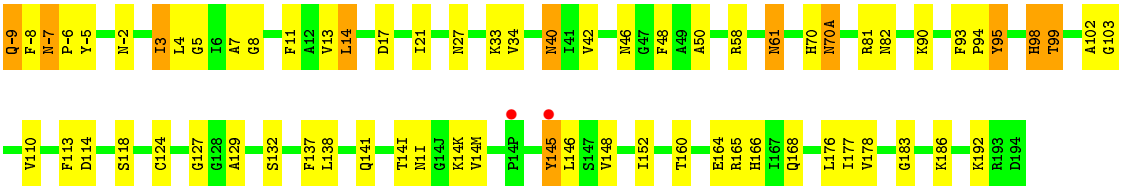
• Molecule 11: Proteasome component PRE2

Chain Y:



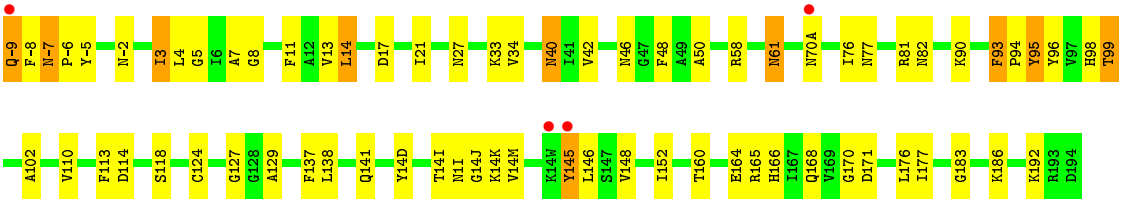
• Molecule 12: Proteasome component C5

Chain L:



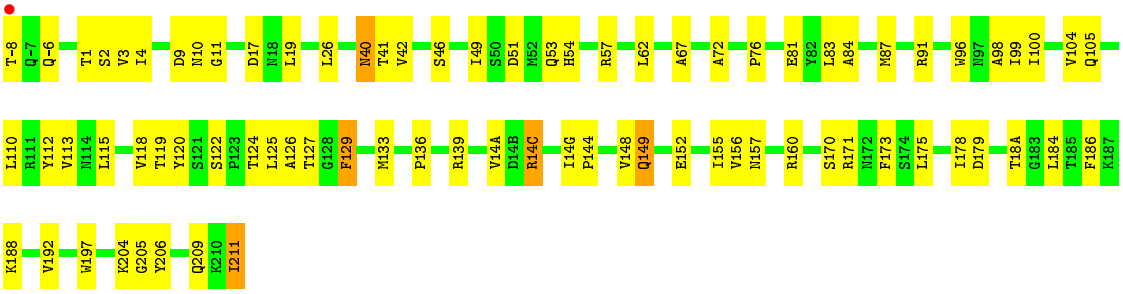
• Molecule 12: Proteasome component C5

Chain Z:

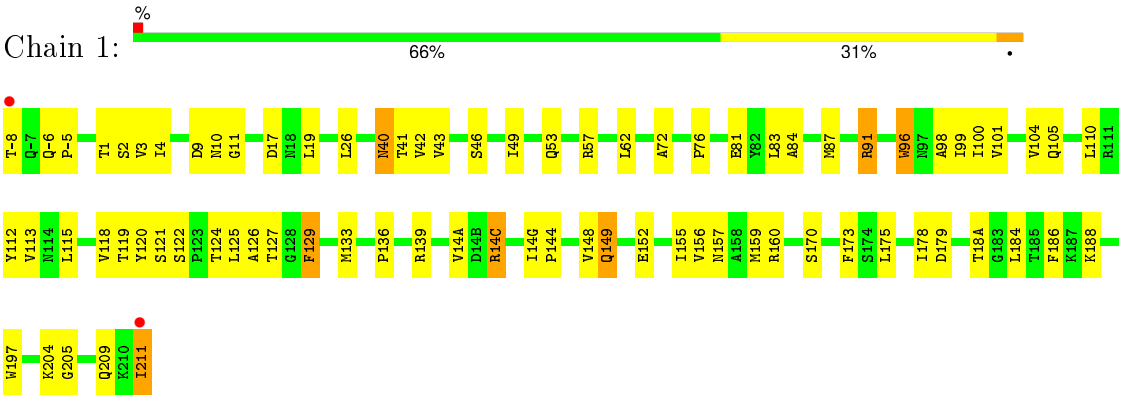


• Molecule 13: Proteasome component PRE4

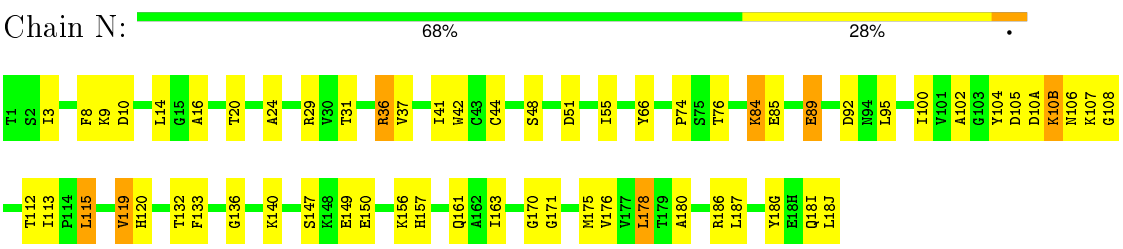
Chain M:



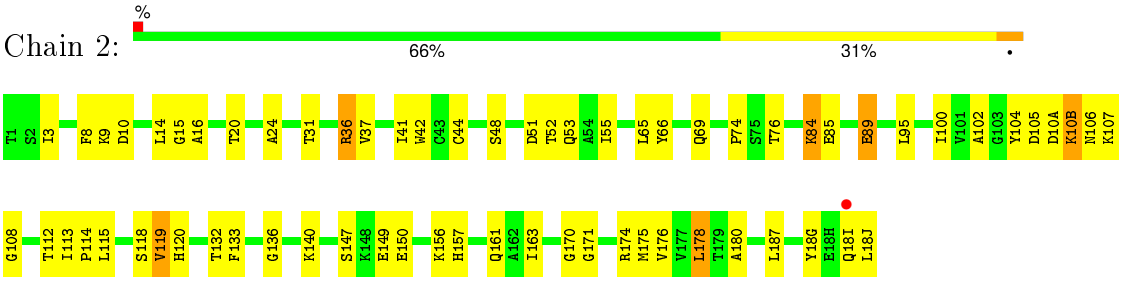
• Molecule 13: Proteasome component PRE4



