Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:36 PM GMT

PDB ID	:	4LQI
Title	:	Yeast 20S Proteasome in complex with Vibralactone
Authors	:	List, A.; Zeiler, E.; Gallastegui, N.; Rusch, M.; Hedberg, C.; Sieber, S.A.; Groll, M.
Deposited on	:	2013-07-18
Resolution	:	2.70 Å(reported)

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

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

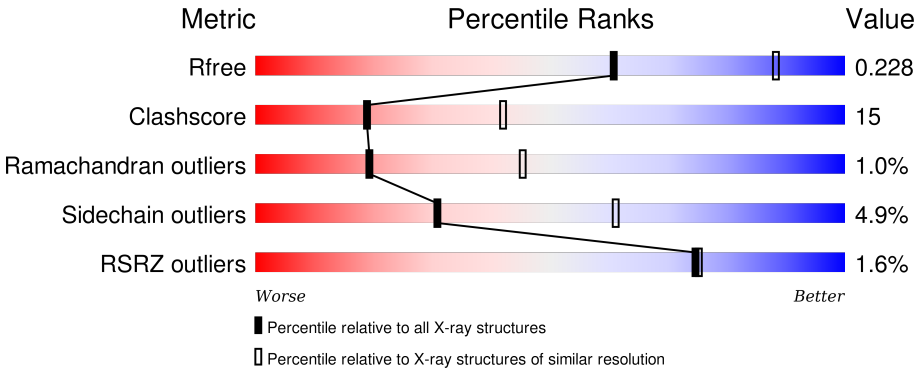
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	76% 23%
1	O	250	74% 25%
2	B	244	64% 31% 5%
2	P	244	3% 66% 30% 5%
3	C	241	60% 37%

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Mol	Chain	Length	Quality of chain
3	Q	241	7% 60% 37%
4	D	242	3% 70% 28%
4	R	242	2% 70% 28%
5	E	233	3% 60% 34% 6%
5	S	233	3% 61% 35% 5%
6	F	244	2% 70% 25% 5%
6	T	244	2% 72% 24% 5%
7	G	243	2% 71% 25%
7	U	243	% 69% 27%
8	H	222	77% 22%
8	V	222	% 74% 24%
9	I	204	80% 19%
9	W	204	76% 22%
10	J	198	2% 70% 29%
10	X	198	3% 70% 29%
11	K	212	74% 23%
11	Y	212	73% 25%
12	L	222	68% 28%
12	Z	222	67% 30%
13	M	233	72% 26%
13	a	233	96%
14	N	196	77% 21%
14	b	196	% 96%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	1Y9	K	301	-	-	-	X
15	1Y9	N	201	-	-	-	X
15	1Y9	Y	301	-	-	-	X
15	1Y9	b	201	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 50942 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 subunit alpha type-2.

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 subunit alpha type-3.

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 subunit alpha type-4.

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 subunit alpha type-5.

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 subunit alpha type-6.

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 subunit alpha type-7.

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 subunit alpha type-1.

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

- Molecule 8 is a protein called Proteasome subunit beta type-2.

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 subunit beta type-3.

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

- Molecule 10 is a protein called Proteasome subunit beta type-4.

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 subunit beta type-5.

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 subunit beta type-6.

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

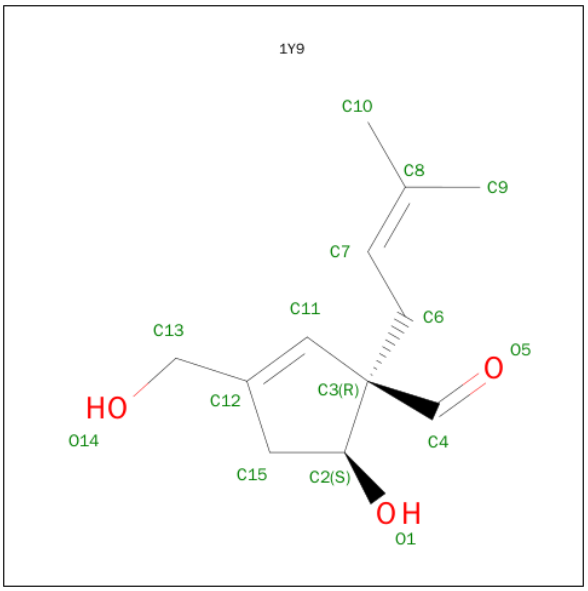
- Molecule 13 is a protein called Proteasome subunit beta type-7.

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

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

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

- Molecule 15 is VIBRALACTONE, BOUND FORM (three-letter code: 1Y9) (formula: $C_{12}H_{18}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total C O 15 12 3	0	0
15	N	1	Total C O 15 12 3	0	0
15	Y	1	Total C O 15 12 3	0	0
15	b	1	Total C O 15 12 3	0	0

- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	56	Total O 56 56	0	0
16	B	36	Total O 36 36	0	0
16	C	42	Total O 42 42	0	0
16	D	38	Total O 38 38	0	0
16	E	23	Total O 23 23	0	0
16	F	49	Total O 49 49	0	0
16	G	61	Total O 61 61	0	0
16	H	49	Total O 49 49	0	0

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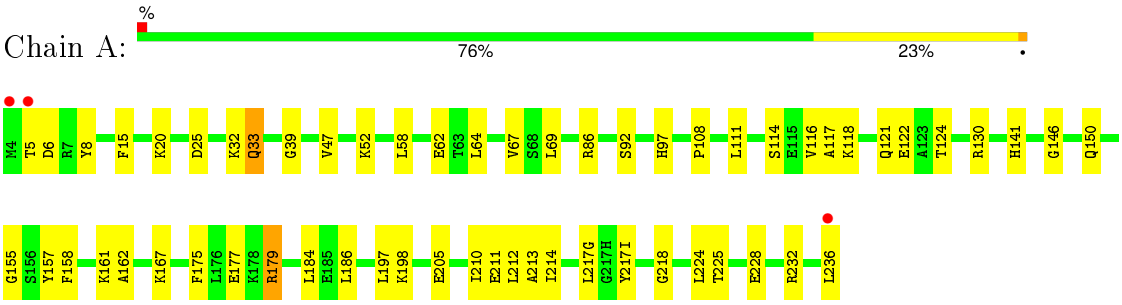
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	I	70	Total O 70 70	0	0
16	J	53	Total O 53 53	0	0
16	K	46	Total O 46 46	0	0
16	L	56	Total O 56 56	0	0
16	M	73	Total O 73 73	0	0
16	N	57	Total O 57 57	0	0
16	O	31	Total O 31 31	0	0
16	P	28	Total O 28 28	0	0
16	Q	28	Total O 28 28	0	0
16	R	31	Total O 31 31	0	0
16	S	20	Total O 20 20	0	0
16	T	38	Total O 38 38	0	0
16	U	62	Total O 62 62	0	0
16	V	46	Total O 46 46	0	0
16	W	61	Total O 61 61	0	0
16	X	52	Total O 52 52	0	0
16	Y	46	Total O 46 46	0	0
16	Z	52	Total O 52 52	0	0
16	a	75	Total O 75 75	0	0
16	b	55	Total O 55 55	0	0

3 Residue-property plots

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.

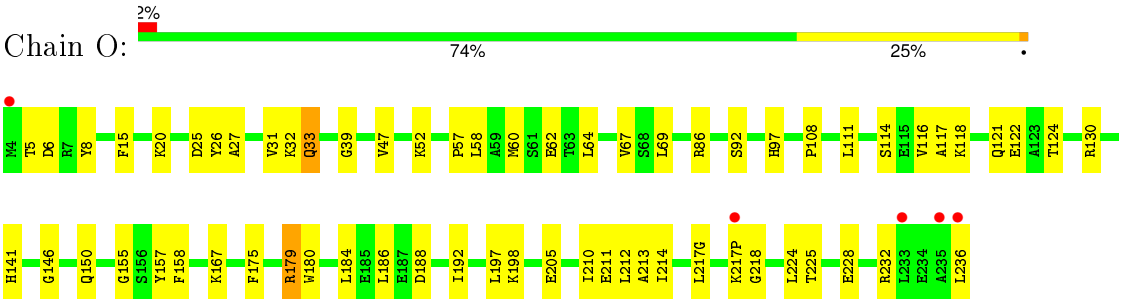
- Molecule 1: Proteasome subunit alpha type-2

Chain A:



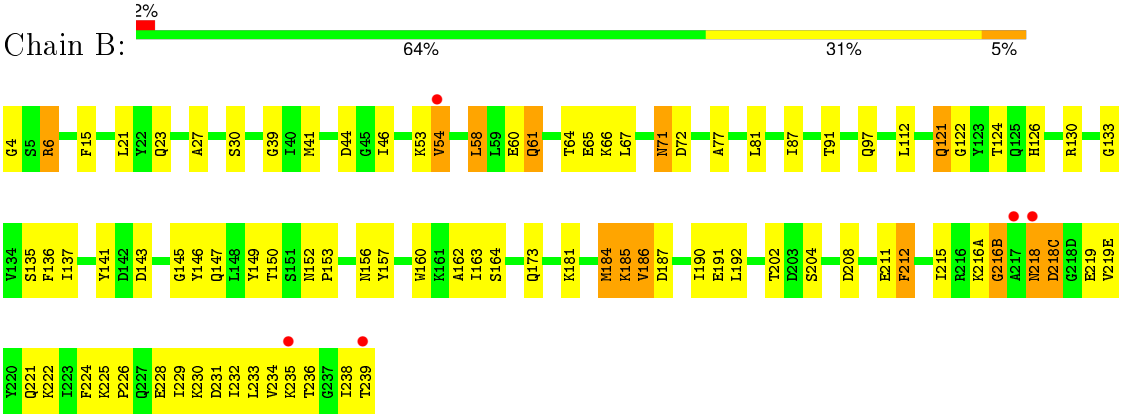
- Molecule 1: Proteasome subunit alpha type-2

Chain O:



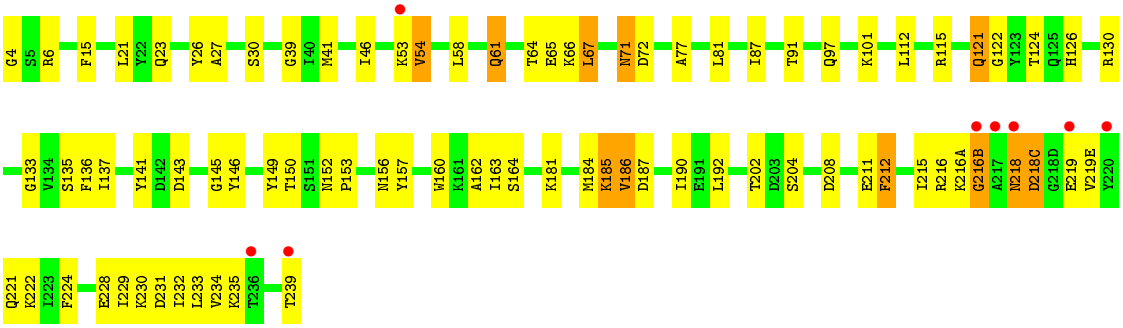
- Molecule 2: Proteasome subunit alpha type-3

Chain B:



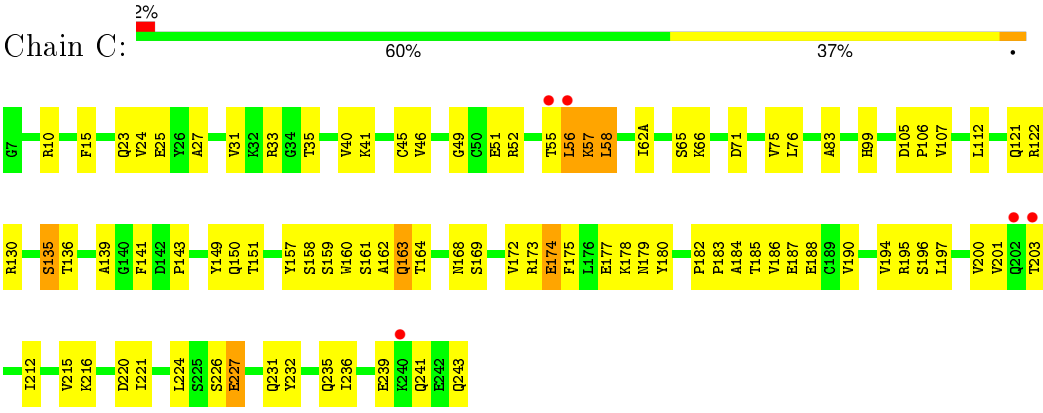
- Molecule 2: Proteasome subunit alpha type-3

Chain P:



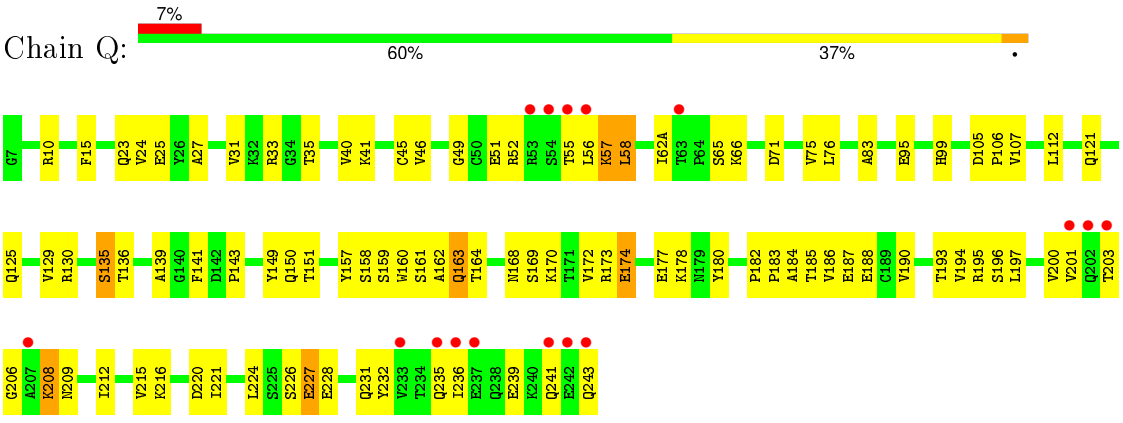
• Molecule 3: Proteasome subunit alpha type-4

Chain C:



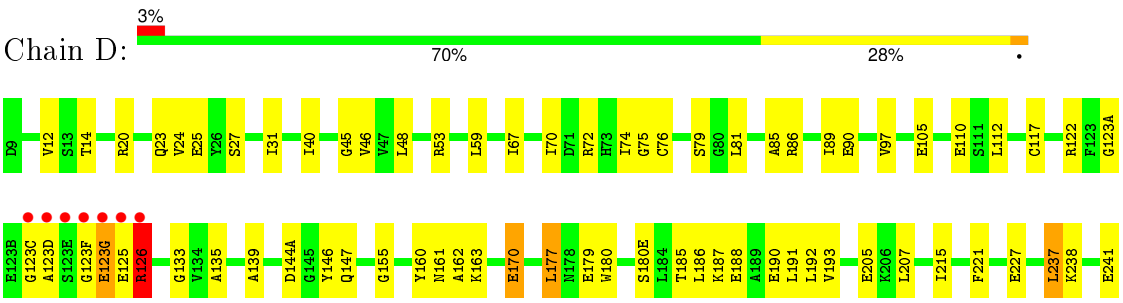
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



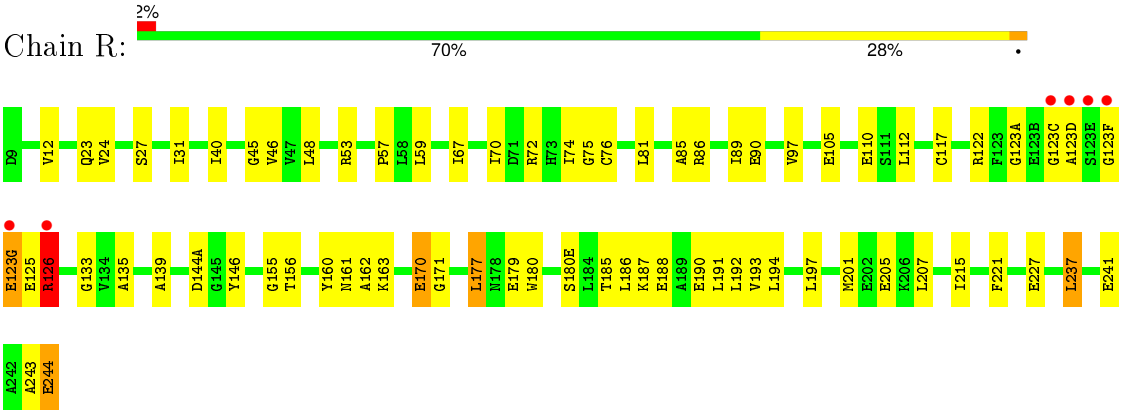
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



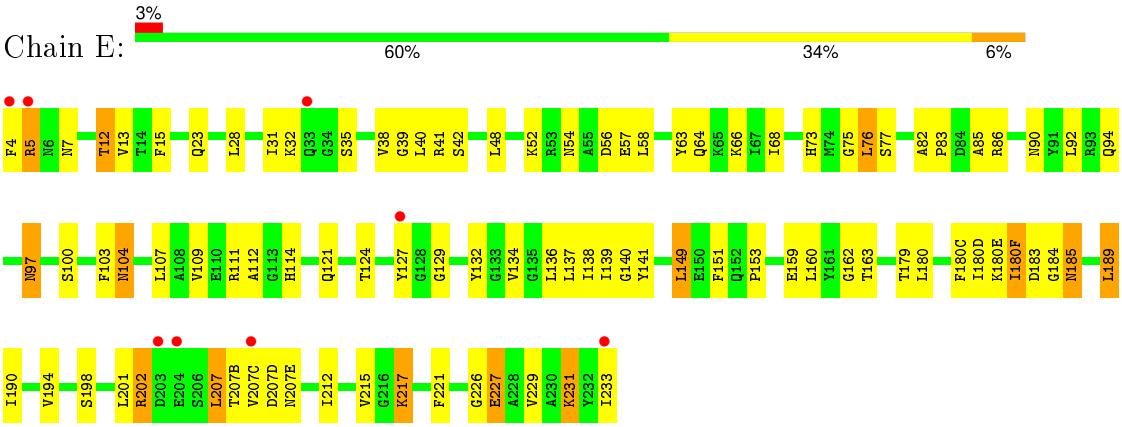
• Molecule 4: Proteasome subunit alpha type-5

Chain R:



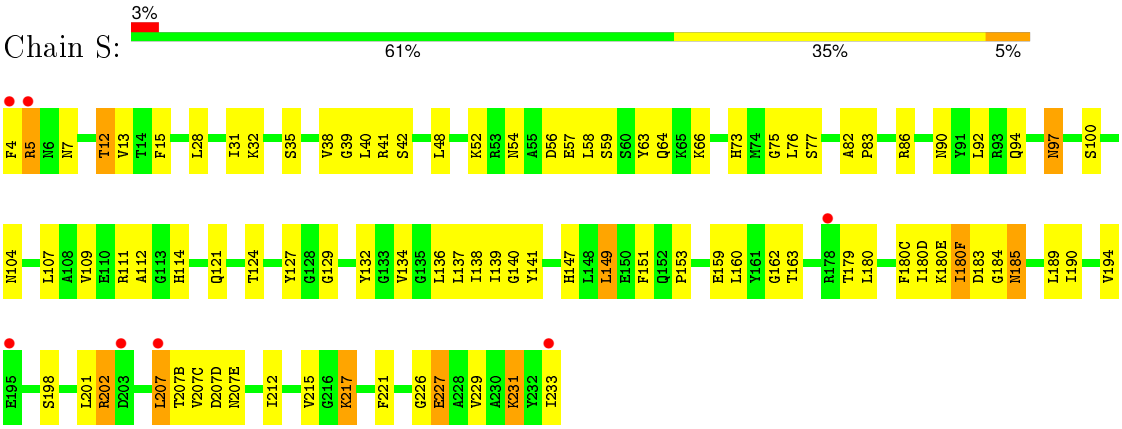
• Molecule 5: Proteasome subunit alpha type-6

Chain E:



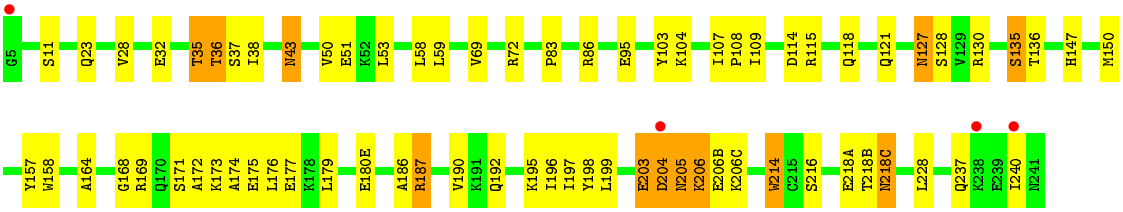
• Molecule 5: Proteasome subunit alpha type-6