• Molecule 14: Proteasome component PRE3



• Molecule 14: Proteasome component PRE3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.17Å 301.16Å 144.14Å 90.00° 112.82° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 20.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-2.80) 98.8 (20.00-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.254 0.229 , 0.253	Depositor DCC
R_{free} test set	12668 reflections (4.95%)	DCC
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	2 of 270489 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	50685	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SA1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.38	0/1952	0.63	0/2642
1	O	0.37	0/1952	0.62	0/2642
2	B	0.37	0/1935	0.62	0/2618
2	P	0.37	0/1935	0.63	0/2618
3	C	0.35	0/1920	0.62	0/2598
3	Q	0.35	0/1920	0.62	0/2598
4	D	0.37	0/1887	0.63	0/2541
4	R	0.37	0/1887	0.63	0/2541
5	E	0.36	0/1823	0.60	0/2463
5	S	0.36	0/1823	0.60	0/2463
6	F	0.37	0/1937	0.60	0/2614
6	T	0.37	0/1937	0.60	0/2614
7	G	0.41	0/1959	0.62	0/2652
7	U	0.41	0/1959	0.62	0/2652
8	H	0.40	0/1716	0.67	0/2326
8	V	0.39	0/1716	0.67	1/2326 (0.0%)
9	I	0.41	0/1611	0.66	0/2174
9	W	0.42	0/1611	0.67	0/2174
10	J	0.39	0/1613	0.64	0/2173
10	X	0.38	0/1613	0.64	0/2173
11	K	0.42	0/1681	0.65	0/2274
11	Y	0.39	0/1681	0.64	0/2274
12	L	0.39	0/1795	0.67	1/2420 (0.0%)
12	Z	0.39	0/1795	0.66	1/2420 (0.0%)
13	1	0.41	0/1855	0.69	0/2514
13	M	0.39	0/1855	0.67	0/2514
14	2	0.40	0/1541	0.64	0/2087
14	N	0.40	0/1541	0.65	0/2087
All	All	0.39	0/50450	0.64	3/68192 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	95	TYR	N-CA-C	-5.27	96.78	111.00
12	Z	95	TYR	N-CA-C	-5.16	97.06	111.00
8	V	100	ILE	N-CA-C	-5.02	97.46	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	55	0
1	O	1915	0	1926	58	0
2	B	1905	0	1901	105	0
2	P	1905	0	1901	99	0
3	C	1891	0	1900	108	0
3	Q	1891	0	1900	97	0
4	D	1862	0	1836	62	0
4	R	1862	0	1836	66	0
5	E	1795	0	1797	88	0
5	S	1795	0	1797	100	0
6	F	1897	0	1886	69	0
6	T	1897	0	1886	76	0
7	G	1921	0	1910	76	0
7	U	1921	0	1910	86	0
8	H	1685	0	1687	45	0
8	V	1685	0	1687	46	0
9	I	1581	0	1574	50	0
9	W	1581	0	1574	51	0
10	J	1585	0	1590	67	0
10	X	1585	0	1590	69	0
11	K	1644	0	1594	46	0
11	Y	1644	0	1594	47	0
12	L	1757	0	1711	61	0
12	Z	1757	0	1711	63	0
13	1	1824	0	1832	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1824	0	1832	66	0
14	2	1512	0	1480	53	0
14	N	1512	0	1480	50	0
15	2	20	0	20	0	0
15	H	20	0	20	0	0
15	K	20	0	20	1	0
15	N	20	0	20	0	0
15	V	20	0	20	0	0
15	Y	20	0	20	1	0
16	1	59	0	0	0	0
16	2	46	0	0	0	0
16	A	42	0	0	1	0
16	B	29	0	0	4	0
16	C	35	0	0	3	0
16	D	27	0	0	1	0
16	E	10	0	0	1	0
16	F	35	0	0	6	0
16	G	50	0	0	1	0
16	H	40	0	0	2	0
16	I	49	0	0	1	0
16	J	43	0	0	2	0
16	K	30	0	0	1	0
16	L	36	0	0	2	0
16	M	49	0	0	4	0
16	N	51	0	0	3	0
16	O	28	0	0	1	0
16	P	20	0	0	2	0
16	Q	20	0	0	5	0
16	R	23	0	0	2	0
16	S	17	0	0	4	0
16	T	31	0	0	4	0
16	U	47	0	0	1	0
16	V	42	0	0	2	0
16	W	41	0	0	3	0
16	X	37	0	0	8	0
16	Y	34	0	0	1	0
16	Z	46	0	0	3	0
All	All	50685	0	49368	1719	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 (1719) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:10(B):LYS:HD2	11:Y:10(B):LYS:H	1.11	1.11
11:K:10(B):LYS:H	11:K:10(B):LYS:HD2	1.11	1.08
2:P:202:THR:HG22	2:P:204:SER:H	1.23	1.04
2:B:202:THR:HG22	2:B:204:SER:H	1.23	1.02
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.20	1.01
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.20	1.00
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.41	0.97
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.11	0.96
1:O:15:PHE:H	2:P:23:GLN:HE22	1.06	0.93
13:1:14(C):ARG:HG3	13:1:14(C):ARG:HH11	1.31	0.93
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.51	0.92
3:C:163:GLN:HE21	3:C:164:THR:H	1.15	0.92
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.14	0.92
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.18	0.91
3:C:163:GLN:NE2	3:C:164:THR:H	1.69	0.91
3:C:15:PHE:H	4:D:23:GLN:HE22	1.12	0.90
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.15	0.90
7:U:96:ALA:HA	7:U:107:MET:HE2	1.52	0.90
1:A:15:PHE:H	2:B:23:GLN:HE22	1.15	0.89
13:M:14(C):ARG:HH11	13:M:14(C):ARG:HG3	1.35	0.89
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.53	0.89
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.37	0.89
6:T:36:THR:HG22	6:T:51:GLU:OE2	1.73	0.89
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.55	0.88
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.56	0.87
2:B:71:ASN:ND2	2:B:72:ASP:H	1.73	0.87
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.56	0.87
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.75	0.87
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.57	0.86
7:G:96:ALA:HA	7:G:107:MET:HE2	1.54	0.86
3:C:185:THR:HB	3:C:188:GLU:HG2	1.57	0.86
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.72	0.86
5:S:15:PHE:H	6:T:23:GLN:HE22	1.23	0.86
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.41	0.86
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.56	0.85
3:C:185:THR:HG22	3:C:187:GLU:H	1.40	0.85
2:P:71:ASN:ND2	2:P:72:ASP:H	1.73	0.85
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.38	0.85
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.89	0.84
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.76	0.83
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.61	0.83
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:243:ALA:O	4:R:244:GLU:HB2	1.80	0.82
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.78	0.82
2:B:15:PHE:H	3:C:23:GLN:HE22	1.25	0.82
2:P:190:ILE:CG2	2:P:232:ILE:HD11	2.08	0.81
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.79	0.81
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.92	0.81
5:S:207:LEU:HA	5:S:2(E):ASN:HD22	1.46	0.81
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.78	0.81
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.80	0.81
5:E:207:LEU:HA	5:E:2(E):ASN:HD22	1.46	0.80
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.46	0.80
4:D:243:ALA:O	4:D:244:GLU:HB2	1.79	0.80
2:B:190:ILE:CG2	2:B:232:ILE:HD11	2.11	0.80
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.81	0.80
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.46	0.80
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.45	0.80
2:P:160:TRP:CE2	2:P:163:ILE:HD12	2.18	0.79
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.63	0.79
2:B:160:TRP:CE2	2:B:163:ILE:HD12	2.18	0.79
3:C:163:GLN:HE21	3:C:164:THR:N	1.80	0.79
2:P:190:ILE:HG21	2:P:232:ILE:HD11	1.65	0.78
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.46	0.78
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.97	0.78
13:1:211:ILE:HD13	13:1:211:ILE:H	1.49	0.78
12:L:33:LYS:HD2	12:L:46:ASN:HD22	1.48	0.78
2:P:219:GLU:HG2	2:P:21(E):VAL:H	1.49	0.78
5:E:15:PHE:H	6:F:23:GLN:HE22	1.32	0.78
2:B:219:GLU:HG2	2:B:21(E):VAL:H	1.46	0.78
14:2:20:THR:HG23	14:2:31:THR:OG1	1.86	0.76
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.51	0.76
4:R:12(D):ALA:HB3	4:R:126:ARG:HD3	1.66	0.76
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.51	0.76
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:H	1.90	0.76
2:B:41:MET:HE3	16:B:240:HOH:O	1.85	0.76
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.68	0.75
3:Q:65:SER:HB2	16:Q:247:HOH:O	1.86	0.75
4:D:12(D):ALA:HB3	4:D:126:ARG:HD3	1.69	0.75
1:O:20:LYS:HE3	1:O:25:ASP:OD1	1.86	0.75
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.17	0.75
2:B:190:ILE:HG21	2:B:232:ILE:HD11	1.69	0.74
6:T:18:ASP:OD1	6:T:20:ARG:HD3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:18:ASP:OD1	6:F:20:ARG:HD3	1.87	0.74
14:N:20:THR:HG23	14:N:31:THR:OG1	1.87	0.74
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.83	0.74
13:M:211:ILE:HD13	13:M:211:ILE:H	1.51	0.74
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.69	0.74
1:A:20:LYS:HE3	1:A:25:ASP:OD1	1.86	0.74
12:Z:33:LYS:HD2	12:Z:46:ASN:HD22	1.53	0.74
2:P:185:LYS:HD3	2:P:186:VAL:N	2.03	0.74
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.70	0.74
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.69	0.74
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.70	0.74
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.02	0.73
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.01	0.73
5:E:132:TYR:O	5:E:153:PRO:HB3	1.88	0.73
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.18	0.73
16:B:258:HOH:O	3:C:33:ARG:HD2	1.89	0.73
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.69	0.73
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.71	0.73
13:1:76:PRO:HD2	13:1:105:GLN:OE1	1.88	0.73
11:K:10(B):LYS:N	11:K:10(B):LYS:HD2	1.97	0.73
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.37	0.73
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.52	0.73
3:Q:52:ARG:HD2	3:Q:208:LYS:O	1.89	0.72
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.70	0.72
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.71	0.72
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.35	0.72
11:Y:10(B):LYS:N	11:Y:10(B):LYS:HD2	1.97	0.72
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.55	0.72
2:B:219:GLU:HG2	2:B:21(E):VAL:N	2.05	0.72
9:W:192:ARG:HG3	16:W:200:HOH:O	1.90	0.72
2:B:185:LYS:HD3	2:B:186:VAL:N	2.05	0.72
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.71	0.72
2:P:6:ARG:HG2	3:Q:10:ARG:HH21	1.53	0.72
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.72	0.71
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.71	0.71
5:S:132:TYR:O	5:S:153:PRO:HB3	1.89	0.71
2:B:202:THR:HG22	2:B:204:SER:N	2.03	0.71
11:K:142:TYR:O	11:K:143:LYS:HD2	1.89	0.71
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.04	0.71
3:C:41:LYS:HG2	3:C:161:SER:O	1.89	0.71
7:U:59:LEU:O	7:U:61:PRO:HD3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:10(B):LYS:H	11:K:10(B):LYS:CD	1.90	0.71
2:P:219:GLU:HG2	2:P:21(E):VAL:N	2.06	0.71
3:C:52:ARG:HD2	3:C:208:LYS:O	1.90	0.71
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.21	0.71
3:C:71:ASP:HA	10:J:68:ILE:HD13	1.72	0.71
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.04	0.70
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.73	0.70
4:R:192:LEU:O	4:R:196:ILE:HG12	1.92	0.70
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.37	0.70
14:2:84:LYS:HG3	14:2:119:VAL:HG22	1.71	0.70
13:M:76:PRO:HD2	13:M:105:GLN:OE1	1.91	0.70
11:Y:142:TYR:O	11:Y:143:LYS:HD2	1.92	0.70
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.92	0.70
9:W:6:MET:HE3	9:W:155:ILE:HD12	1.73	0.69
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.41	0.69
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.72	0.69
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	1.90	0.69
13:1:14(C):ARG:CG	13:1:14(C):ARG:HH11	2.02	0.69
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.75	0.69
13:M:14(C):ARG:CG	13:M:14(C):ARG:HH11	2.05	0.69
12:L:166:HIS:HD2	12:L:168:GLN:H	1.41	0.69
1:O:121:GLN:O	1:O:124:THR:HB	1.92	0.69
2:B:121:GLN:O	2:B:124:THR:HB	1.93	0.69
7:G:59:LEU:O	7:G:61:PRO:HD3	1.93	0.68
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.07	0.68
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.74	0.68
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.40	0.68
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.40	0.68
2:P:202:THR:HG22	2:P:204:SER:N	2.03	0.68
1:A:179:ARG:HB3	1:A:179:ARG:NH1	2.08	0.68
3:C:65:SER:HB2	16:C:253:HOH:O	1.94	0.68
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.27	0.68
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.58	0.68
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.07	0.67
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.42	0.67
4:R:207:LEU:CD2	4:R:233:ILE:HD12	2.24	0.67
5:E:207:LEU:HA	5:E:2(E):ASN:ND2	2.09	0.67
5:E:226:GLY:O	5:E:229:VAL:HG22	1.93	0.67
4:D:207:LEU:CD2	4:D:233:ILE:HD12	2.24	0.67
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.09	0.67
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:220:PRO:O	5:S:222:THR:HG23	1.95	0.67
7:U:96:ALA:CA	7:U:107:MET:HE2	2.23	0.67
5:S:207:LEU:HA	5:S:2(E):ASN:ND2	2.09	0.67
9:I:137:MET:HE3	9:I:141:LEU:HD11	1.77	0.67
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.09	0.67
1:A:4:MET:SD	1:A:5:THR:N	2.60	0.67
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.75	0.67
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.77	0.67
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.75	0.67
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.77	0.67
1:A:121:GLN:O	1:A:124:THR:HB	1.95	0.66
4:D:192:LEU:O	4:D:196:ILE:HG12	1.95	0.66
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	1.96	0.66
9:I:6:MET:HE3	9:I:155:ILE:HD12	1.76	0.66
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.31	0.66
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.25	0.66
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.78	0.66
7:G:121:GLN:O	7:G:124:THR:HB	1.96	0.66
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.76	0.66
1:O:27:ALA:O	1:O:31:VAL:HG23	1.96	0.66
10:J:168:MET:HG2	10:X:168:MET:CE	2.26	0.66
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.43	0.66
2:B:181:LYS:O	2:B:184:MET:HG3	1.95	0.66
7:U:87:ASN:HD22	7:U:87:ASN:C	1.98	0.66
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	2.11	0.66
12:Z:21:ILE:HD12	12:Z:21:ILE:C	2.16	0.66
5:S:226:GLY:O	5:S:229:VAL:HG22	1.96	0.66
7:G:96:ALA:CA	7:G:107:MET:HE2	2.26	0.65
2:P:121:GLN:O	2:P:124:THR:HB	1.96	0.65
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.26	0.65
3:C:105:ASP:OD2	3:C:106:PRO:HD2	1.96	0.65
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.26	0.65
6:F:35:THR:HG21	6:F:51:GLU:O	1.96	0.65
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.11	0.65
10:J:168:MET:CE	10:X:168:MET:HG2	2.25	0.65
7:G:172:ILE:HD11	7:G:201:LEU:HD21	1.78	0.65
3:C:185:THR:HG22	3:C:187:GLU:N	2.10	0.65
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.79	0.65
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.42	0.65
5:E:177:GLU:OE1	6:F:56:SER:HB2	1.96	0.65
2:B:6:ARG:HG2	3:C:10:ARG:HH21	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:161:ASN:N	5:S:58:LEU:O	2.30	0.65
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.77	0.65
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.61	0.65
13:1:40:ASN:HD22	13:1:40:ASN:H	1.44	0.65
6:T:35:THR:HG21	6:T:51:GLU:O	1.97	0.65
3:Q:170:LYS:HB2	16:Q:254:HOH:O	1.97	0.65
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.79	0.65
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.79	0.65
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.32	0.65
2:P:181:LYS:O	2:P:184:MET:HG3	1.97	0.65
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.27	0.64
10:J:-1:MET:HG2	10:J:1:ASP:H	1.62	0.64
5:S:207:LEU:N	5:S:207:LEU:HD23	2.12	0.64
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.43	0.64
7:G:198:ILE:HG23	7:G:203:THR:O	1.97	0.64
9:I:106:GLY:HA2	9:I:181:LYS:HD3	1.79	0.64
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.62	0.64
3:Q:186:VAL:O	3:Q:190:VAL:HG23	1.97	0.64
7:U:121:GLN:O	7:U:124:THR:HB	1.96	0.64
7:U:198:ILE:HG23	7:U:203:THR:O	1.97	0.64
10:J:168:MET:HE3	10:X:168:MET:HG2	1.80	0.64
4:R:102:TYR:O	12:Z:81:ARG:HG3	1.97	0.64
12:L:114:ASP:HB2	12:L:118:SER:HB3	1.80	0.64
7:U:236:ILE:HD12	7:U:237:ALA:N	2.13	0.64
2:B:228:GLU:O	2:B:232:ILE:HG22	1.98	0.64
9:I:48:LEU:HG	9:I:50:THR:HG22	1.80	0.64
1:A:225:THR:OG1	1:A:228:GLU:HG3	1.98	0.64
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.46	0.64
4:R:12(D):ALA:HB3	4:R:126:ARG:CD	2.28	0.63
9:W:48:LEU:HG	9:W:50:THR:HG22	1.79	0.63
3:C:46:VAL:O	3:C:215:VAL:HG12	1.98	0.63
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.80	0.63
6:T:186:ALA:O	6:T:190:VAL:HG23	1.97	0.63
12:L:21:ILE:HD12	12:L:21:ILE:C	2.18	0.63
7:G:87:ASN:C	7:G:87:ASN:HD22	2.02	0.63
5:E:198:SER:HA	5:E:201:LEU:HG	1.79	0.63
2:P:97:GLN:NE2	9:W:64:ASN:HD22	1.96	0.63
13:M:40:ASN:H	13:M:40:ASN:HD22	1.44	0.63
5:S:198:SER:HA	5:S:201:LEU:HG	1.79	0.63
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.81	0.63
5:S:180:LEU:HA	5:S:18(C):PHE:CE2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.79	0.63
3:C:175:PHE:O	3:C:179:ASN:HB2	1.98	0.63
10:X:147:THR:OG1	10:X:150:GLU:HG3	1.99	0.63
2:P:6:ARG:HG2	3:Q:10:ARG:NH2	2.14	0.63
1:A:27:ALA:O	1:A:31:VAL:HG23	1.98	0.63
12:Z:114:ASP:HB2	12:Z:118:SER:HB3	1.78	0.63
10:J:147:THR:OG1	10:J:150:GLU:HG3	1.98	0.63
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.64	0.63
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.47	0.63
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.29	0.63
10:X:-1:MET:HG2	10:X:1:ASP:H	1.63	0.63
12:Z:-9:GLN:HE21	13:1:-8:THR:HG21	1.63	0.63
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.80	0.62
5:E:220:PRO:O	5:E:222:THR:HG23	1.97	0.62
5:S:104:ASN:HB2	13:1:81:GLU:HG2	1.79	0.62
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.80	0.62
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.79	0.62
7:U:18(G):GLU:HG2	7:U:188:LYS:HB2	1.81	0.62
5:S:177:GLU:OE1	6:T:56:SER:HB2	1.99	0.62
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.64	0.62
3:Q:173:ARG:O	3:Q:177:GLU:HG3	1.99	0.62
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.81	0.62
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.81	0.62
12:L:148:VAL:O	12:L:152:ILE:HG12	2.00	0.62
9:W:106:GLY:HA2	9:W:181:LYS:HD3	1.80	0.62
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.00	0.62
12:L:-7:ASN:ND2	12:L:-5:TYR:H	1.98	0.62
10:X:156:LYS:O	10:X:160:GLN:HG3	1.98	0.62
7:U:172:ILE:HD11	7:U:201:LEU:HD21	1.79	0.62
4:D:102:TYR:O	12:L:81:ARG:HG3	1.99	0.62
5:E:207:LEU:HD23	5:E:207:LEU:N	2.14	0.62
1:O:4:MET:SD	1:O:5:THR:N	2.62	0.62
2:B:97:GLN:NE2	9:I:64:ASN:HD22	1.98	0.62
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	1.82	0.62
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.15	0.62
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.82	0.62
3:C:186:VAL:O	3:C:190:VAL:HG23	2.00	0.61
9:W:66:TYR:CE1	9:W:70:GLU:HG3	2.35	0.61
4:R:121:LEU:HB2	16:R:853:HOH:O	1.99	0.61
4:D:154:SER:OG	4:D:156:THR:HG23	2.00	0.61
2:P:71:ASN:ND2	2:P:72:ASP:N	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:12(D):ALA:HB3	4:D:126:ARG:CD	2.30	0.61
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.82	0.61
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.82	0.61
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.82	0.61
4:R:154:SER:OG	4:R:156:THR:HG23	2.00	0.61
11:K:20:ALA:HB2	11:K:31:VAL:HG21	1.83	0.61
11:K:99:THR:HG22	11:K:113:VAL:O	2.01	0.61
1:O:159:PRO:O	2:P:59:LEU:HD12	2.00	0.61
16:P:248:HOH:O	3:Q:87:ILE:HD11	1.98	0.61
13:M:139:ARG:HH11	8:V:165:ASN:ND2	1.99	0.61
3:C:100:ARG:NH1	3:C:106:PRO:HB3	2.16	0.61
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.00	0.61
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.31	0.61
7:G:18(G):GLU:HG2	7:G:188:LYS:HB2	1.83	0.61
10:J:168:MET:HG2	10:X:168:MET:HE3	1.83	0.61
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.65	0.61
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.48	0.60
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.82	0.60
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.36	0.60
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.31	0.60
7:G:172:ILE:HD12	7:G:197:MET:CE	2.31	0.60
3:Q:175:PHE:O	3:Q:179:ASN:HB2	2.00	0.60
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.35	0.60
3:Q:71:ASP:HA	10:X:68:ILE:HD13	1.82	0.60
13:1:19:LEU:HD21	13:1:26:LEU:HD22	1.82	0.60
2:B:71:ASN:ND2	2:B:72:ASP:N	2.47	0.60
5:S:207:LEU:HD23	5:S:207:LEU:H	1.65	0.60
2:B:15:PHE:H	3:C:23:GLN:NE2	1.98	0.60
8:V:172:ASN:ND2	8:V:193:THR:HA	2.17	0.60
2:P:160:TRP:CD2	2:P:163:ILE:HD12	2.37	0.60
12:Z:148:VAL:O	12:Z:152:ILE:HG12	2.00	0.60
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.83	0.60
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.36	0.60
1:A:58:LEU:HD12	7:G:173:THR:HG23	1.84	0.60
6:F:186:ALA:O	6:F:190:VAL:HG23	2.00	0.60
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.82	0.60
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.84	0.60
7:U:172:ILE:HD12	7:U:197:MET:CE	2.31	0.60
16:F:246:HOH:O	7:G:86:ARG:HD2	2.01	0.60
10:J:156:LYS:O	10:J:160:GLN:HG3	2.02	0.60
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.50	0.60
10:J:-1:MET:HG2	10:J:1:ASP:N	2.17	0.60
6:T:127:ASN:HD22	6:T:127:ASN:C	2.05	0.60
6:T:237:GLN:O	6:T:240:ILE:HG22	2.01	0.60
5:S:18(C):PHE:O	5:S:18(F):ILE:HG12	2.02	0.59
7:G:236:ILE:HD12	7:G:237:ALA:N	2.17	0.59
5:E:180:LEU:HA	5:E:18(C):PHE:CE2	2.36	0.59
2:B:160:TRP:CD2	2:B:163:ILE:HD12	2.36	0.59
6:T:127:ASN:HD22	6:T:128:SER:N	2.00	0.59
2:P:41:MET:HE3	16:Q:246:HOH:O	2.02	0.59
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.83	0.59
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.84	0.59
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.83	0.59
14:2:89:GLU:HA	14:2:89:GLU:OE1	2.02	0.59
9:W:97:VAL:HG23	9:W:99:PRO:HD3	1.84	0.59
2:B:141:TYR:CD1	2:B:21(E):VAL:HG21	2.37	0.59
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.85	0.59
2:P:228:GLU:O	2:P:232:ILE:HG22	2.01	0.59
8:H:165:ASN:ND2	13:1:139:ARG:HH11	1.99	0.59
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.84	0.59
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.84	0.59
13:M:14(A):VAL:O	13:M:14(A):VAL:HG23	2.02	0.59
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.16	0.59
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.85	0.59
14:2:112:THR:CG2	14:2:120:HIS:HB2	2.32	0.59
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.15	0.59
10:X:-1:MET:HG2	10:X:1:ASP:N	2.17	0.59
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.33	0.59
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.85	0.59
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.85	0.59
8:V:148:LYS:O	8:V:152:ILE:HG12	2.01	0.59
1:O:184:LEU:HB2	16:O:248:HOH:O	2.02	0.59
5:E:18(C):PHE:O	5:E:18(F):ILE:HG12	2.02	0.59
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.84	0.59
6:F:237:GLN:O	6:F:240:ILE:HG22	2.03	0.59
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.85	0.59
6:F:127:ASN:HD22	6:F:128:SER:N	2.01	0.59
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.84	0.59
12:Z:3:ILE:HD12	12:Z:46:ASN:HB2	1.85	0.59
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.49	0.59
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:244:HOH:O	7:U:86:ARG:HD2	2.02	0.59
1:O:150:GLN:O	1:O:157:TYR:HA	2.03	0.59
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.03	0.59
5:E:207:LEU:HD23	5:E:207:LEU:H	1.68	0.58
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.00	0.58
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.84	0.58
9:I:97:VAL:HG23	9:I:99:PRO:HD3	1.84	0.58
1:A:173:LYS:O	1:A:177:GLU:HG3	2.03	0.58
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.84	0.58
3:Q:159:SER:HB2	16:Q:258:HOH:O	2.03	0.58
14:N:89:GLU:HA	14:N:89:GLU:OE1	2.02	0.58
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.38	0.58
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.84	0.58
7:G:18(G):GLU:HG2	7:G:188:LYS:CB	2.33	0.58
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.68	0.58
2:P:11:ARG:O	2:P:14:ILE:HD12	2.02	0.58
1:O:33:GLN:HA	1:O:33:GLN:HE21	1.66	0.58
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.39	0.58
10:J:64:GLN:NE2	16:J:215:HOH:O	2.34	0.58
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.84	0.58
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.85	0.58
1:A:51:GLU:OE1	1:A:202:VAL:HG22	2.03	0.58
10:J:167:PRO:CB	10:X:168:MET:HE1	2.33	0.58
3:C:173:ARG:O	3:C:177:GLU:HG3	2.03	0.58
7:U:18(G):GLU:HG2	7:U:188:LYS:CB	2.34	0.58
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.85	0.58
11:K:37:ILE:HD12	11:K:59:LEU:HD23	1.86	0.58
7:U:77:VAL:CG1	7:U:137:THR:HB	2.34	0.58
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	2.02	0.57
4:R:68:VAL:HG21	4:R:89:ILE:HD13	1.86	0.57
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.87	0.57
3:C:15:PHE:CE1	3:C:21:ILE:HD11	2.40	0.57
2:P:87:ILE:O	2:P:91:THR:HG23	2.04	0.57
10:J:168:MET:HE1	10:X:167:PRO:CB	2.33	0.57
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.17	0.57
12:Z:99:THR:HG22	16:Z:203:HOH:O	2.04	0.57
6:F:21(B):THR:O	6:F:21(C):ASN:HB2	2.03	0.57
11:Y:37:ILE:HD12	11:Y:59:LEU:HD23	1.86	0.57
7:G:8:TYR:C	7:G:10:ARG:H	2.07	0.57
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.86	0.57
5:E:40:LEU:HD23	5:E:40:LEU:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:77:VAL:CG1	7:G:137:THR:HB	2.34	0.57
8:V:196:VAL:HG23	16:V:246:HOH:O	2.03	0.57
9:W:66:TYR:CZ	9:W:70:GLU:HG3	2.40	0.57
9:I:66:TYR:CE1	9:I:70:GLU:HG3	2.39	0.57
4:D:177:LEU:HD22	5:E:58:LEU:CD1	2.35	0.57
6:F:127:ASN:HD22	6:F:127:ASN:C	2.07	0.57
2:P:46:ILE:HD11	2:P:146:TYR:HB3	1.85	0.57
5:S:38:VAL:HG22	5:S:164:ALA:HB2	1.86	0.57
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.86	0.57
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.70	0.57
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.87	0.57
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.87	0.57
12:Z:3:ILE:HD13	12:Z:127:GLY:O	2.05	0.57
8:V:200:LYS:HE3	9:W:140:SER:O	2.04	0.57
5:E:76:LEU:HD12	5:E:136:LEU:HD22	1.86	0.57
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.40	0.57
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.40	0.57
6:T:21(B):THR:O	6:T:21(C):ASN:HB2	2.05	0.57
1:A:150:GLN:O	1:A:157:TYR:HA	2.05	0.57
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.40	0.57
3:C:235:GLN:O	3:C:239:GLU:HG2	2.05	0.57
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.40	0.57
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.70	0.57
8:V:172:ASN:HD22	8:V:193:THR:HA	1.69	0.56
14:2:104:TYR:OH	14:2:180:ALA:HB2	2.05	0.56
8:H:144:GLN:O	8:H:145:ASP:HB2	2.04	0.56
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.86	0.56
6:F:40:ILE:HD12	6:F:193:ALA:HB2	1.88	0.56
2:B:27:ALA:O	2:B:31:ILE:HG12	2.05	0.56
7:G:107:MET:HE1	7:G:112:LEU:HD13	1.87	0.56
4:R:243:ALA:O	4:R:244:GLU:CB	2.53	0.56
2:P:163:ILE:HG12	2:P:164:SER:N	2.21	0.56
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.18	0.56
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.03	0.56
1:A:97:HIS:HD2	8:H:61:SER:OG	1.88	0.56
4:D:68:VAL:HG21	4:D:89:ILE:HD13	1.88	0.56
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.69	0.56
5:E:231:LYS:HD2	5:E:231:LYS:H	1.69	0.56
7:U:56:ASP:HB3	7:U:59:LEU:HG	1.87	0.56
3:C:57:LYS:O	3:C:58:LEU:HB2	2.06	0.56
8:H:172:ASN:ND2	8:H:193:THR:HA	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:14(A):VAL:O	13:1:14(A):VAL:HG23	2.06	0.56
1:O:51:GLU:OE1	1:O:202:VAL:HG22	2.04	0.56
8:V:144:GLN:O	8:V:145:ASP:HB2	2.06	0.56
12:L:8:GLY:HA3	12:L:11:PHE:CZ	2.40	0.56
9:W:29:ASN:H	9:W:29:ASN:ND2	2.04	0.56
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.70	0.56
4:R:186:LEU:O	4:R:190:GLU:HG3	2.06	0.56
4:R:40:ILE:CD1	4:R:193:VAL:HG23	2.34	0.56
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.21	0.56
8:H:148:LYS:O	8:H:152:ILE:HG12	2.06	0.56
2:B:87:ILE:O	2:B:91:THR:HG23	2.05	0.56
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.71	0.56
5:S:40:LEU:HD23	5:S:40:LEU:N	2.21	0.56
4:D:207:LEU:HD23	4:D:207:LEU:C	2.27	0.56
13:M:4:ILE:HD12	13:M:155:ILE:HD12	1.87	0.56
5:S:231:LYS:H	5:S:231:LYS:HD2	1.71	0.56
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.21	0.55
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.35	0.55
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.86	0.55
3:Q:163:GLN:HA	3:Q:163:GLN:HE21	1.71	0.55
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.07	0.55
5:S:207:LEU:H	5:S:207:LEU:CD2	2.18	0.55
14:2:84:LYS:HG3	14:2:119:VAL:CG2	2.36	0.55
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.88	0.55
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.22	0.55
1:O:173:LYS:O	1:O:177:GLU:HG3	2.05	0.55
2:B:46:ILE:HD11	2:B:146:TYR:HB3	1.87	0.55
2:P:141:TYR:CD1	2:P:21(E):VAL:HG21	2.42	0.55
5:S:18(C):PHE:HA	5:S:18(F):ILE:HG12	1.89	0.55
4:D:186:LEU:O	4:D:190:GLU:HG3	2.06	0.55
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.89	0.55
4:R:177:LEU:HD22	5:S:58:LEU:CD1	2.36	0.55
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.89	0.55
4:D:81:LEU:HD12	4:D:133:GLY:HA3	1.88	0.55
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.88	0.55
2:B:21:LEU:O	2:B:25:GLU:HG2	2.06	0.55
12:Z:33:LYS:HD2	12:Z:46:ASN:ND2	2.21	0.55
2:P:186:VAL:HG21	2:P:216:ARG:HD3	1.87	0.55
2:P:14:ILE:HD13	2:P:14:ILE:H	1.71	0.55
5:E:38:VAL:HG22	5:E:164:ALA:HB2	1.88	0.55
12:Z:14(I):THR:O	12:Z:14(K):LYS:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:67:ILE:CG2	5:E:223:ILE:HD13	2.36	0.55
4:R:160:TYR:HA	5:S:59:SER:HA	1.88	0.55
12:L:3:ILE:HD13	12:L:127:GLY:O	2.06	0.55
6:F:21(B):THR:HG22	6:F:222:LYS:HD3	1.89	0.55
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.89	0.55
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.89	0.55
7:U:8:TYR:C	7:U:10:ARG:H	2.09	0.55
3:Q:15:PHE:CE1	3:Q:21:ILE:HD11	2.41	0.55
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.37	0.55
9:I:66:TYR:CZ	9:I:70:GLU:HG3	2.42	0.55
6:T:21(B):THR:HG22	6:T:222:LYS:HD3	1.88	0.55
2:P:27:ALA:O	2:P:31:ILE:HG12	2.07	0.55
5:E:18(D):ILE:HG23	5:E:18(E):LYS:HG3	1.88	0.55
13:1:152:GLU:O	13:1:156:VAL:HG23	2.07	0.55
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.89	0.55
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.07	0.55
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.89	0.55
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.71	0.55
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.88	0.55
11:K:7:ARG:HD2	11:K:108:PRO:O	2.06	0.55
10:X:6:ILE:CG2	10:X:13:ILE:HB	2.36	0.55
2:P:101:LYS:NZ	10:X:85:GLN:HE22	2.06	0.54
12:Z:8:GLY:HA3	12:Z:11:PHE:CZ	2.42	0.54
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.88	0.54
9:I:137:MET:CE	9:I:141:LEU:HD11	2.36	0.54
8:H:200:LYS:HE3	9:I:140:SER:O	2.07	0.54
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.07	0.54
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.89	0.54
12:L:3:ILE:HD12	12:L:46:ASN:HB2	1.90	0.54
6:T:40:ILE:HD12	6:T:193:ALA:HB2	1.90	0.54
14:2:10(B):LYS:C	14:2:10(B):LYS:HD3	2.27	0.54
6:F:20(B):GLU:HG3	6:F:20(C):LYS:N	2.23	0.54
4:R:207:LEU:C	4:R:207:LEU:HD23	2.27	0.54
12:L:14(I):THR:O	12:L:1(I):ASN:HB3	2.08	0.54
5:S:67:ILE:CG2	5:S:223:ILE:HD13	2.37	0.54
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.89	0.54
5:S:18(D):ILE:HG23	5:S:18(E):LYS:HG3	1.89	0.54
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.22	0.54
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.89	0.54
3:Q:33:ARG:HH11	3:Q:33:ARG:HB2	1.73	0.54
7:U:67:ILE:CD1	7:U:211:GLU:HG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:41:ILE:HD12	14:N:76:THR:HA	1.90	0.54
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.88	0.54
4:R:53:ARG:HG2	4:R:53:ARG:O	2.07	0.54
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.89	0.54
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.43	0.54
6:T:88:LEU:HD11	6:T:116:LEU:HD22	1.89	0.54
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.08	0.54
13:1:4:ILE:HD12	13:1:155:ILE:HD12	1.90	0.54
5:S:15:PHE:H	6:T:23:GLN:NE2	2.00	0.54
12:L:33:LYS:HD2	12:L:46:ASN:ND2	2.20	0.54
2:B:186:VAL:HG21	2:B:216:ARG:HD3	1.89	0.54
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.89	0.54
6:T:20(B):GLU:HG3	6:T:20(C):LYS:N	2.22	0.54
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.38	0.54
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.42	0.54
14:2:14:LEU:O	14:2:175:MET:HA	2.08	0.54
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.08	0.54
8:H:196:VAL:HG23	16:H:245:HOH:O	2.08	0.54
5:E:167:ALA:HB3	16:E:243:HOH:O	2.07	0.54
10:J:6:ILE:CG2	10:J:13:ILE:HB	2.38	0.54
14:N:10(B):LYS:HD3	14:N:10(B):LYS:C	2.28	0.54
2:B:163:ILE:HG12	2:B:164:SER:N	2.24	0.53
7:U:87:ASN:ND2	7:U:87:ASN:C	2.60	0.53
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.23	0.53
13:M:57:ARG:NE	16:M:239:HOH:O	2.40	0.53
13:M:149:GLN:NE2	13:M:149:GLN:H	2.05	0.53
8:V:36:ARG:HG3	8:V:38:SER:O	2.08	0.53
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.90	0.53
12:Z:17:ASP:OD2	12:Z:33:LYS:NZ	2.40	0.53
2:B:11:ARG:O	2:B:14:ILE:HD12	2.08	0.53
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.57	0.53
14:N:92:ASP:HB2	16:N:199:HOH:O	2.08	0.53
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.91	0.53
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.72	0.53
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.24	0.53
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.43	0.53
9:I:29:ASN:H	9:I:29:ASN:ND2	2.06	0.53
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.90	0.53
11:Y:10(A):ARG:HD3	11:Y:180:GLU:OE1	2.09	0.53
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.24	0.53
6:F:176:LEU:O	6:F:180:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.24	0.53
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.91	0.53
5:S:227:GLU:N	5:S:227:GLU:CD	2.62	0.53
1:A:85:TYR:O	1:A:89:VAL:HG23	2.08	0.53
10:J:162:LEU:O	10:J:166:MET:HB2	2.09	0.53
12:Z:-8:PHE:CB	13:1:-8:THR:HG23	2.39	0.53
3:C:190:VAL:O	3:C:194:VAL:HG23	2.08	0.53
5:E:207:LEU:CD2	5:E:207:LEU:H	2.21	0.53
4:R:21:LEU:HD21	5:S:130:ARG:HD2	1.89	0.53
3:C:7:GLY:N	16:C:271:HOH:O	2.41	0.53
12:L:13:VAL:HG12	12:L:177:ILE:HG13	1.91	0.53
3:C:227:GLU:OE1	3:C:227:GLU:N	2.38	0.53
11:K:13:ILE:HG13	11:K:151:ALA:HB1	1.90	0.53
4:D:170:GLU:N	4:D:170:GLU:OE1	2.41	0.53
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.35	0.53
5:S:134:VAL:O	5:S:153:PRO:HG3	2.08	0.53
12:Z:14(I):THR:HG21	12:Z:14(M):VAL:HB	1.91	0.53
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.90	0.53
11:Y:13:ILE:HG13	11:Y:151:ALA:HB1	1.90	0.53
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.90	0.53
7:G:118:ASN:O	7:G:122:ILE:HD12	2.09	0.53
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.38	0.53
10:J:52:THR:CG2	10:J:53:VAL:N	2.72	0.53
14:N:14:LEU:O	14:N:175:MET:HA	2.09	0.53
6:T:41:LYS:HA	6:T:46:VAL:HG12	1.91	0.53
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.74	0.53
1:A:69:LEU:HD23	1:A:69:LEU:C	2.29	0.53
14:2:85:GLU:O	14:2:89:GLU:HB2	2.09	0.53
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.90	0.53
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.90	0.53
3:C:163:GLN:CA	3:C:163:GLN:HE21	2.22	0.53
2:P:185:LYS:HD3	2:P:186:VAL:H	1.74	0.53
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.44	0.53
12:L:61:ASN:ND2	16:L:218:HOH:O	2.41	0.53
9:W:137:MET:CE	9:W:141:LEU:HD11	2.39	0.53
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.38	0.53
13:1:46:SER:OG	13:1:98:ALA:HB3	2.09	0.53
8:H:36:ARG:HG3	8:H:38:SER:O	2.09	0.53
6:T:192:GLN:O	6:T:196:ILE:HG12	2.09	0.53
5:E:227:GLU:CD	5:E:227:GLU:N	2.62	0.53
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:17:ASP:HA	13:M:173:PHE:CB	2.39	0.52
8:V:128:GLY:O	8:V:131:SER:HB2	2.09	0.52
5:S:41:ARG:NH1	5:S:42:SER:O	2.43	0.52
12:Z:14(I):THR:O	12:Z:1(I):ASN:HB3	2.07	0.52
6:T:136:THR:O	6:T:150:MET:HA	2.10	0.52
2:P:77:ALA:HB3	2:P:137:ILE:HB	1.90	0.52
12:Z:27:ASN:HB3	13:1:120:TYR:CZ	2.45	0.52
4:D:112:LEU:C	4:D:112:LEU:HD13	2.30	0.52
14:N:84:LYS:HG3	14:N:119:VAL:CG2	2.38	0.52
12:L:14(I):THR:O	12:L:14(K):LYS:HB2	2.09	0.52
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.90	0.52
11:K:196:PHE:HB3	16:K:215:HOH:O	2.09	0.52
5:S:148:LEU:HD23	5:S:162:GLY:HA2	1.91	0.52
4:R:227:GLU:O	4:R:231:GLU:HG3	2.09	0.52
5:E:41:ARG:NH1	5:E:42:SER:O	2.43	0.52
1:A:21(A):GLU:HG3	16:A:260:HOH:O	2.10	0.52
6:T:176:LEU:O	6:T:180:VAL:HG23	2.08	0.52
12:Z:42:VAL:CG2	12:Z:102:ALA:HB3	2.40	0.52
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.75	0.52
6:F:20(B):GLU:HG3	6:F:20(C):LYS:HG3	1.92	0.52
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.90	0.52
2:B:15:PHE:N	3:C:23:GLN:HE22	2.02	0.52
12:Z:-7:ASN:HD22	12:Z:-7:ASN:C	2.12	0.52
10:X:113:ILE:HA	10:X:118:THR:O	2.10	0.52
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.10	0.52
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.10	0.52
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.90	0.52
5:S:73:HIS:HE1	5:S:107:LEU:O	1.92	0.52
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.22	0.52
5:S:201:LEU:O	5:S:202:ARG:HB2	2.09	0.52
12:L:14(I):THR:HG21	12:L:14(M):VAL:HB	1.92	0.52
2:B:77:ALA:HB3	2:B:137:ILE:HB	1.92	0.52
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.92	0.52
10:X:52:THR:CG2	10:X:53:VAL:N	2.72	0.52
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.92	0.52
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.17	0.52
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.10	0.52
6:T:127:ASN:ND2	6:T:127:ASN:C	2.63	0.52
11:K:4:LEU:HD13	11:K:15:ALA:O	2.09	0.52
16:S:242:HOH:O	6:T:12:ASN:HB2	2.09	0.52
6:F:192:GLN:O	6:F:196:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:239:THR:OXT	2:P:239:THR:HG22	2.09	0.52
6:F:69:VAL:HG12	16:F:249:HOH:O	2.09	0.52
1:O:69:LEU:HD23	1:O:69:LEU:C	2.30	0.52
4:D:243:ALA:O	4:D:244:GLU:CB	2.53	0.52
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.92	0.52
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.91	0.52
2:P:150:THR:O	2:P:157:TYR:HA	2.09	0.52
10:J:113:ILE:HA	10:J:118:THR:O	2.10	0.52
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.75	0.52
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.92	0.52
6:F:216:SER:HB3	6:F:21(A):GLU:HB2	1.91	0.52
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.93	0.52
7:G:87:ASN:ND2	7:G:87:ASN:C	2.64	0.52
11:K:199:VAL:O	11:K:203:GLU:HB3	2.10	0.52
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.92	0.52
3:Q:241:GLN:C	3:Q:243:GLN:H	2.14	0.52
1:O:58:LEU:HD12	7:U:173:THR:HG23	1.92	0.52
3:C:15:PHE:N	4:D:23:GLN:HE22	1.93	0.51
5:E:18(C):PHE:HA	5:E:18(F):ILE:HG12	1.91	0.51
5:E:67:ILE:HG22	5:E:223:ILE:HD13	1.92	0.51
14:2:41:ILE:HD12	14:2:76:THR:HA	1.92	0.51
7:U:140:SER:HA	7:U:215:ALA:HB1	1.92	0.51
7:G:141:VAL:HG21	7:G:216:THR:HA	1.92	0.51
3:C:141:PHE:CE1	3:C:217:PRO:HG3	2.45	0.51
6:T:216:SER:HB3	6:T:21(A):GLU:HB2	1.92	0.51
3:C:241:GLN:C	3:C:243:GLN:H	2.14	0.51
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.09	0.51
5:E:139:ILE:HG22	5:E:148:LEU:HD13	1.93	0.51
5:E:201:LEU:O	5:E:202:ARG:HB2	2.10	0.51
7:U:236:ILE:HD12	7:U:236:ILE:C	2.30	0.51
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.30	0.51
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.92	0.51
5:S:190:ILE:HG23	5:S:212:ILE:HD13	1.91	0.51
8:H:172:ASN:HD22	8:H:193:THR:HA	1.74	0.51
6:T:147:HIS:HD2	16:T:242:HOH:O	1.94	0.51
3:C:232:TYR:O	3:C:236:ILE:HG13	2.10	0.51
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.93	0.51
13:1:149:GLN:NE2	13:1:149:GLN:H	2.07	0.51
4:D:207:LEU:HD21	4:D:233:ILE:HD12	1.93	0.51
13:M:4:ILE:HD11	13:M:155:ILE:HG23	1.93	0.51
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:LYS:HA	6:F:46:VAL:HG12	1.91	0.51
12:L:93:PHE:N	12:L:94:PRO:HD3	2.25	0.51
13:M:175:LEU:HD23	13:M:175:LEU:C	2.30	0.51
2:P:122:GLY:C	2:P:124:THR:H	2.14	0.51
10:J:133:TYR:OH	10:X:24:ILE:HG12	2.10	0.51
5:E:227:GLU:CD	5:E:227:GLU:H	2.14	0.51
4:D:53:ARG:HG2	4:D:53:ARG:O	2.10	0.51
11:K:10(A):ARG:HD3	11:K:180:GLU:OE1	2.10	0.51
4:R:237:LEU:O	4:R:241:GLU:HG3	2.10	0.51
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.46	0.51
4:R:170:GLU:OE1	4:R:170:GLU:N	2.42	0.51
10:J:10(B):LYS:HB2	10:J:10(B):LYS:NZ	2.26	0.51
1:O:177:GLU:HG2	2:P:58:LEU:HD22	1.91	0.51
6:F:203:GLU:C	6:F:205:ASN:H	2.14	0.51
12:L:5:GLY:O	12:L:124:CYS:HA	2.10	0.51
5:E:142:ASP:HB2	16:M:247:HOH:O	2.11	0.51
1:O:232:ARG:HH11	1:O:232:ARG:HG3	1.74	0.51
3:Q:190:VAL:HG13	3:Q:212:ILE:HG21	1.92	0.51
14:N:85:GLU:O	14:N:89:GLU:HB2	2.10	0.51
5:S:67:ILE:HG22	5:S:223:ILE:CD1	2.41	0.51
12:L:145:TYR:CD1	12:L:146:LEU:N	2.79	0.51
5:E:190:ILE:HG23	5:E:212:ILE:HD13	1.93	0.51
5:E:4:PHE:CG	5:E:5:ARG:N	2.79	0.51
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.46	0.51
11:Y:4:LEU:CD1	11:Y:15:ALA:HB3	2.40	0.51
5:S:67:ILE:HG22	5:S:223:ILE:HD13	1.93	0.51
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.26	0.51
8:V:214:LEU:HD21	9:W:190:LYS:HD2	1.92	0.51
10:J:16:SER:HB2	16:J:205:HOH:O	2.10	0.51
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.92	0.51
5:E:148:LEU:HD23	5:E:162:GLY:HA2	1.93	0.51
4:D:227:GLU:O	4:D:231:GLU:HG3	2.10	0.51
4:D:237:LEU:O	4:D:241:GLU:HG3	2.10	0.51
1:A:86:ARG:HH21	7:G:118:ASN:ND2	2.09	0.50
5:S:227:GLU:CD	5:S:227:GLU:H	2.14	0.50
8:H:214:LEU:HD21	9:I:190:LYS:HD2	1.94	0.50
10:X:143:ARG:O	10:X:146:MET:HG3	2.11	0.50
6:T:20(B):GLU:HG3	6:T:20(C):LYS:HG3	1.92	0.50
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.94	0.50
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.93	0.50
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.46	0.50
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.11	0.50
3:C:177:GLU:OE2	4:D:57:PRO:HD2	2.11	0.50
5:S:76:LEU:HD12	5:S:136:LEU:HD22	1.93	0.50
16:F:246:HOH:O	7:G:83:PRO:HA	2.10	0.50
9:I:114:ASP:HB2	16:I:232:HOH:O	2.11	0.50
5:S:82:ALA:CB	16:S:237:HOH:O	2.59	0.50
1:O:85:TYR:O	1:O:89:VAL:HG23	2.11	0.50
8:V:84:LYS:HG3	8:V:85:GLN:N	2.27	0.50
11:Y:40:PHE:HB3	11:Y:73:ARG:NH2	2.26	0.50
5:E:2(C):VAL:O	5:E:226:GLY:HA2	2.12	0.50
11:Y:4:LEU:HD13	11:Y:15:ALA:O	2.11	0.50
2:B:146:TYR:OH	2:B:21(A):LYS:HB2	2.12	0.50
7:G:140:SER:HA	7:G:215:ALA:HB1	1.92	0.50
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.92	0.50
11:Y:199:VAL:O	11:Y:203:GLU:HB3	2.11	0.50
6:T:203:GLU:C	6:T:205:ASN:H	2.14	0.50
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.46	0.50
1:A:225:THR:O	1:A:229:ILE:HG13	2.11	0.50
13:1:17:ASP:HA	13:1:173:PHE:CB	2.42	0.50
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.93	0.50
3:C:57:LYS:HD2	3:C:58:LEU:N	2.27	0.50
2:P:191:GLU:O	2:P:195:LYS:HG2	2.12	0.50
7:U:131:PRO:HB3	16:U:257:HOH:O	2.11	0.50
6:F:88:LEU:HD11	6:F:116:LEU:HD22	1.94	0.50
8:H:73:GLU:HA	8:H:73:GLU:OE1	2.10	0.50
2:B:107:ILE:HD11	2:B:111:ILE:HG22	1.93	0.50
7:U:118:ASN:O	7:U:122:ILE:HD12	2.11	0.50
10:J:133:TYR:HE1	16:X:220:HOH:O	1.95	0.50
10:J:24:ILE:HG12	10:X:133:TYR:OH	2.11	0.50
13:1:4:ILE:HD11	13:1:155:ILE:HG23	1.94	0.50
2:B:150:THR:O	2:B:157:TYR:HA	2.11	0.50
6:F:136:THR:O	6:F:150:MET:HA	2.12	0.50
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.46	0.50
7:U:107:MET:HE1	7:U:112:LEU:HD13	1.93	0.50
14:N:113:ILE:HG12	14:N:119:VAL:HG13	1.93	0.50
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.27	0.50
3:C:35:THR:HB	3:C:51:GLU:HG3	1.93	0.50
13:M:129:PHE:HE2	14:2:24:ALA:HB3	1.76	0.50
7:U:141:VAL:HG21	7:U:216:THR:HA	1.93	0.50
2:P:202:THR:CG2	2:P:204:SER:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.47	0.49
12:Z:-7:ASN:HD22	12:Z:-6:PRO:N	2.09	0.49
11:K:4:LEU:C	11:K:4:LEU:HD22	2.32	0.49
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.11	0.49
10:J:10(B):LYS:HB2	10:J:10(B):LYS:HZ3	1.77	0.49
5:E:194:VAL:HA	5:E:197:ILE:HG22	1.94	0.49
13:M:46:SER:OG	13:M:98:ALA:HB3	2.12	0.49
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.94	0.49
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.47	0.49
3:Q:55:THR:C	3:Q:56:LEU:HD22	2.32	0.49
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.94	0.49
7:G:233:LEU:O	7:G:236:ILE:HG13	2.12	0.49
6:F:127:ASN:ND2	6:F:127:ASN:C	2.65	0.49
2:P:146:TYR:OH	2:P:21(A):LYS:HB2	2.12	0.49
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.93	0.49
6:F:90:ASN:O	6:F:94:GLU:HG3	2.12	0.49
6:F:11:SER:HB3	6:F:14:VAL:HG23	1.94	0.49
5:S:160:LEU:HD13	5:S:163:THR:HB	1.95	0.49
2:B:191:GLU:O	2:B:195:LYS:HG2	2.12	0.49
2:P:112:LEU:HD23	2:P:112:LEU:C	2.32	0.49
12:L:-7:ASN:HD22	12:L:-6:PRO:N	2.11	0.49
5:E:35:SER:O	5:E:66:LYS:NZ	2.45	0.49
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.47	0.49
7:U:12:ILE:HD13	7:U:12:ILE:H	1.76	0.49
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.11	0.49
2:B:202:THR:CG2	2:B:204:SER:HB2	2.42	0.49
10:X:162:LEU:O	10:X:166:MET:HB2	2.12	0.49