Chain S:

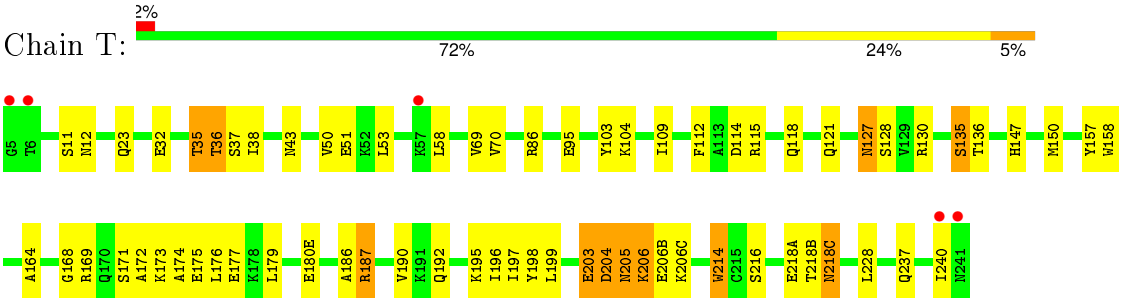


• Molecule 6: Proteasome subunit alpha type-7

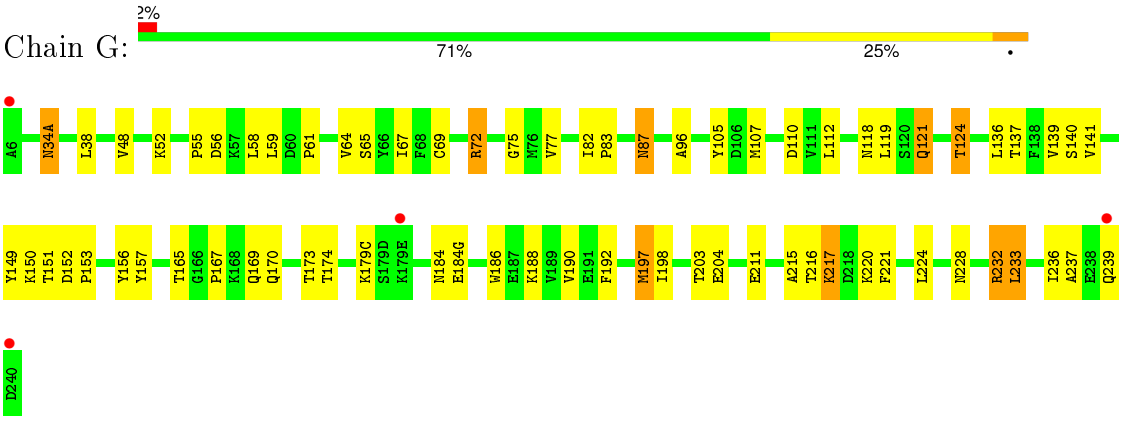
Chain F:



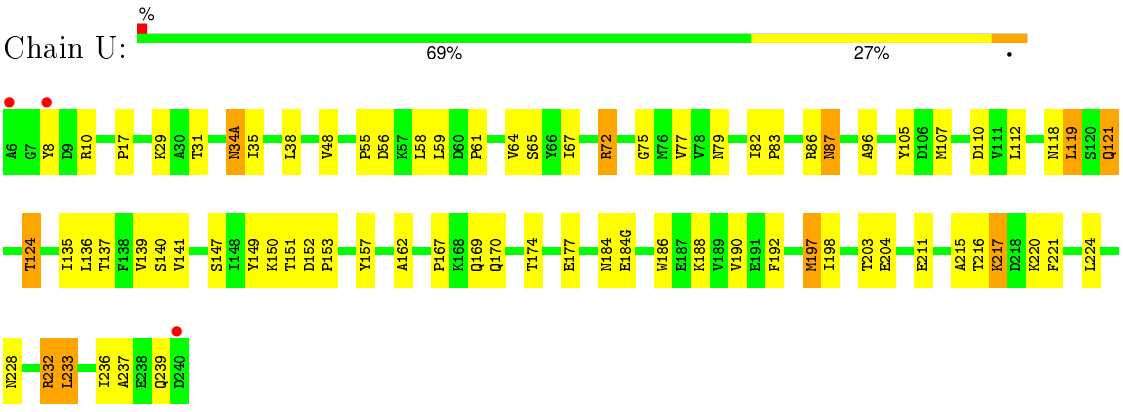
• Molecule 6: Proteasome subunit alpha type-7



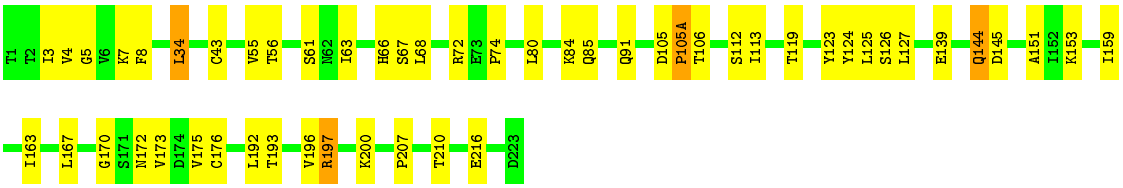
• Molecule 7: Proteasome subunit alpha type-1



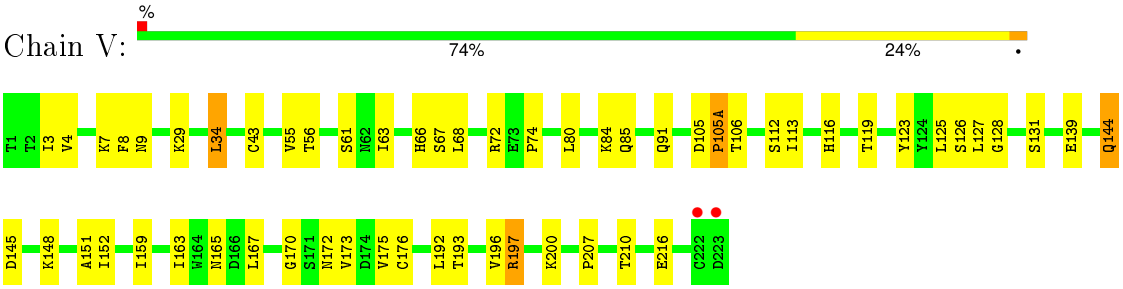
• Molecule 7: Proteasome subunit alpha type-1



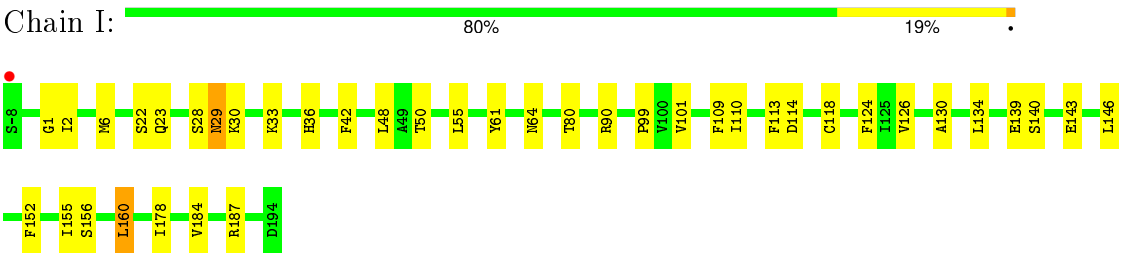
• Molecule 8: Proteasome subunit beta type-2



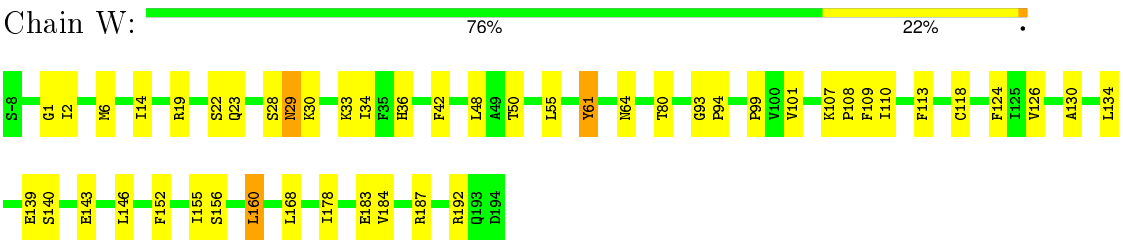
• Molecule 8: Proteasome subunit beta type-2



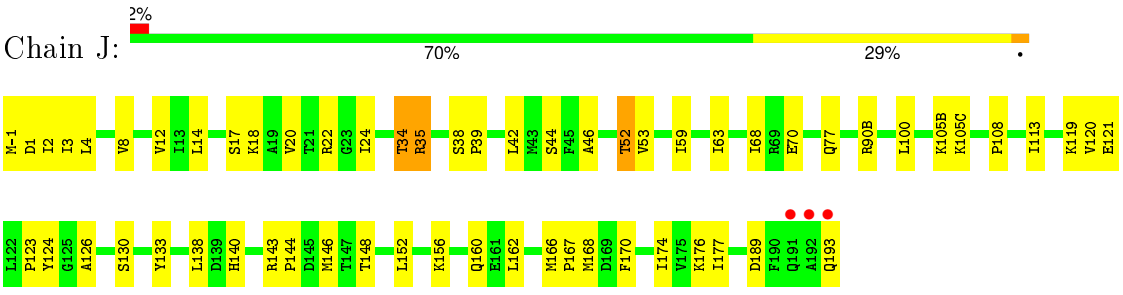
• Molecule 9: Proteasome subunit beta type-3



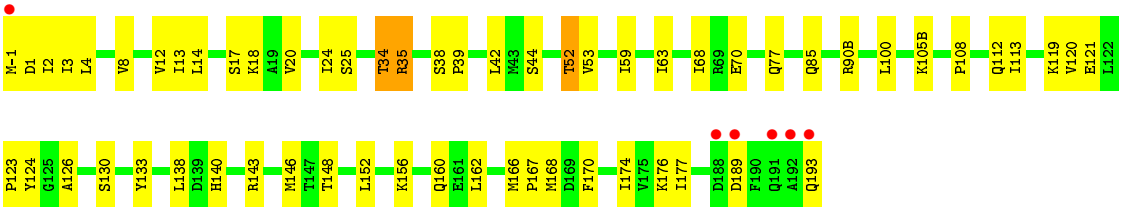
• Molecule 9: Proteasome subunit beta type-3



• Molecule 10: Proteasome subunit beta type-4

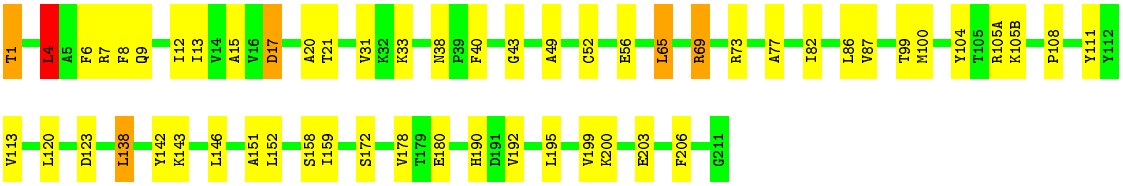


• Molecule 10: Proteasome subunit beta type-4



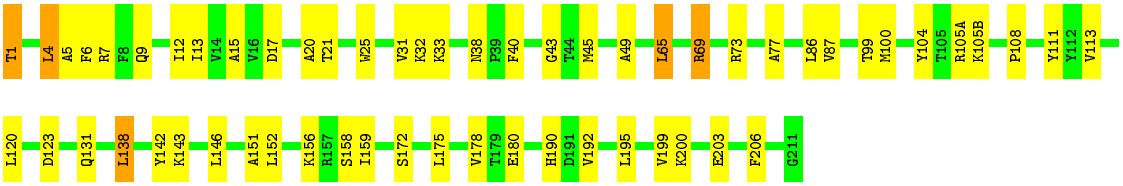
• Molecule 11: Proteasome subunit beta type-5

Chain K:



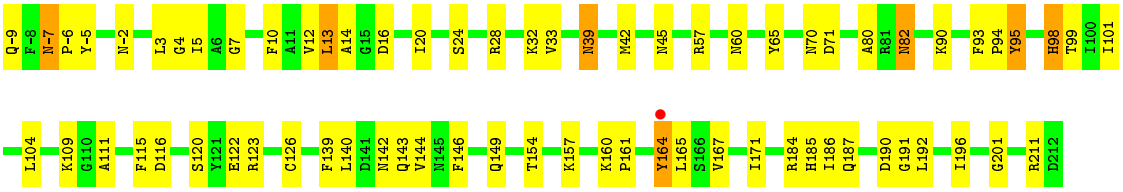
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



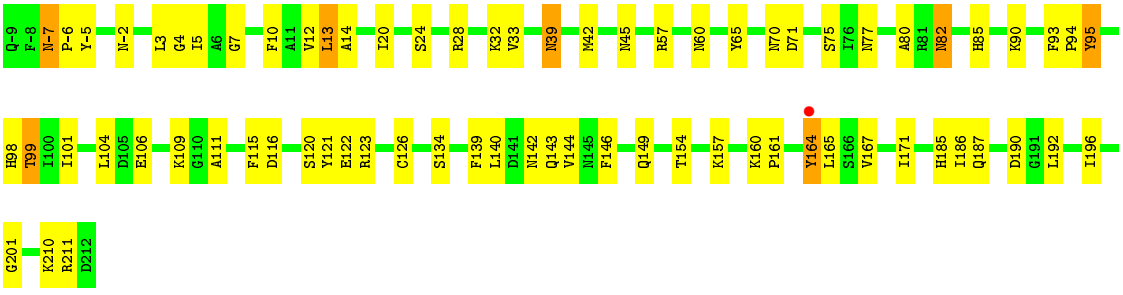
• Molecule 12: Proteasome subunit beta type-6

Chain L:



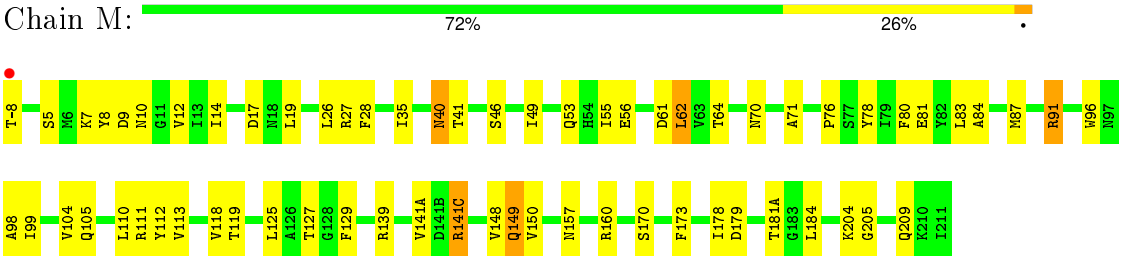
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



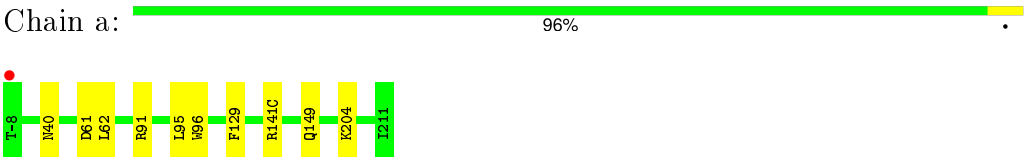
• Molecule 13: Proteasome subunit beta type-7

Chain M:



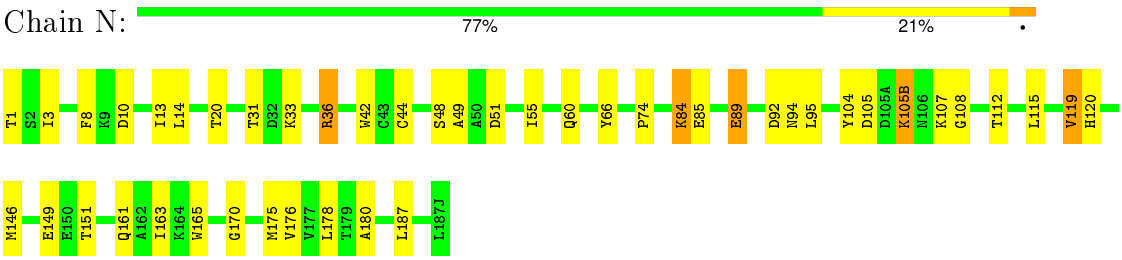
• Molecule 13: Proteasome subunit beta type-7

Chain a:



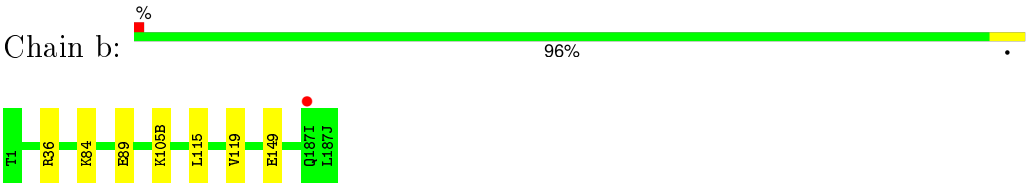
• Molecule 14: Proteasome subunit beta type-1

Chain N:



• Molecule 14: Proteasome subunit beta type-1

Chain b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.86Å 299.40Å 144.99Å 90.00° 113.07° 90.00°	Depositor
Resolution (Å)	14.99 – 2.70 48.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (14.99-2.70) 99.5 (48.95-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.202 , 0.227 0.202 , 0.228	Depositor DCC
R_{free} test set	14275 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.619	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 289175 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	50942	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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: 1Y9

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	95	TYR	N-CA-C	-5.26	96.80	111.00
12	Z	95	TYR	N-CA-C	-5.23	96.89	111.00
6	T	135	SER	N-CA-C	-5.21	96.94	111.00
6	F	135	SER	N-CA-C	-5.20	96.96	111.00
13	a	95	LEU	N-CA-C	-5.18	97.02	111.00
3	C	56	LEU	CA-CB-CG	5.16	127.16	115.30
11	K	4	LEU	CA-CB-CG	5.09	127.00	115.30

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	54	0
1	O	1915	0	1926	58	0
2	B	1905	0	1901	80	0
2	P	1905	0	1901	75	0
3	C	1891	0	1900	95	0
3	Q	1891	0	1900	99	0
4	D	1862	0	1836	51	0
4	R	1862	0	1836	53	0
5	E	1795	0	1797	88	0
5	S	1795	0	1797	85	0
6	F	1897	0	1886	62	0
6	T	1897	0	1886	61	0
7	G	1921	0	1910	66	0
7	U	1921	0	1910	74	0
8	H	1685	0	1688	40	0
8	V	1685	0	1688	42	0
9	I	1581	0	1574	36	0
9	W	1581	0	1574	39	0
10	J	1585	0	1590	64	0
10	X	1585	0	1590	68	0
11	K	1644	0	1594	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	Y	1644	0	1594	51	0
12	L	1757	0	1711	52	0
12	Z	1757	0	1711	54	0
13	M	1824	0	1832	52	0
13	a	1824	0	1832	0	0
14	N	1512	0	1480	36	0
14	b	1512	0	1480	0	0
15	K	15	0	17	2	0
15	N	15	0	17	3	0
15	Y	15	0	17	2	0
15	b	15	0	17	0	0
16	A	56	0	0	0	0
16	B	36	0	0	2	0
16	C	42	0	0	2	0
16	D	38	0	0	2	0
16	E	23	0	0	0	0
16	F	49	0	0	2	0
16	G	61	0	0	3	0
16	H	49	0	0	4	0
16	I	70	0	0	3	0
16	J	53	0	0	3	0
16	K	46	0	0	2	0
16	L	56	0	0	1	0
16	M	73	0	0	1	0
16	N	57	0	0	4	0
16	O	31	0	0	2	0
16	P	28	0	0	2	0
16	Q	28	0	0	4	0
16	R	31	0	0	1	0
16	S	20	0	0	0	0
16	T	38	0	0	3	0
16	U	62	0	0	3	0
16	V	46	0	0	3	0
16	W	61	0	0	2	0
16	X	52	0	0	3	0
16	Y	46	0	0	1	0
16	Z	52	0	0	3	0
16	a	75	0	0	0	0
16	b	55	0	0	0	0
All	All	50942	0	49318	1418	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 15.

All (1418) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:202:THR:HG22	2:P:204:SER:H	1.13	1.09
2:B:202:THR:HG22	2:B:204:SER:H	1.14	1.07
7:G:96:ALA:HA	7:G:107:MET:HE2	1.40	1.03
7:U:96:ALA:HA	7:U:107:MET:HE2	1.43	1.00
11:K:105(B):LYS:HD2	11:K:105(B):LYS:H	1.26	1.00
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.47	0.97
11:Y:105(B):LYS:HD2	11:Y:105(B):LYS:H	1.26	0.97
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.10	0.96
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.32	0.94
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.46	0.94
5:S:207:LEU:HD23	5:S:207:LEU:H	1.32	0.93
2:B:15:PHE:H	3:C:23:GLN:HE22	1.04	0.93
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.34	0.92
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.32	0.92
5:E:207:LEU:HD23	5:E:207:LEU:H	1.33	0.91
1:O:15:PHE:H	2:P:23:GLN:HE22	1.17	0.91
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.53	0.91
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.32	0.90
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.20	0.89
7:U:217:LYS:HE3	7:U:217:LYS:HA	1.54	0.89
3:C:15:PHE:H	4:D:23:GLN:HE22	1.21	0.88
7:G:217:LYS:HA	7:G:217:LYS:HE3	1.54	0.87
5:E:12:THR:HG21	5:E:124:THR:HA	1.56	0.87
2:B:71:ASN:ND2	2:B:72:ASP:H	1.71	0.87
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.40	0.86
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.39	0.86
3:C:185:THR:HB	3:C:188:GLU:HG2	1.57	0.86
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.89	0.86
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.58	0.85
5:S:12:THR:HG21	5:S:124:THR:HA	1.57	0.85
5:E:207:LEU:HA	5:E:207(E):ASN:ND2	1.91	0.85
1:A:15:PHE:H	2:B:23:GLN:HE22	1.21	0.85
3:Q:185:THR:HG22	3:Q:187:GLU:H	1.42	0.85
15:N:201:1Y9:H12	16:N:321:HOH:O	1.76	0.85
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.42	0.85
3:C:185:THR:HG22	3:C:187:GLU:H	1.42	0.84
5:S:207:LEU:HA	5:S:207(E):ASN:ND2	1.90	0.84
2:P:71:ASN:ND2	2:P:72:ASP:H	1.74	0.84
8:H:172:ASN:HD22	8:H:193:THR:HA	1.42	0.84
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:179:ARG:HH11	1:O:179:ARG:HB3	1.43	0.83
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.76	0.83
8:V:172:ASN:HD22	8:V:193:THR:HA	1.41	0.83
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.61	0.82
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.27	0.82
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.60	0.82
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.60	0.82
7:G:184(G):GLU:HG2	7:G:188:LYS:HB2	1.62	0.81
4:R:162:ALA:HB3	5:S:58:LEU:HD23	1.61	0.80
2:B:124:THR:CG2	3:C:130:ARG:HH21	1.93	0.80
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.64	0.80
5:S:207:LEU:HA	5:S:207(E):ASN:HD22	1.45	0.80
13:M:40:ASN:H	13:M:40:ASN:HD22	1.27	0.80
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.80	0.79
10:J:156:LYS:O	10:J:160:GLN:HG3	1.83	0.79
5:E:207:LEU:HA	5:E:207(E):ASN:HD22	1.46	0.79
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.31	0.79
9:W:192:ARG:HG3	16:W:207:HOH:O	1.82	0.78
3:C:163:GLN:NE2	3:C:164:THR:H	1.82	0.78
10:J:2:ILE:HD13	10:J:162:LEU:HD13	1.65	0.78
13:M:141(C):ARG:HH11	13:M:141(C):ARG:HG3	1.47	0.78
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.82	0.78
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.32	0.78
12:L:42:MET:HB2	12:L:101:ILE:HG22	1.66	0.78
4:R:243:ALA:O	4:R:244:GLU:HB2	1.85	0.77
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.66	0.77
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.66	0.77
1:A:124:THR:CG2	2:B:130:ARG:HH21	1.98	0.77
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.98	0.77
10:X:156:LYS:O	10:X:160:GLN:HG3	1.83	0.77
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.65	0.77
2:P:202:THR:HG22	2:P:204:SER:N	1.97	0.76
4:D:243:ALA:O	4:D:244:GLU:HB2	1.85	0.75
3:Q:65:SER:HB2	16:Q:303:HOH:O	1.85	0.75
10:X:2:ILE:HD13	10:X:162:LEU:HD13	1.67	0.75
2:B:15:PHE:N	3:C:23:GLN:HE22	1.84	0.75
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.16	0.75
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.35	0.75
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.69	0.74
2:P:219:GLU:HG2	2:P:219(E):VAL:H	1.52	0.74
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.36	0.74
2:B:219:GLU:HG2	2:B:219(E):VAL:H	1.51	0.74
7:G:184(G):GLU:HG2	7:G:188:LYS:CB	2.17	0.74
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.00	0.73
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.53	0.73
3:C:163:GLN:HE21	3:C:164:THR:H	1.36	0.73
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.18	0.73
3:Q:163:GLN:HA	3:Q:163:GLN:HE21	1.54	0.73
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.69	0.73
12:Z:42:MET:HB2	12:Z:101:ILE:HG22	1.70	0.73
5:S:201:LEU:HD11	5:S:207:LEU:HD22	1.71	0.73
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.85	0.73
12:Z:185:HIS:HD2	12:Z:187:GLN:H	1.35	0.73
4:D:123(D):ALA:HA	5:E:129:GLY:HA2	1.71	0.72
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.19	0.72
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.19	0.72
14:N:107:LYS:HG2	14:N:108:GLY:H	1.53	0.72
10:J:168:MET:HE1	10:X:167:PRO:HB2	1.72	0.72
2:B:219:GLU:HG2	2:B:219(E):VAL:N	2.05	0.72
2:B:173:GLN:HG2	3:C:56:LEU:HD12	1.72	0.72
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.71	0.72
5:E:207:LEU:CD2	5:E:207:LEU:H	2.03	0.71
2:P:219:GLU:HG2	2:P:219(E):VAL:N	2.06	0.71
14:N:1:THR:HG23	14:N:33:LYS:NZ	2.05	0.71
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.72	0.71
5:S:207:LEU:H	5:S:207:LEU:CD2	2.03	0.71
5:E:201:LEU:HD11	5:E:207:LEU:HD22	1.72	0.71
5:S:201:LEU:HD11	5:S:207:LEU:CD2	2.21	0.71
10:J:133:TYR:CE2	10:J:166:MET:HG3	2.26	0.71
12:L:185:HIS:HD2	12:L:187:GLN:H	1.39	0.70
14:N:49:ALA:HB2	15:N:201:1Y9:H13	1.72	0.70
1:A:179:ARG:NH1	1:A:179:ARG:HB3	2.06	0.70
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.27	0.70
1:O:179:ARG:NH1	1:O:179:ARG:HB3	2.05	0.70
5:S:180(C):PHE:HA	5:S:180(F):ILE:HG13	1.73	0.70
2:B:202:THR:HG22	2:B:204:SER:N	1.98	0.69
10:J:167:PRO:HB2	10:X:168:MET:HE1	1.74	0.69
8:V:196:VAL:HG23	16:V:320:HOH:O	1.90	0.69
5:E:180(C):PHE:HA	5:E:180(F):ILE:HG13	1.73	0.69
5:E:201:LEU:HD11	5:E:207:LEU:CD2	2.22	0.69
10:X:133:TYR:CE2	10:X:166:MET:HG3	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:ASP:HA	10:J:68:ILE:HD13	1.74	0.69
14:N:1:THR:HG23	14:N:33:LYS:HZ3	1.56	0.69
6:T:203:GLU:O	6:T:206:LYS:HD2	1.92	0.69
12:L:12:VAL:HG12	12:L:196:ILE:HG13	1.73	0.69
7:U:59:LEU:O	7:U:61:PRO:HD3	1.93	0.69
5:E:207(B):THR:H	5:E:207(E):ASN:HD22	1.40	0.69
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.40	0.69
5:S:132:TYR:O	5:S:153:PRO:HB3	1.92	0.69
7:G:59:LEU:O	7:G:61:PRO:HD3	1.93	0.69
2:P:61:GLN:OE1	2:P:208:ASP:HA	1.93	0.68
6:F:203:GLU:O	6:F:206:LYS:HD2	1.93	0.68
5:S:207(B):THR:H	5:S:207(E):ASN:HD22	1.41	0.68
5:E:132:TYR:O	5:E:153:PRO:HB3	1.94	0.68
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.29	0.68
11:Y:143:LYS:HB2	11:Y:146:LEU:CD1	2.24	0.68
11:Y:105(B):LYS:H	11:Y:105(B):LYS:CD	2.06	0.68
2:B:121:GLN:O	2:B:124:THR:HB	1.95	0.68
1:O:121:GLN:O	1:O:124:THR:HB	1.94	0.68
12:Z:12:VAL:HG12	12:Z:196:ILE:HG13	1.75	0.68
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.29	0.68
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.76	0.67
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.76	0.67
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.30	0.67
13:M:19:LEU:HB2	13:M:170:SER:HB2	1.76	0.67
2:B:61:GLN:OE1	2:B:208:ASP:HA	1.94	0.67
12:L:116:ASP:HB2	12:L:120:SER:HB3	1.77	0.67
5:E:207:LEU:HD23	5:E:207:LEU:N	2.08	0.67
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.75	0.67
12:Z:13:LEU:HD13	12:Z:33:VAL:HG13	1.76	0.67
12:Z:116:ASP:HB2	12:Z:120:SER:HB3	1.76	0.67
3:C:41:LYS:HG2	3:C:161:SER:O	1.94	0.67
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.30	0.67
11:Y:49:ALA:HB2	15:Y:301:1Y9:H13	1.76	0.67
5:S:207:LEU:N	5:S:207:LEU:HD23	2.08	0.67
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.77	0.67
3:Q:41:LYS:HG2	3:Q:161:SER:O	1.95	0.66
1:A:33:GLN:HA	1:A:33:GLN:HE21	1.60	0.66
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.75	0.66
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.31	0.66
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.92	0.66
12:L:13:LEU:HD13	12:L:33:VAL:HG13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:121:GLN:O	7:G:124:THR:HB	1.95	0.66
9:I:6:MET:HE3	9:I:155:ILE:HG13	1.78	0.66
11:K:7:ARG:HG2	11:K:108:PRO:HB2	1.77	0.66
11:K:143:LYS:HB2	11:K:146:LEU:CD1	2.25	0.66
11:K:49:ALA:HB2	15:K:301:1Y9:H13	1.78	0.66
13:M:40:ASN:HD22	13:M:40:ASN:N	1.90	0.66
1:A:121:GLN:O	1:A:124:THR:HB	1.95	0.66
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.07	0.66
6:T:127:ASN:HD22	6:T:127:ASN:C	1.99	0.66
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.43	0.66
11:Y:7:ARG:HG2	11:Y:108:PRO:HB2	1.78	0.65
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.78	0.65
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.26	0.65
8:V:172:ASN:ND2	8:V:193:THR:HG22	2.12	0.65
5:S:15:PHE:H	6:T:23:GLN:HE22	1.45	0.65
3:Q:71:ASP:HA	10:X:68:ILE:HD13	1.77	0.65
1:O:33:GLN:HA	1:O:33:GLN:HE21	1.61	0.65
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.78	0.65
9:I:143:GLU:HG3	9:I:146:LEU:HD21	1.79	0.65
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.79	0.65
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.32	0.65
9:W:6:MET:HE3	9:W:155:ILE:HG13	1.78	0.65
7:U:121:GLN:O	7:U:124:THR:HB	1.97	0.64
12:Z:99:THR:HG23	16:Z:307:HOH:O	1.97	0.64
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.63	0.64
5:E:15:PHE:H	6:F:23:GLN:HE22	1.46	0.64
6:T:35:THR:HG21	6:T:51:GLU:O	1.97	0.64
14:N:112:THR:HG22	14:N:120:HIS:HB2	1.78	0.64
2:B:71:ASN:ND2	2:B:72:ASP:N	2.44	0.64
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.33	0.64
8:V:34:LEU:HB2	16:V:318:HOH:O	1.98	0.64
2:B:15:PHE:H	3:C:23:GLN:NE2	1.88	0.63
3:C:105:ASP:OD2	3:C:106:PRO:HD2	1.98	0.63
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.78	0.63
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.79	0.63
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.81	0.63
5:S:160:LEU:HD13	5:S:163:THR:HB	1.80	0.63
6:F:35:THR:HG21	6:F:51:GLU:O	1.98	0.63
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.62	0.63
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.81	0.63
10:J:-1:MET:HG2	10:J:1:ASP:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.80	0.63
1:O:225:THR:OG1	1:O:228:GLU:HG3	1.99	0.63
6:F:127:ASN:HD22	6:F:127:ASN:C	2.00	0.63
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.12	0.63
7:G:233:LEU:O	7:G:236:ILE:HG13	1.99	0.63
6:T:187:ARG:HG3	6:T:187:ARG:HH11	1.64	0.63
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.63	0.63
16:R:316:HOH:O	12:Z:85:HIS:HD2	1.82	0.62
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.81	0.62
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.79	0.62
2:P:121:GLN:O	2:P:124:THR:HB	1.98	0.62
10:J:166:MET:CE	10:J:168:MET:HB2	2.30	0.62
5:E:160:LEU:HD13	5:E:163:THR:HB	1.80	0.62
7:G:77:VAL:HG12	7:G:137:THR:HB	1.81	0.62
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.82	0.62
5:S:86:ARG:HH11	5:S:86:ARG:HG3	1.65	0.62
2:B:181:LYS:O	2:B:184:MET:HG3	2.00	0.62
2:P:71:ASN:ND2	2:P:72:ASP:N	2.46	0.62
14:N:107:LYS:HG2	14:N:108:GLY:N	2.14	0.62
3:C:163:GLN:CA	3:C:163:GLN:HE21	2.12	0.62
1:A:20:LYS:HE3	1:A:25:ASP:OD1	2.00	0.62
11:K:172:SER:HA	11:K:192:VAL:HG23	1.82	0.62
8:H:172:ASN:ND2	8:H:193:THR:HG22	2.15	0.62
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.64	0.62
9:I:29:ASN:ND2	9:I:30:LYS:HG3	2.15	0.61
7:G:96:ALA:CA	7:G:107:MET:HE2	2.25	0.61
11:K:105(B):LYS:H	11:K:105(B):LYS:CD	2.05	0.61
3:Q:163:GLN:HE21	3:Q:164:THR:N	1.97	0.61
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.00	0.61
13:M:35:ILE:HG12	13:M:56:GLU:HG3	1.82	0.61
4:D:31:ILE:HD13	4:D:135:ALA:HB2	1.83	0.61
14:N:84:LYS:HG3	14:N:119:VAL:HG22	1.83	0.61
11:Y:172:SER:HA	11:Y:192:VAL:HG23	1.82	0.61
3:C:241:GLN:C	3:C:243:GLN:H	2.03	0.61
1:O:20:LYS:HE3	1:O:25:ASP:OD1	2.00	0.61
7:G:198:ILE:HG23	7:G:203:THR:O	2.01	0.61
10:J:168:MET:HG2	10:X:168:MET:CE	2.31	0.61
3:Q:159:SER:HB2	16:Q:322:HOH:O	2.00	0.61
11:K:138:LEU:HD13	11:K:158:SER:OG	2.01	0.61
5:S:198:SER:HA	5:S:201:LEU:HG	1.82	0.61
3:Q:170:LYS:HB2	16:Q:315:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:166:MET:CE	10:X:168:MET:HB2	2.31	0.61
10:X:38:SER:HB2	10:X:39:PRO:HD2	1.83	0.61
5:E:82:ALA:HB3	5:E:83:PRO:HD3	1.83	0.61
3:Q:241:GLN:C	3:Q:243:GLN:H	2.04	0.61
5:E:198:SER:HA	5:E:201:LEU:HG	1.82	0.60
11:Y:138:LEU:HD13	11:Y:158:SER:OG	2.00	0.60
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.83	0.60
4:D:162:ALA:HB3	5:E:58:LEU:HD23	1.83	0.60
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.82	0.60
7:U:198:ILE:HG23	7:U:203:THR:O	2.01	0.60
3:C:65:SER:HB2	16:C:311:HOH:O	2.01	0.60
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.83	0.60
10:X:-1:MET:HG2	10:X:1:ASP:H	1.65	0.60
4:D:205:GLU:HA	4:D:205:GLU:OE2	2.01	0.60
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.83	0.60
2:P:101:LYS:HZ2	10:X:85:GLN:NE2	1.99	0.60
6:F:69:VAL:HG12	16:F:308:HOH:O	2.00	0.60
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.16	0.60
5:E:86:ARG:HH11	5:E:86:ARG:HG3	1.65	0.60
3:C:163:GLN:HE21	3:C:164:THR:N	1.99	0.60
7:U:233:LEU:O	7:U:236:ILE:HG13	2.01	0.60
11:Y:105(B):LYS:HD2	11:Y:105(B):LYS:N	2.06	0.60
10:J:168:MET:CE	10:X:168:MET:HG2	2.31	0.60
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.82	0.60
10:J:4:LEU:HD23	10:J:126:ALA:HB2	1.83	0.60
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.84	0.60
2:B:21:LEU:HD13	2:B:124:THR:HG23	1.83	0.60
1:A:97:HIS:HD2	8:H:61:SER:OG	1.84	0.59