3:C:39:GLY:O	3:C:162:ALA:HA	2.13	0.49
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.42	0.49
12:Z:145:TYR:CD1	12:Z:146:LEU:N	2.80	0.49
12:Z:13:VAL:HG12	12:Z:177:ILE:HG13	1.95	0.49
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.94	0.49
5:S:52:LYS:HD3	5:S:211:SER:HB2	1.94	0.49
14:2:156:LYS:HG2	14:2:18(J):LEU:HD11	1.94	0.49
4:R:85:ALA:HB2	4:R:134:VAL:HG11	1.94	0.49
13:M:-6:GLN:O	13:M:-6:GLN:HG3	2.13	0.49
1:O:225:THR:O	1:O:229:ILE:HG13	2.12	0.49
5:S:139:ILE:HG22	5:S:148:LEU:HD13	1.93	0.49
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.12	0.49
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.94	0.49
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:177:LEU:HA	5:S:58:LEU:HD11	1.94	0.49
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.95	0.49
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.95	0.49
6:T:88:LEU:CD1	6:T:116:LEU:HD22	2.42	0.49
7:G:12:ILE:HG12	7:G:14:ILE:HG23	1.94	0.49
3:C:97:GLN:HG3	10:J:65:LEU:HB2	1.95	0.49
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.27	0.49
5:S:15:PHE:N	6:T:23:GLN:HE22	2.03	0.49
2:P:71:ASN:HD22	2:P:72:ASP:H	1.55	0.49
2:B:160:TRP:HA	3:C:59:GLN:HA	1.95	0.49
3:Q:55:THR:HG22	3:Q:56:LEU:CD2	2.40	0.49
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.93	0.49
7:G:67:ILE:CD1	7:G:211:GLU:HG2	2.40	0.49
7:G:8:TYR:C	7:G:10:ARG:N	2.66	0.49
5:E:38:VAL:HG12	5:E:39:GLY:N	2.28	0.49
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.93	0.49
2:B:49:ALA:HB2	2:B:212:PHE:CE1	2.48	0.49
10:J:148:THR:HG21	10:J:177:ILE:HD13	1.95	0.49
1:A:117:ALA:HB1	1:A:155:GLY:O	2.12	0.49
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.43	0.49
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.94	0.49
7:U:233:LEU:O	7:U:236:ILE:HG13	2.12	0.49
3:C:190:VAL:HG13	3:C:212:ILE:HG21	1.95	0.49
6:F:195:LYS:NZ	16:F:276:HOH:O	2.41	0.49
5:E:73:HIS:HE1	5:E:107:LEU:O	1.96	0.49
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.47	0.49
8:V:105:ASP:HB2	8:V:10(A):PRO:HD2	1.95	0.49
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.95	0.49
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.28	0.49
2:B:14:ILE:H	2:B:14:ILE:HD13	1.77	0.49
7:U:38:LEU:HD23	7:U:197:MET:HE3	1.94	0.49
8:H:128:GLY:O	8:H:131:SER:HB2	2.12	0.49
11:Y:14:VAL:HB	11:Y:176:TYR:HB2	1.95	0.49
14:N:18(G):TYR:HA	14:N:18(J):LEU:HG	1.94	0.49
10:X:110:LEU:O	10:X:121:GLU:HG2	2.13	0.49
11:K:207:ASN:ND2	10:X:144:PRO:CG	2.76	0.49
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.78	0.49
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.95	0.49
2:B:11:ARG:HD2	3:C:10:ARG:NH1	2.28	0.49
6:F:186:ALA:HB3	16:F:264:HOH:O	2.13	0.49
5:E:67:ILE:HG22	5:E:223:ILE:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:10(A):ARG:HH11	11:Y:10(A):ARG:HG2	1.78	0.49
10:J:44:SER:OG	10:J:100:LEU:HB2	2.13	0.49
2:P:235:LYS:N	2:P:235:LYS:HD3	2.28	0.49
11:Y:97:MET:HG2	11:Y:115:SER:HB3	1.94	0.49
6:T:35:THR:HG23	6:T:51:GLU:HB3	1.95	0.48
10:J:168:MET:HE2	10:X:168:MET:HE2	1.94	0.48
10:X:18:LYS:CG	10:X:174:ILE:HG13	2.43	0.48
4:R:24:VAL:O	4:R:27:SER:HB3	2.13	0.48
3:C:44:ASN:O	3:C:45:CYS:HB3	2.13	0.48
5:S:4:PHE:CG	5:S:5:ARG:N	2.80	0.48
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.95	0.48
13:1:9:ASP:OD1	13:1:10:ASN:N	2.46	0.48
10:X:44:SER:OG	10:X:100:LEU:HB2	2.12	0.48
2:B:122:GLY:C	2:B:124:THR:H	2.14	0.48
6:F:35:THR:HG23	6:F:51:GLU:HB3	1.96	0.48
7:G:38:LEU:HD12	7:G:38:LEU:C	2.33	0.48
13:M:100:ILE:HD11	13:M:127:THR:HG23	1.95	0.48
13:1:122:SER:HB3	13:1:124:THR:O	2.13	0.48
7:U:158:VAL:HG22	7:U:159:GLY:N	2.28	0.48
4:D:85:ALA:HB2	4:D:134:VAL:HG11	1.95	0.48
8:H:18:THR:HB	8:H:30:ASN:HD22	1.78	0.48
13:M:9:ASP:OD1	13:M:10:ASN:N	2.46	0.48
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.94	0.48
13:1:175:LEU:HD23	13:1:175:LEU:C	2.34	0.48
12:L:17:ASP:OD2	12:L:33:LYS:NZ	2.44	0.48
13:1:41:THR:OG1	13:1:76:PRO:HG3	2.14	0.48
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.48	0.48
12:L:-8:PHE:CB	13:M:-8:THR:HG23	2.44	0.48
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.28	0.48
7:G:12:ILE:HD13	7:G:12:ILE:H	1.78	0.48
8:H:147:THR:OG1	8:H:150:GLU:HG3	2.13	0.48
12:L:48:PHE:CZ	12:L:50:ALA:HB3	2.48	0.48
5:E:160:LEU:HD13	5:E:163:THR:HB	1.95	0.48
7:G:192:PHE:CD1	7:G:192:PHE:C	2.86	0.48
2:P:163:ILE:HG12	2:P:164:SER:H	1.79	0.48
6:T:18:ASP:N	6:T:18:ASP:OD2	2.39	0.48
12:Z:3:ILE:HD12	12:Z:46:ASN:CB	2.44	0.48
2:B:185:LYS:HD3	2:B:186:VAL:H	1.76	0.48
11:Y:31:VAL:HG11	15:Y:0:SA1:H13	1.95	0.48
9:W:29:ASN:H	9:W:29:ASN:HD22	1.61	0.48
11:K:195:LEU:O	11:K:199:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:44:THR:OG1	11:K:100:MET:HB2	2.13	0.48
13:M:179:ASP:HB3	13:M:18(A):THR:OG1	2.14	0.48
2:B:239:THR:OXT	2:B:239:THR:HG22	2.13	0.48
10:J:110:LEU:O	10:J:121:GLU:HG2	2.13	0.48
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.96	0.48
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.95	0.48
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.40	0.48
7:U:12:ILE:HG12	7:U:14:ILE:HG23	1.96	0.48
2:B:234:VAL:HA	2:B:239:THR:HA	1.96	0.48
5:E:52:LYS:HD3	5:E:211:SER:HB2	1.96	0.48
2:P:224:PHE:N	2:P:224:PHE:HD2	2.11	0.48
6:T:36:THR:HB	6:T:168:GLY:H	1.79	0.48
1:O:122:GLU:C	1:O:124:THR:H	2.17	0.48
6:T:69:VAL:HG12	16:T:262:HOH:O	2.12	0.48
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.14	0.48
5:E:179:THR:O	5:E:179:THR:HG22	2.14	0.48
2:B:71:ASN:HD22	2:B:72:ASP:H	1.54	0.48
5:E:2(B):THR:H	5:E:2(E):ASN:HB3	1.78	0.48
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.96	0.48
5:S:2(C):VAL:O	5:S:226:GLY:HA2	2.13	0.48
2:B:6:ARG:NH1	4:D:12(B):GLU:OE2	2.47	0.48
7:G:203:THR:HG22	7:G:204:GLU:N	2.28	0.48
7:G:177:GLU:O	7:G:17(B):LYS:HG3	2.13	0.48
3:Q:39:GLY:O	3:Q:162:ALA:HA	2.13	0.48
9:W:130:ALA:HB2	9:W:166:ASP:HB2	1.94	0.48
11:K:14:VAL:HB	11:K:176:TYR:HB2	1.95	0.48
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.96	0.48
10:X:10(B):LYS:NZ	10:X:10(B):LYS:HB2	2.28	0.48
2:P:21:LEU:O	2:P:25:GLU:HG2	2.14	0.48
14:2:113:ILE:HG12	14:2:119:VAL:HG13	1.95	0.48
3:Q:41:LYS:HD3	3:Q:160:TRP:O	2.13	0.48
6:T:172:ALA:O	6:T:176:LEU:HD22	2.14	0.48
2:P:224:PHE:N	2:P:224:PHE:CD2	2.81	0.48
8:V:18:THR:HB	8:V:30:ASN:HD22	1.78	0.48
9:W:101:VAL:O	9:W:110:ILE:HA	2.14	0.48
14:N:147:SER:OG	14:N:150:GLU:HG3	2.14	0.48
10:J:133:TYR:HD1	16:Y:232:HOH:O	1.96	0.48
4:R:207:LEU:HD21	4:R:233:ILE:HD12	1.96	0.48
5:E:76:LEU:CD1	5:E:136:LEU:HD22	2.43	0.48
5:S:38:VAL:HG12	5:S:39:GLY:N	2.27	0.48
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:LYS:HG3	8:H:85:GLN:N	2.27	0.48
8:H:105:ASP:HB2	8:H:10(A):PRO:HD2	1.95	0.48
2:B:224:PHE:CD2	2:B:224:PHE:N	2.82	0.48
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.14	0.47
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.95	0.47
2:P:234:VAL:HA	2:P:239:THR:HA	1.96	0.47
7:U:192:PHE:C	7:U:192:PHE:CD1	2.86	0.47
7:G:96:ALA:HA	7:G:107:MET:CE	2.36	0.47
5:E:15:PHE:H	6:F:23:GLN:NE2	2.06	0.47
7:G:151:THR:HG22	7:G:157:TYR:CB	2.44	0.47
14:2:18(G):TYR:HA	14:2:18(J):LEU:HG	1.95	0.47
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.95	0.47
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.50	0.47
10:X:148:THR:HG21	10:X:177:ILE:HD13	1.97	0.47
5:S:179:THR:O	5:S:179:THR:HG22	2.13	0.47
3:C:41:LYS:HD3	3:C:160:TRP:O	2.14	0.47
4:D:177:LEU:HD13	5:E:58:LEU:HD11	1.96	0.47
13:1:113:VAL:HA	13:1:118:VAL:O	2.14	0.47
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.97	0.47
3:C:224:LEU:N	3:C:224:LEU:HD12	2.29	0.47
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.95	0.47
3:C:33:ARG:HB2	3:C:33:ARG:HH11	1.74	0.47
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.77	0.47
7:G:236:ILE:HD12	7:G:236:ILE:C	2.34	0.47
13:1:100:ILE:HD11	13:1:127:THR:HG23	1.95	0.47
14:N:156:LYS:HG2	14:N:18(J):LEU:HD11	1.95	0.47
7:U:82:ILE:N	7:U:83:PRO:HD2	2.30	0.47
12:L:98:HIS:HD2	16:L:199:HOH:O	1.98	0.47
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.49	0.47
2:B:121:GLN:HG3	3:C:83:ALA:HB1	1.95	0.47
3:C:55:THR:C	3:C:56:LEU:HD22	2.35	0.47
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.95	0.47
10:X:34:THR:HG21	10:X:176:LYS:HZ2	1.80	0.47
12:L:42:VAL:HG23	12:L:102:ALA:HB3	1.97	0.47
2:B:224:PHE:HD2	2:B:224:PHE:N	2.12	0.47
13:1:1:THR:OG1	13:1:2:SER:N	2.47	0.47
1:O:97:HIS:HD2	8:V:61:SER:OG	1.97	0.47
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.49	0.47
5:S:58:LEU:N	5:S:58:LEU:HD12	2.30	0.47
1:A:13:THR:O	2:B:130:ARG:HD3	2.14	0.47
5:E:134:VAL:O	5:E:153:PRO:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:40:ASN:HD22	13:M:40:ASN:N	2.06	0.47
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.96	0.47
10:X:100:LEU:CD2	10:X:112:GLN:HG3	2.44	0.47
2:P:44:ASP:N	2:P:44:ASP:OD2	2.45	0.47
12:Z:5:GLY:O	12:Z:124:CYS:HA	2.13	0.47
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.97	0.47
7:U:203:THR:HG22	7:U:204:GLU:N	2.30	0.47
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.95	0.47
6:F:180:VAL:HG21	7:G:58:LEU:HD23	1.95	0.47
13:M:152:GLU:O	13:M:156:VAL:HG23	2.14	0.47
1:O:67:VAL:HB	1:O:223:LYS:NZ	2.29	0.47
6:T:114:ASP:O	6:T:118:GLN:HG2	2.14	0.47
10:J:143:ARG:O	10:J:146:MET:HG3	2.14	0.47
11:K:156:LYS:HB2	11:K:175:LEU:HD11	1.96	0.47
13:1:133:MET:O	13:1:136:PRO:HD2	2.14	0.47
10:J:19:ALA:HB2	10:J:171:LYS:HG2	1.97	0.47
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.12	0.47
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.44	0.47
1:A:141:HIS:HA	1:A:146:GLY:O	2.15	0.47
7:G:158:VAL:HG22	7:G:159:GLY:N	2.30	0.47
4:D:24:VAL:O	4:D:27:SER:HB3	2.15	0.47
2:P:196:THR:O	2:P:200:THR:HG23	2.15	0.47
2:B:229:ILE:O	2:B:233:LEU:HB2	2.15	0.47
9:W:124:PHE:O	9:W:125:ILE:HD12	2.15	0.47
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.50	0.47
8:H:179:GLU:OE2	8:H:182:LYS:HE2	2.14	0.47
2:B:112:LEU:C	2:B:112:LEU:HD23	2.34	0.47
3:Q:224:LEU:HD12	3:Q:224:LEU:N	2.30	0.47
6:F:53:LEU:HD13	6:F:20(C):LYS:HD2	1.97	0.47
5:S:2(B):THR:H	5:S:2(E):ASN:HB3	1.79	0.47
2:B:6:ARG:HG2	3:C:10:ARG:NH2	2.29	0.47
6:T:45:GLY:HA3	6:T:215:CYS:O	2.14	0.47
6:F:114:ASP:O	6:F:118:GLN:HG2	2.15	0.47
5:S:149:LEU:HD12	5:S:159:GLU:HA	1.97	0.47
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.80	0.47
9:W:104:ILE:HD13	9:W:108:PRO:HA	1.97	0.47
6:F:88:LEU:CD1	6:F:116:LEU:HD22	2.44	0.47
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.98	0.47
7:U:46:THR:HG21	7:U:139:VAL:HB	1.96	0.47
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.96	0.47
5:E:188:GLU:OE1	5:E:188:GLU:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.30	0.47
12:L:-7:ASN:C	12:L:-7:ASN:HD22	2.17	0.46
11:Y:10(A):ARG:NH1	11:Y:10(A):ARG:HG2	2.29	0.46
12:L:27:ASN:HB3	13:M:120:TYR:CZ	2.50	0.46
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.50	0.46
1:O:141:HIS:HA	1:O:146:GLY:O	2.15	0.46
4:D:17:PRO:HD2	16:D:268:HOH:O	2.15	0.46
4:R:112:LEU:C	4:R:112:LEU:HD13	2.36	0.46
2:B:196:THR:O	2:B:200:THR:HG23	2.15	0.46
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.15	0.46
12:Z:160:THR:O	12:Z:164:GLU:HG2	2.16	0.46
3:C:97:GLN:NE2	16:C:244:HOH:O	2.47	0.46
7:G:46:THR:HG21	7:G:139:VAL:HB	1.97	0.46
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.50	0.46
1:A:67:VAL:HB	1:A:223:LYS:NZ	2.30	0.46
2:P:190:ILE:HG21	2:P:232:ILE:CD1	2.41	0.46
12:L:3:ILE:HD12	12:L:46:ASN:CB	2.46	0.46
3:C:159:SER:O	4:D:59:LEU:HD22	2.16	0.46
9:I:6:MET:HE3	9:I:155:ILE:HA	1.98	0.46
7:U:234:VAL:O	7:U:237:ALA:HB3	2.15	0.46
7:U:151:THR:HG22	7:U:157:TYR:CB	2.45	0.46
5:E:58:LEU:HD12	5:E:58:LEU:N	2.29	0.46
6:T:90:ASN:O	6:T:94:GLU:HG3	2.15	0.46
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.97	0.46
8:V:208:ARG:HD3	9:W:149:GLU:HB3	1.97	0.46
3:Q:125:GLN:NE2	16:Q:256:HOH:O	2.48	0.46
8:V:179:GLU:OE2	8:V:182:LYS:HE2	2.16	0.46
13:1:-6:GLN:HG3	13:1:-6:GLN:O	2.14	0.46
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.27	0.46
4:R:121:LEU:HD13	5:S:130:ARG:HH21	1.80	0.46
12:L:160:THR:O	12:L:164:GLU:HG2	2.14	0.46
10:J:148:THR:CG2	10:J:177:ILE:HD13	2.45	0.46
11:K:12:ILE:HB	11:K:178:VAL:HB	1.97	0.46
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.98	0.46
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.45	0.46
2:B:39:GLY:O	2:B:162:ALA:HA	2.16	0.46
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.97	0.46
2:B:44:ASP:OD2	2:B:44:ASP:N	2.46	0.46
9:W:27:VAL:HG13	16:W:208:HOH:O	2.16	0.46
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.46	0.46
10:X:100:LEU:HD21	10:X:112:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:110:GLU:HB2	16:R:828:HOH:O	2.15	0.46
5:S:214:ILE:HG12	5:S:215:VAL:N	2.31	0.46
2:P:71:ASN:HD22	2:P:72:ASP:N	2.12	0.46
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.11	0.46
7:U:152:ASP:HB2	7:U:153:PRO:HD2	1.96	0.46
7:U:172:ILE:HD12	7:U:197:MET:HE1	1.96	0.46
14:2:10(B):LYS:HD3	14:2:10(B):LYS:O	2.14	0.46
3:Q:182:PRO:O	3:Q:184:ALA:N	2.49	0.46
11:K:200:LYS:HE3	11:K:206:PHE:O	2.15	0.46
2:P:39:GLY:O	2:P:162:ALA:HA	2.15	0.46
1:A:205:GLU:OE2	1:A:205:GLU:HA	2.15	0.46
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.46	0.46
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.46	0.46
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.97	0.46
13:1:83:LEU:O	13:1:87:MET:HG2	2.16	0.46
8:H:6:VAL:O	8:H:13:VAL:HG12	2.16	0.46
16:V:261:HOH:O	9:W:150:ASP:HA	2.15	0.46
5:E:207:LEU:N	5:E:207:LEU:CD2	2.78	0.46
6:F:18:ASP:N	6:F:18:ASP:OD2	2.40	0.46
5:S:194:VAL:HA	5:S:197:ILE:HG22	1.96	0.46
10:X:124:TYR:CD2	10:X:138:LEU:HD13	2.51	0.46
10:X:112:GLN:NE2	10:X:126:ALA:H	2.14	0.46
14:2:3:ILE:HG22	14:2:16:ALA:HB2	1.97	0.46
13:M:14(G):ILE:N	13:M:144:PRO:HD2	2.31	0.46
10:X:185:ARG:HG2	10:X:185:ARG:HH11	1.81	0.46
14:2:107:LYS:HG2	14:2:108:GLY:N	2.31	0.46
13:1:179:ASP:HB3	13:1:18(A):THR:OG1	2.15	0.46
3:Q:15:PHE:N	4:R:23:GLN:HE22	1.96	0.46
6:F:36:THR:HB	6:F:168:GLY:H	1.79	0.46
12:Z:-7:ASN:ND2	12:Z:-7:ASN:C	2.68	0.46
10:X:85:GLN:HB3	16:X:210:HOH:O	2.16	0.46
7:U:8:TYR:C	7:U:10:ARG:N	2.68	0.46
12:Z:42:VAL:HG23	12:Z:102:ALA:HB3	1.98	0.46
11:K:10(A):ARG:HG2	11:K:10(A):ARG:HH11	1.81	0.46
9:I:101:VAL:O	9:I:110:ILE:HA	2.16	0.46
9:I:124:PHE:O	9:I:125:ILE:HD12	2.15	0.46
13:M:1:THR:OG1	13:M:2:SER:N	2.49	0.46
8:V:73:GLU:OE1	8:V:73:GLU:HA	2.15	0.46
10:J:100:LEU:CD2	10:J:112:GLN:HG3	2.46	0.46
5:S:35:SER:O	5:S:66:LYS:NZ	2.49	0.46
3:C:182:PRO:O	3:C:184:ALA:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:PHE:H	4:D:23:GLN:NE2	1.95	0.45
9:I:104:ILE:HG21	9:I:181:LYS:HG2	1.98	0.45
7:U:38:LEU:C	7:U:38:LEU:HD12	2.37	0.45
13:1:112:TYR:CE1	13:1:127:THR:HG22	2.51	0.45
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.81	0.45
5:E:214:ILE:HG12	5:E:215:VAL:N	2.32	0.45
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.51	0.45
13:1:14(C):ARG:CG	13:1:14(C):ARG:NH1	2.70	0.45
6:T:95:GLU:HG3	6:T:115:ARG:HD2	1.99	0.45
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.17	0.45
7:G:152:ASP:HB2	7:G:153:PRO:HD2	1.98	0.45
1:O:32:LYS:HA	1:O:32:LYS:CE	2.47	0.45
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.51	0.45
3:Q:44:ASN:O	3:Q:45:CYS:HB3	2.15	0.45
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	1.98	0.45
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.52	0.45
10:X:7:ARG:HG2	10:X:7:ARG:HH11	1.81	0.45
6:T:62:GLN:HA	6:T:209:GLU:OE2	2.16	0.45
8:V:139:GLU:OE2	8:V:139:GLU:HA	2.17	0.45
4:D:12(D):ALA:HA	5:E:129:GLY:HA2	1.98	0.45
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.98	0.45
9:I:113:PHE:CD2	9:I:113:PHE:N	2.83	0.45
14:N:37:VAL:HG22	14:N:41:ILE:O	2.17	0.45
4:D:31:ILE:HD13	4:D:135:ALA:HB2	1.98	0.45
6:T:107:ILE:HA	6:T:108:PRO:HD3	1.87	0.45
3:C:163:GLN:HA	3:C:163:GLN:NE2	2.30	0.45
2:P:121:GLN:C	2:P:121:GLN:NE2	2.70	0.45
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.11	0.45
1:A:4:MET:HG2	6:F:126:TYR:CE2	2.51	0.45
9:I:6:MET:HB3	9:I:151:LEU:HD11	1.98	0.45
13:M:40:ASN:ND2	13:M:40:ASN:H	2.13	0.45
11:Y:37:ILE:HB	11:Y:41:LEU:HB2	1.98	0.45
5:E:40:LEU:HD23	5:E:40:LEU:H	1.81	0.45
10:J:100:LEU:HD21	10:J:112:GLN:HG3	1.98	0.45
14:2:107:LYS:HG2	14:2:108:GLY:H	1.82	0.45
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.98	0.45
4:R:120:ALA:CB	4:R:155:GLY:HA2	2.46	0.45
1:O:205:GLU:HA	1:O:205:GLU:OE2	2.16	0.45
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.80	0.45
2:B:163:ILE:HG12	2:B:164:SER:H	1.81	0.45
14:2:20:THR:CG2	14:2:31:THR:OG1	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:211:ILE:H	13:M:211:ILE:CD1	2.26	0.45
3:Q:215:VAL:HG23	3:Q:221:ILE:HG12	1.98	0.45
7:G:173:THR:O	7:G:177:GLU:HG3	2.16	0.45
2:P:21(A):LYS:O	2:P:21(B):GLY:C	2.55	0.45
10:X:185:ARG:NH1	16:X:218:HOH:O	2.50	0.45
12:L:192:LYS:HE3	8:V:195:ASN:HB3	1.99	0.45
2:B:235:LYS:HD3	2:B:235:LYS:N	2.30	0.45
2:P:215:ILE:HG12	2:P:221:GLN:HG2	1.98	0.45
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.51	0.45
3:C:169:SER:HA	3:C:172:VAL:CG1	2.47	0.45
3:Q:163:GLN:HA	3:Q:163:GLN:NE2	2.30	0.45
10:X:119:LYS:HE2	16:X:216:HOH:O	2.16	0.45
1:O:117:ALA:HB1	1:O:155:GLY:O	2.17	0.45
6:T:75:GLY:O	6:T:138:PHE:HA	2.17	0.45
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.52	0.45
14:N:186:ARG:HD2	16:N:229:HOH:O	2.16	0.45
8:V:105:ASP:HB2	8:V:10(A):PRO:CD	2.47	0.45
2:P:235:LYS:C	2:P:237:GLY:H	2.20	0.45
7:U:82:ILE:HG22	7:U:83:PRO:HD3	1.99	0.45
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.52	0.45
16:Z:209:HOH:O	13:1:121:SER:HB2	2.16	0.45
6:F:103:TYR:O	6:F:104:LYS:HB3	2.17	0.45
6:F:119:TYR:O	6:F:122:ALA:HB3	2.16	0.45
10:J:185:ARG:HH11	10:J:185:ARG:HG2	1.82	0.45
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.97	0.45
7:U:18(D):ILE:O	7:U:18(G):GLU:N	2.50	0.45
13:M:4:ILE:CD1	13:M:155:ILE:HG23	2.47	0.45
12:Z:27:ASN:HB3	13:1:120:TYR:CE1	2.52	0.45
6:T:173:LYS:O	6:T:177:GLU:HG3	2.17	0.45
11:K:97:MET:HG2	11:K:115:SER:HB3	1.97	0.45
3:Q:238:GLN:O	3:Q:242:GLU:HG3	2.17	0.45
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.64	0.45
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.99	0.45
7:U:188:LYS:HA	7:U:188:LYS:HD3	1.77	0.45
5:S:18(D):ILE:O	5:S:18(D):ILE:HG12	2.17	0.45
8:H:197:ARG:NH2	9:I:139:GLU:HG3	2.32	0.45
14:N:24:ALA:HB3	13:1:129:PHE:HE2	1.81	0.45
6:F:62:GLN:HA	6:F:209:GLU:OE2	2.16	0.45
7:U:29:LYS:HD2	7:U:29:LYS:HA	1.69	0.45
3:C:106:PRO:HG2	3:C:143:PRO:HG2	1.96	0.45
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:166:HIS:CD2	12:L:168:GLN:H	2.28	0.45
9:I:29:ASN:HD22	9:I:29:ASN:C	2.20	0.45
9:W:113:PHE:CD2	9:W:113:PHE:N	2.85	0.45
9:W:89:GLU:HG2	9:W:90:ARG:NH1	2.32	0.45
1:O:57:PRO:HG3	7:U:177:GLU:OE1	2.17	0.45
6:T:157:TYR:CD1	6:T:157:TYR:C	2.90	0.45
7:U:105:TYR:OH	8:V:66:HIS:HE1	2.00	0.45
13:1:211:ILE:N	13:1:211:ILE:HD13	2.24	0.44
9:W:6:MET:HB3	9:W:151:LEU:HD11	1.99	0.44
14:N:10(B):LYS:O	14:N:10(B):LYS:HD3	2.17	0.44
8:V:128:GLY:O	8:V:131:SER:CB	2.65	0.44
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.37	0.44
11:K:10(A):ARG:HG2	11:K:10(A):ARG:NH1	2.32	0.44
8:H:29:LYS:HE2	12:Z:165:ARG:NH2	2.32	0.44
14:N:29:ARG:HG2	16:N:227:HOH:O	2.16	0.44
11:Y:44:THR:OG1	11:Y:100:MET:HB2	2.17	0.44
6:F:45:GLY:HA3	6:F:215:CYS:O	2.17	0.44
8:H:48:THR:HB	8:H:51:ASP:HB2	2.00	0.44
6:T:53:LEU:HD13	6:T:20(C):LYS:HD2	1.98	0.44
3:C:55:THR:HG22	3:C:56:LEU:CD2	2.42	0.44
2:B:149:TYR:CZ	3:C:62(A):ILE:HD12	2.52	0.44
2:B:21(A):LYS:O	2:B:21(B):GLY:C	2.55	0.44
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.99	0.44
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.81	0.44
10:X:7:ARG:NE	16:X:195:HOH:O	2.42	0.44
7:U:177:GLU:O	7:U:17(B):LYS:HG3	2.17	0.44
2:B:88:LEU:HB3	2:B:116:LEU:HD21	1.98	0.44
6:T:54:ILE:HG13	6:T:208:PHE:HA	1.98	0.44
6:T:11:SER:HB3	6:T:14:VAL:HG23	1.99	0.44
6:F:54:ILE:HG13	6:F:208:PHE:HA	1.98	0.44
7:U:17(C):LYS:HE3	7:U:17(C):LYS:HB2	1.83	0.44
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.48	0.44
5:S:82:ALA:HB1	16:S:237:HOH:O	2.17	0.44
2:B:230:LYS:O	2:B:234:VAL:HG23	2.17	0.44
10:X:148:THR:CG2	10:X:177:ILE:HD13	2.47	0.44
14:2:15:GLY:HA2	14:2:174:ARG:O	2.17	0.44
13:1:49:ILE:O	13:1:53:GLN:HG3	2.18	0.44
14:2:48:SER:HB3	14:2:51:ASP:HB2	1.98	0.44
7:G:218:ASP:O	7:G:220:LYS:HB2	2.17	0.44
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.99	0.44
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:147:THR:HG23	10:X:150:GLU:OE2	2.18	0.44
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.47	0.44
11:K:31:VAL:HG11	15:K:0:SA1:H13	1.99	0.44
1:A:32:LYS:HA	1:A:32:LYS:CE	2.48	0.44
14:2:9:LYS:O	14:2:107:LYS:HD3	2.17	0.44
10:X:35:ARG:NH1	10:X:57:GLU:CG	2.81	0.44
12:L:103:GLY:HA2	12:L:178:VAL:HG11	1.99	0.44
13:1:211:ILE:H	13:1:211:ILE:CD1	2.24	0.44
12:Z:-8:PHE:HB2	13:1:-8:THR:HG23	2.00	0.44
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.31	0.44
6:T:119:TYR:O	6:T:122:ALA:HB3	2.17	0.44
3:C:85:SER:O	3:C:89:ILE:HD13	2.18	0.44
12:Z:48:PHE:CZ	12:Z:50:ALA:HB3	2.53	0.44
2:P:141:TYR:C	2:P:141:TYR:CD1	2.91	0.44
4:R:59:LEU:HD13	4:R:59:LEU:C	2.38	0.44
5:S:40:LEU:HD23	5:S:40:LEU:H	1.81	0.44
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.82	0.44
8:H:128:GLY:O	8:H:131:SER:CB	2.66	0.44
8:H:30:ASN:O	8:H:189:ARG:NH2	2.49	0.44
2:B:101:LYS:HG3	9:I:57:GLU:HB3	2.00	0.44
10:X:12:VAL:HG22	10:X:108:PRO:HB2	1.99	0.44
7:U:218:ASP:O	7:U:220:LYS:HB2	2.18	0.44
5:S:172:ALA:HB2	5:S:196:ALA:O	2.17	0.44
8:V:147:THR:OG1	8:V:150:GLU:HG3	2.17	0.44
13:1:14(G):ILE:N	13:1:144:PRO:HD2	2.32	0.44
7:U:186:TRP:O	7:U:190:VAL:HG23	2.18	0.44
6:F:95:GLU:HG3	6:F:115:ARG:HD2	2.00	0.44
10:J:147:THR:HG23	10:J:150:GLU:OE2	2.16	0.44
11:K:37:ILE:HB	11:K:41:LEU:HB2	1.99	0.44
10:J:124:TYR:CD2	10:J:138:LEU:HD13	2.53	0.44
8:V:3:ILE:HG22	8:V:16:ALA:HB2	2.00	0.44
14:N:157:HIS:HD2	14:2:140:LYS:NZ	2.15	0.44
10:J:88:ALA:O	10:J:90(A):ILE:HG22	2.17	0.44
5:S:188:GLU:OE1	5:S:188:GLU:HA	2.17	0.44
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.52	0.44
12:Z:-8:PHE:HB3	13:1:-8:THR:HG23	1.99	0.44
6:T:126:TYR:HE1	7:U:129:MET:SD	2.40	0.44
7:G:234:VAL:O	7:G:237:ALA:HB3	2.17	0.44
7:U:119:LEU:HA	7:U:119:LEU:HD12	1.87	0.44
13:M:83:LEU:O	13:M:87:MET:HG2	2.18	0.44
11:K:86:LEU:HD13	11:K:86:LEU:C	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:SER:CB	4:D:59:LEU:HD21	2.48	0.44