10:X:4:LEU:HD23	10:X:126:ALA:HB2	1.84	0.59
12:L:93:PHE:N	12:L:94:PRO:HD3	2.17	0.59
9:W:6:MET:HE1	9:W:155:ILE:HA	1.85	0.59
10:J:-1:MET:HG2	10:J:1:ASP:N	2.17	0.59
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.84	0.59
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.83	0.59
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.83	0.59
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.85	0.59
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.84	0.59
14:N:85:GLU:O	14:N:89:GLU:HB2	2.03	0.59
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.85	0.59
4:D:177:LEU:HD22	5:E:58:LEU:HD13	1.84	0.59
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:149:GLN:HG2	8:V:210:THR:CG2	2.32	0.59
14:N:20:THR:HG23	14:N:31:THR:OG1	2.02	0.59
5:S:180(D):ILE:HG23	5:S:180(E):LYS:HG3	1.85	0.59
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.85	0.59
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.85	0.59
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.67	0.59
2:B:224:PHE:HD2	2:B:224:PHE:H	1.51	0.59
9:W:29:ASN:ND2	9:W:30:LYS:HG3	2.18	0.58
11:K:105(B):LYS:HD2	11:K:105(B):LYS:N	2.07	0.58
7:U:77:VAL:HG12	7:U:137:THR:HB	1.83	0.58
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.84	0.58
7:G:69:CYS:HB3	16:G:341:HOH:O	2.02	0.58
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.85	0.58
4:D:24:VAL:O	4:D:27:SER:HB3	2.03	0.58
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.39	0.58
2:B:141:TYR:CD1	2:B:219(E):VAL:HG21	2.38	0.58
4:D:123(D):ALA:HB3	4:D:126:ARG:HD3	1.85	0.58
5:E:180(D):ILE:HG23	5:E:180(E):LYS:HG3	1.86	0.58
4:D:45:GLY:HA2	4:D:146:TYR:CD1	2.38	0.58
3:C:232:TYR:O	3:C:236:ILE:HG13	2.03	0.58
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.86	0.58
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.85	0.58
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.86	0.58
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.86	0.58
4:R:177:LEU:HD22	5:S:58:LEU:HD13	1.85	0.58
7:G:184(G):GLU:CG	7:G:188:LYS:HB2	2.33	0.58
8:V:216:GLU:HG3	9:W:187:ARG:HG2	1.85	0.58
3:Q:169:SER:HA	3:Q:172:VAL:CG1	2.34	0.57
3:Q:232:TYR:O	3:Q:236:ILE:HG13	2.04	0.57
10:X:143:ARG:O	10:X:146:MET:HG3	2.03	0.57
4:R:207:LEU:C	4:R:207:LEU:HD23	2.25	0.57
3:C:206:GLY:HA3	3:C:209:ASN:HB2	1.87	0.57
2:B:228:GLU:O	2:B:232:ILE:HG22	2.04	0.57
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.52	0.57
10:J:143:ARG:O	10:J:146:MET:HG3	2.04	0.57
10:X:20:VAL:HG11	11:Y:120:LEU:HD11	1.86	0.57
4:R:205:GLU:OE2	4:R:205:GLU:HA	2.04	0.57
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.86	0.57
7:G:77:VAL:CG1	7:G:137:THR:HB	2.35	0.57
10:X:-1:MET:HG2	10:X:1:ASP:N	2.18	0.57
2:P:181:LYS:O	2:P:184:MET:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.34	0.57
2:B:230:LYS:O	2:B:234:VAL:HG23	2.04	0.57
1:A:177:GLU:HG2	2:B:58:LEU:HD22	1.87	0.57
12:L:98:HIS:HD2	16:L:305:HOH:O	1.86	0.57
14:N:105(B):LYS:C	14:N:105(B):LYS:HD3	2.24	0.57
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.34	0.57
9:W:6:MET:CE	9:W:155:ILE:HA	2.35	0.57
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.87	0.57
12:L:20:ILE:C	12:L:20:ILE:HD12	2.24	0.57
14:N:107:LYS:CG	14:N:108:GLY:H	2.18	0.57
6:T:127:ASN:HD22	6:T:128:SER:N	2.02	0.57
5:S:52:LYS:HB3	5:S:63:TYR:HB3	1.85	0.57
4:R:160:TYR:CE2	4:R:163:LYS:HD3	2.40	0.57
4:R:123(D):ALA:HB3	4:R:126:ARG:HD3	1.86	0.57
10:J:168:MET:HE1	10:X:167:PRO:CB	2.34	0.56
1:A:177:GLU:HG2	2:B:58:LEU:CD2	2.35	0.56
12:L:-2:ASN:HA	12:L:20:ILE:O	2.05	0.56
5:E:48:LEU:HG	5:E:139:ILE:HD13	1.86	0.56
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.05	0.56
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.05	0.56
12:Z:20:ILE:HD12	12:Z:20:ILE:C	2.26	0.56
12:Z:-2:ASN:HA	12:Z:20:ILE:O	2.04	0.56
12:Z:116:ASP:CB	12:Z:120:SER:HB3	2.36	0.56
9:W:29:ASN:H	9:W:29:ASN:ND2	2.03	0.56
7:U:136:LEU:O	7:U:150:LYS:HA	2.05	0.56
16:B:319:HOH:O	3:C:33:ARG:HD2	2.05	0.56
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.87	0.56
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.70	0.56
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.86	0.56
3:Q:206:GLY:HA3	3:Q:209:ASN:HB2	1.86	0.56
2:P:224:PHE:H	2:P:224:PHE:HD2	1.52	0.56
3:C:169:SER:HA	3:C:172:VAL:CG1	2.36	0.56
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.40	0.56
8:H:197:ARG:NH2	9:I:139:GLU:HG3	2.21	0.56
2:P:228:GLU:O	2:P:232:ILE:HG22	2.04	0.56
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.87	0.56
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.20	0.56
10:J:189:ASP:O	10:J:193:GLN:HB2	2.04	0.56
11:K:82:ILE:HG13	16:K:439:HOH:O	2.05	0.56
3:Q:31:VAL:HG11	3:Q:135:SER:HB2	1.88	0.56
12:L:111:ALA:HB2	12:L:123:ARG:NH2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:185:THR:HG22	3:C:187:GLU:N	2.18	0.56
6:F:127:ASN:HD22	6:F:128:SER:N	2.04	0.56
5:S:111:ARG:HG2	5:S:111:ARG:HH11	1.70	0.56
8:V:105:ASP:HB2	8:V:105(A):PRO:HD2	1.87	0.56
1:O:197:LEU:HD23	1:O:210:ILE:HD12	1.87	0.56
5:S:97:ASN:HD21	12:Z:60:ASN:ND2	2.03	0.56
13:M:141(A):VAL:HG23	13:M:141(A):VAL:O	2.06	0.56
13:M:141(C):ARG:HH11	13:M:141(C):ARG:CG	2.17	0.56
5:S:134:VAL:O	5:S:153:PRO:HG3	2.06	0.56
9:W:6:MET:HG2	9:W:124:PHE:HB3	1.88	0.56
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.88	0.56
10:X:189:ASP:O	10:X:193:GLN:HB2	2.06	0.56
6:T:38:ILE:HG22	6:T:164:ALA:HB2	1.87	0.56
7:U:170:GLN:NE2	7:U:174:THR:HG23	2.21	0.56
10:J:14:LEU:HD12	10:J:42:LEU:HD23	1.88	0.56
1:A:150:GLN:O	1:A:157:TYR:HA	2.06	0.56
7:G:136:LEU:O	7:G:150:LYS:HA	2.05	0.56
3:C:52:ARG:HB2	3:C:209:ASN:HA	1.88	0.56
10:J:20:VAL:HG11	11:K:120:LEU:HD11	1.87	0.56
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.36	0.56
8:H:210:THR:CG2	12:Z:149:GLN:HG2	2.36	0.56
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.88	0.56
1:A:197:LEU:HD23	1:A:210:ILE:HD12	1.87	0.56
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.88	0.56
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.71	0.56
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.21	0.55
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.41	0.55
5:S:41:ARG:NH1	5:S:42:SER:O	2.39	0.55
11:K:99:THR:HG22	11:K:113:VAL:O	2.05	0.55
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.71	0.55
4:D:160:TYR:CE2	4:D:163:LYS:HD3	2.41	0.55
1:A:32:LYS:HE2	1:A:32:LYS:HA	1.89	0.55
2:P:141:TYR:CD1	2:P:219(E):VAL:HG21	2.41	0.55
2:B:218:ASN:O	2:B:218(C):ASP:HB2	2.06	0.55
12:L:3:LEU:HD11	12:L:140:LEU:HD21	1.89	0.55
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.71	0.55
4:R:45:GLY:HA2	4:R:146:TYR:CD1	2.40	0.55
8:V:4:VAL:HG22	8:V:159:ILE:HD11	1.89	0.55
7:U:96:ALA:CA	7:U:107:MET:HE2	2.27	0.55
8:H:105:ASP:HB2	8:H:105(A):PRO:HD2	1.87	0.55
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:ARG:HB2	3:C:33:ARG:NH1	2.22	0.55
11:K:1:THR:HG23	11:K:33:LYS:NZ	2.20	0.55
7:U:86:ARG:HD2	16:U:309:HOH:O	2.07	0.55
10:X:124:TYR:CD2	10:X:138:LEU:HD13	2.41	0.55
12:L:116:ASP:CB	12:L:120:SER:HB3	2.36	0.55
9:I:6:MET:HG2	9:I:124:PHE:HB3	1.89	0.55
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	1.87	0.55
12:Z:111:ALA:HB2	12:Z:123:ARG:NH2	2.22	0.55
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.89	0.55
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.37	0.55
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.88	0.55
10:X:105(B):LYS:HB2	10:X:105(B):LYS:NZ	2.22	0.55
3:Q:33:ARG:HH11	3:Q:33:ARG:CB	2.19	0.55
3:Q:46:VAL:HG11	3:Q:139:ALA:HB1	1.87	0.55
12:Z:28:ARG:NH1	12:Z:190:ASP:OD1	2.36	0.55
9:I:6:MET:CE	9:I:155:ILE:HA	2.36	0.55
5:S:227:GLU:CD	5:S:227:GLU:H	2.09	0.55
7:U:77:VAL:CG1	7:U:137:THR:HB	2.37	0.55
3:Q:46:VAL:HB	3:Q:215:VAL:CG1	2.37	0.55
2:P:230:LYS:O	2:P:234:VAL:HG23	2.06	0.55
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.89	0.54
3:Q:163:GLN:HA	3:Q:163:GLN:NE2	2.22	0.54
4:R:24:VAL:O	4:R:27:SER:HB3	2.08	0.54
11:Y:1:THR:HG23	11:Y:33:LYS:NZ	2.22	0.54
1:O:150:GLN:O	1:O:157:TYR:HA	2.07	0.54
14:N:105:ASP:HB2	16:N:334:HOH:O	2.08	0.54
11:Y:99:THR:HG22	11:Y:113:VAL:O	2.07	0.54
4:R:123(D):ALA:HA	5:S:129:GLY:HA2	1.89	0.54
3:C:57:LYS:O	3:C:58:LEU:HB2	2.07	0.54
12:Z:3:LEU:HD11	12:Z:140:LEU:HD21	1.89	0.54
4:D:207:LEU:HD23	4:D:207:LEU:C	2.28	0.54
14:N:161:GLN:NE2	14:N:165:TRP:HE1	2.05	0.54
5:S:109:VAL:HG12	5:S:149:LEU:HD22	1.89	0.54
5:E:227:GLU:CD	5:E:227:GLU:H	2.09	0.54
6:T:69:VAL:HG12	16:T:324:HOH:O	2.07	0.54
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.36	0.54
3:C:33:ARG:CB	3:C:33:ARG:HH11	2.21	0.54
3:C:197:LEU:O	3:C:201:VAL:HG23	2.07	0.54
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.37	0.54
8:H:175:VAL:HG12	8:H:176:CYS:N	2.22	0.54
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.88	0.54
2:P:71:ASN:HD22	2:P:72:ASP:N	2.05	0.54
2:P:218:ASN:O	2:P:218(C):ASP:HB2	2.06	0.54
5:E:109:VAL:HG12	5:E:149:LEU:HD22	1.90	0.54
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.71	0.54
1:O:57:PRO:HG2	7:U:177:GLU:HG2	1.89	0.54
10:J:167:PRO:CB	10:X:168:MET:HE1	2.37	0.54
14:N:14:LEU:O	14:N:175:MET:HA	2.08	0.54
9:W:156:SER:O	9:W:160:LEU:HB2	2.08	0.54
2:B:4:GLY:HA3	5:E:127:TYR:CE1	2.42	0.54
1:O:232:ARG:HG3	1:O:232:ARG:HH11	1.73	0.54
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.88	0.54
1:A:186:LEU:HD21	1:A:214:ILE:HD12	1.90	0.54
8:V:175:VAL:HG12	8:V:176:CYS:N	2.23	0.54
3:Q:185:THR:HG22	3:Q:187:GLU:N	2.18	0.54
3:C:31:VAL:HG11	3:C:135:SER:HB2	1.89	0.54
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.89	0.54
10:J:124:TYR:CD2	10:J:138:LEU:HD13	2.42	0.54
13:M:41:THR:OG1	13:M:76:PRO:HG3	2.08	0.54
13:M:149:GLN:NE2	13:M:149:GLN:H	2.06	0.54
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.90	0.54
6:F:192:GLN:HE21	6:F:195:LYS:HE3	1.73	0.54
7:U:96:ALA:HA	7:U:107:MET:CE	2.30	0.53
3:C:57:LYS:HD2	3:C:58:LEU:N	2.24	0.53
1:A:69:LEU:HD23	1:A:69:LEU:C	2.28	0.53
2:B:71:ASN:HD22	2:B:72:ASP:N	2.03	0.53
14:N:105(B):LYS:O	14:N:105(B):LYS:HD3	2.09	0.53
3:Q:75:VAL:HG13	3:Q:221:ILE:HD13	1.89	0.53
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.89	0.53
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.23	0.53
7:U:224:LEU:HB3	7:U:228:ASN:HB2	1.91	0.53
10:J:18:LYS:HD3	10:J:174:ILE:HG13	1.91	0.53
3:C:169:SER:HA	3:C:172:VAL:HG12	1.90	0.53
3:Q:169:SER:HA	3:Q:172:VAL:HG12	1.89	0.53
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.39	0.53
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.73	0.53
5:E:41:ARG:NH1	5:E:42:SER:O	2.42	0.53
7:U:55:PRO:HG2	7:U:56:ASP:H	1.73	0.53
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.39	0.53
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.39	0.53
4:D:187:LYS:O	4:D:191:LEU:HD22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:32:LYS:HD2	12:Z:45:ASN:HD22	1.73	0.53
10:J:168:MET:HE2	10:X:168:MET:HE2	1.90	0.53
6:T:206(B):GLU:HG3	6:T:206(C):LYS:H	1.72	0.53
2:P:239:THR:HG22	2:P:239:THR:OXT	2.09	0.53
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.07	0.53
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.23	0.53
6:F:206(B):GLU:HG3	6:F:206(C):LYS:H	1.72	0.53
3:Q:45:CYS:HA	3:Q:141:PHE:HZ	1.74	0.53
5:S:162:GLY:O	6:T:58:LEU:HD13	2.08	0.53
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.21	0.53
6:F:179:LEU:HD11	6:F:192:GLN:HG3	1.90	0.53
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.74	0.53
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.21	0.53
3:C:45:CYS:HA	3:C:141:PHE:HZ	1.74	0.53
11:Y:4:LEU:CD1	11:Y:159:ILE:HD11	2.39	0.53
10:J:105(B):LYS:NZ	10:J:105(B):LYS:HB2	2.23	0.53
13:M:46:SER:OG	13:M:98:ALA:HB3	2.09	0.53
9:I:29:ASN:H	9:I:29:ASN:ND2	2.07	0.52
2:P:41:MET:HE2	16:P:305:HOH:O	2.08	0.52
5:E:134:VAL:O	5:E:153:PRO:HG3	2.08	0.52
11:Y:4:LEU:CD1	11:Y:15:ALA:HB3	2.40	0.52
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.39	0.52
11:K:1:THR:HG23	11:K:33:LYS:HZ3	1.74	0.52
12:L:7:GLY:HA3	12:L:10:PHE:CE2	2.44	0.52
12:L:32:LYS:HD2	12:L:45:ASN:HD22	1.74	0.52
11:Y:195:LEU:O	11:Y:199:VAL:HG23	2.09	0.52
6:T:127:ASN:ND2	6:T:127:ASN:C	2.63	0.52
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.39	0.52
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.90	0.52
12:Z:82:ASN:HD22	12:Z:82:ASN:C	2.12	0.52
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.73	0.52
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.09	0.52
3:C:186:VAL:O	3:C:190:VAL:HG23	2.10	0.52
3:C:75:VAL:HG13	3:C:221:ILE:HD13	1.91	0.52
12:Z:7:GLY:HA3	12:Z:10:PHE:CE2	2.44	0.52
2:P:87:ILE:O	2:P:91:THR:HG23	2.09	0.52
10:J:123:PRO:HB2	10:J:124:TYR:CD1	2.45	0.52
11:K:190:HIS:HA	16:K:444:HOH:O	2.10	0.52
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.10	0.52
7:U:184(G):GLU:CG	7:U:188:LYS:HB2	2.34	0.52
3:C:163:GLN:HA	3:C:163:GLN:NE2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.56	0.52
12:Z:-7:ASN:ND2	12:Z:-5:TYR:H	2.06	0.52
13:M:76:PRO:HD2	13:M:105:GLN:OE1	2.10	0.52
9:I:156:SER:O	9:I:160:LEU:HB2	2.10	0.52
1:O:175:PHE:O	1:O:179:ARG:HG2	2.09	0.52
13:M:40:ASN:ND2	13:M:40:ASN:N	2.57	0.52
3:Q:215:VAL:HG23	3:Q:221:ILE:HG12	1.92	0.52
5:S:227:GLU:N	5:S:227:GLU:CD	2.63	0.52
6:T:176:LEU:HB3	7:U:58:LEU:HD21	1.91	0.52
5:S:54:ASN:ND2	5:S:56:ASP:O	2.43	0.52
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.93	0.52
3:C:46:VAL:O	3:C:215:VAL:HG12	2.10	0.52
13:M:17:ASP:HA	13:M:173:PHE:CB	2.40	0.52
1:O:97:HIS:HD2	8:V:61:SER:OG	1.93	0.52
7:U:141:VAL:HG21	7:U:216:THR:HA	1.92	0.52
7:U:151:THR:HG22	7:U:157:TYR:CB	2.40	0.52
2:P:101:LYS:HZ1	10:X:85:GLN:HE22	1.58	0.52
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.92	0.52
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.92	0.52
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.45	0.52
5:S:66:LYS:O	5:S:77:SER:HA	2.09	0.52
1:A:232:ARG:HG3	1:A:232:ARG:HH11	1.72	0.52