4:D:179:GLU:HG3	4:D:192:LEU:HD11	1.99	0.44
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.26	0.44
13:M:99:ILE:C	13:M:100:ILE:HD12	2.38	0.44
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.79	0.44
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.99	0.44
14:N:9:LYS:O	14:N:107:LYS:HD3	2.17	0.44
6:F:75:GLY:O	6:F:138:PHE:HA	2.16	0.44
2:B:63:THR:O	2:B:63:THR:HG22	2.18	0.44
2:B:69:LYS:HE3	2:B:69:LYS:HB2	1.77	0.44
6:T:203:GLU:O	6:T:206:LYS:HD2	2.18	0.43
3:Q:55:THR:O	3:Q:56:LEU:HD22	2.18	0.43
5:E:40:LEU:CD2	5:E:40:LEU:N	2.81	0.43
13:1:99:ILE:C	13:1:100:ILE:HD12	2.38	0.43
13:M:113:VAL:HA	13:M:118:VAL:O	2.17	0.43
10:J:111:TYR:CE1	10:J:121:GLU:HG3	2.53	0.43
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.53	0.43
14:N:107:LYS:HG2	14:N:108:GLY:N	2.33	0.43
10:J:105:ASP:O	10:J:106:ASN:N	2.48	0.43
5:S:74:MET:CE	5:S:96:CYS:SG	3.06	0.43
1:O:15:PHE:N	2:P:23:GLN:HE22	1.91	0.43
7:G:107:MET:CE	7:G:112:LEU:HD13	2.47	0.43
2:B:141:TYR:C	2:B:141:TYR:CD1	2.92	0.43
13:M:211:ILE:HD11	14:2:36:ARG:HD3	2.00	0.43
2:B:184:MET:HE2	2:B:189:ALA:N	2.33	0.43
5:S:38:VAL:HG22	5:S:164:ALA:CB	2.47	0.43
4:D:51:GLU:HG2	4:D:53:ARG:HB2	1.99	0.43
10:X:143:ARG:HG2	10:X:143:ARG:HH11	1.83	0.43
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.54	0.43
13:M:133:MET:C	13:M:136:PRO:HD2	2.39	0.43
2:P:63:THR:HG22	2:P:63:THR:O	2.18	0.43
2:P:144:ARG:O	2:P:144:ARG:HG2	2.18	0.43
13:M:14(C):ARG:CG	13:M:14(C):ARG:NH1	2.72	0.43
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.49	0.43
9:I:29:ASN:HD22	9:I:29:ASN:H	1.65	0.43
7:G:173:THR:HG22	7:G:177:GLU:OE2	2.17	0.43
4:R:51:GLU:HG2	4:R:53:ARG:HB2	2.00	0.43
14:2:156:LYS:HG2	14:2:18(J):LEU:CD1	2.49	0.43
9:I:89:GLU:HG2	9:I:90:ARG:NH1	2.32	0.43
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.48	0.43
4:R:160:TYR:HA	5:S:58:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:163:GLN:NE2	3:C:164:THR:N	2.48	0.43
7:U:107:MET:CE	7:U:112:LEU:HD13	2.49	0.43
1:A:122:GLU:C	1:A:124:THR:H	2.19	0.43
14:2:20:THR:HG23	14:2:31:THR:HG1	1.82	0.43
3:Q:206:GLY:CA	3:Q:209:ASN:HB2	2.47	0.43
5:S:39:GLY:O	5:S:162:GLY:HA2	2.18	0.43
5:S:5:ARG:HG3	5:S:22:PHE:CZ	2.53	0.43
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.53	0.43
16:X:211:HOH:O	11:Y:88:TYR:HB2	2.18	0.43
6:F:173:LYS:O	6:F:177:GLU:HG3	2.18	0.43
12:L:176:LEU:HG	12:L:186:LYS:HG2	2.00	0.43
1:A:185:GLU:OE1	1:A:187:GLU:HB2	2.19	0.43
2:B:71:ASN:HD22	2:B:72:ASP:N	2.12	0.43
10:X:166:MET:HA	10:X:167:PRO:HD3	1.82	0.43
10:J:52:THR:HG23	10:J:53:VAL:N	2.34	0.43
2:P:49:ALA:HB2	2:P:212:PHE:CE1	2.54	0.43
2:P:229:ILE:O	2:P:233:LEU:HB2	2.18	0.43
11:K:6:PHE:HA	11:K:123:ASP:O	2.19	0.43
10:X:90(B):ARG:NH1	16:X:204:HOH:O	2.49	0.43
10:J:168:MET:CE	10:X:168:MET:CE	2.97	0.43
3:Q:159:SER:O	4:R:59:LEU:HD22	2.19	0.43
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.54	0.43
13:M:42:VAL:CG2	13:M:178:ILE:HD11	2.48	0.43
8:V:30:ASN:O	8:V:189:ARG:NH2	2.45	0.43
11:K:200:LYS:HG3	11:K:206:PHE:HB2	2.00	0.43
7:U:31:THR:HG21	7:U:135:ILE:HG13	2.01	0.43
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.53	0.43
2:P:69:LYS:HE3	2:P:69:LYS:HB2	1.78	0.43
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.84	0.43
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.81	0.43
12:Z:99:THR:CG2	16:Z:203:HOH:O	2.65	0.43
7:G:82:ILE:HG22	7:G:83:PRO:HD3	1.99	0.43
5:S:40:LEU:CD2	5:S:40:LEU:N	2.82	0.43
5:E:18(D):ILE:O	5:E:18(D):ILE:HG12	2.17	0.43
5:E:190:ILE:O	5:E:194:VAL:HG23	2.18	0.43
8:H:105:ASP:HB2	8:H:10(A):PRO:CD	2.48	0.43
13:1:133:MET:C	13:1:136:PRO:HD2	2.38	0.43
10:J:171:LYS:HE3	16:X:223:HOH:O	2.19	0.43
2:B:235:LYS:C	2:B:237:GLY:H	2.22	0.43
4:R:12(G):GLU:HG2	4:R:125:GLU:H	1.83	0.43
10:X:19:ALA:HB2	10:X:171:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:18(A):ASP:OD2	3:Q:18(C):LYS:HG2	2.18	0.43
2:P:88:LEU:HB3	2:P:116:LEU:HD21	1.99	0.43
14:N:133:PHE:HA	14:2:132:THR:O	2.18	0.43
13:M:67:ALA:HB3	16:M:254:HOH:O	2.18	0.43
5:E:85:ALA:HB2	5:E:134:VAL:HG21	2.00	0.43
9:I:33:LYS:O	9:I:44:GLY:HA2	2.17	0.43
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.49	0.43
12:L:-8:PHE:HB2	13:M:-8:THR:HG23	2.01	0.43
13:M:112:TYR:CE1	13:M:127:THR:HG22	2.51	0.43
11:Y:99:THR:HG22	11:Y:113:VAL:HB	2.00	0.43
13:M:113:VAL:HG23	13:M:119:THR:HG22	2.00	0.43
5:S:190:ILE:O	5:S:194:VAL:HG23	2.19	0.43
5:E:5:ARG:HG3	5:E:22:PHE:CZ	2.54	0.43
6:F:50:VAL:HB	6:F:77:VAL:HG21	2.01	0.43
7:U:213:GLY:HA2	7:U:223:THR:HA	2.01	0.43
7:U:224:LEU:HB3	7:U:228:ASN:HB2	2.00	0.43
4:D:120:ALA:CB	4:D:155:GLY:HA2	2.48	0.43
5:S:47:VAL:HG23	5:S:189:LEU:HD13	2.00	0.43
1:O:185:GLU:OE1	1:O:187:GLU:HB2	2.19	0.43
8:H:208:ARG:HD3	9:I:149:GLU:HB3	1.99	0.43
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.66	0.43
9:I:6:MET:CE	9:I:155:ILE:HA	2.48	0.43
13:1:40:ASN:HD22	13:1:40:ASN:N	2.07	0.43
5:S:76:LEU:CD1	5:S:136:LEU:HD22	2.49	0.43
3:Q:215:VAL:O	3:Q:215:VAL:HG13	2.19	0.43
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.82	0.43
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.99	0.43
10:J:144:PRO:CG	11:Y:207:ASN:ND2	2.82	0.43
8:V:3:ILE:O	8:V:126:SER:HA	2.19	0.43
14:N:3:ILE:HG22	14:N:16:ALA:HB2	2.01	0.43
1:O:60:MET:HB2	1:O:63:THR:HG23	2.01	0.43
14:N:140:LYS:NZ	14:2:157:HIS:HD2	2.16	0.43
3:C:134:VAL:HG12	3:C:135:SER:N	2.34	0.43
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.19	0.43
1:A:177:GLU:CG	2:B:58:LEU:HD22	2.36	0.43
6:F:51:GLU:OE1	6:F:53:LEU:HD21	2.19	0.43
10:J:166:MET:HA	10:J:167:PRO:HD3	1.83	0.43
10:X:24:ILE:HG12	10:X:24:ILE:O	2.18	0.43
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.49	0.43
11:K:99:THR:HG22	11:K:113:VAL:HB	2.00	0.43
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.54	0.43
2:B:218:ASN:O	2:B:21(C):ASP:HB2	2.18	0.43
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.18	0.43
3:C:20:HIS:HB3	3:C:25:GLU:OE1	2.19	0.43
6:T:103:TYR:O	6:T:104:LYS:HB3	2.18	0.43
6:T:187:ARG:HG3	6:T:187:ARG:HH11	1.83	0.43
12:Z:129:ALA:HB1	12:Z:166:HIS:NE2	2.34	0.42
12:L:-2:ASN:HA	12:L:21:ILE:O	2.18	0.42
12:L:164:GLU:CD	8:V:197:ARG:HG3	2.39	0.42
7:G:224:LEU:HB3	7:G:228:ASN:HB2	2.01	0.42
13:1:186:PHE:CE1	13:1:188:LYS:HG3	2.54	0.42
2:B:17:PRO:HA	3:C:26:TYR:CE1	2.53	0.42
6:F:157:TYR:C	6:F:157:TYR:CD1	2.92	0.42
10:J:7:ARG:HG2	10:J:7:ARG:HH11	1.84	0.42
13:M:115:LEU:HD23	13:M:115:LEU:N	2.34	0.42
9:I:104:ILE:HD13	9:I:108:PRO:HA	2.00	0.42
7:G:82:ILE:N	7:G:83:PRO:HD2	2.33	0.42
2:P:230:LYS:O	2:P:234:VAL:HG23	2.19	0.42
5:E:143:LYS:HB2	16:M:247:HOH:O	2.19	0.42
2:B:213:ALA:HA	2:B:222:LYS:O	2.19	0.42
10:X:140:HIS:HD2	10:X:141:HIS:CE1	2.36	0.42
5:E:15:PHE:N	6:F:23:GLN:HE22	2.09	0.42
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.54	0.42
13:1:11:GLY:HA3	13:1:178:ILE:O	2.20	0.42
9:W:29:ASN:C	9:W:29:ASN:HD22	2.23	0.42
2:P:27:ALA:O	2:P:30:SER:HB3	2.19	0.42
6:T:90:ASN:ND2	16:T:248:HOH:O	2.52	0.42
1:O:60:MET:HE2	1:O:63:THR:HG21	2.00	0.42
9:I:93:GLY:N	9:I:94:PRO:CD	2.83	0.42
2:P:213:ALA:HA	2:P:222:LYS:O	2.19	0.42
7:G:186:TRP:O	7:G:190:VAL:HG23	2.19	0.42
5:E:149:LEU:HD12	5:E:159:GLU:HA	2.00	0.42
9:W:23:GLN:HB2	16:W:229:HOH:O	2.18	0.42
11:Y:10(B):LYS:CD	11:Y:10(B):LYS:N	2.69	0.42
7:G:34(A):ASN:HA	7:G:167:PRO:HG2	2.01	0.42
13:1:40:ASN:ND2	13:1:40:ASN:H	2.14	0.42
12:L:27:ASN:HB3	13:M:120:TYR:CE1	2.54	0.42
1:O:112:LEU:O	1:O:116:VAL:HG23	2.19	0.42
7:G:136:LEU:O	7:G:150:LYS:HA	2.19	0.42
10:J:12:VAL:HG22	10:J:108:PRO:HB2	2.02	0.42
3:C:238:GLN:O	3:C:242:GLU:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:115:ARG:HH12	7:G:119:LEU:HD13	1.85	0.42
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.40	0.42
10:J:24:ILE:HG12	10:J:24:ILE:O	2.19	0.42
4:D:59:LEU:C	4:D:59:LEU:HD13	2.40	0.42
12:Z:166:HIS:CD2	12:Z:168:GLN:H	2.29	0.42
12:L:-7:ASN:ND2	12:L:-7:ASN:C	2.72	0.42
3:C:215:VAL:O	3:C:215:VAL:HG13	2.19	0.42
1:O:33:GLN:HA	1:O:33:GLN:NE2	2.34	0.42
5:S:194:VAL:O	5:S:197:ILE:HG22	2.20	0.42
5:E:194:VAL:O	5:E:197:ILE:HG22	2.19	0.42
14:N:132:THR:O	14:2:133:PHE:HA	2.20	0.42
1:O:236:LEU:C	1:O:236:LEU:HD13	2.39	0.42
1:O:92:SER:O	1:O:95:VAL:HG12	2.19	0.42
12:Z:176:LEU:HG	12:Z:186:LYS:HG2	2.02	0.42
4:D:76:CYS:HB2	4:D:137:LEU:O	2.19	0.42
3:Q:85:SER:O	3:Q:89:ILE:HD13	2.19	0.42
1:A:109:THR:O	1:A:113:VAL:HG23	2.20	0.42
2:B:202:THR:HG21	2:B:204:SER:HB2	2.02	0.42
1:O:4:MET:HG2	6:T:126:TYR:CE2	2.54	0.42
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.49	0.42
13:1:4:ILE:CD1	13:1:155:ILE:HG23	2.48	0.42
7:U:115:ARG:HH12	7:U:119:LEU:HD13	1.83	0.42
5:E:74:MET:CE	5:E:96:CYS:SG	3.08	0.42
3:C:18(A):ASP:OD2	3:C:18(C):LYS:HG2	2.19	0.42
14:N:115:LEU:HD12	14:N:115:LEU:HA	1.77	0.42
2:B:209:ARG:HH11	2:B:209:ARG:HG2	1.84	0.42
13:1:57:ARG:HH11	13:1:57:ARG:HG2	1.83	0.42
1:A:236:LEU:HD13	1:A:236:LEU:C	2.40	0.42
11:Y:114:ASP:C	11:Y:114:ASP:OD1	2.57	0.42
1:O:225:THR:HG23	1:O:228:GLU:OE1	2.20	0.42
10:J:112:GLN:NE2	10:J:126:ALA:H	2.17	0.42
5:S:109:VAL:HG12	5:S:149:LEU:HD22	2.00	0.42
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	2.02	0.42
14:2:105:ASP:OD2	14:2:106:ASN:N	2.47	0.42
4:D:91:HIS:CG	4:D:119:LEU:HD11	2.55	0.42
13:M:186:PHE:CE1	13:M:188:LYS:HG3	2.55	0.42
4:D:12(G):GLU:HG2	4:D:125:GLU:H	1.85	0.42
3:C:125:GLN:HG3	3:C:125:GLN:O	2.20	0.42
6:T:53:LEU:HD11	6:T:205:ASN:OD1	2.20	0.42
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.85	0.42
2:P:185:LYS:HD2	2:P:187:ASP:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:GLN:NE2	16:B:246:HOH:O	2.46	0.42
5:E:38:VAL:HG22	5:E:164:ALA:CB	2.50	0.42
6:F:172:ALA:O	6:F:176:LEU:HD22	2.20	0.42
9:W:130:ALA:HB2	9:W:166:ASP:CB	2.50	0.42
6:F:41:LYS:HD2	16:F:248:HOH:O	2.20	0.42
9:I:89:GLU:HG2	9:I:90:ARG:HH12	1.85	0.42
4:R:12(F):GLY:O	4:R:12(G):GLU:HB2	2.20	0.42
7:U:110:ASP:HB3	7:U:149:TYR:CE2	2.55	0.42
10:J:35:ARG:NH1	10:J:57:GLU:CG	2.83	0.42
6:F:28:VAL:O	6:F:32:GLU:HG3	2.20	0.42
3:Q:79:SER:OG	3:Q:165:ILE:HG13	2.20	0.42
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.20	0.42
8:V:72:ARG:HG3	8:V:72:ARG:HH11	1.84	0.42
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.55	0.42
3:C:75:VAL:HG13	3:C:221:ILE:HD13	2.02	0.42
14:N:107:LYS:HG2	14:N:108:GLY:H	1.85	0.42
14:2:44:CYS:HB2	14:2:100:ILE:HB	2.01	0.42
2:P:218:ASN:O	2:P:21(C):ASP:HB2	2.19	0.42
8:H:139:GLU:OE2	8:H:139:GLU:HA	2.19	0.42
9:W:61:TYR:C	9:W:61:TYR:CD1	2.93	0.42
4:D:170:GLU:CD	4:D:170:GLU:H	2.22	0.42
10:J:143:ARG:HG2	10:J:143:ARG:HH11	1.84	0.42
3:Q:224:LEU:N	3:Q:224:LEU:CD1	2.83	0.42
13:M:3:VAL:O	13:M:126:ALA:HA	2.20	0.42
4:R:236:GLU:O	4:R:240:LYS:HG3	2.19	0.42
11:K:25:TRP:CH2	12:L:132:SER:HA	2.54	0.42
4:R:238:LYS:HE2	4:R:238:LYS:HB3	1.84	0.42
4:D:238:LYS:HE2	4:D:238:LYS:HB3	1.81	0.42
4:R:215:ILE:HD13	4:R:215:ILE:C	2.40	0.42
8:V:80:LEU:HD12	8:V:113:ILE:CD1	2.46	0.41
6:F:126:TYR:HE1	7:G:129:MET:SD	2.42	0.41
9:I:155:ILE:HG23	9:I:156:SER:N	2.35	0.41
7:U:233:LEU:HD12	7:U:233:LEU:HA	1.89	0.41
14:N:14:LEU:HD11	14:N:102:ALA:HB3	2.01	0.41
1:A:92:SER:O	1:A:95:VAL:HG12	2.20	0.41
13:1:3:VAL:O	13:1:126:ALA:HA	2.20	0.41
14:2:66:TYR:CD2	14:2:74:PRO:HB3	2.55	0.41
12:Z:170:GLY:O	12:Z:171:ASP:HB2	2.20	0.41
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	2.01	0.41
1:A:112:LEU:O	1:A:116:VAL:HG23	2.19	0.41
7:G:232:ARG:NE	7:G:232:ARG:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:96:ALA:HA	7:U:107:MET:CE	2.36	0.41
7:U:34(A):ASN:HA	7:U:167:PRO:HG2	2.01	0.41
7:G:172:ILE:HD12	7:G:197:MET:HE1	2.03	0.41
7:U:168:LYS:O	7:U:172:ILE:HG12	2.19	0.41
2:B:27:ALA:O	2:B:30:SER:HB3	2.21	0.41
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.83	0.41
13:1:43:VAL:HG22	13:1:101:VAL:HG22	2.01	0.41
9:I:88:TYR:CE1	9:I:91:ARG:HD3	2.55	0.41
2:B:10:SER:HB2	16:B:248:HOH:O	2.20	0.41
3:Q:97:GLN:HG3	10:X:65:LEU:HB2	2.01	0.41
7:U:232:ARG:NE	7:U:232:ARG:HA	2.35	0.41
2:B:51:GLU:OE2	2:B:202:THR:HG23	2.21	0.41
3:Q:163:GLN:NE2	3:Q:163:GLN:CA	2.84	0.41
1:A:179:ARG:CB	1:A:179:ARG:HH11	2.25	0.41
12:L:129:ALA:HB1	12:L:166:HIS:NE2	2.35	0.41
2:B:181:LYS:HG3	2:B:184:MET:HG3	2.03	0.41
2:P:181:LYS:HG3	2:P:184:MET:HG3	2.02	0.41
2:P:184:MET:HE2	2:P:189:ALA:N	2.35	0.41
13:M:100:ILE:CD1	13:M:127:THR:HG23	2.51	0.41
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.50	0.41
9:I:130:ALA:HB2	9:I:166:ASP:CB	2.51	0.41
6:F:203:GLU:O	6:F:206:LYS:HD2	2.20	0.41
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.35	0.41
8:H:3:ILE:HG22	8:H:16:ALA:HB2	2.03	0.41
9:W:19:ARG:HB2	9:W:171:TRP:HB2	2.02	0.41
11:Y:172:SER:HA	11:Y:192:VAL:HG23	2.03	0.41
13:M:122:SER:HB3	13:M:124:THR:O	2.20	0.41
4:R:159:ARG:O	5:S:60:SER:N	2.53	0.41
13:1:42:VAL:CG2	13:1:178:ILE:HD11	2.50	0.41
13:1:113:VAL:HG23	13:1:119:THR:HG22	2.01	0.41
11:Y:174:ASN:ND2	11:Y:186:TYR:OH	2.53	0.41
3:C:197:LEU:O	3:C:201:VAL:HG23	2.21	0.41
14:2:114:PRO:HD2	14:2:118:SER:O	2.20	0.41
8:V:103:GLY:HA2	8:V:178:MET:SD	2.61	0.41
2:B:122:GLY:C	2:B:124:THR:N	2.74	0.41
5:S:85:ALA:HB2	5:S:134:VAL:HG21	2.03	0.41
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.50	0.41
2:P:136:PHE:O	2:P:150:THR:HA	2.21	0.41
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.19	0.41
9:W:89:GLU:HG2	9:W:90:ARG:HH12	1.85	0.41
10:J:35:ARG:HA	10:J:35:ARG:HD3	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.56	0.41
5:E:36:VAL:HG22	5:E:37:THR:N	2.35	0.41
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.20	0.41
2:P:202:THR:HG21	2:P:204:SER:HB2	2.02	0.41
2:B:185:LYS:HD2	2:B:187:ASP:H	1.84	0.41
12:L:21:ILE:CD1	12:L:21:ILE:C	2.86	0.41
3:Q:75:VAL:HG13	3:Q:221:ILE:HD13	2.02	0.41
7:U:164:ALA:CB	7:U:172:ILE:HB	2.50	0.41
5:E:227:GLU:OE2	5:E:227:GLU:N	2.54	0.41
3:C:224:LEU:N	3:C:224:LEU:CD1	2.82	0.41
14:2:48:SER:O	14:2:52:THR:HG23	2.21	0.41
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.56	0.41
8:H:3:ILE:O	8:H:126:SER:HA	2.21	0.41
5:S:36:VAL:HG22	5:S:37:THR:N	2.36	0.41
10:J:140:HIS:HD2	10:J:141:HIS:CE1	2.39	0.41
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.86	0.41
9:W:115:LEU:HD23	9:W:115:LEU:N	2.35	0.41
2:P:121:GLN:NE2	16:P:248:HOH:O	2.53	0.41
1:O:175:PHE:O	1:O:179:ARG:HG2	2.20	0.41
14:N:36:ARG:HD3	13:1:211:ILE:HD11	2.03	0.41
7:G:77:VAL:HG12	7:G:137:THR:HB	2.02	0.41
12:Z:14(I):THR:O	12:Z:1(I):ASN:CB	2.69	0.41
14:2:37:VAL:HG22	14:2:41:ILE:O	2.19	0.41
4:D:237:LEU:HD22	4:D:241:GLU:HG3	2.02	0.41
4:D:12(F):GLY:O	4:D:12(G):GLU:HB2	2.20	0.41
2:P:194:LEU:O	2:P:198:SER:HB2	2.21	0.41
3:C:99:HIS:CG	3:C:107:VAL:HG12	2.56	0.41
9:W:45:ILE:HB	9:W:52:VAL:HG13	2.02	0.41
7:U:136:LEU:O	7:U:150:LYS:HA	2.20	0.41
13:M:171:ARG:HG3	13:M:192:VAL:HB	2.02	0.41
14:2:147:SER:OG	14:2:150:GLU:HG3	2.21	0.41
7:G:171:GLU:OE1	7:G:171:GLU:N	2.53	0.41
4:D:142:ASP:OD2	4:D:142:ASP:C	2.59	0.41
3:C:163:GLN:CA	3:C:163:GLN:NE2	2.83	0.41
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.28	0.41
5:S:51:LEU:HD11	5:S:2(E):ASN:HD21	1.85	0.41
3:C:55:THR:O	3:C:56:LEU:HD22	2.21	0.41
1:O:100:TYR:CG	1:O:107:PRO:HB3	2.55	0.41
4:R:107:ILE:CD1	4:R:111:SER:HB2	2.51	0.41
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.56	0.41
8:V:6:VAL:O	8:V:13:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:159:MET:HB3	13:1:159:MET:HE2	1.90	0.41
4:D:185:THR:HG23	4:D:188:GLU:OE1	2.20	0.41
1:A:15:PHE:N	2:B:23:GLN:HE22	1.98	0.41
6:T:20(B):GLU:HG3	6:T:20(C):LYS:H	1.85	0.41
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.35	0.41
2:P:122:GLY:C	2:P:124:THR:N	2.74	0.41
9:W:6:MET:CE	9:W:155:ILE:HA	2.50	0.41
12:L:61:ASN:HA	12:L:61:ASN:HD22	1.72	0.41
2:P:101:LYS:HG3	9:W:57:GLU:HB3	2.03	0.41
5:S:77:SER:OG	5:S:137:LEU:HB2	2.21	0.41
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.56	0.41
4:R:68:VAL:HG21	4:R:89:ILE:CD1	2.50	0.41
13:M:11:GLY:HA3	13:M:178:ILE:O	2.21	0.41
5:E:100:SER:O	5:E:104:ASN:HA	2.21	0.41
9:W:29:ASN:N	9:W:29:ASN:ND2	2.66	0.41
13:1:100:ILE:CD1	13:1:127:THR:HG23	2.50	0.41
10:X:6:ILE:HG23	10:X:13:ILE:HB	2.02	0.41
10:X:18:LYS:CD	10:X:174:ILE:HG13	2.51	0.41
14:2:14:LEU:N	14:2:14:LEU:HD12	2.36	0.41
13:M:57:ARG:HH11	13:M:57:ARG:HG2	1.86	0.41
6:T:196:ILE:HG12	6:T:196:ILE:H	1.66	0.41
6:T:50:VAL:HB	6:T:77:VAL:HG21	2.02	0.41
5:S:82:ALA:HB3	16:S:237:HOH:O	2.19	0.41
2:P:235:LYS:C	2:P:237:GLY:N	2.73	0.41
10:X:126:ALA:HB1	10:X:130:SER:HB2	2.03	0.41
3:Q:201:VAL:HG21	3:Q:210:ILE:HD11	2.02	0.41
8:H:63:ILE:HD13	8:H:63:ILE:HA	1.94	0.41
4:R:99:HIS:CG	4:R:107:ILE:HG12	2.56	0.41
10:X:14:LEU:HD12	10:X:42:LEU:HD23	2.03	0.41
11:K:17:ASP:CG	11:K:33:LYS:HZ2	2.24	0.41
5:S:12:THR:HG21	5:S:124:THR:HA	2.03	0.41
12:L:70:HIS:O	12:L:70(A):ASN:C	2.59	0.41
9:I:15:ALA:HB1	9:I:159:LEU:HD22	2.03	0.41
14:N:105:ASP:HB3	14:N:106:ASN:HB2	2.02	0.41
6:T:63:LYS:O	6:T:65:VAL:N	2.54	0.41
4:R:185:THR:HG23	4:R:188:GLU:OE1	2.21	0.41
1:A:60:MET:HB2	1:A:63:THR:HG23	2.03	0.41
7:G:75:GLY:HA3	7:G:221:PHE:CE2	2.56	0.41
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.56	0.41
6:T:95:GLU:CG	6:T:115:ARG:HD2	2.51	0.41
12:L:114:ASP:CB	12:L:118:SER:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:76:LEU:HB3	5:S:138:ILE:HG13	2.03	0.41
9:I:113:PHE:HA	9:I:118:CYS:O	2.20	0.41
7:U:77:VAL:HG12	7:U:137:THR:HB	2.03	0.41
4:D:68:VAL:HG21	4:D:89:ILE:CD1	2.50	0.41
6:T:109:ILE:HG21	6:T:147:HIS:HB2	2.03	0.41
4:R:237:LEU:HD22	4:R:241:GLU:HG3	2.03	0.41
9:I:159:LEU:HD21	9:I:173:ALA:HB1	2.02	0.41
8:V:1:THR:CG2	8:V:2:THR:N	2.84	0.41
6:F:49:ALA:HA	6:F:211:GLU:O	2.20	0.41
9:W:12(A):LYS:HG3	9:W:123:ASP:N	2.35	0.41
13:M:49:ILE:O	13:M:53:GLN:HG3	2.21	0.41
6:F:63:LYS:O	6:F:65:VAL:N	2.53	0.41
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.35	0.41
13:M:51:ASP:O	13:M:54:HIS:HB3	2.21	0.41
9:W:93:GLY:N	9:W:94:PRO:CD	2.82	0.41
9:W:159:LEU:HD21	9:W:173:ALA:HB1	2.03	0.41
9:I:20:LEU:C	9:I:20:LEU:HD13	2.41	0.41
11:K:142:TYR:C	11:K:143:LYS:HD2	2.42	0.40
9:W:104:ILE:HG21	9:W:181:LYS:HG2	2.04	0.40
9:I:29:ASN:N	9:I:29:ASN:ND2	2.68	0.40
5:E:76:LEU:HA	5:E:137:LEU:O	2.22	0.40
4:D:177:LEU:HD22	5:E:58:LEU:HD11	2.03	0.40
14:N:156:LYS:HG2	14:N:18(J):LEU:CD1	2.50	0.40
10:J:143:ARG:HA	10:J:144:PRO:HD3	1.94	0.40
13:M:206:TYR:CZ	14:2:53:GLN:HG2	2.55	0.40
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.51	0.40
4:D:215:ILE:HD13	4:D:215:ILE:C	2.41	0.40
1:A:169:SER:O	1:A:173:LYS:HG3	2.21	0.40
1:A:175:PHE:O	1:A:179:ARG:HG2	2.21	0.40
3:Q:38:VAL:HG22	3:Q:39:GLY:N	2.36	0.40
1:O:35:VAL:HG11	1:O:51:GLU:HB3	2.03	0.40
11:K:5:ALA:HA	11:K:13:ILE:O	2.21	0.40
5:S:5:ARG:HG3	5:S:22:PHE:CE1	2.56	0.40
12:L:48:PHE:CE2	12:L:50:ALA:HB3	2.56	0.40
12:Z:14(D):TYR:CG	12:Z:14(J):GLY:HA2	2.57	0.40
5:E:82:ALA:HB3	5:E:83:PRO:HD3	2.03	0.40
13:1:115:LEU:N	13:1:115:LEU:HD23	2.35	0.40
11:K:114:ASP:OD1	11:K:114:ASP:C	2.60	0.40
3:C:206:GLY:CA	3:C:209:ASN:HB2	2.49	0.40
5:S:130:ARG:HG3	5:S:130:ARG:HH11	1.86	0.40
7:G:18(G):GLU:HG2	7:G:188:LYS:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:4:LEU:O	12:L:14:LEU:HD23	2.21	0.40
9:I:70:GLU:O	9:I:71:GLU:HB2	2.22	0.40
14:N:14:LEU:N	14:N:14:LEU:HD12	2.36	0.40
7:U:139:VAL:HA	7:U:147:SER:O	2.21	0.40
4:R:52:LYS:HB2	4:R:20(B):ASN:C	2.42	0.40
12:Z:76:ILE:HG23	12:Z:77:ASN:N	2.35	0.40
7:U:35:ILE:HA	7:U:35:ILE:HD13	1.79	0.40
3:Q:206:GLY:HA2	3:Q:209:ASN:HD22	1.86	0.40
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.56	0.40
5:S:18(C):PHE:HA	5:S:18(F):ILE:CG1	2.52	0.40
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.89	0.40
1:O:32:LYS:HE2	1:O:32:LYS:CA	2.51	0.40
3:C:241:GLN:O	3:C:243:GLN:N	2.50	0.40
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.51	0.40
6:T:49:ALA:HA	6:T:211:GLU:O	2.21	0.40
14:2:65:LEU:HG	14:2:69:GLN:HE21	1.87	0.40
9:I:28:SER:HB2	10:J:120:VAL:HG21	2.03	0.40
1:O:17:PRO:HA	2:P:26:TYR:CD1	2.56	0.40
9:W:88:TYR:CE1	9:W:91:ARG:HD3	2.56	0.40
4:D:236:GLU:O	4:D:240:LYS:HG3	2.21	0.40
14:N:44:CYS:HB2	14:N:100:ILE:HB	2.03	0.40
3:C:29:GLU:OE2	3:C:32:LYS:HE2	2.22	0.40
6:T:121:GLN:HE21	6:T:121:GLN:HB3	1.64	0.40
2:P:209:ARG:HH11	2:P:209:ARG:HG2	1.86	0.40
6:F:20(B):GLU:HG3	6:F:20(C):LYS:H	1.86	0.40
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.78	0.40
12:Z:-5:TYR:CE2	12:Z:96:TYR:HB2	2.57	0.40
5:E:97:ASN:HD22	5:E:97:ASN:HA	1.72	0.40
5:S:76:LEU:HA	5:S:137:LEU:O	2.21	0.40
10:X:111:TYR:CE1	10:X:121:GLU:HG3	2.56	0.40
1:O:195:LEU:HD23	1:O:236:LEU:HD21	2.03	0.40
9:W:15:ALA:HB1	9:W:159:LEU:HD22	2.04	0.40
7:G:131:PRO:HB3	16:G:244:HOH:O	2.20	0.40
11:Y:78:ALA:O	11:Y:82:ILE:HG12	2.21	0.40
1:A:52:LYS:HG3	1:A:211:GLU:HB2	2.04	0.40
8:H:62:ASN:ND2	16:H:227:HOH:O	2.50	0.40
7:U:171:GLU:N	7:U:171:GLU:OE1	2.54	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%)	235 (95%)	10 (4%)	3 (1%)	16 47
1	O	248/250 (99%)	236 (95%)	9 (4%)	3 (1%)	16 47
2	B	242/244 (99%)	219 (90%)	18 (7%)	5 (2%)	9 29
2	P	242/244 (99%)	219 (90%)	17 (7%)	6 (2%)	7 24
3	C	239/241 (99%)	220 (92%)	16 (7%)	3 (1%)	15 44
3	Q	239/241 (99%)	219 (92%)	17 (7%)	3 (1%)	15 44
4	D	240/242 (99%)	225 (94%)	10 (4%)	5 (2%)	9 29
4	R	240/242 (99%)	224 (93%)	11 (5%)	5 (2%)	9 29
5	E	231/233 (99%)	211 (91%)	13 (6%)	7 (3%)	5 18
5	S	231/233 (99%)	210 (91%)	14 (6%)	7 (3%)	5 18
6	F	242/244 (99%)	226 (93%)	15 (6%)	1 (0%)	39 74
6	T	242/244 (99%)	228 (94%)	12 (5%)	2 (1%)	24 58
7	G	241/243 (99%)	226 (94%)	13 (5%)	2 (1%)	24 58
7	U	241/243 (99%)	225 (93%)	13 (5%)	3 (1%)	16 47
8	H	220/222 (99%)	208 (94%)	12 (6%)	0	100 100
8	V	220/222 (99%)	208 (94%)	12 (6%)	0	100 100
9	I	202/204 (99%)	194 (96%)	7 (4%)	1 (0%)	34 69
9	W	202/204 (99%)	194 (96%)	7 (4%)	1 (0%)	34 69
10	J	196/198 (99%)	185 (94%)	10 (5%)	1 (0%)	34 69
10	X	196/198 (99%)	185 (94%)	10 (5%)	1 (0%)	34 69
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100 100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100 100
12	L	220/222 (99%)	208 (94%)	12 (6%)	0	100 100
12	Z	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	34 69
13	1	231/233 (99%)	216 (94%)	13 (6%)	2 (1%)	21 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	M	231/233 (99%)	215 (93%)	14 (6%)	2 (1%)	21 55
14	2	194/196 (99%)	187 (96%)	7 (4%)	0	100 100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100 100
All	All	6312/6368 (99%)	5929 (94%)	319 (5%)	64 (1%)	19 52