7:U:107:MET:HE3	7:U:112:LEU:HB2	1.91	0.51
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.45	0.51
10:J:52:THR:CG2	10:J:53:VAL:N	2.73	0.51
6:F:186:ALA:O	6:F:190:VAL:HG23	2.10	0.51
11:Y:190:HIS:CD2	11:Y:190:HIS:N	2.78	0.51
4:R:243:ALA:O	4:R:244:GLU:CB	2.57	0.51
11:K:190:HIS:CD2	11:K:190:HIS:N	2.78	0.51
6:F:127:ASN:ND2	6:F:127:ASN:C	2.63	0.51
12:L:164:TYR:CD1	12:L:165:LEU:N	2.78	0.51
5:E:190:ILE:CG2	5:E:212:ILE:HD13	2.40	0.51
6:F:237:GLN:O	6:F:240:ILE:HG22	2.10	0.51
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.46	0.51
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.30	0.51
1:O:186:LEU:HD21	1:O:214:ILE:HD12	1.92	0.51
6:T:237:GLN:O	6:T:240:ILE:HG22	2.09	0.51
4:R:187:LYS:O	4:R:191:LEU:HD22	2.10	0.51
7:G:55:PRO:HG2	7:G:56:ASP:H	1.74	0.51
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.46	0.51
13:M:205:GLY:HA3	13:M:209:GLN:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.45	0.51
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.92	0.51
11:Y:12:ILE:HB	11:Y:178:VAL:HB	1.93	0.51
4:D:112:LEU:C	4:D:112:LEU:HD13	2.31	0.51
11:K:142:TYR:O	11:K:143:LYS:HD2	2.11	0.51
5:E:97:ASN:HD21	12:L:60:ASN:ND2	2.09	0.51
3:Q:235:GLN:O	3:Q:239:GLU:HG2	2.10	0.51
6:T:95:GLU:CG	6:T:115:ARG:HB3	2.32	0.51
5:S:190:ILE:CG2	5:S:212:ILE:HD13	2.41	0.51
3:Q:182:PRO:O	3:Q:184:ALA:N	2.44	0.51
10:X:14:LEU:HD12	10:X:42:LEU:HD23	1.92	0.51
12:Z:164:TYR:CD1	12:Z:165:LEU:N	2.79	0.51
4:R:85:ALA:O	4:R:89:ILE:HG12	2.10	0.51
7:G:217:LYS:CA	7:G:217:LYS:HE3	2.36	0.51
14:N:89:GLU:HA	14:N:89:GLU:OE1	2.09	0.51
5:E:162:GLY:O	6:F:58:LEU:HD13	2.11	0.51
4:R:112:LEU:C	4:R:112:LEU:HD13	2.31	0.51
9:I:50:THR:HG22	16:I:207:HOH:O	2.11	0.51
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.46	0.51
12:L:149:GLN:HG2	8:V:210:THR:HG21	1.92	0.51
3:C:158:SER:HB2	4:D:59:LEU:HD21	1.92	0.51
3:C:46:VAL:HG11	3:C:139:ALA:HB1	1.92	0.51
3:C:46:VAL:HB	3:C:215:VAL:CG1	2.40	0.51
10:X:52:THR:HG23	10:X:53:VAL:N	2.26	0.51
6:T:147:HIS:HD2	16:T:302:HOH:O	1.94	0.51
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.93	0.51
11:K:12:ILE:HB	11:K:178:VAL:HB	1.92	0.51
5:E:54:ASN:ND2	5:E:56:ASP:O	2.43	0.51
2:B:239:THR:OXT	2:B:239:THR:HG22	2.11	0.51
5:E:201:LEU:O	5:E:202:ARG:HB2	2.11	0.50
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.26	0.50
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.26	0.50
7:G:141:VAL:HG21	7:G:216:THR:HA	1.93	0.50
7:G:151:THR:HG22	7:G:157:TYR:CB	2.41	0.50
1:A:212:LEU:HD22	1:A:224:LEU:HD12	1.93	0.50
2:B:41:MET:HE2	16:B:302:HOH:O	2.09	0.50
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.93	0.50
1:O:69:LEU:HD23	1:O:69:LEU:C	2.31	0.50
8:H:139:GLU:HA	8:H:139:GLU:OE2	2.11	0.50
1:A:197:LEU:CD2	1:A:210:ILE:HD12	2.41	0.50
13:M:83:LEU:O	13:M:87:MET:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:THR:HG22	3:C:56:LEU:HD22	1.94	0.50
10:J:44:SER:OG	10:J:100:LEU:HB2	2.11	0.50
4:R:186:LEU:O	4:R:190:GLU:HG3	2.12	0.50
3:C:235:GLN:O	3:C:239:GLU:HG2	2.11	0.50
5:S:201:LEU:O	5:S:202:ARG:HB2	2.12	0.50
7:U:65:SER:HA	7:U:211:GLU:OE2	2.11	0.50
5:E:227:GLU:CD	5:E:227:GLU:N	2.64	0.50
3:C:215:VAL:HG23	3:C:221:ILE:HG12	1.93	0.50
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.93	0.50
10:J:52:THR:HG23	10:J:53:VAL:N	2.25	0.50
2:P:101:LYS:NZ	10:X:85:GLN:HE22	2.09	0.50
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.42	0.50
3:Q:46:VAL:O	3:Q:215:VAL:HG12	2.12	0.50
10:X:52:THR:CG2	10:X:53:VAL:N	2.75	0.50
11:K:195:LEU:O	11:K:199:VAL:HG23	2.11	0.50
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.10	0.50
5:E:66:LYS:O	5:E:77:SER:HA	2.11	0.50
8:V:139:GLU:OE2	8:V:139:GLU:HA	2.11	0.50
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.15	0.50
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.94	0.50
9:W:29:ASN:H	9:W:29:ASN:HD22	1.60	0.50
1:O:141:HIS:HA	1:O:146:GLY:O	2.12	0.50
8:V:72:ARG:HH11	8:V:72:ARG:HG3	1.77	0.50
11:K:86:LEU:HD13	11:K:86:LEU:C	2.32	0.50
1:A:175:PHE:O	1:A:179:ARG:HG2	2.10	0.50
3:Q:41:LYS:HD3	3:Q:161:SER:HA	1.93	0.50
5:S:149:LEU:HD12	5:S:159:GLU:HA	1.94	0.50
10:J:18:LYS:HG2	10:J:174:ILE:HG13	1.93	0.50
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.77	0.50
7:G:107:MET:HE3	7:G:112:LEU:HB2	1.94	0.50
11:Y:143:LYS:O	11:Y:146:LEU:HD13	2.12	0.50
11:Y:13:ILE:HD12	11:Y:152:LEU:HD23	1.93	0.50
7:G:184(G):GLU:HG2	7:G:188:LYS:HB3	1.94	0.49
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.94	0.49
5:S:77:SER:OG	5:S:137:LEU:HB2	2.12	0.49
5:S:97:ASN:HD21	12:Z:60:ASN:HD21	1.59	0.49
5:S:73:HIS:HE1	5:S:107:LEU:O	1.94	0.49
8:V:172:ASN:HB3	8:V:192:LEU:O	2.12	0.49
1:O:197:LEU:CD2	1:O:210:ILE:HD12	2.42	0.49
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.48	0.49
3:C:182:PRO:O	3:C:184:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:227:GLU:OE2	4:D:227:GLU:N	2.42	0.49
11:Y:142:TYR:O	11:Y:143:LYS:HD2	2.13	0.49
2:B:185:LYS:HE2	2:B:187:ASP:OD1	2.12	0.49
3:C:35:THR:HB	3:C:51:GLU:HG3	1.94	0.49
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.94	0.49
9:I:178:ILE:HG23	9:I:184:VAL:HG22	1.95	0.49
4:D:53:ARG:HG2	4:D:53:ARG:O	2.12	0.49
8:H:172:ASN:HB3	8:H:192:LEU:O	2.13	0.49
5:S:180(C):PHE:HA	5:S:180(F):ILE:CG1	2.43	0.49
3:C:41:LYS:HD3	3:C:161:SER:HA	1.95	0.49
5:E:77:SER:OG	5:E:137:LEU:HB2	2.13	0.49
3:Q:149:TYR:CE1	3:Q:159:SER:HB3	2.47	0.49
7:U:236:ILE:HD12	7:U:236:ILE:C	2.33	0.49
9:W:113:PHE:HA	9:W:118:CYS:O	2.13	0.49
6:F:198:TYR:HE2	6:F:237:GLN:HE21	1.61	0.49
6:T:198:TYR:HE2	6:T:237:GLN:HE21	1.60	0.49
3:Q:125:GLN:NE2	16:Q:318:HOH:O	2.45	0.49
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.95	0.49
11:Y:1:THR:HG23	11:Y:33:LYS:HZ3	1.78	0.49
5:E:149:LEU:HD12	5:E:159:GLU:HA	1.94	0.49
13:M:112:TYR:CE1	13:M:127:THR:HG22	2.48	0.49
4:D:85:ALA:O	4:D:89:ILE:HG12	2.13	0.49
6:T:186:ALA:O	6:T:190:VAL:HG23	2.13	0.49
12:L:82:ASN:C	12:L:82:ASN:HD22	2.15	0.49
3:Q:173:ARG:O	3:Q:177:GLU:HG3	2.13	0.48
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.94	0.48
5:E:73:HIS:HE1	5:E:107:LEU:O	1.96	0.48
3:C:227:GLU:OE1	3:C:227:GLU:N	2.46	0.48
12:L:39:ASN:HD21	12:L:201:GLY:HA2	1.78	0.48
12:L:28:ARG:NH1	12:L:190:ASP:OD1	2.38	0.48
4:D:243:ALA:O	4:D:244:GLU:CB	2.58	0.48
13:M:104:VAL:CG2	13:M:178:ILE:HG22	2.39	0.48
7:G:65:SER:HA	7:G:211:GLU:OE2	2.13	0.48
7:U:236:ILE:HD12	7:U:237:ALA:N	2.27	0.48
3:Q:49:GLY:HA2	3:Q:212:ILE:HD13	1.95	0.48
6:T:36:THR:HB	6:T:168:GLY:H	1.79	0.48
2:P:163:ILE:HG13	2:P:164:SER:N	2.29	0.48
10:X:18:LYS:HG2	10:X:174:ILE:HG13	1.94	0.48
1:A:141:HIS:HA	1:A:146:GLY:O	2.14	0.48
4:R:170:GLU:OE1	4:R:170:GLU:N	2.46	0.48
10:X:44:SER:OG	10:X:100:LEU:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:226:SER:HB2	3:Q:227:GLU:OE1	2.14	0.48
10:J:133:TYR:HD1	16:Y:422:HOH:O	1.94	0.48
10:J:168:MET:CE	10:X:168:MET:CE	2.92	0.48
6:T:176:LEU:HB3	7:U:58:LEU:CD2	2.43	0.48
2:B:87:ILE:O	2:B:91:THR:HG23	2.14	0.48
4:R:227:GLU:OE2	4:R:227:GLU:N	2.43	0.48
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.60	0.48
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.77	0.48
10:J:166:MET:HE2	10:J:168:MET:HB2	1.96	0.48
1:O:33:GLN:CA	1:O:33:GLN:HE21	2.22	0.48
6:T:35:THR:CG2	6:T:36:THR:N	2.76	0.48
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.44	0.48
5:E:111:ARG:NH1	5:E:111:ARG:HG2	2.29	0.48
8:H:105:ASP:HB2	8:H:105(A):PRO:CD	2.43	0.48
1:A:33:GLN:HE21	1:A:33:GLN:CA	2.22	0.48
5:S:64:GLN:NE2	5:S:82:ALA:HB2	2.29	0.48
5:S:207(C):VAL:CG1	5:S:207(D):ASP:N	2.76	0.48
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.94	0.48
7:U:186:TRP:O	7:U:190:VAL:HG23	2.13	0.48
7:U:72:ARG:HB2	7:U:72:ARG:NH1	2.28	0.48
8:V:173:VAL:HB	8:V:192:LEU:HB2	1.96	0.48
2:P:141:TYR:CE2	2:P:145:GLY:HA2	2.49	0.48
5:S:111:ARG:HG2	5:S:111:ARG:NH1	2.28	0.48
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.48	0.48
1:A:232:ARG:HG3	1:A:232:ARG:NH1	2.29	0.48
4:D:117:CYS:HB3	4:D:155:GLY:O	2.14	0.48
1:O:205:GLU:HA	1:O:205:GLU:OE2	2.13	0.48
4:R:40:ILE:CD1	4:R:193:VAL:HG23	2.42	0.48
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.28	0.48
2:P:216(A):LYS:O	2:P:216(B):GLY:C	2.52	0.48
9:W:178:ILE:HG23	9:W:184:VAL:HG22	1.94	0.48
7:G:220:LYS:HG2	7:G:221:PHE:N	2.28	0.48
7:G:236:ILE:HD12	7:G:237:ALA:N	2.29	0.48
7:U:203:THR:HG22	7:U:204:GLU:N	2.29	0.48
2:P:81:LEU:HD23	2:P:133:GLY:HA3	1.95	0.48
5:E:207(C):VAL:CG1	5:E:207(D):ASP:N	2.77	0.48
9:W:126:VAL:HG11	9:W:134:LEU:HB3	1.96	0.48
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.96	0.47
3:C:106:PRO:HG2	3:C:143:PRO:HG2	1.95	0.47
2:B:216(A):LYS:O	2:B:216(B):GLY:C	2.52	0.47
5:S:136:LEU:HB2	5:S:151:PHE:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:217(P):LYS:HE3	16:O:315:HOH:O	2.13	0.47
13:M:70:ASN:ND2	13:M:71:ALA:HA	2.29	0.47
4:D:170:GLU:N	4:D:170:GLU:OE1	2.46	0.47
7:U:107:MET:CE	7:U:112:LEU:HD13	2.44	0.47
1:O:86:ARG:NE	7:U:118:ASN:HD21	2.07	0.47
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.42	0.47
9:I:152:PHE:CE1	9:I:187:ARG:HD2	2.49	0.47
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.29	0.47
7:G:48:VAL:HG23	7:G:48:VAL:O	2.14	0.47
12:L:-9:GLN:HG2	13:M:-8:THR:HG21	1.96	0.47
1:A:205:GLU:OE2	1:A:205:GLU:HA	2.13	0.47
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.14	0.47
12:L:-9:GLN:HE21	13:M:-8:THR:HG21	1.79	0.47
7:U:220:LYS:HG2	7:U:221:PHE:N	2.29	0.47
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.95	0.47
4:D:237:LEU:HD22	4:D:241:GLU:HG3	1.94	0.47
9:I:6:MET:HE3	9:I:155:ILE:HA	1.94	0.47
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.39	0.47
11:Y:32:LYS:O	11:Y:45:MET:HE1	2.15	0.47
3:C:149:TYR:CE1	3:C:159:SER:HB3	2.49	0.47
6:F:114:ASP:O	6:F:118:GLN:HG2	2.13	0.47
4:R:53:ARG:HG2	4:R:53:ARG:O	2.15	0.47
5:S:207(B):THR:N	5:S:207(E):ASN:HD22	2.11	0.47
14:N:49:ALA:CB	15:N:201:1Y9:H13	2.43	0.47
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.77	0.47
8:H:210:THR:HG21	12:Z:149:GLN:HG2	1.96	0.47
5:S:73:HIS:H	5:S:73:HIS:CD2	2.33	0.47
6:T:32:GLU:HB3	6:T:169:ARG:NH2	2.30	0.47
6:F:136:THR:O	6:F:150:MET:HA	2.15	0.47
1:O:179:ARG:HH11	1:O:179:ARG:CB	2.23	0.47
3:Q:227:GLU:N	3:Q:227:GLU:OE1	2.47	0.47
2:P:67:LEU:HD22	2:P:211:GLU:HB3	1.96	0.47
4:R:123(G):GLU:HG2	4:R:125:GLU:H	1.80	0.47
4:R:237:LEU:HD22	4:R:241:GLU:HG3	1.96	0.47
12:Z:185:HIS:CD2	12:Z:187:GLN:H	2.24	0.47
5:S:35:SER:HB3	5:S:66:LYS:NZ	2.30	0.47
1:A:67:VAL:HG11	1:A:213:ALA:HB3	1.95	0.47
8:H:72:ARG:HH11	8:H:72:ARG:HG3	1.78	0.47
1:O:124:THR:HG22	2:P:130:ARG:NH2	2.15	0.47
5:E:73:HIS:H	5:E:73:HIS:CD2	2.32	0.47
1:A:92:SER:OG	1:A:116:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:186:TRP:O	7:G:190:VAL:HG23	2.15	0.47
2:P:235:LYS:N	2:P:235:LYS:HD3	2.29	0.47
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.47	0.47
7:U:232:ARG:HA	7:U:232:ARG:NE	2.30	0.47
5:S:12:THR:CG2	5:S:124:THR:HA	2.38	0.47
11:Y:49:ALA:HB2	15:Y:301:1Y9:C10	2.45	0.47
9:W:143:GLU:CG	9:W:146:LEU:HD21	2.44	0.47
7:G:203:THR:HG22	7:G:204:GLU:N	2.29	0.47
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.36	0.47
2:B:190:ILE:HG23	2:B:212:PHE:CE2	2.49	0.47
7:U:75:GLY:HA3	7:U:221:PHE:CE2	2.50	0.47
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.45	0.47
10:J:46:ALA:HA	16:J:221:HOH:O	2.14	0.47
14:N:8:PHE:HB2	14:N:146:MET:O	2.15	0.47
3:C:49:GLY:HA2	3:C:212:ILE:HD13	1.96	0.47
4:R:117:CYS:HB3	4:R:155:GLY:O	2.14	0.47
7:G:96:ALA:HA	7:G:107:MET:CE	2.29	0.47
2:P:121:GLN:C	2:P:121:GLN:NE2	2.69	0.47
10:J:166:MET:HA	10:J:167:PRO:HD3	1.76	0.47
6:T:203:GLU:HG3	6:T:206:LYS:NZ	2.30	0.47
2:B:112:LEU:C	2:B:112:LEU:HD23	2.35	0.47
5:E:64:GLN:NE2	5:E:82:ALA:HB2	2.30	0.47
10:X:18:LYS:HD3	10:X:174:ILE:CG1	2.45	0.47
9:W:152:PHE:CE1	9:W:187:ARG:HD2	2.50	0.47
2:B:6:ARG:HB2	5:E:127:TYR:OH	2.15	0.47
11:K:13:ILE:HD12	11:K:152:LEU:HD23	1.96	0.47
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.49	0.46
6:T:114:ASP:O	6:T:118:GLN:HG2	2.15	0.46
14:N:13:ILE:HD12	14:N:151:THR:CG2	2.45	0.46
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.97	0.46
3:Q:163:GLN:NE2	3:Q:163:GLN:CA	2.79	0.46
2:B:141:TYR:CE2	2:B:145:GLY:HA2	2.50	0.46
3:C:33:ARG:CB	3:C:33:ARG:NH1	2.79	0.46
9:I:113:PHE:HA	9:I:118:CYS:O	2.15	0.46
13:M:104:VAL:HG23	13:M:178:ILE:CG2	2.42	0.46
6:F:203:GLU:HG3	6:F:206:LYS:NZ	2.30	0.46
6:F:36:THR:HB	6:F:168:GLY:H	1.79	0.46
10:J:152:LEU:HD13	10:J:193:GLN:HE22	1.81	0.46
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.97	0.46
12:L:186:ILE:O	8:V:167:LEU:HD22	2.15	0.46
6:T:175:GLU:OE1	6:T:199:LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:167:LEU:HD22	12:Z:186:ILE:O	2.15	0.46
5:E:136:LEU:HB2	5:E:151:PHE:HB3	1.96	0.46
5:S:190:ILE:O	5:S:194:VAL:HG23	2.16	0.46
11:K:172:SER:CA	11:K:192:VAL:HG23	2.45	0.46
9:I:29:ASN:HD22	9:I:30:LYS:HG3	1.79	0.46
1:O:232:ARG:HG3	1:O:232:ARG:NH1	2.29	0.46
2:B:146:TYR:OH	2:B:216(A):LYS:HB2	2.14	0.46
11:K:105(A):ARG:HG2	11:K:105(A):ARG:HH11	1.79	0.46
14:N:3:ILE:HB	14:N:44:CYS:HB3	1.96	0.46
7:G:72:ARG:NH1	7:G:72:ARG:HB2	2.30	0.46
2:B:136:PHE:O	2:B:150:THR:HA	2.16	0.46
2:P:121:GLN:CG	3:Q:83:ALA:HB1	2.46	0.46
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.08	0.46
4:D:123(D):ALA:HA	5:E:129:GLY:CA	2.42	0.46
5:E:31:ILE:HD11	5:E:153:PRO:CG	2.46	0.46
11:K:143:LYS:O	11:K:146:LEU:HD13	2.16	0.46
12:Z:82:ASN:C	12:Z:82:ASN:ND2	2.67	0.46
5:E:35:SER:HB3	5:E:66:LYS:NZ	2.30	0.46
12:Z:80:ALA:HA	12:Z:115:PHE:HZ	1.80	0.46
1:O:67:VAL:HG11	1:O:213:ALA:HB3	1.96	0.46
3:C:122:ARG:NH2	16:C:327:HOH:O	2.47	0.46
4:D:70:ILE:HD12	4:D:74:ILE:HG22	1.96	0.46
2:B:163:ILE:HG13	2:B:164:SER:N	2.30	0.46
4:D:12:VAL:HG23	4:D:123(A):GLY:HA2	1.98	0.46
7:U:217:LYS:CA	7:U:217:LYS:HE3	2.36	0.46
4:D:205:GLU:OE2	4:D:205:GLU:CA	2.64	0.46
2:B:149:TYR:CZ	3:C:62(A):ILE:HD12	2.50	0.46
10:X:3:ILE:HG22	10:X:100:LEU:CD1	2.45	0.46