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	20(A)	SER
3	C	58	LEU
4	D	12(G)	GLU
3	Q	58	LEU
4	R	12(G)	GLU
1	A	5	THR
1	A	53	LYS
1	A	167	LYS
2	B	54	VAL
2	B	21(B)	GLY
2	B	21(C)	ASP
3	C	183	PRO
3	C	203	THR
4	D	18(D)	SER
5	E	5	ARG
5	E	202	ARG
10	J	192	ALA
13	M	96	TRP
1	O	5	THR
1	O	53	LYS
1	O	167	LYS
2	P	54	VAL
2	P	20(A)	SER
2	P	21(B)	GLY
2	P	21(C)	ASP
3	Q	183	PRO
3	Q	203	THR
4	R	18(D)	SER
5	S	5	ARG
5	S	202	ARG
10	X	192	ALA
5	E	203	ASP
5	E	231	LYS

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Mol	Chain	Res	Type
6	F	64	ASN
5	S	203	ASP
5	S	231	LYS
6	T	64	ASN
7	U	184	ASN
13	1	96	TRP
2	B	184	MET
4	D	12(F)	GLY
4	D	128	MET
5	E	180	LEU
5	E	217	LYS
9	I	93	GLY
4	R	12(F)	GLY
4	R	128	MET
5	S	180	LEU
5	S	217	LYS
9	W	93	GLY
7	G	184	ASN
7	G	239	GLN
13	M	72	ALA
7	U	239	GLN
13	1	72	ALA
2	P	6	ARG
2	P	184	MET
6	T	206	LYS
12	Z	93	PHE
5	E	18(F)	ILE
5	S	18(F)	ILE
4	D	12(C)	GLY
4	R	12(C)	GLY
7	U	61	PRO