7:U:82:ILE:N	7:U:83:PRO:HD2	2.31	0.46
4:R:70:ILE:HD12	4:R:74:ILE:HG22	1.96	0.46
7:U:38:LEU:HD23	7:U:197:MET:HE3	1.98	0.46
11:Y:172:SER:CA	11:Y:192:VAL:HG23	2.45	0.46
6:T:192:GLN:O	6:T:196:ILE:HG13	2.15	0.46
10:J:3:ILE:HG22	10:J:100:LEU:CD1	2.45	0.46
11:K:13:ILE:HG13	11:K:151:ALA:HB1	1.98	0.46
2:P:115:ARG:HG2	16:P:304:HOH:O	2.15	0.46
8:H:173:VAL:HB	8:H:192:LEU:HB2	1.97	0.46
5:S:31:ILE:HD11	5:S:153:PRO:CG	2.46	0.46
1:A:97:HIS:CD2	8:H:61:SER:OG	2.66	0.46
14:N:66:TYR:CD2	14:N:74:PRO:HB3	2.51	0.46
2:P:215:ILE:HG12	2:P:221:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:218(B):THR:O	6:F:218(C):ASN:HB2	2.16	0.46
9:I:29:ASN:HD22	9:I:29:ASN:H	1.64	0.46
10:X:105(B):LYS:HB2	10:X:105(B):LYS:HZ3	1.80	0.46
5:E:97:ASN:HD21	12:L:60:ASN:HD21	1.63	0.46
1:O:217(P):LYS:HB2	16:O:315:HOH:O	2.16	0.46
10:X:148:THR:HG21	10:X:177:ILE:HD13	1.98	0.46
1:A:62:GLU:H	1:A:62:GLU:CD	2.19	0.46
10:J:168:MET:HE3	10:X:168:MET:HE3	1.97	0.46
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	1.96	0.46
7:G:75:GLY:HA3	7:G:221:PHE:CE2	2.51	0.46
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.99	0.46
2:P:136:PHE:O	2:P:150:THR:HA	2.16	0.46
6:F:35:THR:CG2	6:F:36:THR:N	2.78	0.45
7:U:203:THR:HG22	7:U:204:GLU:O	2.17	0.45
2:B:186:VAL:O	2:B:190:ILE:HG13	2.16	0.45
6:F:192:GLN:O	6:F:196:ILE:HG13	2.16	0.45
8:H:7:LYS:HG3	8:H:123:TYR:HA	1.98	0.45
5:E:40:LEU:HD23	5:E:40:LEU:N	2.31	0.45
4:D:90:GLU:OE2	11:K:69:ARG:NH1	2.49	0.45
11:K:200:LYS:HE3	11:K:206:PHE:O	2.17	0.45
7:G:82:ILE:N	7:G:83:PRO:HD2	2.31	0.45
8:H:196:VAL:HG23	16:H:324:HOH:O	2.15	0.45
6:F:95:GLU:CG	6:F:115:ARG:HB3	2.32	0.45
10:X:166:MET:HE2	10:X:168:MET:HB2	1.97	0.45
9:I:143:GLU:CG	9:I:146:LEU:HD21	2.46	0.45
3:C:241:GLN:C	3:C:243:GLN:N	2.69	0.45
12:L:154:THR:O	12:L:157:LYS:HB2	2.16	0.45
6:F:109:ILE:HG21	6:F:147:HIS:HB2	1.98	0.45
10:J:148:THR:HG21	10:J:177:ILE:HD13	1.98	0.45
12:Z:210:LYS:HG3	16:Z:334:HOH:O	2.15	0.45
2:P:101:LYS:HZ1	10:X:85:GLN:NE2	2.12	0.45
14:N:112:THR:CG2	14:N:120:HIS:HB2	2.46	0.45
7:G:236:ILE:HD12	7:G:236:ILE:C	2.37	0.45
3:Q:241:GLN:C	3:Q:243:GLN:N	2.69	0.45
11:K:4:LEU:C	11:K:4:LEU:HD22	2.37	0.45
1:A:212:LEU:HD22	1:A:224:LEU:CD1	2.46	0.45
2:P:185:LYS:HD3	2:P:186:VAL:N	2.32	0.45
2:P:231:ASP:O	2:P:235:LYS:HG2	2.17	0.45
13:M:9:ASP:OD1	13:M:10:ASN:N	2.49	0.45
10:J:24:ILE:HG12	10:X:133:TYR:OH	2.16	0.45
2:P:222:LYS:NZ	2:P:228:GLU:OE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:152:LEU:HD13	10:X:193:GLN:HE22	1.81	0.45
2:B:185:LYS:HD3	2:B:186:VAL:N	2.31	0.45
5:E:190:ILE:O	5:E:194:VAL:HG23	2.16	0.45
3:C:150:GLN:HG2	3:C:151:THR:N	2.32	0.45
6:T:173:LYS:O	6:T:177:GLU:HG3	2.17	0.45
9:I:55:LEU:HA	9:I:55:LEU:HD23	1.80	0.45
1:O:62:GLU:CD	1:O:62:GLU:H	2.19	0.45
3:Q:106:PRO:HG2	3:Q:143:PRO:HG2	1.95	0.45
3:Q:158:SER:HB2	4:R:59:LEU:HD21	1.99	0.45
12:L:140:LEU:O	12:L:144:VAL:HB	2.16	0.45
12:L:82:ASN:C	12:L:82:ASN:ND2	2.70	0.45
10:X:3:ILE:N	16:X:247:HOH:O	2.44	0.45
2:P:146:TYR:OH	2:P:216(A):LYS:HB2	2.16	0.45
9:W:101:VAL:O	9:W:110:ILE:HA	2.17	0.45
9:I:90:ARG:HD2	16:I:266:HOH:O	2.17	0.45
7:U:110:ASP:HB3	7:U:149:TYR:CZ	2.52	0.45
11:K:6:PHE:HA	11:K:123:ASP:O	2.17	0.45
10:J:35:ARG:HA	10:J:35:ARG:HD3	1.83	0.45
2:B:235:LYS:HD3	2:B:235:LYS:N	2.31	0.45
1:A:217(G):LEU:HD13	1:A:218:GLY:HA2	1.99	0.45
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.98	0.45
3:C:174:GLU:O	3:C:178:LYS:HD2	2.17	0.45
4:R:86:ARG:HA	4:R:86:ARG:HD3	1.82	0.45
14:N:36:ARG:HH21	14:N:60:GLN:HE21	1.65	0.45
5:S:226:GLY:O	5:S:229:VAL:HG22	2.17	0.45
9:I:101:VAL:O	9:I:110:ILE:HA	2.16	0.45
1:O:60:MET:HE1	16:U:318:HOH:O	2.16	0.45
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.52	0.45
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.51	0.45
6:F:173:LYS:O	6:F:177:GLU:HG3	2.17	0.45
12:Z:154:THR:O	12:Z:157:LYS:HB2	2.17	0.45
12:Z:39:ASN:ND2	16:Z:326:HOH:O	2.49	0.45
3:Q:136:THR:O	3:Q:150:GLN:HA	2.16	0.45
7:G:232:ARG:NE	7:G:232:ARG:HA	2.32	0.45
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.65	0.45
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.52	0.45
10:J:35:ARG:NH2	16:J:239:HOH:O	2.50	0.45
10:J:105(C):LYS:NZ	16:J:248:HOH:O	2.49	0.45
4:R:46:VAL:HG11	4:R:139:ALA:HB1	1.99	0.45
4:D:123(G):GLU:HG2	4:D:125:GLU:H	1.82	0.45
7:U:48:VAL:CG1	7:U:139:VAL:HG11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:157:TYR:C	6:F:157:TYR:CD1	2.90	0.45
5:E:100:SER:O	5:E:104:ASN:HA	2.17	0.45
13:M:7:LYS:HB3	13:M:12:VAL:HG12	1.98	0.45
11:Y:6:PHE:HA	11:Y:123:ASP:O	2.17	0.45
6:T:157:TYR:CD1	6:T:157:TYR:C	2.90	0.45
2:B:121:GLN:C	2:B:121:GLN:NE2	2.70	0.45
1:A:179:ARG:CB	1:A:179:ARG:HH11	2.22	0.45
2:B:218(C):ASP:OD2	2:B:219:GLU:HB3	2.16	0.45
6:T:187:ARG:NH1	6:T:228:LEU:HD13	2.32	0.45
5:E:226:GLY:O	5:E:229:VAL:HG22	2.17	0.45
9:W:48:LEU:HG	9:W:50:THR:HG22	1.99	0.45
2:P:39:GLY:O	2:P:162:ALA:HA	2.17	0.45
5:S:179:THR:O	5:S:179:THR:HG22	2.16	0.45
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.52	0.44
2:P:224:PHE:N	2:P:224:PHE:CD2	2.85	0.44
3:Q:33:ARG:HG2	3:Q:33:ARG:O	2.16	0.44
10:J:18:LYS:HD3	10:J:174:ILE:CG1	2.47	0.44
5:S:207(C):VAL:HA	5:S:233:ILE:HD11	1.99	0.44
4:D:186:LEU:O	4:D:190:GLU:HG3	2.16	0.44
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.52	0.44
10:X:25:SER:HB2	11:Y:131:GLN:NE2	2.32	0.44
6:T:109:ILE:HG21	6:T:147:HIS:HB2	1.99	0.44
12:Z:139:PHE:CE1	12:Z:143:GLN:HG3	2.52	0.44
8:V:7:LYS:HG3	8:V:123:TYR:HA	1.99	0.44
5:E:38:VAL:HG12	5:E:39:GLY:N	2.32	0.44
6:F:176:LEU:HB3	7:G:58:LEU:HD21	1.99	0.44
4:D:46:VAL:HG11	4:D:139:ALA:HB1	1.99	0.44
1:O:58:LEU:HB3	7:U:162:ALA:O	2.17	0.44
1:O:26:TYR:CD1	7:U:17:PRO:HA	2.52	0.44
2:B:122:GLY:C	2:B:124:THR:H	2.19	0.44
5:E:207(B):THR:N	5:E:207(E):ASN:HD22	2.10	0.44
5:E:180(C):PHE:HA	5:E:180(F):ILE:CG1	2.44	0.44
11:K:143:LYS:HB2	11:K:146:LEU:HD13	1.99	0.44
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.47	0.44
2:B:143:ASP:OD2	10:J:105(B):LYS:HE2	2.18	0.44
7:U:48:VAL:O	7:U:48:VAL:HG23	2.16	0.44
6:T:216:SER:HB3	6:T:218(A):GLU:HB2	1.99	0.44
8:H:144:GLN:O	8:H:145:ASP:HB2	2.17	0.44
6:F:175:GLU:OE1	6:F:199:LEU:HD23	2.17	0.44
6:F:216:SER:HB3	6:F:218(A):GLU:HB2	2.00	0.44
8:H:200:LYS:HE3	9:I:140:SER:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:179:THR:HG22	5:E:179:THR:O	2.17	0.44
3:C:163:GLN:CA	3:C:163:GLN:NE2	2.79	0.44
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.32	0.44
12:Z:167:VAL:O	12:Z:171:ILE:HG13	2.18	0.44
5:S:140:GLY:HA2	5:S:215:VAL:HG11	1.98	0.44
12:Z:5:ILE:HG12	12:Z:126:CYS:HB2	1.99	0.44
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.34	0.44
12:L:185:HIS:CD2	12:L:187:GLN:H	2.27	0.44
5:S:86:ARG:NH1	5:S:86:ARG:HG3	2.32	0.44
8:V:105:ASP:O	8:V:106:THR:N	2.51	0.44
2:B:160:TRP:CD2	2:B:163:ILE:HD13	2.52	0.44
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.52	0.44
4:R:194:LEU:HA	4:R:194:LEU:HD12	1.83	0.44
10:J:133:TYR:OH	10:X:24:ILE:HG12	2.17	0.44
5:S:207(C):VAL:HG13	5:S:207(D):ASP:N	2.31	0.44
12:L:80:ALA:HA	12:L:115:PHE:HZ	1.82	0.44
11:Y:105(A):ARG:HH11	11:Y:105(A):ARG:HG2	1.81	0.44
3:Q:224:LEU:N	3:Q:224:LEU:HD12	2.33	0.44
2:B:124:THR:HG22	3:C:130:ARG:NH2	2.15	0.44
5:S:180(F):ILE:O	5:S:180(F):ILE:HG22	2.18	0.44
12:L:93:PHE:N	12:L:94:PRO:CD	2.81	0.44
7:G:48:VAL:CG1	7:G:139:VAL:HG11	2.47	0.44
8:V:67:SER:HB2	8:V:74:PRO:HG3	2.00	0.44
9:I:126:VAL:HG11	9:I:134:LEU:HB3	1.99	0.44
4:D:86:ARG:HD3	4:D:86:ARG:HA	1.83	0.44
5:S:40:LEU:HD23	5:S:40:LEU:N	2.32	0.44
2:B:150:THR:O	2:B:157:TYR:HA	2.17	0.44
10:X:17:SER:HB2	10:X:170:PHE:HB2	1.98	0.44
5:S:180(C):PHE:HA	5:S:180(F):ILE:CD1	2.48	0.44
6:T:187:ARG:HH12	6:T:228:LEU:HD13	1.83	0.44
5:E:86:ARG:NH1	5:E:86:ARG:HG3	2.33	0.44
12:Z:140:LEU:O	12:Z:144:VAL:HB	2.18	0.44
5:E:207(C):VAL:HG13	5:E:207(D):ASP:N	2.31	0.44
12:Z:39:ASN:HD21	12:Z:201:GLY:HA2	1.82	0.44
12:L:139:PHE:CE1	12:L:143:GLN:HG3	2.52	0.44
4:R:185:THR:HG23	4:R:188:GLU:OE1	2.17	0.44
2:P:112:LEU:HD23	2:P:112:LEU:C	2.38	0.44
3:Q:112:LEU:HD13	3:Q:112:LEU:O	2.18	0.44
5:E:12:THR:CG2	5:E:124:THR:HA	2.38	0.44
2:P:122:GLY:C	2:P:124:THR:H	2.21	0.44
2:P:143:ASP:OD2	10:X:105(B):LYS:HE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.47	0.44
12:L:14:ALA:HB1	12:L:192:LEU:HD11	2.00	0.44
13:M:80:PHE:CE1	13:M:111:ARG:HD3	2.53	0.44
12:Z:14:ALA:HB1	12:Z:192:LEU:HD11	1.99	0.44
7:G:192:PHE:CD1	7:G:192:PHE:C	2.90	0.44
10:J:2:ILE:HB	10:J:17:SER:HB3	1.99	0.43
2:P:218(C):ASP:OD2	2:P:219:GLU:HB3	2.18	0.43
3:C:136:THR:O	3:C:150:GLN:HA	2.17	0.43
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.48	0.43
7:G:38:LEU:HD12	7:G:38:LEU:C	2.39	0.43
4:D:14:THR:HG23	5:E:23:GLN:NE2	2.33	0.43
7:G:140:SER:HA	7:G:215:ALA:HB1	1.98	0.43
1:A:198:LYS:HE3	1:A:236:LEU:HD11	1.99	0.43
7:U:140:SER:HA	7:U:215:ALA:HB1	1.99	0.43
9:W:36:HIS:HB3	9:W:42:PHE:CD2	2.53	0.43
6:T:204:ASP:OD1	6:T:204:ASP:N	2.51	0.43
7:U:87:ASN:HD22	7:U:87:ASN:C	2.21	0.43
9:W:55:LEU:HA	9:W:55:LEU:HD23	1.82	0.43
7:U:192:PHE:CD1	7:U:192:PHE:C	2.90	0.43
2:B:121:GLN:CG	3:C:83:ALA:HB1	2.48	0.43
7:G:184(G):GLU:CG	7:G:188:LYS:CB	2.94	0.43
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.53	0.43
3:Q:40:VAL:HG22	3:Q:193:THR:OG1	2.18	0.43
3:C:33:ARG:O	3:C:33:ARG:HG2	2.16	0.43
5:E:207(C):VAL:HA	5:E:233:ILE:HD11	2.00	0.43
2:P:150:THR:O	2:P:157:TYR:HA	2.18	0.43
7:G:110:ASP:HB3	7:G:149:TYR:CE2	2.53	0.43
3:Q:24:VAL:O	3:Q:27:ALA:HB3	2.18	0.43
6:T:171:SER:O	6:T:174:ALA:HB3	2.19	0.43
7:G:179(C):LYS:HB2	7:G:179(C):LYS:HE3	1.72	0.43
4:D:122:ARG:HG2	4:D:122:ARG:HH11	1.83	0.43
2:B:222:LYS:NZ	2:B:228:GLU:OE2	2.50	0.43
6:T:38:ILE:HG12	6:T:197:ILE:HD11	2.00	0.43
8:H:207:PRO:HG2	8:H:210:THR:OG1	2.19	0.43
2:P:186:VAL:O	2:P:190:ILE:HG13	2.18	0.43
3:C:227:GLU:O	3:C:231:GLN:HG3	2.18	0.43
2:B:46:ILE:HD11	2:B:146:TYR:HB3	2.00	0.43
6:T:218(B):THR:O	6:T:218(C):ASN:HB2	2.17	0.43
6:T:136:THR:O	6:T:150:MET:HA	2.17	0.43
7:U:29:LYS:HA	7:U:29:LYS:HD2	1.85	0.43
5:E:138:ILE:HD12	5:E:138:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.53	0.43
13:M:113:VAL:HA	13:M:118:VAL:O	2.19	0.43
11:K:105(A):ARG:HD3	11:K:180:GLU:OE1	2.18	0.43
12:L:160:LYS:HG3	12:L:161:PRO:HD2	2.00	0.43
7:U:119:LEU:HA	7:U:119:LEU:HD12	1.88	0.43
4:D:185:THR:HG23	4:D:188:GLU:OE1	2.18	0.43
3:Q:177:GLU:OE2	4:R:57:PRO:HD2	2.19	0.43
11:K:142:TYR:C	11:K:143:LYS:HD2	2.39	0.43
10:J:126:ALA:HB1	10:J:130:SER:HB2	2.01	0.43
3:Q:215:VAL:O	3:Q:215:VAL:HG13	2.19	0.43
11:Y:13:ILE:HG13	11:Y:151:ALA:HB1	2.00	0.43
1:O:212:LEU:HD22	1:O:224:LEU:CD1	2.48	0.43
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.54	0.43
1:O:118:LYS:HE2	1:O:122:GLU:OE1	2.19	0.43
12:L:5:ILE:HG12	12:L:126:CYS:HB2	2.01	0.43
6:F:103:TYR:O	6:F:104:LYS:HB3	2.19	0.43
14:N:104:TYR:OH	14:N:180:ALA:HB2	2.19	0.43
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.54	0.43
6:T:103:TYR:O	6:T:104:LYS:HB3	2.18	0.43
10:X:90(B):ARG:HG2	10:X:90(B):ARG:HH11	1.84	0.43
7:U:107:MET:HE3	7:U:112:LEU:HD13	2.00	0.43
3:Q:31:VAL:CG1	3:Q:135:SER:HB2	2.48	0.43
3:C:227:GLU:CD	3:C:227:GLU:H	2.22	0.43
11:K:105(A):ARG:HG2	11:K:105(A):ARG:NH1	2.34	0.43
1:A:217(G):LEU:HG	1:A:217(I):TYR:CE1	2.54	0.43
4:R:12:VAL:HG23	4:R:123(A):GLY:HA2	2.00	0.43
4:D:105:GLU:OE1	12:L:65:TYR:OH	2.29	0.43
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.54	0.43
14:N:48:SER:HB3	14:N:51:ASP:HB2	2.00	0.43
4:R:81:LEU:HD12	4:R:133:GLY:HA3	2.01	0.43
1:O:39:GLY:HA2	1:O:47:VAL:O	2.18	0.43
3:C:224:LEU:N	3:C:224:LEU:HD12	2.34	0.43
12:Z:116:ASP:HB3	12:Z:120:SER:H	1.83	0.43
9:I:28:SER:CB	10:J:120:VAL:HG21	2.48	0.43
14:N:13:ILE:HD12	14:N:151:THR:HG22	2.00	0.43
6:T:12:ASN:HB2	16:T:301:HOH:O	2.17	0.43
2:P:77:ALA:HB3	2:P:137:ILE:HB	1.99	0.43
7:U:8:TYR:C	7:U:10:ARG:H	2.22	0.43
13:M:184:LEU:HD23	13:M:184:LEU:C	2.38	0.43
3:Q:76:LEU:HD23	3:Q:76:LEU:C	2.38	0.43
1:A:184:LEU:C	1:A:184:LEU:HD23	4.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.53	0.43
5:E:180(C):PHE:HA	5:E:180(F):ILE:CD1	2.49	0.43
1:A:118:LYS:HE2	1:A:122:GLU:OE1	2.19	0.43
8:H:105:ASP:O	8:H:106:THR:N	2.51	0.43
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.53	0.43
11:K:40:PHE:CD1	11:K:73:ARG:CZ	3.02	0.43
1:A:39:GLY:HA2	1:A:47:VAL:O	2.19	0.43
9:W:14:ILE:HG23	9:W:34:ILE:HD13	2.00	0.43
12:L:167:VAL:O	12:L:171:ILE:HG13	2.18	0.43
1:O:92:SER:OG	1:O:116:VAL:HG22	2.18	0.43
11:K:43:GLY:HA2	11:K:100:MET:O	2.19	0.43
13:M:5:SER:HB3	13:M:14:ILE:HG13	2.00	0.43
13:M:179:ASP:HB3	13:M:181(A):THR:OG1	2.19	0.43
4:R:105:GLU:OE1	12:Z:65:TYR:OH	2.30	0.43
11:Y:40:PHE:CD1	11:Y:73:ARG:CZ	3.02	0.43
10:X:126:ALA:HB1	10:X:130:SER:HB2	2.00	0.42
8:H:3:ILE:O	8:H:126:SER:HA	2.19	0.42
7:U:110:ASP:HB3	7:U:149:TYR:CE2	2.54	0.42
8:V:63:ILE:HG23	8:V:74:PRO:HB3	2.01	0.42
7:U:79:ASN:HA	16:U:312:HOH:O	2.19	0.42
2:P:27:ALA:O	2:P:30:SER:HB3	2.18	0.42
9:I:6:MET:HE1	9:I:155:ILE:HA	2.00	0.42
1:O:33:GLN:CA	1:O:33:GLN:NE2	2.82	0.42
6:F:187:ARG:NH1	6:F:228:LEU:HD13	2.33	0.42
2:B:224:PHE:N	2:B:224:PHE:CD2	2.85	0.42
9:W:29:ASN:HD22	9:W:30:LYS:HG3	1.84	0.42
10:J:52:THR:CG2	10:J:53:VAL:H	2.32	0.42
3:Q:227:GLU:O	3:Q:231:GLN:HG3	2.19	0.42
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.83	0.42
5:S:38:VAL:HG12	5:S:39:GLY:N	2.33	0.42
5:S:100:SER:O	5:S:104:ASN:HA	2.19	0.42
5:E:160:LEU:CD2	6:F:59:LEU:HD12	2.49	0.42
3:C:186:VAL:HG21	3:C:216:LYS:HE2	2.00	0.42
5:S:207(C):VAL:HG22	5:S:226:GLY:C	2.40	0.42
11:Y:105(A):ARG:HD3	11:Y:180:GLU:OE1	2.20	0.42
11:K:77:ALA:HA	11:K:111:TYR:CE2	2.54	0.42
8:V:144:GLN:O	8:V:145:ASP:HB2	2.19	0.42
8:H:34:LEU:HB2	16:H:325:HOH:O	2.19	0.42
6:F:72:ARG:HD2	13:M:64:THR:OG1	2.19	0.42
5:E:140:GLY:HA2	5:E:215:VAL:HG11	2.01	0.42
13:M:27:ARG:HD3	13:M:28:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.82	0.42
7:U:87:ASN:ND2	7:U:87:ASN:C	2.73	0.42
2:B:77:ALA:HB3	2:B:137:ILE:HB	2.00	0.42
11:Y:25:TRP:CH2	12:Z:134:SER:HA	2.54	0.42