5.3.2 Protein sidechains (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	204 (98%)	5 (2%)	57	87
1	O	209/209 (100%)	204 (98%)	5 (2%)	57	87
2	B	203/203 (100%)	187 (92%)	16 (8%)	15	40
2	P	203/203 (100%)	187 (92%)	16 (8%)	15	40
3	C	213/213 (100%)	203 (95%)	10 (5%)	32	67
3	Q	213/213 (100%)	203 (95%)	10 (5%)	32	67
4	D	198/198 (100%)	186 (94%)	12 (6%)	23	55
4	R	198/198 (100%)	186 (94%)	12 (6%)	23	55
5	E	192/192 (100%)	174 (91%)	18 (9%)	11	31
5	S	192/192 (100%)	174 (91%)	18 (9%)	11	31
6	F	201/201 (100%)	184 (92%)	17 (8%)	13	36
6	T	201/201 (100%)	183 (91%)	18 (9%)	12	34
7	G	207/207 (100%)	195 (94%)	12 (6%)	25	57
7	U	207/207 (100%)	194 (94%)	13 (6%)	22	53
8	H	181/181 (100%)	175 (97%)	6 (3%)	45	79
8	V	181/181 (100%)	175 (97%)	6 (3%)	45	79
9	I	172/172 (100%)	167 (97%)	5 (3%)	50	83
9	W	172/172 (100%)	167 (97%)	5 (3%)	50	83
10	J	175/175 (100%)	168 (96%)	7 (4%)	38	73
10	X	175/175 (100%)	168 (96%)	7 (4%)	38	73
11	K	169/169 (100%)	162 (96%)	7 (4%)	37	72
11	Y	169/169 (100%)	162 (96%)	7 (4%)	37	72
12	L	185/185 (100%)	173 (94%)	12 (6%)	21	52
12	Z	185/185 (100%)	173 (94%)	12 (6%)	21	52
13	1	199/199 (100%)	189 (95%)	10 (5%)	30	64
13	M	199/199 (100%)	189 (95%)	10 (5%)	30	64
14	2	162/162 (100%)	152 (94%)	10 (6%)	23	54
14	N	162/162 (100%)	152 (94%)	10 (6%)	23	54
All	All	5332/5332 (100%)	5036 (94%)	296 (6%)	26	59

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	124	THR
1	A	158	PHE
1	A	179	ARG
2	B	14	ILE
2	B	46	ILE
2	B	58	LEU
2	B	62	ASP
2	B	71	ASN
2	B	116	LEU
2	B	121	GLN
2	B	135	SER
2	B	150	THR
2	B	156	ASN
2	B	158	THR
2	B	185	LYS
2	B	187	ASP
2	B	192	LEU
2	B	212	PHE
2	B	218	ASN
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	61	THR
3	C	121	GLN
3	C	135	SER
3	C	150	GLN
3	C	163	GLN
3	C	174	GLU
3	C	208	LYS
4	D	28	LEU
4	D	48	LEU
4	D	107	ILE
4	D	110	GLU
4	D	126	ARG
4	D	156	THR
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU

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Mol	Chain	Res	Type
5	E	12	THR
5	E	13	VAL
5	E	32	LYS
5	E	57	GLU
5	E	97	ASN
5	E	104	ASN
5	E	111	ARG
5	E	117	CYS
5	E	121	GLN
5	E	149	LEU
5	E	185	ASN
5	E	189	LEU
5	E	199	GLN
5	E	207	LEU
5	E	2(D)	ASP
5	E	223	ILE
5	E	227	GLU
5	E	231	LYS
6	F	11	SER
6	F	18	ASP
6	F	35	THR
6	F	43	ASN
6	F	98	SER
6	F	105	THR
6	F	121	GLN
6	F	127	ASN
6	F	144	ASN
6	F	169	ARG
6	F	176	LEU
6	F	18(E)	GLU
6	F	187	ARG
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
7	G	12	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	157	TYR

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Mol	Chain	Res	Type
7	G	169	GLN
7	G	184	ASN
7	G	197	MET
7	G	232	ARG
7	G	233	LEU
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	121	VAL
8	H	197	ARG
9	I	29	ASN
9	I	61	TYR
9	I	113	PHE
9	I	155	ILE
9	I	160	LEU
10	J	34	THR
10	J	35	ARG
10	J	52	THR
10	J	70	GLU
10	J	77	GLN
10	J	121	GLU
10	J	155	LEU
11	K	4	LEU
11	K	9	GLN
11	K	87	VAL
11	K	99	THR
11	K	100	MET
11	K	104	TYR
11	K	10(B)	LYS
12	L	-9	GLN
12	L	-7	ASN
12	L	3	ILE
12	L	14	LEU
12	L	40	ASN
12	L	58	ARG
12	L	61	ASN
12	L	70(A)	ASN
12	L	82	ASN
12	L	98	HIS
12	L	99	THR
12	L	145	TYR

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Mol	Chain	Res	Type
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	129	PHE
13	M	14(C)	ARG
13	M	148	VAL
13	M	149	GLN
13	M	184	LEU
13	M	204	LYS
13	M	211	ILE
14	N	36	ARG
14	N	84	LYS
14	N	89	GLU
14	N	10(A)	ASP
14	N	10(B)	LYS
14	N	115	LEU
14	N	119	VAL
14	N	149	GLU
14	N	178	LEU
14	N	18(I)	GLN
1	O	33	GLN
1	O	64	LEU
1	O	124	THR
1	O	158	PHE
1	O	179	ARG
2	P	14	ILE
2	P	46	ILE
2	P	58	LEU
2	P	62	ASP
2	P	71	ASN
2	P	116	LEU
2	P	121	GLN
2	P	135	SER
2	P	150	THR
2	P	156	ASN
2	P	158	THR
2	P	185	LYS
2	P	187	ASP
2	P	192	LEU
2	P	212	PHE
2	P	218	ASN
3	Q	10	ARG

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Mol	Chain	Res	Type
3	Q	25	GLU
3	Q	57	LYS
3	Q	61	THR
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	163	GLN
3	Q	174	GLU
3	Q	208	LYS
4	R	28	LEU
4	R	48	LEU
4	R	107	ILE
4	R	110	GLU
4	R	126	ARG
4	R	156	THR
4	R	170	GLU
4	R	177	LEU
4	R	191	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
5	S	12	THR
5	S	13	VAL
5	S	32	LYS
5	S	57	GLU
5	S	97	ASN
5	S	104	ASN
5	S	111	ARG
5	S	117	CYS
5	S	121	GLN
5	S	149	LEU
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	207	LEU
5	S	2(D)	ASP
5	S	223	ILE
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	18	ASP
6	T	35	THR

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Mol	Chain	Res	Type
6	T	43	ASN
6	T	98	SER
6	T	105	THR
6	T	121	GLN
6	T	127	ASN
6	T	135	SER
6	T	144	ASN
6	T	169	ARG
6	T	176	LEU
6	T	18(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
7	U	12	ILE
7	U	48	VAL
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	157	TYR
7	U	169	GLN
7	U	184	ASN
7	U	197	MET
7	U	232	ARG
7	U	233	LEU
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	121	VAL
8	V	197	ARG
9	W	29	ASN
9	W	61	TYR
9	W	113	PHE
9	W	155	ILE
9	W	160	LEU
10	X	34	THR
10	X	35	ARG
10	X	52	THR

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Mol	Chain	Res	Type
10	X	70	GLU
10	X	77	GLN
10	X	121	GLU
10	X	155	LEU
11	Y	4	LEU
11	Y	9	GLN
11	Y	87	VAL
11	Y	99	THR
11	Y	100	MET
11	Y	104	TYR
11	Y	10(B)	LYS
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	3	ILE
12	Z	14	LEU
12	Z	40	ASN
12	Z	58	ARG
12	Z	61	ASN
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	145	TYR
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	129	PHE
13	1	14(C)	ARG
13	1	148	VAL
13	1	149	GLN
13	1	184	LEU
13	1	204	LYS
13	1	211	ILE
14	2	36	ARG
14	2	84	LYS
14	2	89	GLU
14	2	10(A)	ASP
14	2	10(B)	LYS
14	2	115	LEU
14	2	119	VAL
14	2	149	GLU
14	2	178	LEU

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Mol	Chain	Res	Type
14	2	18(I)	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (202) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	238	GLN
3	C	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	114	GLN
4	D	161	ASN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	7	ASN
5	E	33	GLN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	156	ASN
5	E	185	ASN
5	E	199	GLN
5	E	2(E)	ASN

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Mol	Chain	Res	Type
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	11	HIS
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	10	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
10	J	36	GLN
10	J	54	GLN
10	J	62	ASN
10	J	64	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	141	HIS
10	J	186	GLN
11	K	9	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN

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Mol	Chain	Res	Type
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	85	HIS
12	L	98	HIS
12	L	123	GLN
12	L	1(I)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	69	GLN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	238	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN

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Mol	Chain	Res	Type
4	R	114	GLN
4	R	161	ASN
4	R	211	GLN
4	R	218	GLN
4	R	226	ASN
5	S	7	ASN
5	S	64	GLN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	125	GLN
5	S	156	ASN
5	S	185	ASN
5	S	199	GLN
5	S	2(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	192	GLN
7	U	11	HIS
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	170	GLN
7	U	178	ASN
7	U	184	ASN
7	U	228	ASN
8	V	10	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	64	ASN

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Mol	Chain	Res	Type
9	W	81	GLN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	141	HIS
10	X	186	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	131	GLN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	82	ASN
12	Z	85	HIS
12	Z	123	GLN
12	Z	1(I)	ASN
12	Z	166	HIS
13	1	10	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	69	GLN
14	2	145	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
15	SA1	2	0	14	18,22,22	1.44	3 (16%)	21,34,34	1.98	3 (14%)
15	SA1	H	0	8	18,22,22	1.46	1 (5%)	21,34,34	1.85	2 (9%)
15	SA1	K	0	11	18,22,22	1.38	2 (11%)	21,34,34	1.85	3 (14%)
15	SA1	N	0	14	18,22,22	1.25	2 (11%)	21,34,34	2.05	3 (14%)
15	SA1	V	0	8	18,22,22	1.44	2 (11%)	21,34,34	2.07	2 (9%)
15	SA1	Y	0	11	18,22,22	1.31	1 (5%)	21,34,34	1.86	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SA1	2	0	14	-	0/4/52/52	0/3/3/3
15	SA1	H	0	8	-	0/4/52/52	0/3/3/3
15	SA1	K	0	11	-	0/4/52/52	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SA1	N	0	14	-	0/4/52/52	0/3/3/3
15	SA1	V	0	8	-	0/4/52/52	0/3/3/3
15	SA1	Y	0	11	-	0/4/52/52	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	2	0	SA1	O17-C10	2.01	1.47	1.42
15	2	0	SA1	O2-C3	2.27	1.47	1.45
15	N	0	SA1	O2-C3	2.50	1.47	1.45
15	K	0	SA1	C4-C3	2.75	1.56	1.51
15	K	0	SA1	O2-C3	2.84	1.48	1.45
15	V	0	SA1	O17-C10	2.90	1.48	1.42
15	Y	0	SA1	C4-C3	2.94	1.56	1.51
15	N	0	SA1	C4-C3	3.12	1.57	1.51
15	H	0	SA1	C4-C3	3.75	1.58	1.51
15	V	0	SA1	C4-C3	3.76	1.58	1.51
15	2	0	SA1	C4-C3	3.81	1.58	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	V	0	SA1	C3-C5-C6	-5.30	99.97	104.30
15	N	0	SA1	C3-C5-C6	-5.27	99.99	104.30
15	2	0	SA1	C3-C5-C6	-5.08	100.15	104.30
15	Y	0	SA1	C3-C5-C6	-4.41	100.70	104.30
15	H	0	SA1	C3-C5-C6	-4.22	100.85	104.30
15	K	0	SA1	C3-C5-C6	-3.66	101.31	104.30
15	N	0	SA1	O7-C6-C5	-2.21	123.58	126.07
15	2	0	SA1	O7-C6-C5	-2.03	123.79	126.07
15	K	0	SA1	O7-C6-C5	-2.01	123.81	126.07
15	Y	0	SA1	C9-C10-C11	6.41	122.14	114.09
15	2	0	SA1	C9-C10-C11	6.54	122.30	114.09
15	H	0	SA1	C9-C10-C11	6.55	122.32	114.09
15	K	0	SA1	C9-C10-C11	6.64	122.43	114.09
15	N	0	SA1	C9-C10-C11	6.69	122.49	114.09
15	V	0	SA1	C9-C10-C11	7.31	123.27	114.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	0	SA1	1	0
15	Y	0	SA1	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.27	4 (1%)	74	66	32, 45, 74, 99	0
1	O	250/250 (100%)	-0.22	9 (3%)	46	34	35, 51, 80, 100	0
2	B	244/244 (100%)	-0.05	11 (4%)	37	26	32, 50, 84, 116	0
2	P	244/244 (100%)	0.00	15 (6%)	25	15	34, 52, 87, 116	0
3	C	241/241 (100%)	0.02	13 (5%)	29	19	30, 54, 105, 122	0
3	Q	241/241 (100%)	0.20	16 (6%)	22	13	36, 59, 109, 121	0
4	D	242/242 (100%)	0.02	11 (4%)	37	26	32, 54, 88, 117	0
4	R	242/242 (100%)	0.12	13 (5%)	29	19	35, 57, 90, 120	0
5	E	233/233 (100%)	-0.08	6 (2%)	59	47	39, 58, 82, 109	0
5	S	233/233 (100%)	0.19	17 (7%)	18	10	37, 62, 86, 107	0
6	F	244/244 (100%)	-0.23	5 (2%)	68	58	33, 51, 85, 101	0
6	T	244/244 (100%)	-0.08	6 (2%)	61	48	31, 53, 89, 102	0
7	G	243/243 (100%)	-0.29	3 (1%)	81	73	28, 44, 72, 106	0
7	U	243/243 (100%)	-0.19	4 (1%)	74	66	28, 47, 73, 105	0
8	H	222/222 (100%)	-0.44	3 (1%)	78	69	23, 41, 61, 91	0
8	V	222/222 (100%)	-0.41	2 (0%)	85	79	30, 44, 61, 89	0
9	I	204/204 (100%)	-0.55	1 (0%)	91	88	29, 42, 57, 75	0
9	W	204/204 (100%)	-0.51	1 (0%)	91	88	29, 41, 61, 78	0
10	J	198/198 (100%)	-0.29	4 (2%)	68	58	26, 45, 62, 115	0
10	X	198/198 (100%)	-0.32	6 (3%)	54	41	30, 46, 62, 116	0
11	K	212/212 (100%)	-0.52	0	100	100	26, 42, 61, 70	0
11	Y	212/212 (100%)	-0.48	0	100	100	30, 44, 63, 73	0
12	L	222/222 (100%)	-0.44	2 (0%)	85	79	26, 44, 64, 85	0
12	Z	222/222 (100%)	-0.42	4 (1%)	71	61	27, 44, 67, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1	233/233 (100%)	-0.44	2 (0%) 85 79	28, 43, 57, 64	0
13	M	233/233 (100%)	-0.46	1 (0%) 93 90	28, 44, 58, 66	0
14	2	196/196 (100%)	-0.46	1 (0%) 91 88	23, 41, 61, 74	0
14	N	196/196 (100%)	-0.49	0 100 100	25, 39, 61, 73	0
All	All	6368/6368 (100%)	-0.24	160 (2%) 61 48	23, 47, 81, 122	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	R	12(E)	SER	10.7
4	R	12(F)	GLY	10.1
7	U	240	ASP	9.9
7	U	6	ALA	9.1
4	D	12(D)	ALA	9.0
3	C	55	THR	8.9
3	C	56	LEU	8.2
2	B	218	ASN	8.0
4	D	12(E)	SER	7.6
2	P	217	ALA	7.6
10	X	193	GLN	7.1
4	D	12(C)	GLY	7.0
7	G	6	ALA	7.0
4	R	12(D)	ALA	6.8
10	X	192	ALA	6.6
2	B	217	ALA	6.6
2	P	218	ASN	6.5
1	O	4	MET	6.2
4	D	126	ARG	6.2
10	J	192	ALA	6.1
3	Q	56	LEU	6.1
2	P	21(B)	GLY	6.0
10	J	193	GLN	5.8
2	P	21(C)	ASP	5.7
1	A	4	MET	5.5
3	Q	55	THR	5.5
4	R	12(C)	GLY	5.4
6	F	5	GLY	5.1
8	V	223	ASP	5.0
3	Q	63	THR	4.9
4	D	12(F)	GLY	4.9
7	G	240	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
4	D	12(G)	GLU	4.7
2	B	54	VAL	4.7
6	F	204	ASP	4.7
5	S	5	ARG	4.5
9	W	-8	SER	4.5
10	J	191	GLN	4.5
13	M	-8	THR	4.4
3	Q	242	GLU	4.3
2	P	54	VAL	4.3
5	E	4	PHE	4.3
3	Q	54	SER	4.3
5	S	203	ASP	4.1
2	B	21(C)	ASP	4.1
4	R	9	ASP	4.1
5	S	233	ILE	4.1
3	Q	203	THR	4.1
8	V	222	CYS	4.0
3	Q	243	GLN	4.0
5	S	206	SER	3.9
2	B	21(B)	GLY	3.9
13	1	-8	THR	3.9
1	O	55	SER	3.9
6	T	241	ASN	3.8
2	P	62	ASP	3.8
2	P	239	THR	3.7
4	D	125	GLU	3.6
1	O	236	LEU	3.6
1	A	5	THR	3.6
3	Q	241	GLN	3.6
5	E	203	ASP	3.5
3	C	241	GLN	3.5
9	I	-8	SER	3.5
2	P	219	GLU	3.5
1	O	5	THR	3.5
6	F	206	LYS	3.5
4	R	12(G)	GLU	3.4
2	B	239	THR	3.4
8	H	223	ASP	3.4
3	C	240	LYS	3.3
3	C	243	GLN	3.3
4	R	125	GLU	3.2
8	H	222	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
14	2	18(I)	GLN	3.2
6	T	6	THR	3.2
12	Z	14(W)	LYS	3.1
2	P	20(A)	SER	3.1
5	S	6	ASN	3.1
4	R	126	ARG	3.1
4	R	12(B)	GLU	3.1
1	O	235	ALA	3.1
5	S	60	SER	3.1
5	S	178	ARG	3.1
5	S	4	PHE	3.0
10	X	191	GLN	3.0
6	T	240	ILE	2.9
3	C	242	GLU	2.9
2	B	21(A)	LYS	2.9
4	R	127	LEU	2.8
1	O	21(P)	LYS	2.8
3	Q	64	PRO	2.8
6	T	203	GLU	2.7
5	E	6	ASN	2.7
5	S	174	THR	2.7
5	E	57	GLU	2.7
5	S	54	ASN	2.7
12	L	14(P)	PRO	2.7
5	S	63	TYR	2.7
10	X	-1	MET	2.7
13	1	211	ILE	2.7
3	C	59	GLN	2.7
1	A	236	LEU	2.7
2	P	21(A)	LYS	2.6
12	Z	145	TYR	2.6
5	S	59	SER	2.6
3	Q	58	LEU	2.6
12	L	145	TYR	2.6
5	S	195	GLU	2.6
3	C	202	GLN	2.6
2	P	63	THR	2.6
4	D	127	LEU	2.6
3	Q	18(D)	GLU	2.6
3	Q	187	GLU	2.6
6	F	241	ASN	2.6
8	H	220	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	O	21(O)	ASP	2.6
5	S	55	ALA	2.6
10	X	189	ASP	2.5
3	C	18(D)	GLU	2.5
3	C	203	THR	2.5
3	C	54	SER	2.5
4	D	244	GLU	2.5
2	B	219	GLU	2.5
6	T	18(B)	HIS	2.5
6	F	20(B)	GLU	2.5
2	B	20(A)	SER	2.4
7	U	239	GLN	2.4
3	C	239	GLU	2.4
3	C	237	GLU	2.4
5	E	127	TYR	2.3
1	A	234	GLU	2.3
3	Q	202	GLN	2.3
7	U	7	GLY	2.3
4	R	19	GLY	2.3
12	Z	70(A)	ASN	2.3
3	Q	238	GLN	2.3
7	G	239	GLN	2.3
5	S	2(E)	ASN	2.3
4	D	218	GLN	2.3
5	S	57	GLU	2.2
1	O	64	LEU	2.2
2	P	21(D)	GLY	2.2
10	J	189	ASP	2.2
4	R	242	ALA	2.2
2	P	63(A)	SER	2.2
2	P	220	TYR	2.2
10	X	188	ASP	2.1
6	T	18(E)	GLU	2.1
2	B	53	LYS	2.1
5	S	56	ASP	2.1
5	E	33	GLN	2.1
12	Z	-9	GLN	2.1
4	D	9	ASP	2.0
1	O	234	GLU	2.0
3	Q	239	GLU	2.0
2	B	227	GLN	2.0
4	R	218	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
3	Q	44	ASN	2.0
2	P	53	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	SA1	N	0	20/20	0.95	0.17	1.72	22,34,37,38	0
15	SA1	2	0	20/20	0.94	0.17	1.68	28,33,36,38	0
15	SA1	H	0	20/20	0.94	0.17	1.19	37,40,42,44	0
15	SA1	K	0	20/20	0.93	0.18	0.95	26,33,37,37	0
15	SA1	V	0	20/20	0.96	0.16	0.66	35,39,42,42	0
15	SA1	Y	0	20/20	0.95	0.17	0.59	34,36,38,39	0

6.5 Other polymers (i)

There are no such residues in this entry.