3:C:173:ARG:O	3:C:177:GLU:HG3	2.19	0.42
11:K:49:ALA:HB2	15:K:301:1Y9:C10	2.46	0.42
6:F:187:ARG:CG	6:F:187:ARG:HH11	2.32	0.42
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.18	0.42
12:Z:10:PHE:CE1	12:Z:167:VAL:HA	2.54	0.42
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.54	0.42
3:Q:174:GLU:O	3:Q:178:LYS:HD2	2.18	0.42
13:M:150:VAL:HG21	16:M:360:HOH:O	2.20	0.42
4:R:122:ARG:HH11	4:R:122:ARG:HG2	1.85	0.42
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	2.01	0.42
10:X:2:ILE:HB	10:X:17:SER:HB3	2.01	0.42
6:F:203:GLU:HA	6:F:203:GLU:OE1	2.19	0.42
6:F:187:ARG:HH12	6:F:228:LEU:HD13	1.85	0.42
3:Q:241:GLN:O	3:Q:243:GLN:N	2.48	0.42
5:E:90:ASN:O	5:E:94:GLN:HG3	2.19	0.42
6:F:38:ILE:HG12	6:F:197:ILE:HD11	2.01	0.42
6:F:192:GLN:NE2	6:F:195:LYS:HE3	2.35	0.42
13:M:112:TYR:O	13:M:119:THR:HA	2.20	0.42
8:H:196:VAL:HA	16:H:344:HOH:O	2.19	0.42
12:Z:4:GLY:O	12:Z:126:CYS:HA	2.20	0.42
12:L:4:GLY:O	12:L:126:CYS:HA	2.19	0.42
1:O:108:PRO:CG	1:O:111:LEU:HD12	2.50	0.42
8:H:153:LYS:HD2	16:H:328:HOH:O	2.19	0.42
13:M:49:ILE:O	13:M:53:GLN:HG3	2.19	0.42
11:K:17:ASP:OD2	11:K:33:LYS:NZ	2.49	0.42
6:F:172:ALA:O	6:F:176:LEU:CD2	2.68	0.42
6:F:172:ALA:O	6:F:176:LEU:HD23	2.19	0.42
12:L:16:ASP:HA	12:L:191:GLY:O	2.19	0.42
8:H:84:LYS:HG3	8:H:85:GLN:N	2.34	0.42
8:V:200:LYS:HE3	9:W:140:SER:O	2.19	0.42
1:A:52:LYS:HG3	1:A:211:GLU:HB2	2.01	0.42
1:O:198:LYS:HE3	1:O:236:LEU:HD11	2.02	0.42
10:J:140:HIS:CE1	11:Y:203:GLU:OE2	2.73	0.42
1:O:6:ASP:OD2	1:O:8:TYR:HB2	2.19	0.42
4:R:160:TYR:HA	5:S:58:LEU:O	2.20	0.42
1:A:86:ARG:NE	7:G:118:ASN:HD21	2.11	0.42
1:A:6:ASP:OD2	1:A:8:TYR:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.54	0.42
6:F:51:GLU:OE1	6:F:53:LEU:HD21	2.19	0.42
5:S:97:ASN:ND2	12:Z:60:ASN:HD21	2.16	0.42
10:X:13:ILE:HD13	10:X:152:LEU:HD23	2.01	0.42
6:F:32:GLU:HB3	6:F:169:ARG:NH2	2.35	0.42
3:Q:99:HIS:CG	3:Q:107:VAL:HG12	2.55	0.42
3:C:112:LEU:HD13	3:C:112:LEU:O	2.19	0.42
1:A:111:LEU:O	1:A:114:SER:HB3	2.20	0.42
2:B:71:ASN:CG	2:B:72:ASP:H	2.23	0.42
10:J:-1:MET:CG	10:J:1:ASP:H	2.31	0.42
10:X:38:SER:HA	16:X:224:HOH:O	2.18	0.42
5:S:183:ASP:O	5:S:185:ASN:N	2.53	0.42
3:Q:125:GLN:HG3	3:Q:125:GLN:O	2.20	0.42
3:Q:227:GLU:H	3:Q:227:GLU:CD	2.22	0.42
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.01	0.42
4:R:179:GLU:HB3	4:R:192:LEU:HD21	2.02	0.42
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	2.00	0.42
14:N:163:ILE:HG23	14:N:170:GLY:HA2	2.02	0.42
4:D:81:LEU:HD12	4:D:133:GLY:HA3	2.02	0.42
14:N:176:VAL:HG12	14:N:178:LEU:HD13	2.01	0.42
12:L:104:LEU:HA	12:L:109:LYS:O	2.19	0.42
2:B:121:GLN:HG3	3:C:83:ALA:HB1	2.01	0.42
2:B:141:TYR:C	2:B:141:TYR:CD1	2.94	0.42
5:E:85:ALA:HB2	5:E:134:VAL:HG21	2.02	0.42
1:A:33:GLN:NE2	1:A:33:GLN:CA	2.83	0.42
3:C:190:VAL:O	3:C:194:VAL:HG23	2.20	0.42
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.85	0.42
3:Q:150:GLN:HG2	3:Q:151:THR:N	2.34	0.42
11:Y:105(A):ARG:HG2	11:Y:105(A):ARG:NH1	2.35	0.42
8:H:5:GLY:O	8:H:124:TYR:HA	2.20	0.42
11:K:52:CYS:O	11:K:56:GLU:HB2	2.20	0.42
4:D:79:SER:HA	16:D:305:HOH:O	2.18	0.42
2:B:39:GLY:O	2:B:162:ALA:HA	2.20	0.42
11:Y:200:LYS:HE3	11:Y:206:PHE:O	2.20	0.42
3:C:24:VAL:O	3:C:27:ALA:HB3	2.19	0.42
5:S:90:ASN:O	5:S:94:GLN:HG3	2.20	0.42
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.35	0.41
6:T:51:GLU:OE1	6:T:53:LEU:HD21	2.20	0.41
9:I:48:LEU:HG	9:I:50:THR:HG22	2.01	0.41
2:P:186:VAL:HG21	2:P:216:ARG:HD3	2.01	0.41
9:W:93:GLY:N	9:W:94:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:38:ASN:OD1	11:K:38:ASN:C	2.57	0.41
7:G:107:MET:CE	7:G:112:LEU:HD13	2.49	0.41
10:J:168:MET:HE3	10:X:168:MET:CE	2.51	0.41
2:P:126:HIS:CB	3:Q:129:VAL:HG12	2.47	0.41
5:E:160:LEU:HD23	6:F:59:LEU:HA	2.02	0.41
4:R:156:THR:HG22	5:S:82:ALA:HB3	2.02	0.41
3:Q:33:ARG:HH11	3:Q:33:ARG:HB3	1.85	0.41
10:J:12:VAL:CG2	10:J:108:PRO:HB2	2.51	0.41
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.32	0.41
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.55	0.41
1:O:111:LEU:O	1:O:114:SER:HB3	2.21	0.41
8:V:116:HIS:HB2	16:V:344:HOH:O	2.20	0.41
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.94	0.41
3:C:99:HIS:CG	3:C:107:VAL:HG12	2.55	0.41
4:D:147:GLN:HA	16:D:324:HOH:O	2.19	0.41
10:J:90(B):ARG:HG2	10:J:90(B):ARG:HH11	1.85	0.41
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.67	0.41
7:G:203:THR:HG22	7:G:204:GLU:O	2.21	0.41
10:X:20:VAL:HA	16:X:232:HOH:O	2.19	0.41
3:C:31:VAL:CG1	3:C:135:SER:HB2	2.49	0.41
8:V:3:ILE:O	8:V:126:SER:HA	2.21	0.41
5:E:207(C):VAL:HG22	5:E:226:GLY:C	2.40	0.41
12:Z:115:PHE:CD2	12:Z:121:TYR:HB3	2.55	0.41
13:M:55:ILE:HD13	13:M:99:ILE:HD11	2.03	0.41
9:I:114:ASP:HB2	16:I:252:HOH:O	2.19	0.41
1:O:27:ALA:O	1:O:31:VAL:HG23	2.19	0.41
1:O:180:TRP:HA	1:O:184:LEU:HD11	2.02	0.41
3:C:125:GLN:O	3:C:125:GLN:HG3	2.21	0.41
9:W:61:TYR:C	9:W:61:TYR:CD1	2.94	0.41
5:S:207(B):THR:H	5:S:207(E):ASN:HB3	1.84	0.41
5:E:207(B):THR:H	5:E:207(E):ASN:HB3	1.86	0.41
5:S:139:ILE:HA	5:S:147:HIS:O	2.20	0.41
10:J:143:ARG:HA	10:J:144:PRO:HD3	1.95	0.41
2:B:231:ASP:O	2:B:235:LYS:HG2	2.20	0.41
4:D:20:ARG:HD3	4:D:25:GLU:OE2	2.19	0.41
11:K:20:ALA:HB2	11:K:31:VAL:HG21	2.01	0.41
14:N:92:ASP:HB2	16:N:309:HOH:O	2.20	0.41
2:B:229:ILE:O	2:B:233:LEU:HB2	2.21	0.41
9:I:22:SER:O	9:I:23:GLN:HB2	2.20	0.41
11:Y:77:ALA:HA	11:Y:111:TYR:CE2	2.56	0.41
3:C:76:LEU:HD23	3:C:76:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:22:SER:O	9:W:23:GLN:HB2	2.21	0.41
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	2.02	0.41
2:P:46:ILE:HD11	2:P:146:TYR:HB3	2.01	0.41
6:F:214:TRP:CH2	6:F:218(A):GLU:HB3	2.55	0.41
1:A:39:GLY:O	1:A:162:ALA:HA	2.21	0.41
2:B:191:GLU:HG3	2:B:236:THR:HG22	2.02	0.41
7:G:165:THR:HG23	16:G:335:HOH:O	2.21	0.41
8:V:148:LYS:O	8:V:152:ILE:HG13	2.21	0.41
12:Z:75:SER:HB2	12:Z:77:ASN:OD1	2.20	0.41
5:E:103:PHE:CE2	13:M:62:LEU:HD21	2.56	0.41
5:S:138:ILE:N	5:S:138:ILE:HD12	2.35	0.41
7:G:87:ASN:HD22	7:G:87:ASN:C	2.23	0.41
6:F:204:ASP:N	6:F:204:ASP:OD1	2.53	0.41
3:Q:190:VAL:O	3:Q:194:VAL:HG23	2.21	0.41
1:O:86:ARG:NE	7:U:118:ASN:ND2	2.62	0.41
11:Y:142:TYR:C	11:Y:143:LYS:HD2	2.40	0.41
11:Y:17:ASP:OD2	11:Y:33:LYS:NZ	2.49	0.41
10:X:25:SER:HB2	11:Y:131:GLN:HE22	1.86	0.41
12:Z:5:ILE:HG12	12:Z:126:CYS:CB	2.50	0.41
12:L:5:ILE:HG12	12:L:126:CYS:CB	2.50	0.41
5:E:103:PHE:O	13:M:78:TYR:HA	2.21	0.41
9:W:183:GLU:HA	16:W:243:HOH:O	2.21	0.41
1:O:217(G):LEU:HD13	1:O:218:GLY:HA2	2.02	0.41
1:A:58:LEU:HD12	7:G:173:THR:HG23	2.03	0.41
2:B:238:ILE:O	2:B:238:ILE:HG22	2.20	0.41
11:Y:38:ASN:OD1	11:Y:38:ASN:C	2.58	0.41
13:M:19:LEU:HD12	13:M:28:PHE:O	2.20	0.41
6:F:192:GLN:HE21	6:F:195:LYS:CE	2.33	0.41
6:T:172:ALA:O	6:T:176:LEU:HD23	2.21	0.41
10:X:148:THR:CG2	10:X:177:ILE:HD13	2.50	0.41
1:A:108:PRO:CG	1:A:111:LEU:HD12	2.51	0.41
4:D:179:GLU:HB3	4:D:192:LEU:HD21	2.01	0.41
4:R:197:LEU:O	4:R:201:MET:HG3	2.20	0.41
8:V:128:GLY:O	8:V:131:SER:HB2	2.20	0.41
2:P:229:ILE:O	2:P:233:LEU:HB2	2.20	0.41
11:Y:43:GLY:HA2	11:Y:100:MET:O	2.20	0.41
2:B:27:ALA:O	2:B:30:SER:HB3	2.21	0.41
3:C:175:PHE:O	3:C:179:ASN:HB2	2.21	0.41
5:E:114:HIS:HB3	6:F:86:ARG:NH2	2.36	0.41
3:Q:95:GLU:OE2	3:Q:95:GLU:HA	2.21	0.41
12:L:196:ILE:HD12	12:L:196:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.12	0.41
12:Z:196:ILE:HD12	12:Z:196:ILE:N	2.36	0.41
10:X:12:VAL:CG2	10:X:108:PRO:HB2	2.48	0.41
6:F:192:GLN:NE2	6:F:195:LYS:CE	2.84	0.41
7:U:38:LEU:C	7:U:38:LEU:HD12	2.41	0.41
8:H:67:SER:HB2	8:H:74:PRO:HG3	2.02	0.41
1:O:117:ALA:HB1	1:O:155:GLY:O	2.20	0.41
2:P:53:LYS:O	2:P:54:VAL:O	2.39	0.41
14:N:94:ASN:ND2	16:N:346:HOH:O	2.30	0.41
12:Z:160:LYS:HG3	12:Z:161:PRO:HD2	2.03	0.41
10:X:59:ILE:O	10:X:63:ILE:HG12	2.21	0.41
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.88	0.41
1:O:188:ASP:O	1:O:192:ILE:HG13	2.21	0.41
12:Z:104:LEU:HA	12:Z:109:LYS:O	2.20	0.41
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.99	0.41
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.56	0.41
3:Q:159:SER:O	4:R:59:LEU:HD22	2.21	0.41
3:C:195:ARG:HG3	3:C:236:ILE:HD13	2.03	0.41
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.21	0.41
5:S:35:SER:HB3	5:S:66:LYS:HZ3	1.85	0.41
4:R:112:LEU:O	4:R:112:LEU:HD13	2.20	0.41
7:G:151:THR:HA	7:G:156:TYR:O	2.21	0.41
7:G:151:THR:HG22	7:G:157:TYR:HB3	2.01	0.41
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.85	0.41
1:A:161:LYS:HE3	2:B:60:GLU:HA	2.03	0.41
6:T:214:TRP:CH2	6:T:218(A):GLU:HB3	2.55	0.41
1:A:111:LEU:HA	1:A:111:LEU:HD23	1.87	0.41
7:U:35:ILE:HA	7:U:35:ILE:HD13	1.92	0.41
10:J:59:ILE:O	10:J:63:ILE:HG12	2.20	0.41
2:P:149:TYR:CZ	3:Q:62(A):ILE:HD12	2.56	0.41
10:X:35:ARG:HD3	10:X:35:ARG:HA	1.84	0.41
4:D:238:LYS:HB3	4:D:238:LYS:HE2	1.89	0.41
8:V:207:PRO:HG2	8:V:210:THR:OG1	2.20	0.41
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	2.03	0.41
12:Z:28:ARG:NH1	12:Z:211:ARG:HB3	2.36	0.41
7:U:151:THR:HG22	7:U:157:TYR:HB3	2.03	0.41
2:P:160:TRP:CD2	2:P:163:ILE:HD13	2.55	0.41
3:Q:150:GLN:O	3:Q:157:TYR:HA	2.21	0.41
6:F:28:VAL:O	6:F:32:GLU:HG3	2.21	0.41
12:L:142:ASN:O	12:L:146:PHE:HA	2.20	0.41
12:L:184:ARG:NH2	8:V:29:LYS:HE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:84:LYS:HG3	8:V:85:GLN:N	2.36	0.41
9:W:80:THR:HG1	9:W:109:PHE:HE2	1.66	0.41
13:M:141(C):ARG:NH1	13:M:141(C):ARG:CG	2.79	0.40
14:N:107:LYS:CG	14:N:108:GLY:N	2.81	0.40
5:E:180(F):ILE:O	5:E:180(F):ILE:HG22	2.20	0.40
5:S:31:ILE:HD11	5:S:153:PRO:HG2	2.03	0.40
6:T:36:THR:CG2	6:T:51:GLU:OE2	2.69	0.40
10:J:18:LYS:CG	10:J:174:ILE:HG13	2.52	0.40
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.21	0.40
12:L:28:ARG:NH1	12:L:211:ARG:HB3	2.36	0.40
3:C:150:GLN:O	3:C:157:TYR:HA	2.22	0.40
7:U:139:VAL:HA	7:U:147:SER:O	2.21	0.40
11:K:40:PHE:HB3	11:K:73:ARG:NH2	2.36	0.40
5:S:114:HIS:HB3	6:T:86:ARG:NH2	2.36	0.40
12:Z:142:ASN:O	12:Z:146:PHE:HA	2.20	0.40
7:U:31:THR:HG21	7:U:135:ILE:HG13	2.03	0.40
9:I:80:THR:HG1	9:I:109:PHE:HE2	1.66	0.40
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	2.03	0.40
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.03	0.40
6:F:83:PRO:HB2	16:F:343:HOH:O	2.20	0.40
6:T:35:THR:CG2	6:T:51:GLU:O	2.67	0.40
1:O:32:LYS:HA	1:O:32:LYS:CE	2.51	0.40
10:J:105(B):LYS:HZ3	10:J:105(B):LYS:HB2	1.86	0.40
3:C:215:VAL:O	3:C:215:VAL:HG13	2.20	0.40
4:R:170:GLU:HG2	4:R:171:GLY:N	2.36	0.40
11:K:8:PHE:CE2	11:K:13:ILE:HG12	2.56	0.40
2:B:44:ASP:OD2	2:B:44:ASP:N	2.54	0.40
2:B:225:LYS:O	2:B:226:PRO:C	2.60	0.40
11:K:203:GLU:OE2	10:X:140:HIS:CE1	2.74	0.40
5:S:207(B):THR:OG1	5:S:207(E):ASN:HB3	2.22	0.40
2:P:15:PHE:N	3:Q:23:GLN:HE22	2.05	0.40
13:M:139:ARG:HD2	8:V:165:ASN:ND2	2.35	0.40
5:E:180(E):LYS:O	5:E:183:ASP:N	2.52	0.40
8:H:126:SER:O	8:H:127:LEU:HD23	2.21	0.40
6:T:172:ALA:O	6:T:176:LEU:CD2	2.70	0.40
10:X:52:THR:CG2	10:X:53:VAL:H	2.34	0.40
10:X:100:LEU:HD21	10:X:112:GLN:HG3	2.04	0.40
6:F:171:SER:O	6:F:174:ALA:HB3	2.21	0.40
1:O:52:LYS:HG3	1:O:211:GLU:HB2	2.02	0.40
6:F:43:ASN:N	6:F:43:ASN:ND2	2.70	0.40
3:C:33:ARG:HH11	3:C:33:ARG:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:193:GLN:OXT	10:X:193:GLN:HG2	2.22	0.40
4:D:112:LEU:O	4:D:112:LEU:HD13	2.22	0.40
2:B:53:LYS:O	2:B:54:VAL:O	2.40	0.40
5:E:4:PHE:CG	5:E:5:ARG:N	2.89	0.40
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.51	0.40
5:S:4:PHE:CG	5:S:5:ARG:N	2.88	0.40
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.03	0.40
1:A:117:ALA:HB1	1:A:155:GLY:O	2.21	0.40
10:J:22:ARG:HA	10:J:22:ARG:HD3	1.98	0.40
5:S:194:VAL:CG1	5:S:207:LEU:HD11	2.52	0.40
6:T:203:GLU:OE1	6:T:203:GLU:HA	2.21	0.40
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.22	0.40
6:T:35:THR:HG23	6:T:51:GLU:HB3	2.03	0.40
6:F:36:THR:CG2	6:F:51:GLU:OE2	2.69	0.40
5:E:86:ARG:O	5:E:90:ASN:HB2	2.22	0.40
12:L:90:LYS:HE3	12:L:93:PHE:O	2.22	0.40
5:S:180(E):LYS:O	5:S:183:ASP:N	2.52	0.40
9:W:29:ASN:N	9:W:29:ASN:ND2	2.65	0.40
5:E:183:ASP:O	5:E:185:ASN:N	2.54	0.40
3:Q:228:GLU:O	3:Q:232:TYR:HD1	2.05	0.40
5:E:40:LEU:HG	5:E:189:LEU:HD22	2.03	0.40
7:G:87:ASN:ND2	7:G:87:ASN:C	2.75	0.40
9:W:19:ARG:HD3	9:W:168:LEU:O	2.21	0.40
7:G:52:LYS:HA	16:G:320:HOH:O	2.22	0.40
2:P:26:TYR:CD1	2:P:26:TYR:N	2.87	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%)	11 (4%)	2 (1%)	24 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	O	248/250 (99%)	235 (95%)	11 (4%)	2 (1%)	24 51
2	B	242/244 (99%)	219 (90%)	16 (7%)	7 (3%)	6 14
2	P	242/244 (99%)	219 (90%)	17 (7%)	6 (2%)	7 18
3	C	239/241 (99%)	226 (95%)	10 (4%)	3 (1%)	15 37
3	Q	239/241 (99%)	225 (94%)	11 (5%)	3 (1%)	15 37
4	D	240/242 (99%)	223 (93%)	13 (5%)	4 (2%)	11 29
4	R	240/242 (99%)	221 (92%)	15 (6%)	4 (2%)	11 29
5	E	231/233 (99%)	208 (90%)	16 (7%)	7 (3%)	5 13
5	S	231/233 (99%)	208 (90%)	16 (7%)	7 (3%)	5 13
6	F	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	24 51
6	T	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	24 51
7	G	241/243 (99%)	227 (94%)	13 (5%)	1 (0%)	39 69
7	U	241/243 (99%)	227 (94%)	13 (5%)	1 (0%)	39 69
8	H	220/222 (99%)	209 (95%)	9 (4%)	2 (1%)	21 49
8	V	220/222 (99%)	209 (95%)	8 (4%)	3 (1%)	14 35
9	I	202/204 (99%)	193 (96%)	9 (4%)	0	100 100
9	W	202/204 (99%)	193 (96%)	9 (4%)	0	100 100
10	J	196/198 (99%)	186 (95%)	9 (5%)	1 (0%)	34 63
10	X	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	34 63
11	K	210/212 (99%)	202 (96%)	8 (4%)	0	100 100
11	Y	210/212 (99%)	203 (97%)	7 (3%)	0	100 100
12	L	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	34 63
12	Z	220/222 (99%)	207 (94%)	12 (6%)	1 (0%)	34 63
13	M	231/233 (99%)	219 (95%)	11 (5%)	1 (0%)	39 69
13	a	231/233 (99%)	219 (95%)	11 (5%)	1 (0%)	39 69
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100 100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100 100
All	All	6312/6368 (99%)	5946 (94%)	304 (5%)	62 (1%)	19 45

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL

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Mol	Chain	Res	Type
2	B	218(C)	ASP
3	C	58	LEU
3	C	203	THR
4	D	123(G)	GLU
12	L	71	ASP
2	P	54	VAL
2	P	218(C)	ASP
3	Q	58	LEU
3	Q	203	THR
4	R	123(G)	GLU
12	Z	71	ASP
1	A	5	THR
1	A	167	LYS
2	B	6	ARG
2	B	216(B)	GLY
3	C	183	PRO
5	E	5	ARG
5	E	180	LEU
5	E	202	ARG
6	F	205	ASN
1	O	5	THR
1	O	167	LYS
2	P	6	ARG
2	P	216(B)	GLY
3	Q	183	PRO
5	S	5	ARG
5	S	180	LEU
5	S	202	ARG
6	T	205	ASN
4	D	123(C)	GLY
6	F	206	LYS
8	H	91	GLN
4	R	123(C)	GLY
6	T	206	LYS
8	V	91	GLN
13	a	96	TRP
2	B	184	MET
5	E	217	LYS
13	M	96	TRP
5	S	217	LYS
2	B	64	THR
5	E	231	LYS

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Mol	Chain	Res	Type
7	G	239	GLN
5	S	231	LYS
7	U	239	GLN
4	D	123(F)	GLY
4	D	126	ARG
10	J	8	VAL
2	P	64	THR
4	R	123(F)	GLY
4	R	126	ARG
8	V	9	ASN
10	X	8	VAL
2	B	186	VAL
2	P	186	VAL
5	S	184	GLY
8	V	105(A)	PRO
8	H	105(A)	PRO
5	E	180(F)	ILE
5	E	184	GLY
5	S	180(F)	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	205 (98%)	4 (2%)	65	88
1	O	209/209 (100%)	205 (98%)	4 (2%)	65	88
2	B	203/203 (100%)	193 (95%)	10 (5%)	31	61
2	P	203/203 (100%)	192 (95%)	11 (5%)	27	56
3	C	213/213 (100%)	203 (95%)	10 (5%)	32	63
3	Q	213/213 (100%)	203 (95%)	10 (5%)	32	63
4	D	198/198 (100%)	186 (94%)	12 (6%)	23	49
4	R	198/198 (100%)	186 (94%)	12 (6%)	23	49
5	E	192/192 (100%)	176 (92%)	16 (8%)	14	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	S	192/192 (100%)	177 (92%)	15 (8%)	16 35
6	F	201/201 (100%)	186 (92%)	15 (8%)	17 38
6	T	201/201 (100%)	186 (92%)	15 (8%)	17 38
7	G	207/207 (100%)	195 (94%)	12 (6%)	25 52
7	U	207/207 (100%)	195 (94%)	12 (6%)	25 52
8	H	181/181 (100%)	174 (96%)	7 (4%)	39 70
8	V	181/181 (100%)	174 (96%)	7 (4%)	39 70
9	I	172/172 (100%)	169 (98%)	3 (2%)	68 90
9	W	172/172 (100%)	169 (98%)	3 (2%)	68 90
10	J	175/175 (100%)	169 (97%)	6 (3%)	44 75
10	X	175/175 (100%)	169 (97%)	6 (3%)	44 75
11	K	169/169 (100%)	159 (94%)	10 (6%)	24 51
11	Y	169/169 (100%)	160 (95%)	9 (5%)	28 57
12	L	185/185 (100%)	174 (94%)	11 (6%)	24 51
12	Z	185/185 (100%)	173 (94%)	12 (6%)	21 46
13	M	199/199 (100%)	191 (96%)	8 (4%)	38 69
13	a	199/199 (100%)	191 (96%)	8 (4%)	38 69
14	N	162/162 (100%)	155 (96%)	7 (4%)	35 66
14	b	162/162 (100%)	155 (96%)	7 (4%)	35 66
All	All	5332/5332 (100%)	5070 (95%)	262 (5%)	31 61

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	64	LEU
1	A	158	PHE
1	A	179	ARG
2	B	58	LEU
2	B	61	GLN
2	B	71	ASN
2	B	121	GLN
2	B	135	SER
2	B	156	ASN
2	B	185	LYS

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Mol	Chain	Res	Type
2	B	192	LEU
2	B	212	PHE
2	B	218	ASN
3	C	10	ARG
3	C	25	GLU
3	C	57	LYS
3	C	66	LYS
3	C	121	GLN
3	C	135	SER
3	C	163	GLN
3	C	174	GLU
3	C	208	LYS
3	C	227	GLU
4	D	48	LEU
4	D	72	ARG
4	D	76	CYS
4	D	110	GLU
4	D	126	ARG
4	D	144(A)	ASP
4	D	170	GLU
4	D	177	LEU
4	D	180(E)	SER
4	D	215	ILE
4	D	237	LEU
4	D	244	GLU
5	E	7	ASN
5	E	12	THR
5	E	13	VAL
5	E	28	LEU
5	E	32	LYS
5	E	57	GLU
5	E	76	LEU
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	149	LEU
5	E	185	ASN
5	E	189	LEU
5	E	207	LEU
5	E	227	GLU
5	E	231	LYS
6	F	11	SER

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Mol	Chain	Res	Type
6	F	35	THR
6	F	36	THR
6	F	43	ASN
6	F	121	GLN
6	F	127	ASN
6	F	130	ARG
6	F	135	SER
6	F	180(E)	GLU
6	F	187	ARG
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	214	TRP
6	F	218(C)	ASN
7	G	34(A)	ASN
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	169	GLN
7	G	184	ASN
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	34	LEU
8	H	43	CYS
8	H	55	VAL
8	H	56	THR
8	H	68	LEU
8	H	144	GLN
8	H	197	ARG
9	I	29	ASN
9	I	61	TYR
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

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Mol	Chain	Res	Type
11	K	1	THR
11	K	4	LEU
11	K	9	GLN
11	K	17	ASP
11	K	21	THR
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL
11	K	104	TYR
11	K	138	LEU
12	L	-7	ASN
12	L	13	LEU
12	L	24	SER
12	L	39	ASN
12	L	57	ARG
12	L	70	ASN
12	L	82	ASN
12	L	98	HIS
12	L	99	THR
12	L	122	GLU
12	L	164	TYR
13	M	40	ASN
13	M	61	ASP
13	M	62	LEU
13	M	91	ARG
13	M	129	PHE
13	M	141(C)	ARG
13	M	149	GLN
13	M	204	LYS
14	N	36	ARG
14	N	84	LYS
14	N	89	GLU
14	N	105(B)	LYS
14	N	115	LEU
14	N	119	VAL
14	N	149	GLU
1	O	33	GLN
1	O	64	LEU
1	O	158	PHE
1	O	179	ARG
2	P	58	LEU
2	P	61	GLN

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Mol	Chain	Res	Type
2	P	67	LEU
2	P	71	ASN
2	P	121	GLN
2	P	135	SER
2	P	156	ASN
2	P	185	LYS
2	P	192	LEU
2	P	212	PHE
2	P	218	ASN
3	Q	10	ARG
3	Q	25	GLU
3	Q	57	LYS
3	Q	66	LYS
3	Q	121	GLN
3	Q	135	SER
3	Q	163	GLN
3	Q	174	GLU
3	Q	208	LYS
3	Q	227	GLU
4	R	48	LEU
4	R	72	ARG
4	R	76	CYS
4	R	110	GLU
4	R	126	ARG
4	R	144(A)	ASP
4	R	170	GLU
4	R	177	LEU
4	R	180(E)	SER
4	R	215	ILE
4	R	237	LEU
4	R	244	GLU
5	S	7	ASN
5	S	12	THR
5	S	13	VAL
5	S	28	LEU
5	S	32	LYS
5	S	57	GLU
5	S	76	LEU
5	S	97	ASN
5	S	121	GLN
5	S	149	LEU
5	S	185	ASN

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Mol	Chain	Res	Type
5	S	189	LEU
5	S	207	LEU
5	S	227	GLU
5	S	231	LYS
6	T	11	SER
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	121	GLN
6	T	127	ASN
6	T	130	ARG
6	T	135	SER
6	T	180(E)	GLU
6	T	187	ARG
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	214	TRP
6	T	218(C)	ASN
7	U	34(A)	ASN
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	124	THR
7	U	169	GLN
7	U	184	ASN
7	U	197	MET
7	U	217	LYS
7	U	232	ARG
7	U	233	LEU
8	V	34	LEU
8	V	43	CYS
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	144	GLN
8	V	197	ARG
9	W	29	ASN
9	W	61	TYR
9	W	160	LEU
10	X	34	THR

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Mol	Chain	Res	Type
10	X	35	ARG
10	X	52	THR
10	X	70	GLU
10	X	77	GLN
10	X	121	GLU
11	Y	1	THR
11	Y	4	LEU
11	Y	9	GLN
11	Y	21	THR
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
11	Y	104	TYR
11	Y	138	LEU
12	Z	-7	ASN
12	Z	13	LEU
12	Z	24	SER
12	Z	39	ASN
12	Z	57	ARG
12	Z	70	ASN
12	Z	82	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	106	GLU
12	Z	122	GLU
12	Z	164	TYR
13	a	40	ASN
13	a	61	ASP
13	a	62	LEU
13	a	91	ARG
13	a	129	PHE
13	a	141(C)	ARG
13	a	149	GLN
13	a	204	LYS
14	b	36	ARG
14	b	84	LYS
14	b	89	GLU
14	b	105(B)	LYS
14	b	115	LEU
14	b	119	VAL
14	b	149	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (201) 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	243	GLN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	161	ASN
4	D	211	GLN
4	D	226	ASN
5	E	7	ASN
5	E	64	GLN
5	E	73	HIS
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	185	ASN
5	E	199	GLN
5	E	207(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
6	F	192	GLN
6	F	205	ASN
7	G	11	HIS

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Mol	Chain	Res	Type
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
7	G	228	ASN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
8	H	220	ASN
9	I	29	ASN
10	J	36	GLN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	186	GLN
10	J	193	GLN
11	K	9	GLN
11	K	85	ASN
11	K	131	GLN
11	K	174	ASN
11	K	207	ASN
12	L	-9	GLN
12	L	-7	ASN
12	L	39	ASN
12	L	45	ASN
12	L	60	ASN
12	L	70	ASN
12	L	82	ASN
12	L	125	GLN
12	L	142	ASN
12	L	143	GLN
12	L	148	ASN

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Mol	Chain	Res	Type
12	L	155	ASN
12	L	185	HIS
13	M	-7	GLN
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	38	HIS
14	N	60	GLN
14	N	69	GLN
14	N	141	ASN
14	N	145	ASN
14	N	161	GLN
1	O	33	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	82	ASN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	211	GLN
4	R	226	ASN
5	S	7	ASN

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Mol	Chain	Res	Type
5	S	64	GLN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	125	GLN
5	S	185	ASN
5	S	199	GLN
5	S	207(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	192	GLN
6	T	205	ASN
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	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
8	V	220	ASN
9	W	29	ASN
9	W	145	ASN
10	X	36	GLN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	141	HIS

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Mol	Chain	Res	Type
10	X	186	GLN
10	X	193	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	39	ASN
12	Z	45	ASN
12	Z	60	ASN
12	Z	70	ASN
12	Z	125	GLN
12	Z	142	ASN
12	Z	143	GLN
12	Z	148	ASN
12	Z	155	ASN
12	Z	185	HIS
13	a	10	ASN
13	a	18	ASN
13	a	40	ASN
13	a	89	GLN
13	a	93	ASN
13	a	149	GLN
13	a	157	ASN
13	a	172	ASN
13	a	191	GLN
14	b	38	HIS
14	b	60	GLN
14	b	141	ASN
14	b	145	ASN
14	b	161	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	1Y9	K	301	11	11,15,15	2.49	1 (9%)	5,21,21	0.68	0
15	1Y9	N	201	14	11,15,15	2.41	1 (9%)	5,21,21	0.79	0
15	1Y9	Y	301	11	11,15,15	2.38	1 (9%)	5,21,21	0.66	0
15	1Y9	b	201	14	11,15,15	2.42	1 (9%)	5,21,21	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	1Y9	K	301	11	-	0/10/26/26	0/1/1/1
15	1Y9	N	201	14	-	0/10/26/26	0/1/1/1
15	1Y9	Y	301	11	-	0/10/26/26	0/1/1/1
15	1Y9	b	201	14	-	0/10/26/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	301	1Y9	O5-C4	7.48	1.43	1.20
15	b	201	1Y9	O5-C4	7.52	1.43	1.20
15	N	201	1Y9	O5-C4	7.63	1.44	1.20
15	K	301	1Y9	O5-C4	7.86	1.44	1.20

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	K	301	1Y9	2	0
15	N	201	1Y9	3	0
15	Y	301	1Y9	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.23	3 (1%) 81 81	44, 58, 89, 114	0
1	O	250/250 (100%)	-0.19	5 (2%) 68 69	44, 59, 91, 114	0
2	B	244/244 (100%)	-0.12	5 (2%) 68 69	42, 62, 102, 124	0
2	P	244/244 (100%)	-0.03	8 (3%) 50 50	42, 63, 103, 124	0
3	C	241/241 (100%)	-0.03	5 (2%) 67 68	45, 67, 117, 132	0
3	Q	241/241 (100%)	0.17	16 (6%) 22 20	47, 69, 118, 133	0
4	D	242/242 (100%)	0.01	7 (2%) 55 55	45, 66, 98, 133	0
4	R	242/242 (100%)	-0.07	6 (2%) 61 61	46, 67, 97, 133	0
5	E	233/233 (100%)	0.04	8 (3%) 49 49	49, 69, 95, 121	0
5	S	233/233 (100%)	0.01	7 (3%) 54 54	49, 70, 95, 120	0
6	F	244/244 (100%)	-0.22	4 (1%) 74 75	45, 62, 99, 114	0
6	T	244/244 (100%)	-0.04	5 (2%) 68 69	46, 63, 99, 115	0
7	G	243/243 (100%)	-0.29	4 (1%) 74 75	40, 57, 87, 123	0
7	U	243/243 (100%)	-0.30	3 (1%) 81 81	39, 57, 86, 124	0
8	H	222/222 (100%)	-0.30	0 100 100	41, 55, 77, 108	0
8	V	222/222 (100%)	-0.37	2 (0%) 85 86	42, 56, 78, 110	0
9	I	204/204 (100%)	-0.37	1 (0%) 91 93	39, 53, 71, 84	0
9	W	204/204 (100%)	-0.27	0 100 100	40, 53, 72, 85	0
10	J	198/198 (100%)	-0.30	3 (1%) 76 76	42, 55, 74, 133	0
10	X	198/198 (100%)	-0.29	6 (3%) 54 54	43, 56, 73, 133	0
11	K	212/212 (100%)	-0.38	0 100 100	39, 54, 73, 83	0
11	Y	212/212 (100%)	-0.41	0 100 100	40, 54, 74, 84	0
12	L	222/222 (100%)	-0.38	1 (0%) 91 93	38, 55, 78, 97	0
12	Z	222/222 (100%)	-0.33	1 (0%) 91 93	39, 55, 76, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/233 (100%)	-0.41	1 (0%) 93 94	39, 56, 71, 79	0
13	a	233/233 (100%)	-0.45	1 (0%) 93 94	39, 55, 71, 79	0
14	N	196/196 (100%)	-0.46	0 100 100	39, 51, 72, 85	0
14	b	196/196 (100%)	-0.38	1 (0%) 91 93	40, 51, 72, 85	0
All	All	6368/6368 (100%)	-0.22	103 (1%) 74 75	38, 58, 91, 133	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	U	6	ALA	11.3
4	D	123(E)	SER	11.0
4	D	123(D)	ALA	11.0
4	D	123(F)	GLY	9.4
10	X	193	GLN	9.3
10	X	192	ALA	8.4
5	E	4	PHE	8.2
4	R	123(D)	ALA	8.2
10	J	193	GLN	7.2
7	G	6	ALA	6.7
4	R	123(F)	GLY	6.7
3	C	55	THR	6.7
7	U	240	ASP	6.4
4	R	123(E)	SER	6.2
4	D	123(G)	GLU	5.8
3	C	56	LEU	5.8
10	J	192	ALA	5.6
4	D	123(C)	GLY	5.4
2	P	217	ALA	5.2
4	D	126	ARG	5.1
1	A	4	MET	5.0
3	Q	56	LEU	5.0
1	O	4	MET	4.8
1	O	236	LEU	4.7
5	S	4	PHE	4.5
4	R	123(C)	GLY	4.4
4	R	126	ARG	4.4
3	Q	203	THR	4.2
8	V	223	ASP	4.1
5	E	203	ASP	3.9
5	E	233	ILE	3.9
2	P	218	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
13	M	-8	THR	3.9
5	S	5	ARG	3.8
6	T	5	GLY	3.8
3	Q	55	THR	3.7
8	V	222	CYS	3.7
5	S	203	ASP	3.7
5	S	233	ILE	3.6
7	G	240	ASP	3.6
1	O	235	ALA	3.5
6	F	204	ASP	3.5
6	F	5	GLY	3.5
2	B	217	ALA	3.5
3	C	203	THR	3.5
6	F	240	ILE	3.5
12	L	164	TYR	3.5
3	Q	235	GLN	3.4
5	E	5	ARG	3.4
2	B	218	ASN	3.3
6	T	6	THR	3.3
10	X	189	ASP	3.2
5	E	204	GLU	3.2
3	Q	242	GLU	3.2
3	C	202	GLN	3.1
10	X	191	GLN	3.1
3	Q	233	VAL	3.0
3	C	240	LYS	3.0
7	G	239	GLN	2.9
6	T	240	ILE	2.9
3	Q	207	ALA	2.9
3	Q	201	VAL	2.8
4	D	125	GLU	2.8
3	Q	54	SER	2.7
3	Q	241	GLN	2.7
1	A	236	LEU	2.7
2	P	53	LYS	2.6
3	Q	243	GLN	2.6
2	P	220	TYR	2.5
6	T	57	LYS	2.5
3	Q	202	GLN	2.5
3	Q	237	GLU	2.5
1	A	5	THR	2.4
2	P	216(B)	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
6	T	241	ASN	2.4
6	F	238	LYS	2.4
2	B	54	VAL	2.4
2	B	235	LYS	2.4
2	P	236	THR	2.4
1	O	217(P)	LYS	2.4
3	Q	236	ILE	2.3
5	S	207	LEU	2.3
4	R	123(G)	GLU	2.3
2	P	219	GLU	2.3
3	Q	63	THR	2.3
5	E	33	GLN	2.3
2	P	239	THR	2.2
13	a	-8	THR	2.2
1	O	233	LEU	2.2
3	Q	53	ARG	2.2
5	S	178	ARG	2.2
7	U	8	TYR	2.2
7	G	179(E)	LYS	2.1
10	X	-1	MET	2.1
12	Z	164	TYR	2.1
10	J	191	GLN	2.1
2	B	239	THR	2.1
5	E	207(C)	VAL	2.0
5	E	127	TYR	2.0
9	I	-8	SER	2.0
5	S	195	GLU	2.0
14	b	187(I)	GLN	2.0
10	X	188	ASP	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

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	1Y9	N	201	15/15	0.92	0.26	4.16	65,71,74,75	0
15	1Y9	Y	301	15/15	0.90	0.25	3.83	67,75,78,80	0
15	1Y9	b	201	15/15	0.92	0.26	2.72	65,73,76,80	0
15	1Y9	K	301	15/15	0.91	0.23	2.60	68,74,78,79	0

6.5 Other polymers

There are no such residues in this entry.